LAMMPS - a flexible simulation tool for particle-based remeso, and continuum scales

Computer Physics Communications 271, 108171

DOI: 10.1016/j.cpc.2021.108171

Citation Report

#	Article	IF	CITATIONS
1	Probing the Size-Dependent Polarizability of Mesoscopic Ionic Clusters and Their Induced-Dipole Interactions. Journal of Chemical Physics, 2021, 155, 194901.	3.0	2
2	Understanding creep in TiAl alloys on the nanosecond scale by molecular dynamics simulations. Materials and Design, 2021, 212, 110282.	7.0	5
3	Physical property and interface binding energy calculation of polyimide/boron nitride nanosheets thermally conductive composite insulating materials. Computational Materials Science, 2022, 210, 111051.	3.0	7
4	Nanoconfined Fluids: Uniqueness of Water Compared to Other Liquids. ACS Nano, 2021, 15, 19864-19876.	14.6	26
5	Insights from Computational Studies on the Anisotropic Volume Change of Li <sub><i>x</i></sub> NiO <sub>2</sub> at High States of Charge ( <i>x</i> < 0.25). Journal of Physical Chemistry C, 2021, 125, 27130-27139.	3.1	3
6	Atomistic studies of the responses of composites with thermal residual stresses and defects under uniaxial loading. Journal of Alloys and Compounds, 2022, 901, 163664.	5.5	2
7	Nucleation kinetics of the <mml:math altimg="si5.svg" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>β</mml:mi><mml:mrow><mml:mo>″</mml:mo></mml:mrow><td>nl:n<b>ss2</b>p&gt;&lt;</td><td>/mាសា:math&gt;</td></mml:msup></mml:math>	nl:n <b>ss2</b> p><	/mាសា:math>
8	Correlation between plastic rearrangements and local structure in a cyclically driven glass. Journal of Chemical Physics, 2022, 156, 074503.	3.0	5
9	Coarse-grained molecular models of the surface of hair. Soft Matter, 2022, 18, 1779-1792.	2.7	7
10	The Impact of the Surface Modification on Tin-Doped Indium Oxide Nanocomposite Properties. Nanomaterials, 2022, 12, 155.	4.1	2
11	Artificial neural network potential for Au <sub>20</sub> clusters based on the first-principles. Journal of Physics Condensed Matter, 2022, 34, 174005.	1.8	3
12	Temperature- and vacancy-concentration-dependence of heat transport in Li3ClO from multi-method numerical simulations. Npj Computational Materials, 2022, 8, .	8.7	16
13	Hybrid parallelization of molecular dynamics simulations to reduce load imbalance. Journal of Supercomputing, 2022, 78, 9184-9215.	3.6	3
14	Multi-scale modeling of ionic electrospray emission. Journal of Applied Physics, 2022, 131, .	2.5	7
15	Negligible contribution of inter-dot coherent modes to heat conduction in quantum-dot superlattice. Materials Today Physics, 2022, 22, 100601.	6.0	3
16	The Impact of Foaming Effect on the Physical and Mechanical Properties of Foam Glasses with Molecular-Level Insights. Molecules, 2022, 27, 876.	3.8	6
17	Critical assessment of machine-learned repulsive potentials for the density functional based tight-binding method: A case study for pure silicon. Journal of Chemical Physics, 2022, 156, 064101.	3.0	4
18	Guided self-assembly of polyethene on graphene. , 2022, , .		1

#	Article	IF	CITATIONS
20	Polycrystalline morphology and mechanical strength of nanotube fibers. Npj Computational Materials, 2022, 8, .	8.7	0
21	Molecular Dynamics of Solids at Constant Pressure and Stress Using Anisotropic Stochastic Cell Rescaling. Applied Sciences (Switzerland), 2022, 12, 1139.	2.5	1
22	Simple structure descriptors quantifying the diffusion of ethene in small-pore zeolites: insights from molecular dynamic simulations. Inorganic Chemistry Frontiers, 2022, 9, 1590-1602.	6.0	4
23	Effects of Coarse-Graining on Molecular Simulation of Craze Formation in Polymer Glass. Macromolecules, 2022, 55, 1267-1278.	4.8	5
24	Transport coefficients of gel electrolytes: A molecular dynamics simulation study. Journal of Chemical Physics, 2022, 156, 084905.	3.0	0
25	Human Learning for Molecular Simulations: The Collective Variables Dashboard in VMD. Journal of Chemical Theory and Computation, 2022, 18, 1945-1956.	5.3	8
26	Molecular dynamics simulation of the shock response of materials: A tutorial. Journal of Applied Physics, 2022, 131, .	2.5	32
27	Adsorption of Polymer-Tethered Particles on Solid Surfaces. Journal of Physical Chemistry B, 2022, , .	2.6	3
28	Kinetics and nucleation dynamics in ion-seeded atomic clusters. Physical Review A, 2022, 105, .	2.5	1
29	Molecular investigation on COâ,,-CHâ,,, displacement and kerogen deformation in enhanced shale gas recovery. Fuel, 2022, 315, 123208.	6.4	21
30	Cyclic Photoisomerization of Azobenzene in Atomistic Simulations: Modeling the Effect of Light on Columnar Aggregates of Azo Stars. Molecules, 2021, 26, 7674.	3.8	5
31	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	3.2	29
32	Shear Is Not Always Simple: Rate-Dependent Effects of Flow Type on Granular Rheology. Physical Review Letters, 2021, 127, 268003.	7.8	5
33	Columnar Aggregates of Azobenzene Stars: Exploring Intermolecular Interactions, Structure, and Stability in Atomistic Simulations. Molecules, 2021, 26, 7598.	3.8	2
34	Condensation and growth of amorphous aluminosilicate nanoparticles <i>via</i> an aggregation process. Physical Chemistry Chemical Physics, 2022, 24, 9229-9235.	2.8	2
35	Effect of ring stiffness and ambient pressure on the dynamical slowdown in ring polymers. Soft Matter, 2022, 18, 2959-2967.	2.7	5
36	Critical Peeling of Tethered Nanoribbons. Nanoscale, 2022, , .	5.6	1
37	Computational Modelling of the Local Structure and Thermophysical Properties of Ternary Mgcl2-Nacl-Kcl Salt for Thermal Energy Storage Applications. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	Citations
38	Significance of atomic-scale defects in flexible surfaces on local solvent and ion behaviour. Faraday Discussions, 2022, , .	3.2	1
39	Featurization strategies for polymer sequence or composition design by machine learning. Molecular Systems Design and Engineering, 2022, 7, 661-676.	3.4	43
40	Computational Insights into Mg <sup>2+</sup> Dehydration in the Presence of Carbonate. ACS Earth and Space Chemistry, 2022, 6, 733-745.	2.7	11
41	Elucidating Curvature-Capacitance Relationships in Carbon-Based Supercapacitors. Physical Review Letters, 2022, 128, 086001.	7.8	14
43	Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics. Thermo, 2022, 2, 56-73.	1.3	1
44	Hydrogen adsorption in phase and grain boundaries of pearlitic steels and its effects on tensile strength. MRS Advances, 2022, 7, 383-387.	0.9	3
45	High-throughput screening of tribological properties of monolayer films using molecular dynamics and machine learning. Journal of Chemical Physics, 2022, 156, 154902.	3.0	5
47	Layer-dependent fracture strength of few-layer WS <sub>2</sub> induced by interlayer sliding: a molecular dynamics study. Journal Physics D: Applied Physics, 2022, 55, 205301.	2.8	1
48	Apatite–Graphene Interface Channel-Aided Rapid and Selective H <sub>2</sub> Permeation. Journal of Physical Chemistry C, 2022, 126, 3653-3660.	3.1	0
49	Sink versus tilt penetration into shaken dry granular matter: The role of the foundation. Physical Review E, 2022, 105, 024903.	2.1	0
50	Simulation Study on the Defect Generation, Accumulation Mechanism and Mechanical Response of GaAs Nanowires under Heavy-Ion Irradiation. Nanomaterials, 2022, 12, 611.	4.1	5
51	Understanding the Role of SEI Layer in Low-Temperature Performance of Lithium-Ion Batteries. ACS Applied Materials & Samp; Interfaces, 2022, 14, 11910-11918.	8.0	29
52	Dual-Force Zone Nonequilibrium Molecular Dynamics Simulations on Nanoporous Metal–Organic Framework Membranes for Separation of H <sub>2</sub> /CH <sub>4</sub> Mixtures. ACS Applied Nano Materials, 2022, 5, 4048-4061.	5.0	9
53	Rigorous expressions for thermodynamic properties in the <i>NpH</i> ensemble. Physical Review E, 2022, 105, 035301.	2.1	7
54	Reentrant transitions in a mixture of small and big particles interacting via soft repulsive potential. Physical Review E, 2022, 105, L032604.	2.1	0
55	Fracture behaviors of double network elastomers with dynamic non-covalent linkages: A molecular dynamics study. Polymer, 2022, 244, 124670.	3.8	4
56	Subnanometer Topological Tuning of the Liquid Intrusion/Extrusion Characteristics of Hydrophobic Micropores. Nano Letters, 2022, 22, 2164-2169.	9.1	11
57	Hybrid Monte Carlo method with potential scaling for sampling from the canonical multimodal distribution and imitating the relaxation process. Journal of Chemical Physics, 2022, 156, 104111.	3.0	1

#	Article	IF	Citations
58	Elucidating size effects on the yield strength of single-crystal Cu via the Richtmyer–Meshkov instability. Journal of Applied Physics, 2022, 131, .	2.5	4
59	Effect of Twin Boundary Density on Mechanical Behavior of Al0.1CoCrFeNi High-Entropy Alloy by Molecular Dynamics Simulation. Frontiers in Materials, 2022, 9, .	2.4	0
60	High-pressure hydrogen decompression in sulfur crosslinked elastomers. International Journal of Hydrogen Energy, 2022, 47, 15094-15106.	7.1	14
62	From Data to Knowledge: Systematic Review of Tools for Automatic Analysis of Molecular Dynamics Output. Frontiers in Pharmacology, 2022, 13, 844293.	3.5	1
63	Anti-sintering behavior and combustion process of aluminum nano particles coated with PTFE: A molecular dynamics study. Defence Technology, 2023, 24, 46-57.	4.2	4
64	Strong reduction of thermal conductivity of WSe <sub>2</sub> with introduction of atomic defects. Nanotechnology, 2022, 33, 275706.	2.6	4
65	Molecular dynamics investigation of a one-component model for the stacking motif in complex alloy structures. Journal of Applied Crystallography, 2022, 55, 284-288.	4.5	0
66	Nanoarchitectonics of Illite-Based Materials: Effect of Metal Oxides Intercalation on the Mechanical Properties. Nanomaterials, 2022, 12, 997.	4.1	2
67	The Dislocation- and Cracking-Mediated Deformation of Single Asperity GaAs during Plowing Using Molecular Dynamics Simulation. Micromachines, 2022, 13, 502.	2.9	4
68	Molecular dynamic simulation on temperature evolution of SiC under directional microwave radiation. Journal of Physics Condensed Matter, 2022, 34, 195701.	1.8	1
69	Devising Bone Molecular Models at the Nanoscale: From Usual Mineralized Collagen Fibrils to the First Bone Fibers Including Hydroxyapatite in the Extra-Fibrillar Volume. Materials, 2022, 15, 2274.	2.9	4
70	The Role of Cross-Linkers in the Mechanical Responses of Gold Nanoparticle Assemblies. Journal of Physical Chemistry C, 2022, 126, 6456-6464.	3.1	2
71	DLPGEN: Preparing Molecular Dynamics Simulations with Support for Polarizable Force Fields. Journal of Chemical Information and Modeling, 2022, 62, 1471-1478.	5.4	3
72	Morphology and Dynamics in Hydroxide-Conducting Polysulfones. ACS Applied Polymer Materials, 2022, 4, 2470-2480.	4.4	12
73	Origin of Enhanced Performance in Nanoporous Electrical Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors. ACS Applied Materials & Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors: Insights on Materials & Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors: Insights on Micropore Structure and Electrolyte Composition from Molecular Simulations. ACS Applied Materials & Double Layer Capacitors and Micropore Structure and Micropore Structure and Micropore Structure and Micropore Acceptance and Micropore Acceptance Ac	8.0	9
74	Modeling swelling effects during coffee extraction with smoothed particle hydrodynamics. Physics of Fluids, 2022, 34, .	4.0	11
75	Adaptive stochastic morphology simulation and mesh generation of high-quality 3D particulate composite microstructures with complex surface texture. Computer Methods in Applied Mechanics and Engineering, 2022, 393, 114811.	6.6	1
76	Investigating finite-size effects in molecular dynamics simulations of ion diffusion, heat transport, and thermal motion in superionic materials. Journal of Chemical Physics, 2022, 156, 134705.	3.0	11

#	ARTICLE	IF	CITATIONS
77	Predicting Melt Curves of Energetic Materials Using Molecular Models. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	2
78	Dynamically Formed Surfactant Assembly at the Electrified Electrode–Electrolyte Interface Boosting CO <sub>2</sub> Electroreduction. Journal of the American Chemical Society, 2022, 144, 6613-6622.	13.7	106
79	Examination of critical grain size of isotropic nanocrystalline iron through molecular dynamics analysis. Molecular Simulation, 2022, 48, 976-990.	2.0	2
80	Effects of Fe atoms on hardening of a nickel matrix: Nanoindentation experiments and atom-scale numerical modeling. Materials and Design, 2022, 217, 110639.	7.0	25
81	The study of polydimethylsiloxane nanocone distortion in the demolding process using molecular dynamics method. AIP Advances, 2022, 12, 045011.	1.3	3
82	Effects of interatomic potential on fracture behaviour in single- and bicrystalline tungsten. Computational Materials Science, 2022, 207, 111283.	3.0	16
83	Reactive scattering of water group ions on ice surfaces with relevance to Saturn's icy moons. Icarus, 2022, 379, 114967.	2.5	0
84	Influence of vacancies on the temperature-dependent magnetism of bulk Fe: A spin-lattice dynamics approach. Computational Condensed Matter, 2022, 31, e00662.	2.1	4
85	Post irradiated microstructure and mechanical properties of pure V. Journal of Nuclear Materials, 2022, 564, 153648.	2.7	4
86	Heat-current filtering for Greenat Kubo and Helfand-moment molecular dynamics predictions of thermal conductivity: Application to the organic crystal <mml:math altimg="si21.svg" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>(2) 432643</mml:mi></mml:math>	4.8	6
87	Enhancing the foaming effects and mechanical strength of foam glasses sintered at low temperatures. Journal of Physics and Chemistry of Solids, 2022, 165, 110698.	4.0	4
88	LAMMPS lb/fluid fix version 2: Improved hydrodynamic forces implemented into LAMMPS through a lattice-Boltzmann fluid. Computer Physics Communications, 2022, 275, 108318.	7.5	2
89	Effect of axial electric field on confined water in carbon nanotube: Enhancement of thermophoresis. International Journal of Heat and Mass Transfer, 2022, 190, 122751.	4.8	6
90	Comparative Stability Analysis of Boron Nitride Nanotube using MD Simulation and Nonlocal Elasticity Theory. International Journal of Engineering and Applied Sciences, 2021, 13, 189-200.	0.1	2
91	Water in an External Electric Field: Comparing Charge Distribution Methods Using ReaxFF Simulations. Journal of Chemical Theory and Computation, 2022, 18, 580-594.	5.3	7
92	CSPTH: A Crystal Structure Prediction Framework on Tianhe-2 Supercomputer. Computer Science and Application, 2022, 12, 866-878.	0.1	0
93	<i>Ab initio</i> neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT. Physical Chemistry Chemical Physics, 2022, 24, 11801-11811.	2.8	13
94	Unravelling pore network and gas dynamics in highly adaptive rubbery organic frameworks. Chemical Science, 0, , .	7.4	0

#	Article	IF	CITATIONS
95	Molecular dynamics simulation of carbon nanotubes diffusion in water. Molecular Simulation, 0, , $1-8$ .	2.0	1
96	Density Scaling of Translational and Rotational Molecular Dynamics in a Simple Ellipsoidal Model near the Glass Transition. International Journal of Molecular Sciences, 2022, 23, 4546.	4.1	3
97	Study on deprotonation from radiation-induced ionized acrylate polymers including acid-generation promoters for improving chemically amplified resists. Japanese Journal of Applied Physics, 2022, 61, 066505.	1.5	3
98	High-Density Nanowells Formation in Ultrafast Laser-Irradiated Thin Film Metallic Glass. Nano-Micro Letters, 2022, 14, 103.	27.0	8
99	Modeling atomic layer deposition of alumina using reactive force field molecular dynamics. MRS Advances, 2022, 7, 185-189.	0.9	1
100	Mechanical properties of fullerene embedded silicon nanowires. Archive of Applied Mechanics, 0, , 1.	2.2	1
101	Simulating the complete pyrolysis and charring process of phenol–formaldehyde resins using reactive molecular dynamics. Journal of Materials Science, 2022, 57, 7600-7620.	3.7	10
102	Molecular simulations for improved process modeling of an acid gas removal unit. Fluid Phase Equilibria, 2022, 560, 113478.	2.5	7
103	Slip and stress from low shear rate nonequilibrium molecular dynamics: The transient-time correlation function technique. Journal of Chemical Physics, 2022, 156, 184111.	3.0	4
104	Generative design, manufacturing, and molecular modeling of 3D architected materials based on natural language input. APL Materials, 2022, 10, .	5.1	20
105	Optimization of Monolayer MoS2 with Prescribed Mechanical Properties. Materials, 2022, 15, 2812.	2.9	0
106	Molecular dynamics inferred transfer learning models for finiteâ€strain hyperelasticity of monoclinic crystals: Sobolev training and validations against physical constraints. International Journal for Numerical Methods in Engineering, 2022, 123, 3922-3949.	2.8	13
107	Thermophysical properties of chloropropanes in liquid phase: experiments and simulations. Journal of Molecular Liquids, 2022, , 119137.	4.9	0
108	Accurate Sequence-Dependent Coarse-Grained Model for Conformational and Elastic Properties of Double-Stranded DNA. Journal of Chemical Theory and Computation, 2022, 18, 3239-3256.	5.3	13
109	Fully periodic, computationally efficient constant potential molecular dynamics simulations of ionic liquid supercapacitors. Journal of Chemical Physics, 2022, 156, 184101.	3.0	20
110	Deformation and film formation mechanisms during high velocity impact of silicon carbide nanoparticles. Journal of Aerosol Science, 2022, 163, 105997.	3.8	5
111	Constructing composite membranes from functionalized metal organic frameworks integrated MXene intended for ultrafast oil/water emulsion separation. Separation and Purification Technology, 2022, 293, 121052.	7.9	62
112	Two-photon absorption induced dangling bonds in amorphous silica revealed by molecular dynamics simulations. Journal of Non-Crystalline Solids, 2022, 588, 121590.	3.1	3

#	ARTICLE	IF	CITATIONS
113	Unusual High Hardness and Load-Dependent Mechanical Characteristics of Hydrogenated Carbon–Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon–Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon—Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon—Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon†"Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon—Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon†"Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics of Hydrogenated Carbon—Nitrogen Hybrid Films. ACS Applied Materials & Dependent Mechanical Characteristics (Naterials & Dependent Mechanical Characteristics (Na	8.0	3
114	A Martini 3 coarse-grain model for the simulation of the photopolymerizable organic phase in dental composites. RSC Advances, 2022, 12, 12053-12059.	3.6	0
115	Headâ€Toâ€Head Comparison of Molecular and Continuum Simulations of Shockâ€Induced Collapse of an Elongated Pore in an Energetic Molecular Crystal. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	5
116	Effect of Radiation Defects on Thermo–Mechanical Properties of UO2 Investigated by Molecular Dynamics Method. Metals, 2022, 12, 761.	2.3	1
117	Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment, and Adsorption Potential Theory. Langmuir, 2022, 38, 5428-5438.	3.5	8
118	Direct simulation of blood flow with heterogeneous cell suspensions in a patient-specific capillary network. Physics of Fluids, 2022, 34, 041912.	4.0	4
119	Normalizing flows for atomic solids. Machine Learning: Science and Technology, 2022, 3, 025009.	<b>5.</b> 0	12
120	Intrusion and extrusion of liquids in highly confining media: bridging fundamental research to applications. Advances in Physics: X, 2022, 7, .	4.1	9
121	Nanoporous SiOx plasma polymer films as carrier for liquidâ€infused surfaces. Plasma Processes and Polymers, 2022, 19, .	3.0	4
122	Relating Dry Friction to Interdigitation of Surface Passivation Species: A Molecular Dynamics Study on Amorphous Carbon. Materials, 2022, 15, 3247.	2.9	8
123	Atomistic simulations of magnetoelastic effects on sound velocity. Physical Review B, 2022, 105, .	<b>3.2</b>	5
124	Ultra-high liquid–solid thermal resistance using nanostructured gold surfaces coated with graphene. Applied Physics Letters, 2022, 120, .	3.3	7
125	Fracture of single crystal silicon caused by nonlinear evolution of surface acoustic waves. Engineering Fracture Mechanics, 2022, 269, 108505.	4.3	3
126	Molecular Dynamics Simulation of Chip Morphology in Nanogrinding of Monocrystalline Nickel. Coatings, 2022, 12, 647.	2.6	1
127	Molecular dynamics study of fatigue behavior of nickel single-crystal under cyclic shear deformation and hyper-gravity condition. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 055006.	2.0	3
128	Molecular Dynamics Simulations of Nitrate/MgO Interfaces and Understanding Metastability of Thermochemical Materials. ACS Omega, 2022, 7, 16371-16379.	3.5	2
129	Subdiffusive High-Pressure Hydrogen Gas Dynamics in Elastomers. Macromolecules, 2022, 55, 3788-3800.	4.8	6
130	Examination of computed aluminum grain boundary structures and energies that span the 5D space of crystallographic character. Acta Materialia, 2022, 234, 118006.	7.9	19

#	Article	IF	CITATIONS
131	Universal density of low-frequency states in silica glass at finite temperatures. Physical Review E, 2022, 105, .	2.1	3
132	Cellulose Nanocrystals: Tensile Strength and Failure Mechanisms Revealed Using Reactive Molecular Dynamics. Biomacromolecules, 2022, 23, 2243-2254.	5.4	4
133	Discovery of Highâ€Performing Metal–Organic Frameworks for Onâ€Board Methane Storage and Delivery via LNG–ANG Coupling: Highâ€Throughput Screening, Machine Learning, and Experimental Validation. Advanced Science, 2022, 9, e2201559.	11.2	14
134	Atomistic simulations of <mml:math altimg="si56.svg" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow></mml:mrow><mml:mrow></mml:mrow></mml:msup></mml:mrow></mml:math> Ar diffusion in muscovite. Geochimica Et Cosmochimica Acta, 2022, 331, 123-142.	3.9	8
135	Elucidating the Atomic Structures of the Gel Layer Formed during Aluminoborosilicate Glass Dissolution: An Integrated Experimental and Simulation Study. Journal of Physical Chemistry C, 2022, 126, 7999-8015.	3.1	4
136	Molecular Dynamics Predictions of Shockâ€Induced Pore Collapse in (010)â€Oriented <i>β</i> àêHMX: Effects of Sample Thickness and Transverse Orientation, and Runâ€Toâ€Run Variability among Statistically Equivalent Samples. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	1
137	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics. Journal of Physical Chemistry C, 2022, 126, 8121-8133.	3.1	8
138	Unveiling the mechanism of the triethyl phosphate hydrolysis reaction in the synthesis of the sol-gel-derived 58S bioactive glass. Materials Today Chemistry, 2022, 24, 100929.	3.5	2
139	Atomevo: a web server combining protein modelling, docking, molecular dynamic simulation and MMPBSA analysis of Candida antarctica lipase B (CalB) fusion protein. Bioresources and Bioprocessing, 2022, 9, .	4.2	2
140	Mechanical properties of 2D materials: A review on molecular dynamics based nanoindentation simulations. Materials Today Communications, 2022, 31, 103623.	1.9	12
141	Reactive molecular dynamics and DFT simulations of FTDO explosive. Computational and Theoretical Chemistry, 2022, 1212, 113723.	2.5	8
142	Interfacial characteristics and their impact on the indentation behavior of CuTa/CuTa amorphous/amorphous nanolaminates. International Journal of Mechanical Sciences, 2022, 223, 107297.	6.7	8
143	Molecular dynamics simulation of thermophysical properties of binary RP-3 surrogate fuel mixtures containing trimethylbenzene, n-decane, and n-dodecane. Journal of Molecular Liquids, 2022, 359, 119258.	4.9	5
144	A spatial upscaling method for describing the three-body potential of a diamond lattice structure. Applied Mathematical Modelling, 2022, 108, 502-511.	4.2	6
145	Reactive molecular simulation of shockwave propagation in calcium–silicate–hydrate gels. Journal of Non-Crystalline Solids, 2022, 590, 121677.	3.1	1
146	Nonlinear Elongation Flows in Associating Polymer Melts: From Homogeneous to Heterogeneous Flow. Physical Review X, 2022, 12, .	8.9	7
147	Molecular dynamics study on surface formation and phase transformation in nanometric cutting of $\hat{l}^2$ -Sn. Advances in Manufacturing, 2022, 10, 356-367.	6.1	4
148	Geometric percolation of hard-sphere dispersions in shear flow. Soft Matter, 2022, , .	2.7	0

#	Article	IF	CITATIONS
149	Multiscale modeling of electrospray ion emission. Journal of Applied Physics, 2022, 131, .	2.5	16
150	Flexible machine-learning interatomic potential for simulating structural disordering behavior of Li7La3Zr2O12 solid electrolytes. Journal of Chemical Physics, 2022, 156, .	3.0	8
151	Kinetic analysis of wetting and spreading at high temperatures: A review. Advances in Colloid and Interface Science, 2022, 305, 102698.	14.7	15
152	Structured globules with twisted arrangement of helical blocks: Computer simulation. Polymer, 2022, , 124974.	3.8	0
153	The Critical Diameter for Continuous Evaporation Is between 3 and 4 nm for Hydrophilic Nanopores. Langmuir, 2022, 38, 6550-6560.	3.5	0
154	Recipes for superior ionic conductivities in thin-film ceria-based electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 12926-12936.	2.8	3
155	Connection between water's dynamical and structural properties: Insights from ab initio simulations. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2121641119.	7.1	9
156	Ultrapermeable 2D-channeled graphene-wrapped zeolite molecular sieving membranes for hydrogen separation. Science Advances, 2022, 8, eabl3521.	10.3	21
157	Molecular dynamics study of shear-induced long-range correlations in simple fluids. Physical Review Research, 2022, 4, .	3.6	3
158	Approximating the impact of nuclear quantum effects on thermodynamic properties of crystalline solids by temperature remapping. Physical Review B, 2022, 105, .	3.2	2
159	Formation of Liquid Film in Heterogeneous Condensation of Water Vapor: Effects of Solid–Fluid Interaction and Sulfuric Acid Component. Langmuir, 2022, 38, 7085-7097.	3.5	3
160	Electromechanical response of stacked h-BN layers: A computational study. Diamond and Related Materials, 2022, , 109126.	3.9	1
161	The combined effect of carbon and chromium enrichment on $\tilde{a} \in \hat{1} 0 0 \tilde{a} \in \infty$ loop absorption in iron. Computational Materials Science, 2022, 211, 111533.	3.0	4
162	A fast atomistic approach to finite-temperature surface elasticity of crystalline solids. Computational Materials Science, 2022, 211, 111511.	3.0	2
163	Mechanisms of Strength and Hardening in Austenitic Stainless 310s Steel: Nanoindentation Experiments and Multiscale Modeling. SSRN Electronic Journal, 0, , .	0.4	0
164	NVIDIA's Quantum InfiniBand Network Congestion Control Technology andÂlts Impact onÂApplication Performance. Lecture Notes in Computer Science, 2022, , 26-43.	1.3	0
165	Modeling the Effects of Pulse Plating on Dendrite Growth in Lithium Metal Batteries. SSRN Electronic Journal, 0, , .	0.4	0
166	Energy Deposition around Swift Carbon-lon Tracks in Liquid Water. International Journal of Molecular Sciences, 2022, 23, 6121.	4.1	7

#	Article	IF	Citations
167	Gravity enables selfâ€assembly. Natural Sciences, 2022, 2, .	2.1	1
168	Effects of Interfacial Solvation Structures on the Morphological Stability of Potassium Metal Anodes Revealed by <i>Operando</i> I > Diagnosis. ACS Applied Energy Materials, 2022, 5, 7124-7133.	5.1	6
169	Edge dislocations in multicomponent solid solution alloys: Beyond traditional elastic depinning. Physical Review Research, 2022, 4, .	3.6	8
170	Mixing Thermodynamics and Flory–Huggins Interaction Parameter of Polyethylene Oxide/Polyethylene Oligomeric Blends from Kirkwood–Buff Theory and Molecular Simulations. Macromolecules, 2022, 55, 4852-4862.	4.8	12
171	Prediction of flexoelectricity in BaTiO <sub>3</sub> using molecular dynamics simulations. Chinese Physics B, 2023, 32, 017701.	1.4	1
172	Sub-surface granular dynamics in the context of oblique, low-velocity impacts into angular granular media. Icarus, 2022, 385, 115089.	2.5	0
173	Extending $\langle i \rangle$ ab initio $\langle  i \rangle$ simulations for the ion-ion structure factor of warm dense aluminum to the hydrodynamic limit using neural network potentials. Physical Review B, 2022, 105, .	3.2	6
174	Zwitterionization of common hemodialysis membranes: assessment of different immobilized structure impact on hydrophilicity and biocompatibility of poly aryl ether sulfone (PAES) and cellulose triacetate (CTA) hemodialysis membranes. Structural Chemistry, 2022, 33, 1965-1982.	2.0	6
175	Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale. Journal of Fluid Mechanics, 2022, 942, .	3.4	3
176	Pore formation in simple systems simulated by molecular dynamics. Journal of Physics: Conference Series, 2022, 2270, 012043.	0.4	0
177	Development of a ReaxFF Force Field for Aqueous Phosphoenolpyruvate as a Novel Biomimetic Carbon Capture Absorbent. Journal of Physical Chemistry C, 0, , .	3.1	2
178	Improved Random Batch Ewald Method in Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2022, 126, 3583-3593.	2.5	2
180	Chemical Decomposition of the TFSI Anion under Aqueous Basic Conditions. , 2022, 1, .		3
181	Adamantanes as White-Light Emitters: Controlling the Arrangement and Functionality by External Coulomb Forces. Journal of Physical Chemistry C, O, , .	3.1	2
182	Modified Poisson–Boltzmann theory for polyelectrolytes in monovalent salt solutions with finite-size ions. Journal of Chemical Physics, 2022, 156, .	3.0	4
183	Characterization and visualization of grain boundary disconnections. Acta Materialia, 2022, 237, 118067.	7.9	4
184	End-to-end prediction of multimaterial stress fields and fracture patterns using cycle-consistent adversarial and transformer neural networks. Biomedical Engineering Advances, 2022, 4, 100038.	3.8	19
185	Molecular Simulations Probing the Adsorption and Diffusion of Ammonia, Nitrogen, Hydrogen, and Their Mixtures in Bulk MFI Zeolite and MFI Nanosheets at High Temperature and Pressure. Journal of Chemical & Chem	1.9	4

#	Article	IF	CITATIONS
186	Molecular Simulation Analyses of Polymorphism Control Factors by the Example of Carbamazepine Forms I-IV: A Blueprint for Industrial Drug Formulation?. Journal of Pharmaceutical Sciences, 2022, 111, 2898-2906.	3.3	1
187	When mechanisms of coalescence and sintering at the nanoscale fundamentally differ: Molecular dynamics study. Journal of Chemical Physics, 2022, 156, .	3.0	11
188	Vorotis: Software for Voronoi tessellation analysis using the polyhedron code. Computer Physics Communications, 2022, 278, 108418.	7.5	3
189	Prediction of atomic stress fields using cycle-consistent adversarial neural networks based on unpaired and unmatched sparse datasets. Materials Advances, 2022, 3, 6280-6290.	5 <b>.</b> 4	7
190	On the mechanical response in nanoalloys: the case of NiCo. Faraday Discussions, 0, 242, 23-34.	3.2	4
191	Deep neural network based quantum simulations and quasichemical theory for accurate modeling of molten salt thermodynamics. Chemical Science, 2022, 13, 8265-8273.	7.4	3
192	Atomistic Asphalt Model Development and Molecular Dynamics Simulation of Rejuvenating Aged Asphalt by Waste Cooking Oil. SSRN Electronic Journal, 0, , .	0.4	0
193	Structure and correlations for harmonically confined charges. Advances in Quantum Chemistry, 2022, , .	0.8	0
194	Premelting layer during ice growth: role of clusters. Physical Chemistry Chemical Physics, 2022, 24, 15330-15339.	2.8	2
195	A machine learning protocol for revealing ion transport mechanisms from dynamic NMR shifts in paramagnetic battery materials. Chemical Science, 2022, 13, 7863-7872.	7.4	10
196	Bilayer Graphene Kirigami. SSRN Electronic Journal, 0, , .	0.4	0
197	Developing a nitrile-based lithium-conducting electrolyte for low temperature operation. Journal of Materials Chemistry A, 2022, 10, 19972-19983.	10.3	2
198	Failure mechanism of graphene kirigami under nanoindentation. Nanotechnology, 2022, 33, 375703.	2.6	2
199	Anisotropic Mechanics of 2D Materials. Advanced Engineering Materials, 2022, 24, .	3.5	8
200	Elucidation of Cu–Zn Surface Alloying on Cu(997) by Machine-Learning Molecular Dynamics. ACS Physical Chemistry Au, 0, , .	4.0	4
201	A Transfer Free Energy Based Implicit Solvent Model for Protein Simulations in Solvent Mixtures: Urea-Induced Denaturation as a Case Study. Journal of Physical Chemistry B, 2022, 126, 4472-4482.	2.6	3
202	Rectified and Salt Concentration Dependent Wetting of Hydrophobic Nanopores. Journal of the American Chemical Society, 2022, 144, 11693-11705.	13.7	8
203	Polymer Vesicles in a Nanochannel under Flow Fields: A DPD Simulation Study. Macromolecular Theory and Simulations, 2022, 31, .	1.4	8

#	Article	IF	CITATIONS
204	Thermal Activation of Gold Atom Diffusion in Au@Pt Nanorods. ACS Nano, 2022, 16, 9608-9619.	14.6	8
205	The Origin of Moiréâ€Level Stickâ€Slip Behavior on Graphene/ <i>h</i> hà€BN Heterostructures. Advanced Functional Materials, 2022, 32, .	14.9	20
206	Modeling cell biological features of meiotic chromosome pairing to study interlock resolution. PLoS Computational Biology, 2022, 18, e1010252.	3.2	5
207	Atomistic modelling approaches to understanding the interfaces of ionic liquid electrolytes for batteries and electrochemical devices. Current Opinion in Electrochemistry, 2022, 35, 101086.	4.8	5
208	Role of the double-glow plasma pre-sputtering in the growth mechanisms and metal–insulator transition of VO2 film. Applied Surface Science, 2022, 603, 154043.	6.1	4
209	Mechanisms of CdTe(100) sublimation. Surface Science, 2022, , 122147.	1.9	0
210	Reversible Al Metal Anodes Enabled by Amorphization for Aqueous Aluminum Batteries. Journal of the American Chemical Society, 2022, 144, 11444-11455.	13.7	63
211	Theoretical methods for structural phase transitions in elemental solids at extreme conditions: statics and dynamics. Journal of Physics Condensed Matter, 2022, 34, 363001.	1.8	1
212	Gas Adsorption and Diffusion Behaviors in Interfacial Systems Composed of a Polymer of Intrinsic Microporosity and Amorphous Silica: A Molecular Simulation Study. Langmuir, 2022, 38, 7567-7579.	<b>3.</b> 5	4
213	Pyrolysis Mechanism of Wheat Straw Based on ReaxFF Molecular Dynamics Simulations. ACS Omega, 2022, 7, 21075-21085.	3.5	5
214	Fractional calculus & machine learning methods based rubber stress-strain relationship prediction. Molecular Simulation, 2022, 48, 944-954.	2.0	1
215	Developing a force field for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ba</mml:mi><mml:m .<="" 105,="" 2022,="" a="" alloy:="" b,="" ferroelectric="" of="" physical="" prediction="" review="" structure.="" superlattice="" td=""><td>ro‰o≥ &lt; mm</td><td>า<b>l:ฮ</b>าท&gt;1</td></mml:m></mml:msub></mml:mrow></mml:math>	ro‰o≥ < mm	า <b>l:ฮ</b> าท>1
216	Machine-learning effective many-body potentials for anisotropic particles using orientation-dependent symmetry functions. Journal of Chemical Physics, 2022, 157, .	3.0	10
217	CO <sub>2</sub> â€Induced Twoâ€Dimensional Amorphous TiO <sub>2</sub> and Its Excellent Filmâ€Forming Properties. ChemNanoMat, 2022, 8, .	2.8	2
218	Surface wettability effects on evaporating meniscus in nanochannels. International Communications in Heat and Mass Transfer, 2022, 136, 106166.	5.6	4
219	Numerical investigation of flow characteristics and packing structure of binary-sized pebble flow in a circulating pebble bed. Progress in Nuclear Energy, 2022, 150, 104312.	2.9	3
220	Elucidating atomistic mechanisms underlying water diffusion in amorphous polymers: An autonomous basin climbing-based simulation method. Computational Materials Science, 2022, 212, 111565.	3.0	3
221	Asphaltene aggregation and deposition in pipeline: Insight from multiscale simulation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 649, 129394.	4.7	8

#	ARTICLE	IF	CITATIONS
222	NiO nanowire-containing heat transfer nanofluids for CSP plants: Experiments and simulations to promote their application. Journal of Molecular Liquids, 2022, 361, 119593.	4.9	3
223	Diffusion of fluids confined in carbonate minerals: A molecular dynamics simulation study for carbon dioxide and methane–ethane mixture within calcite. Fuel, 2022, 325, 124800.	6.4	4
224	Effect of sorption-induced deformation on methane flow in kerogen slit pores. Fuel, 2022, 325, 124886.	6.4	14
225	Structural Rearrangements During Sub-Tg Relaxation and Nucleation in Lithium Disilicate Glass Revealed by a Solid-State NMR and MD Strategy. SSRN Electronic Journal, 0, , .	0.4	O
226	Interaction of divalent cations and amino acids in bulk water: Molecular simulations with neural network potentials. Chinese Journal of Chemical Physics, 2023, 36, 162.	1.3	0
227	On Cyclic Plasticity of Nanostructured Dual-Phase Cocrfenial High-Entropy Alloy: An Atomistic Study. SSRN Electronic Journal, 0, , .	0.4	0
228	"Smarter―NICs for faster molecular dynamics: a case study. , 2022, , .		5
229	Towards General-Purpose Long-Timescale Molecular Dynamics Simulation on Exascale Supercomputers with Data Processing Units. , 2022, , .		0
230	Mesoscale Modeling of Micellization and Adsorption of Surfactants and Surfactant-Like Polymers in Solution: Challenges and Opportunities. Industrial & Engineering Chemistry Research, 0, , .	3.7	4
231	Configurational entropy significantly influences point defect thermodynamics and diffusion in crystalline silicon. Physical Review Materials, 2022, 6, .	2.4	1
232	C/H/O/F/Al ReaxFF Force Field Development and Application to Study the Condensed-Phase Poly(vinylidene fluoride) and Reaction Mechanisms with Aluminum. Journal of Physical Chemistry C, 2022, 126, 11058-11074.	3.1	7
233	On the relative contributions of point defect clusters to macroscopic swelling of metals. Journal of Applied Physics, 2022, 131, 225103.	2.5	3
235	Superstretchable Elastomer from Cross-linked Ring Polymers. Physical Review Letters, 2022, 128, .	7.8	13
236	FieldPerceiver: Domain agnostic transformer model to predict multiscale physical fields and nonlinear material properties through neural ologs. Materials Today, 2022, 57, 9-25.	14.2	31
237	Probing electrolyte–silica interactions through simulations of the infrared spectroscopy of nanoscale pores. Journal of Chemical Physics, 2022, 157, .	3.0	2
238	Local inversion of the chemical environment representations. Physical Review B, 2022, 106, .  Molecular dynamics study of the ionic liquid 1-n-hexyl-3-methylimidazolium	3.2	2
239	tris(pentaflúoroethyl)trifluorophosphate ([ <mml:máth) (xmlns:mml<="" 0="" 10="" 117="" 50="" etóq0="" overlock="" rgbt="" td="" tf="" tj=""><td>="http://w 2.7</td><td>ww.w3.org/1</td></mml:máth)>	="http://w 2.7	ww.w3.org/1
240	fiel Distribution Cutoff for Clusters near the Gel Point. ACS Polymers Au, 2022, 2, 361-370.	4.1	4

#	ARTICLE	IF	CITATIONS
241	Shape Transformations and Self-Assembly of Hairy Particles under Confinement. International Journal of Molecular Sciences, 2022, 23, 7919.	4.1	2
242	Interatomic Potential for InP. Materials, 2022, 15, 4960.	2.9	0
243	The Microstructural Evolution of Nickel Single Crystal under Cyclic Deformation and Hyper-Gravity Conditions: A Molecular Dynamics Study. Metals, 2022, 12, 1128.	2.3	3
244	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	3.0	8
245	Molecular dynamics simulation for quantitative characterization of wettability transition on silica surface. Journal of Materials Research and Technology, 2022, 19, 4371-4380.	5.8	14
247	Sequence Effects on the Glass Transition of a Model Copolymer System. Macromolecules, 2022, 55, 5926-5937.	4.8	3
248	Molecular Dynamics Simulation on the Wettability of Nanoscale Wrinkles: High Water Adhesion of Rose Petals. Langmuir, 2022, 38, 8854-8861.	3.5	3
249	Method to determine the electron–ion temperature relaxation rate from test particle distributions. Physics of Plasmas, 2022, 29, .	1.9	2
250	Viscosity in water from first-principles and deep-neural-network simulations. Npj Computational Materials, 2022, 8, .	8.7	23
251	Predicting pullout strength of pedicle screws in broken bones from X-ray images. Journal of the Mechanical Behavior of Biomedical Materials, 2022, 134, 105366.	3.1	3
252	Cross-correlation corrected friction in generalized Langevin models: Application to the continuous Asakura–Oosawa model. Journal of Chemical Physics, 2022, 157, .	3.0	7
253	Rayleigh–Taylor instability in strongly coupled plasma. Scientific Reports, 2022, 12, .	3.3	2
254	Atomistic origin of nano-silver paracrystalline structure: molecular dynamics and x-ray diffraction studies. Journal of Physics Condensed Matter, 2022, 34, 375401.	1.8	0
255	Energetically deposited cluster assembly of metallic glasses. Acta Materialia, 2022, 237, 118152.	7.9	4
256	Thermophoresis and thermal orientation of Janus nanoparticles in thermal fields. European Physical Journal E, 2022, 45, .	1.6	3
257	Molecular dynamics study of domain switching dynamics in KNbO3 and BaTiO3. Journal of Materials Science, 2022, 57, 12929-12946.	3.7	0
258	Liquid–Liquid Phase Separation and Assembly of Silk-like Proteins is Dependent on the Polymer Length. Biomacromolecules, 2022, 23, 3142-3153.	5.4	10
259	Focusing frustration for self-limiting assembly of flexible, curved particles. Physical Review Research, 2022, 4, .	3.6	5

#	Article	IF	CITATIONS
260	Spontaneous Crystallization for Tailoring Polymorphic Nanoscale Nickel with Superior Hardness. Journal of Physical Chemistry C, 2022, 126, 12301-12312.	3.1	3
261	Thermal Conductivity of Semicrystalline Polymer Networks: Crystallinity or Cross-Linking?. ACS Macro Letters, 2022, 11, 925-929.	4.8	5
262	Drag on a circular intruder traversing a shape-heterogeneous granular mixture. Physical Review E, 2022, 106, .	2.1	1
263	A triatomic carbon and derived pentacarbides with superstrong mechanical properties. IScience, 2022, 25, 104712.	4.1	6
264	Uniaxial ratcheting behavior and molecular dynamics simulation evaluation of 316LN stainless steel. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2022, 849, 143535.	5.6	6
265	Atomistic simulations of plasticity heterogeneity in gradient nano-grained FCC metals. Materials and Design, 2022, 221, 110929.	7.0	11
266	Molecular Dynamics study of the effect on the interfacial activity of Alkylamine-Modified graphene oxide. Journal of Molecular Liquids, 2022, 362, 119724.	4.9	0
267	Atomistically-informed modeling of point defect clustering and evolution in irradiated ThO2. Chemical Physics, 2022, 562, 111645.	1.9	2
268	Molecular simulations on the continuous methane desorption in illite nanoslits. Fuel, 2022, 328, 125207.	6.4	2
269	In situ inelastic neutron scattering of mixed CH4–CO2 hydrates. Fuel, 2022, 327, 125197.	6.4	1
270	A dilemma in calculating ethane absolute adsorption in shale gas reservoirs: A theoretical approach. Chemical Engineering Journal, 2022, 450, 138242.	12.7	15
271	Atomistic insights into early stage corrosion of bcc Fe surfaces in oxygen dissolved liquid lead-bismuth eutectic (LBE-O). Chinese Physics B, 2023, 32, 036801.	1.4	2
272	Atomic order evolution on the length scale in metallic glasses. Materials Today Communications, 2022, 32, 104125.	1.9	0
273	Data Specifications for Battery Manufacturing Digitalization: Current Status, Challenges, and Opportunities. Batteries and Supercaps, 2022, 5, .	4.7	26
274	Effects of Ca substitution on the local structure and oxide–ion behavior of layered perovskite lanthanum nickelate. Frontiers in Materials, 0, 9, .	2.4	1
275	Phase Separation and Correlated Motions in Motorized Genome. Journal of Physical Chemistry B, 2022, 126, 5619-5628.	2.6	12
276	Symmetry Breaking and Anomalous Conductivity in a Double-Moir $\tilde{A}$ $\tilde{\mathbb{Q}}$ Superlattice. Nano Letters, 2022, 22, 6215-6222.	9.1	11
277	Solid-state bonding behavior between surface-nanostructured Cu and Au: a molecular dynamics simulation. Scientific Reports, 2022, 12, .	3.3	2

#	Article	IF	CITATIONS
278	Effects of interdiffusion on shear response of semi-coherent $\{111\}$ interfaces in Ni/Cu. International Journal of Plasticity, 2022, 157, 103393.	8.8	5
279	Unusual Glass Transition Breadths of Ionomers: Effects of Thermal Treatment and Charge-Carrying Side Chains. Macromolecules, 2022, 55, 6536-6546.	4.8	5
280	Cooperative Reaction of Hydrogen-Networked Water Molecules at the SiCâ€"H <sub>2</sub> O <sub>2</sub> Solution Interface: Microscopic Insights from <i>Ab Initio</i> Molecular Dynamics. Journal of Physical Chemistry C, O, , .	3.1	3
281	Computational modelling of the local structure and thermophysical properties of ternary MgCl2-NaCl-KCl salt for thermal energy storage applications. International Journal of Heat and Mass Transfer, 2022, 196, 123273.	4.8	0
282	Highly Portable C++ Based Simulator with Dual Parallelism and Spatial Decomposition of Simulation Domain using Floating Point Operations and More Flops Per Watt for Better Time-To-Solution on Particle Simulation., 2022,,.		0
283	Material Property Recovery by Controlling the Melt Memory Effects on Recrystallization and on Crystal Deformation: An Approach by the Molecular Dynamics Simulation for Polyethylene. Polymers, 2022, 14, 3082.	4.5	1
285	Classical Molecular Dynamics Simulations of Surface Modifications Triggered by a Femtosecond Laser Pulse. Modelling, 2022, 3, 333-343.	1.4	1
288	Anisotropic atomistic shock response mechanisms of aramid crystals. Journal of Chemical Physics, 2022, 157, .	3.0	2
289	Highâ€Throughput Generation of 3D Graphene Metamaterials and Property Quantification Using Machine Learning. Small Methods, 2022, 6, .	8.6	12
290	Designing Adsorptive Gating via Linker Side-Chain Functionalization in a Honeycomb-MOF. Journal of Physical Chemistry C, 2022, 126, 12755-12764.	3.1	4
291	An Integrated Experimental and Computational Platform to Explore Gas Hydrate Promotion, Inhibition, Rheology, and Mechanical Properties at McGill University: A Review. Energies, 2022, 15, 5532.	3.1	4
292	DP Compress: A Model Compression Scheme for Generating Efficient Deep Potential Models. Journal of Chemical Theory and Computation, 2022, 18, 5559-5567.	5.3	25
293	Embedding functions for Pt and Pd: recalculation and verification on properties of bulk phases, Pt, Pd, and Pt–Pd nanoparticles. Applied Physics A: Materials Science and Processing, 2022, 128, .	2.3	4
294	Leveraging Theory for Enhanced Machine Learning. ACS Macro Letters, 2022, 11, 1117-1122.	4.8	5
295	Computational Modeling of Molecular Mechanics for the Experimentally Inclined. Chemistry of Materials, 2022, 34, 7620-7634.	6.7	1
296	Stability and distortion of fcc <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>10<td>:m<b>ឆា2</b> <td>ml:<b>:</b>ansub&gt;</td></td></mml:mn></mml:msub></mml:math>	:m <b>ឆា2</b> <td>ml:<b>:</b>ansub&gt;</td>	ml: <b>:</b> ansub>
297	GPUMD: A package for constructing accurate machine-learned potentials and performing highly efficient atomistic simulations. Journal of Chemical Physics, 2022, 157, .	3.0	66
298	Effect of Tethering Anions in Block Copolymer Electrolytes via Molecular Dynamics Simulations. Macromolecules, 2022, 55, 7945-7955.	4.8	3

#	Article	IF	CITATIONS
299	On the origin of amorphous nanobridge formation behind the crack tip in an fcc-structured high-entropy alloy: A molecular dynamics simulation study. Journal of Materials Research, 2022, 37, 2803-2814.	2.6	1
300	Vacancy Energetics and Diffusivities in the Equiatomic Multielement Nb-Mo-Ta-W Alloy. Materials, 2022, 15, 5468.	2.9	10
301	Understanding the role of cross-link density in the segmental dynamics and elastic properties of cross-linked thermosets. Journal of Chemical Physics, 2022, $157$ , .	3.0	13
302	Determining the threshold displacement energy of magnesium using molecular dynamics simulations. Bulletin of Materials Science, 2022, 45, .	1.7	1
303	The origin of jerky dislocation motion in high-entropy alloys. Nature Communications, 2022, 13, .	12.8	28
304	Nucleation and growth of crystals inside polyethylene nano-droplets. Journal of Chemical Physics, 2022, 157, .	3.0	1
305	Continuum Modeling with Functional Lennard-Jones Parameters for Methane Storage inside Various Carbon Nanostructures. ACS Omega, 2022, 7, 29773-29786.	3.5	4
306	Investigating the strength of Ti/TiB interfaces at multiple scales using density functional theory, molecular dynamics, and cohesive zone modeling. Ceramics International, 2022, 48, 33185-33199.	4.8	5
307	Porous amorphous nitinol synthesized by argon injection: a molecular dynamics study. Journal of Physics Condensed Matter, 2022, 34, 414003.	1.8	1
308	Biodegradable Block Copolymer–Tannic Acid Glue. Jacs Au, 2022, 2, 1978-1988.	7.9	4
309	Revealing Temperature-Dependent Noise Sources in Aluminum Oxide Josephson Junctions Using Topological Analysis. Journal of Physical Chemistry C, 2022, 126, 14297-14304.	3.1	2
310	Physical Insight into the Conditions Required in the Solid-Phase Molecular Self-Assembly of SDS Revealed by Coarse-Grained Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2022, 126, 6345-6353.	2.6	3
311	Molecular Dynamic Simulation of Crude Oil (SARA) Water Flooding Mechanisms under Different Driving Forces in Oleophilic Pore Channels. Geofluids, 2022, 2022, 1-15.	0.7	1
312	Rapid water dynamics structures the OH-stretching spectra of solitary water in ionic liquids and dipolar solvents. Journal of Chemical Physics, 2022, 157, .	3.0	6
313	Molecular dynamics of preferential adsorption in mixed alkali–halide electrolytes at graphene electrodes. Journal of Chemical Physics, 2022, 157, .	3.0	4
314	Deriving force fields with a multiscale approach: From <i>ab initio</i> calculations to molecular-based equations of state. Journal of Chemical Physics, 2022, 157, .	3.0	2
315	Critical Scaling of Solid Fragmentation at Quasistatic and Finite Strain Rates. Physical Review Letters, 2022, 129, .	7.8	5
316	All-Atom Molecular Dynamics of Pure Water–Methane Gas Hydrate Systems under Pre-Nucleation Conditions: A Direct Comparison between Experiments and Simulations of Transport Properties for the Tip4p/Ice Water Model. Molecules, 2022, 27, 5019.	3.8	8

#	Article	IF	CITATIONS
317	Thermal transport properties of monolayer GeS and SnS: A comparative study based on machine learning and SW interatomic potential models. AIP Advances, 2022, 12, .	1.3	6
318	ELECTRODE: An electrochemistry package for atomistic simulations. Journal of Chemical Physics, 2022, 157, .	3.0	13
319	Effect of <scp>GO </scp> agglomeration on the mechanical properties of graphene oxide and nylon 66 composites and micromechanical analysis. Polymer Composites, 2022, 43, 8356-8367.	4.6	5
320	Atomistic simulation of phonon heat transport across metallic vacuum nanogaps. Physical Review B, 2022, 106, .	3.2	14
321	Statistical perspective on embrittling potency for intergranular fracture. Physical Review Materials, 2022, 6, .	2.4	0
322	A multiscale approach to modeling the frictional behavior of the materials produced by additive manufacturing technologies. Continuum Mechanics and Thermodynamics, 2023, 35, 1353-1385.	2.2	2
323	Fluctuations and power-law scaling of dry, frictionless granular rheology near the hard-particle limit. Physical Review Fluids, 2022, 7, .	2.5	3
324	Efficient lattice Green's function method for bounded domain problems. International Journal for Numerical Methods in Engineering, 0, , .	2.8	0
325	High temperature stability and transport characteristics of hydrogen in alumina via multiscale computation. International Journal of Hydrogen Energy, 2022, , .	7.1	1
326	In silico study of liquid crystalline phases formed by bent-shaped molecules with excluded volume type interactions. Journal of Molecular Liquids, 2022, 367, 120156.	4.9	4
327	Shape Entropy of a Reconfigurable Ising Surface. Physical Review Letters, 2022, 129, .	7.8	0
328	Fluid flow at interfaces driven by thermal gradients. Physical Review E, 2022, 106, .	2.1	3
329	Rapid mechanical property prediction and <i>de novo</i> design of three-dimensional spider webs through graph and GraphPerceiver neural networks. Journal of Applied Physics, 2022, 132, .	2.5	11
330	Transport of thin water films: from thermally activated random walks to hydrodynamics. Journal of Chemical Physics, 0, , .	3.0	3
331	Creep and Recovery Behavior of Vitrimers with Fast Bond Exchange Rate. Macromolecular Rapid Communications, 2023, 44, .	3.9	11
332	Cancer immune therapy using engineered †tail-flipping' nanoliposomes targeting alternatively activated macrophages. Nature Communications, 2022, 13, .	12.8	13
333	Molecular dynamics analysis of elastic properties and new phase formation during amorphous ices transformations. Scientific Reports, 2022, 12, .	3.3	4
334	Simple machine-learned interatomic potentials for complex alloys. Physical Review Materials, 2022, 6, .	2.4	7

#	Article	IF	CITATIONS
335	JAX-ReaxFF: A Gradient-Based Framework for Fast Optimization of Reactive Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 5181-5194.	5.3	8
336	Microscopic Origins of the Viscosity of a Lennard-Jones Liquid. Physical Review Letters, 2022, 129, .	7.8	6
337	Molecular dynamics study on the role of Ar ions in the sputter deposition of Al thin films. Journal of Applied Physics, 2022, 132, 063302.	2.5	4
338	Importance of feature construction in machine learning for phase transitions. Journal of Chemical Physics, 2022, 157, .	3.0	0
339	Atomic level simulations of the phase stability and stacking fault energy of FeCoCrMnSi high entropy alloy. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 075002.	2.0	9
340	<i>Ab initio</i> study of shock-compressed copper. Physical Review B, 2022, 106, .	3.2	9
341	Inelastic phonon transport across atomically sharp metal/semiconductor interfaces. Nature Communications, 2022, $13$ , .	12.8	15
342	Local Thermodynamic Description of Isothermal Single-Phase Flow in Simple Porous Media. Transport in Porous Media, 0, , .	2.6	1
343	Revealing Phosphorus Nitrides up to the Megabar Regime: Synthesis of α′â€P <sub>3</sub> N <sub>5,</sub> Î'â€P <sub>3</sub> N <sub>5</sub> and PN <sub>2</sub> . Chemistry - A European Journal, 2022, 28, .	3.3	6
344	Investigation on mechanism of ultraprecision three-body polishing of single-crystal silicon carbide with voids by molecular dynamics simulation. Applied Physics A: Materials Science and Processing, 2022, 128 Bond-order potential for the surface-terminated titanium carbide MXene monolayers <mml:math< td=""><td>2.3</td><td>2</td></mml:math<>	2.3	2
345	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mi></mml:mi></mml:msub> </td <td></td> <td></td>		

#	Article	IF	CITATIONS
353	Energy storage under high-rate compression of single crystal tantalum. Acta Materialia, 2022, 239, 118253.	7.9	4
354	Improving electric field strength of interfacial electric double layer and cycle stability of Li-ion battery via LiCl additive. Electrochimica Acta, 2022, 429, 141060.	5.2	3
355	Diffusion and thermo-driven migration of silver, palladium, and ruthenium nanoparticles in cubic SiC matrix using molecular dynamics. International Journal of Heat and Mass Transfer, 2022, 197, 123359.	4.8	3
356	MEAM interatomic potential for thermodynamic and mechanical properties of lithium allotropes. Computational Materials Science, 2022, 214, 111706.	3.0	3
357	Microstructure evolution of Si nanoparticles during the melting process: Insights from molecular dynamics simulation. Materials Science in Semiconductor Processing, 2022, 152, 107038.	4.0	0
358	ReaxFF simulations on the combustion of Al and n-butanol nanofluid. Fuel, 2022, 330, 125465.	6.4	12
359	Influence of grain boundary density on the surface energy of nanocrystalline metal thin films. Applied Surface Science, 2022, 604, 154463.	6.1	1
360	Anomalous water transport in narrow-diameter carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	4
361	Indirect learning and physically guided validation of interatomic potential models. Journal of Chemical Physics, 2022, 157, .	3.0	3
362	Shock resistance capability of multi-principal elemental alloys as a function of lattice distortion and grain size. Journal of Applied Physics, 2022, 132, .	2.5	12
363	Large-scale frictionless jamming with power-law particle size distributions. Physical Review E, 2022, 106, .	2.1	9
364	Molecular dynamics simulation on fabrication of chiral nanoneedle by optical vortex. Japanese Journal of Applied Physics, 0, , .	1.5	0
365	The multicomponent oxide glass as a statistical ensemble of neighboring glassy compounds in the composition space. Journal of the American Ceramic Society, 0, , .	3.8	1
366	A Study of the Critical Velocity of the Droplet Transition from the Cassie to Wenzel State on the Symmetric Pillared Surface. Symmetry, 2022, 14, 1891.	2.2	2
367	Hybridization and deconfinement in colloidal quantum dot molecules. Journal of Chemical Physics, 0,	3.0	3
368	Molecular Dynamics Simulation of Solar Wind Implantation in the Permanently Shadowed Regions on the Lunar Surface. Geophysical Research Letters, 2022, 49, .	4.0	2
369	Modeling Atomistic Dynamic Fracture Mechanisms Using a Progressive Transformer Diffusion Model. Journal of Applied Mechanics, Transactions ASME, 2022, 89, .	2.2	25
370	Dynamic characterization of shock wave responses of bicontinuous nanoporous amorphous alloys: Microstructure effects. Mechanics of Materials, 2022, 173, 104410.	3.2	5

#	ARTICLE	IF	CITATIONS
371	Mechanical properties of phenine nanotubes. Extreme Mechanics Letters, 2022, 56, 101893.	4.1	3
372	Atomistic simulations of the enhanced creep resistance and underlying mechanisms of nanograined-nanotwinned copper. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2022, 855, 143912.	5.6	3
373	Effect of lattice distortion and grain size on the crack tip behaviour in Co-Cr-Cu-Fe-Ni under mode-I and mode-II loading. Engineering Fracture Mechanics, 2022, 274, 108809.	4.3	12
374	Study of dielectric properties of meta-aramid fibers by molecular dynamics methods using modified OPLSAA force field. Polymer, 2022, 259, 125331.	3.8	2
375	Modeling the effects of pulse plating on dendrite growth in lithium metal batteries. Electrochimica Acta, 2022, 433, 141227.	5.2	5
376	Temperature-dependent multiscale modeling of graphene sheet under finite deformation. Diamond and Related Materials, 2022, 129, 109334.	3.9	3
377	Structural rearrangements during sub-Tg relaxation and nucleation in lithium disilicate glass revealed by a solid-state NMR and MD strategy. Acta Materialia, 2022, 240, 118318.	7.9	12
378	Crystallization behavior and defect analysis on induction growth of hexagonal GaN in isothermal relaxation. Vacuum, 2022, 205, 111475.	3.5	4
379	Shear-induced amorphization in nanocrystalline NiTi micropillars under large plastic deformation. Acta Materialia, 2022, 241, 118358.	7.9	20
380	Couette flow of pentane in clay nanopores: Molecular dynamics simulation. Journal of Molecular Liquids, 2022, 366, 120290.	4.9	6
381	Atomic fast dynamic motion on the Cu nanoparticle's surface before melting: A molecular dynamics study. Applied Surface Science, 2022, 606, 154901.	6.1	7
382	Evolution of bubble in tungsten irradiated by deuterium of low energy and high flux by molecular dynamics simulations. Applied Surface Science, 2022, 606, 154715.	6.1	6
383	Atomic-level sintering mechanism of silica aerogels at high temperatures: structure evolution and solid thermal conductivity. International Journal of Heat and Mass Transfer, 2022, 199, 123456.	4.8	7
384	Lattice dynamics and elastic properties of $\hat{l}$ ±-U at high-temperature and high-pressure by machine learning potential simulations. Journal of Nuclear Materials, 2022, 572, 154029.	2.7	6
385	Mechanochemically driven formation of protective carbon films from ethanol environment. Materials Today Chemistry, 2022, 26, 101112.	3.5	8
386	Exploring reaction mechanism for ammonia/methane combustion via reactive molecular dynamics simulations. Fuel, 2023, 331, 125806.	6.4	21
387	Molecular dynamics simulation of droplet evaporation in a one-dimensional standing wave acoustic field. International Journal of Thermal Sciences, 2023, 184, 107939.	4.9	6
388	Investigation of Fibrin Fiber Deformation Theories: Insights from Phenomenological Modeling to Molecular Details. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	Citations
389	Integrative structural modelling and visualisation of a cellular organelle. QRB Discovery, 2022, 3, .	1.6	3
390	Atomistic simulation of helium diffusion and clustering in plutonium dioxide. Physical Chemistry Chemical Physics, 2022, 24, 20709-20720.	2.8	3
391	Structure and stability of 7-mercapto-4-methylcoumarin self-assembled monolayers on gold: an experimental and computational analysis. Physical Chemistry Chemical Physics, 2022, 24, 22083-22090.	2.8	2
392	Simulation of calcium-ion Coulomb crystal structure and motion trajectory in linear ion traps. Wuli Xuebao/Acta Physica Sinica, 2022, .	0.5	0
393	Revealing the thermal decomposition mechanism of RDX crystals by a neural network potential. Physical Chemistry Chemical Physics, 2022, 24, 25885-25894.	2.8	3
394	Deformation Behavior of Single-Crystal Magnesium During Nano-Ecap Simulation. SSRN Electronic Journal, 0, , .	0.4	0
395	Interaction between two polyelectrolytes in monovalent aqueous salt solutions. Physical Chemistry Chemical Physics, 2022, 24, 21112-21121.	2.8	2
396	The Nature of Deformation-Induced Dislocations in SrTiO <sub>3</sub> : Insights from Atomistic Simulations. SSRN Electronic Journal, 0, , .	0.4	0
397	Size-dependent shape distributions of platinum nanoparticles. Nanoscale Advances, 2022, 4, 3978-3986.	4.6	5
398	An Atomistic Model of Aged Asphalt Guided by the Oxidation Chemistry of Benzylic Carbon with Application to Asphalt Rejuvenated with a Triglyceride. SSRN Electronic Journal, 0, , .	0.4	0
399	Elastogranular Sheets. SSRN Electronic Journal, 0, , .	0.4	0
400	Deep learning potential of mean force between polymer grafted nanoparticles. Soft Matter, 2022, 18, 7909-7916.	2.7	6
401	Room temperature bilayer water structures on a rutile TiO <sub>2</sub> (110) surface: hydrophobic or hydrophilic?. Chemical Science, 2022, 13, 10546-10554.	7.4	11
402	Force-driven active dynamics of thin nanorods in unentangled polymer melts. Soft Matter, 2022, 18, 6582-6591.	2.7	3
403	Removal of Sic at Atomic and Close-to-Atomic Scale by Nanosecond Ultraviolet Laser. SSRN Electronic Journal, 0, , .	0.4	0
404	Gradient copolymers <i>versus</i> block copolymers: self-assembly in solution and surface adsorption. Soft Matter, 2022, 18, 6538-6549.	2.7	2
405	A meso-scale model of clay matrix: Role of hydration transitions in the geomechanical behavior. Soft Matter, 0, , .	2.7	0
406	Introduction to Molecular Dynamics Simulations. Lecture Notes in Applied and Computational Mechanics, 2022, , 1-19.	2.2	16

#	Article	IF	CITATIONS
407	Molecular investigations of the prenucleation mechanism of bone-like apatite assisted by type I collagen nanofibrils: insights into intrafibrillar mineralization. Physical Chemistry Chemical Physics, 2022, 24, 18931-18942.	2.8	3
408	Computational Study of Graphene Flakes for Carbon Capture. SSRN Electronic Journal, 0, , .	0.4	0
409	Understanding asymmetry effects at low grafting density on the self-assembly of polyion grafted nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 22724-22735.	2.8	0
410	A polymer-tethered particle confined in a slit. Condensed Matter Physics, 2022, 25, 33604.	0.7	0
411	Size-Tunable Graphitized Carbon Spheres for Water Defluoridation. SSRN Electronic Journal, 0, , .	0.4	0
412	Simulation of calcium-ion Coulomb crystal structure and motion trajectory in linear ion traps. Wuli Xuebao/Acta Physica Sinica, 2023, .	0.5	0
413	Eccrine Sweat Molecular Model for Development of de novo Biosensors. , 2022, , .		0
414	Sensitivity Analysis of ReaxFF Potential: The Case of Si/O System. Journal of Physical Chemistry B, 2022, 126, 7027-7036.	2.6	3
415	A Multistage Analysis of Asphalt Binder Nanocrack Generation and Self-Healing Behavior Based on Molecular Dynamics. Polymers, 2022, 14, 3581.	4.5	2
416	Evolution of Symmetrical Grain Boundaries under External Strain in Iron Investigated by Molecular Dynamics Method. Metals, 2022, 12, 1448.	2.3	3
417	Diffusion coefficient of ions through graphene nanopores. AIP Advances, 2022, 12, .	1.3	5
418	Stabilizing the Unstable: Chromium Coating on NiMo Electrode for Enhanced Stability in Intermittent Water Electrolysis. ACS Applied Materials & Samp; Interfaces, 2022, 14, 40822-40833.	8.0	8
419	Evaluating the performance of ReaxFF potentials for sp2 carbon systems (graphene, carbon nanotubes,) Tj ETQq0	)	/Overlock 10
420	Relaxation effects in twisted bilayer graphene: A multiscale approach. Physical Review B, 2022, 106, .	3.2	14
421	Impacts of various interfacial nanostructures on spectral phonon thermal boundary conductance. Journal of Applied Physics, 2022, 132, .	2.5	5
422	Xponge: A Python package to perform pre- and post-processing of molecular simulations. Journal of Open Source Software, 2022, 7, 4467.	4.6	0
423	Role of Short Chain Branching in Crystalline Model Polyethylenes. Macromolecules, 2022, 55, 8438-8450.	4.8	5
424	Structure and Surface Relaxation of CeO2 Nanoparticles Unveiled by Combining Real and Reciprocal Space Total Scattering Analysis. Nanomaterials, 2022, 12, 3385.	4.1	1

#	Article	IF	Citations
425	Interaction confinement and electronic screening in two-dimensional nanofluidic channels. Journal of Chemical Physics, 2022, $157$ , .	3.0	8
426	Virtual Angstrom-Beam Electron Diffraction Analysis for Zr80Pt20 Metallic Glasses. Quantum Beam Science, 2022, 6, 28.	1.2	1
427	Modeling Solution Drying by Moving a Liquid-Vapor Interface: Method and Applications. Polymers, 2022, 14, 3996.	4.5	3
429	Comparison of glancing-angle scatterings on different materials in a high aspect ratio plasma etching process using molecular dynamics simulation. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, 053007.	2.1	4
430	Composition Engineering on the Local Structure and Viscosity of the CaO-SiO2-Al2O3-P2O5-FeO Slag by Machine Learning Methods. Crystals, 2022, 12, 1338.	2.2	0
431	Data-Driven Many-Body Potential Energy Functions for Generic Molecules: Linear Alkanes as a Proof-of-Concept Application. Journal of Chemical Theory and Computation, 2023, 19, 4494-4509.	5.3	11
432	Effect of initial temperature on compaction and strength of porous silica under shock compression. Physical Review B, 2022, 106, .	3.2	1
433	Energy loss in low energy nuclear recoils in dark matter detector materials. Physical Review D, 2022, 106, .	4.7	7
434	VELAS: An open-source toolbox for visualization and analysis of elastic anisotropy. Computer Physics Communications, 2023, 283, 108540.	7.5	9
435	Centroid Molecular Dynamics Can Be Greatly Accelerated through Neural Network Learned Centroid Forces Derived from Path Integral Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 5856-5863.	5.3	2
436	Many-Body Correlations Are Non-negligible in Both Fragile and Strong Glassformers. Physical Review Letters, 2022, 129, .	7.8	7
437	Structural, vibrational and transport properties of liquid and amorphous alumina: A molecular dynamics simulation study. Frontiers in Materials, 0, 9, .	2.4	0
438	Antifouling Bilayer Graphene Slit Membrane for Desalination of Nanoplastic-Infested Seawater: A Molecular Dynamics Simulation Study. ACS Applied Materials & Samp; Interfaces, 2022, 14, 43965-43974.	8.0	4
439	Unexpected Ductility in Semiflexible Polymer Glasses with Entanglement Length Equal to Their Kuhn Length. Physical Review Letters, 2022, 129, .	7.8	4
440	Collective diffusion in a two-dimensional liquid composed of Janus particles. Communications in Theoretical Physics, 2022, 74, 105602.	2.5	1
441	Review of Electrostatic Force Calculation Methods and Their Acceleration in Molecular Dynamics Packages Using Graphics Processors. ACS Omega, 2022, 7, 32877-32896.	3.5	1
442	The importance of long-timescale simulations for driven systems: An example of He bubble growth at a W GB. MRS Communications, 2022, 12, 1103-1110.	1.8	3
443	Training data selection for accuracy and transferability of interatomic potentials. Npj Computational Materials, 2022, 8, .	8.7	16

#	Article	IF	Citations
444	Predicting hot-electron free energies from ground-state data. Physical Review B, 2022, 106, .	3.2	4
445	Guiding the self-assembly of colloidal diamond. Journal of Chemical Physics, 2022, 157, .	3.0	5
446	Accurate p <i>K</i> <sub>a</sub> Calculations in Proteins with Reactive Molecular Dynamics Provide Physical Insight Into the Electrostatic Origins of Their Values. Journal of Physical Chemistry B, 2022, 126, 7321-7330.	2.6	2
447	Inhomogeneity Effects on Reactions in Supercritical Fluids: A Computational Study on the Pyrolysis of <i>n</i> -Decane. Jacs Au, 2022, 2, 2081-2088.	7.9	2
448	Atomic and Electronic Structure of the Al <sub>2</sub> O <sub>3</sub> /Al Interface during Oxide Propagation Probed by Ab Initio Grand Canonical Monte Carlo. ACS Applied Materials & Samp; Interfaces, 2022, 14, 42613-42627.	8.0	2
449	Bypassing backmapping: Coarse-grained electronic property distributions using heteroscedastic Gaussian processes. Journal of Chemical Physics, 2022, 157, .	3.0	12
450	Adjustment of high-energy ion flux in BP-HiPIMS via pulsed coil magnetic field: plasma dynamics and film deposition. Plasma Sources Science and Technology, 2022, 31, 095015.	3.1	2
451	Systematic research on gallium atom-doped neutral small- and medium-sized gas-phase magnesium clusters: A DFT study of GaMg⟨i⟩n⟨/i⟩ (n=2–12) clusters. Journal of Chemical Physics, 2022, 157, .	3.0	8
452	Methane Diffusion Through Nanopore-Throat Geometry: A Molecular Dynamics Simulation Study. SPE Journal, 2023, 28, 819-830.	3.1	1
454	Water Uptake in an Anion Exchange Membrane Based on Polyamine: A First-Principles Study. Journal of Physical Chemistry B, 2022, 126, 7418-7428.	2.6	5
455	Effects of self-irradiation on deuterium retention and reflectivity of molybdenum, fusion plasma-facing material: Combined experimental and modeling study. Journal of Applied Physics, 2022, 132, 125902.	2.5	2
456	Ultrafast nano generation of acoustic waves in water via a single carbon nanotube. Photoacoustics, 2022, 28, 100407.	7.8	8
457	Analysis of Inhibitory Mechanisms of Ammonia Addition on Soot Formation: A Combined ReaxFF MD Simulations and Experimental Study. Energy & Simulations and Experimental Study. Energy & Simulations and Experimental Study.	5.1	11
458	Optimal experiment design for element specific atom counting using multiple annular dark field scanning transmission electron microscopy detectors. Ultramicroscopy, 2022, 242, 113626.	1.9	4
459	Mechanical Behavior of Polymer Nanocomposites via Atomistic Simulations: Conformational Heterogeneity and the Role of Strain Rate. Journal of Physical Chemistry B, 2022, 126, 7429-7444.	2.6	2
460	Pinning of domain walls by strontium layer in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3perovskite: An atomic-scale study. Physical Review B, 2022, 106, .</mml:mn></mml:msub></mml:math>	ml:man2> <td>nm<b>l</b>zmsub&gt;&lt;</td>	nm <b>l</b> zmsub><
461	Dislocation glide driven interstitial shuffling of oxygen interstitials in titanium. Physical Review Materials, 2022, 6, .	2.4	1
462	Element Specific Atom Counting at the Atomic Scale by Combining High Angle Annular Dark Field Scanning Transmission Electron Microscopy and Energy Dispersive Xâ€ray Spectroscopy. Small Methods, 2022, 6, .	8.6	5

#	Article	IF	CITATIONS
464	Molecular insights into the adsorption of chloride ions in calcium silicate hydrate gels: The synergistic effect of calcium to silicon ratio and sulfate ion. Microporous and Mesoporous Materials, 2022, 345, 112248.	4.4	39
465	Effects of minimum uncut chip thickness on tungsten nano-cutting mechanism. International Journal of Mechanical Sciences, 2023, 237, 107790.	6.7	11
468	Atomistic modeling of LiF microstructure ionic conductivity and its influence on nucleation and plating. Physical Review Materials, 2022, 6, .	2.4	4
469	Theoretical study of the thermal conductivity of silica glass–crystal composites. Journal of the American Ceramic Society, 2023, 106, 977-987.	3.8	2
470	Modeling Oxygen Tricluster Formation in Calcium Aluminosilicate Supercooled Liquids and Glasses. Journal of Physical Chemistry B, 2022, 126, 8039-8047.	2.6	2
471	Number-resolved detection of dark ions in Coulomb crystals. Physical Review A, 2022, 106, .	2.5	1
472	Molecular Dynamics Study on the Demulsification Mechanism of Water-In-Oil Emulsion with SDS Surfactant under a DC Electric Field. Langmuir, 2022, 38, 12717-12730.	3.5	3
473	Development of a novel ReaxFF reactive potential for organochloride molecules. Journal of Chemical Physics, 2022, 157, .	3.0	1
474	Polar vs nematic unjamming: Distinct impacts of polar and nematic self-propulsion on active unjamming Journal of Chemical Physics, 0, , .	3.0	0
475	Experimentsâ€Guided Modeling of MCMâ€41: Impact of Pore Symmetry on Gas Adsorption. Advanced Materials Interfaces, 2022, 9, .	3.7	4
476	Pullout Strength of Triply Periodic Minimal Surface-Structured Bone Implants. International Journal of Mechanical Sciences, 2023, 237, 107795.	6.7	8
477	Structure and Dynamics of Hydrofluorocarbon/Ionic Liquid Mixtures: An Experimental and Molecular Dynamics Study. Journal of Physical Chemistry B, 2022, 126, 8309-8321.	2.6	12
478	Newton-X Platform: New Software Developments for Surface Hopping and Nuclear Ensembles. Journal of Chemical Theory and Computation, 2022, 18, 6851-6865.	5.3	18
479	Modeling the Solvation and Acidity of Carboxylic Acids Using an <i>Ab Initio</i> Deep Neural Network Potential. Journal of Physical Chemistry A, 2022, 126, 7283-7290.	2.5	3
480	Defining the pressures of a fluid in a nanoporous, heterogeneous medium. Frontiers in Physics, 0, 10, .	2.1	2
481	Quantifying the dynamic spreading of a molten sand droplet using multiphase mesoscopic simulations. Physical Review Fluids, 2022, 7, .	2.5	3
483	Shock melting of lamellae-forming block copolymers. Physical Review E, 2022, 106, .	2.1	3
484	MateriApps LIVE! and MateriApps Installer: Environment for starting and scaling up materials science simulations. SoftwareX, 2022, 20, 101210.	2.6	1

#	Article	IF	CITATIONS
485	Interatomic potentials: achievements and challenges. Advances in Physics: X, 2023, 8, .	4.1	11
486	Polymer solution structure and dynamics within pores of hexagonally close-packed nanoparticles. Soft Matter, 2022, 18, 8175-8187.	2.7	2
487	Exploring the configurational space of amorphous graphene with machine-learned atomic energies. Chemical Science, 2022, 13, 13720-13731.	7.4	8
488	Density-tunable pathway complexity in a minimalistic self-assembly model. Soft Matter, 2022, 18, 8106-8116.	2.7	2
489	Enhanced vapor sorption in block and random copolymer brushes. Soft Matter, 2022, 18, 8398-8405.	2.7	3
490	LONGITUDINAL THERMAL CONDUCTIVITY OF CU-SWCNT CORE-SHELL NANOWIRE: MOLECULAR DYNAMICS SIMULATIONS. Heat Transfer Research, 2023, 54, 77-89.	1.6	2
491	Substituent engineering of the diboron molecular architecture for a nondoped and ultrathin emitting layer. Chemical Science, 2022, 13, 12996-13005.	7.4	6
492	Percolation of co-continuous domains in tapered copolymer networks. Molecular Systems Design and Engineering, 0, , .	3.4	1
493	Molecular dynamics simulations of cold welding of nanoporous amorphous alloys: effects of welding conditions and microstructures. Physical Chemistry Chemical Physics, 2022, 24, 25462-25479.	2.8	6
494	Role of tilt grain boundaries on the structural integrity of WSe <sub>2</sub> monolayers. Physical Chemistry Chemical Physics, 2022, 24, 27241-27249.	2.8	5
495	Spatio-temporal Model Checking forÂ3D Individual-Based Biofilm Simulations. Lecture Notes in Computer Science, 2022, , 157-174.	1.3	0
496	Security labeling and optical information encryption enabled by laser-printed silicon Mie resonators. Nanoscale, 2022, 14, 16618-16626.	5.6	3
497	Lattice Boltzmann simulation of the ERCOFTAC pump impeller. IOP Conference Series: Earth and Environmental Science, 2022, 1079, 012074.	0.3	0
498	Data-Driven Machine Learning to Predict Mechanical Properties of Monolayer Transition-Metal Dichalcogenides for Applications in Flexible Electronics. ACS Applied Nano Materials, 2022, 5, 16489-16499.	5.0	9
499	High performance of carbon nanotube elastocaloric refrigerators over a large temperature span. Physical Review B, 2022, 106, .	3.2	5
500	Dislocation nucleation mechanisms during nanoindentation of concentrated FeNiCr alloys: unveiling the effects of Cr through molecular simulations. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 085010.	2.0	5
501	Bulk and Point Defect Properties in $\hat{l}$ ±-Zr: Uncertainty Quantification on a Semi-Empirical Potential $\hat{a}$ €. , 0, , .		0
502	Phase Behavior and Morphology of Blends Containing Associating Polymers: Insights from Liquid-State Theory and Molecular Simulations. Macromolecules, 2022, 55, 9297-9311.	4.8	2

#	Article	IF	CITATIONS
503	ReaxFF molecular dynamics simulation of nickel catalysed gasification of cellulose in supercritical water. International Journal of Hydrogen Energy, 2023, 48, 123-137.	7.1	2
504	A review of thermal rectification in solid-state devices. Journal of Semiconductors, 2022, 43, 103101.	3.7	8
505	Evaluation of the Reax Force-Field for Studying the Collision of an Energetic Proton with the DNA. Journal of Chemical Theory and Computation, 2022, 18, 6463-6471.	5.3	1
506	Effect of Layer Orientation and Pore Morphology on Water Transport in Multilayered Porous Graphene. Micromachines, 2022, 13, 1786.	2.9	0
507	A fluorescent multi-domain protein reveals the unfolding mechanism of Hsp70. Nature Chemical Biology, 2023, 19, 198-205.	8.0	14
508	Reticular chemistry for the rational design of mechanically robust mesoporous merged-net metal-organic frameworks. Matter, 2023, 6, 285-295.	10.0	12
509	Scalable training of graph convolutional neural networks for fast and accurate predictions of HOMO-LUMO gap in molecules. Journal of Cheminformatics, 2022, 14, .	6.1	5
510	Stability and formation process of hydrogen-bonded organic porous thin films: A molecular dynamics study. AIP Advances, 2022, 12, 105109.	1.3	0
511	Accurate Quantum-Mechanically Derived Force-Fields through a Fragment-Based Approach: Balancing Specificity and Transferability in the Prediction of Self-Assembly in Soft Matter. Journal of Chemical Theory and Computation, 2022, 18, 6905-6919.	5.3	4
512	Crowding-Induced Spatial Organization of Gene Expression in Cell-Sized Vesicles. ACS Synthetic Biology, 2022, 11, 3733-3742.	3.8	9
513	Low-energy moiré phonons in twisted bilayer van der Waals heterostructures. Physical Review B, 2022, 106, .	3.2	5
514	On the Evolution of Nano-Structures at the Al–Cu Interface and the Influence of Annealing Temperature on the Interfacial Strength. Nanomaterials, 2022, 12, 3658.	4.1	2
515	Supersonic Motion of Atoms in an Octahedral Channel of fcc Copper. Materials, 2022, 15, 7260.	2.9	1
516	Machine learning interatomic potentials for aluminium: application to solidification phenomena. Journal of Physics Condensed Matter, 2023, 35, 035402.	1.8	3
517	Systematic Identification of Atom-Centered Symmetry Functions for the Development of Neural Network Potentials. Journal of Physical Chemistry A, 2022, 126, 8337-8347.	2.5	1
518	Topological gelation of reconnecting polymers. Proceedings of the National Academy of Sciences of the United States of America, 2022, $119,\ldots$	7.1	5
519	Potential of Mean Force for Face–Face Interactions between Pairs of 2:1 Clay Mineral Platelets. Langmuir, 2022, 38, 13065-13074.	3.5	6
520	Effect of the <i>N</i> -Alkyl Side Chain on the Amide–Water Interactions. Journal of Physical Chemistry B, 2022, 126, 8290-8299.	2.6	3

#	ARTICLE	IF	CITATIONS
521	A random batch Ewald method for charged particles in the isothermal–isobaric ensemble. Journal of Chemical Physics, 2022, 157, .	3.0	3
522	Understanding the mechanisms of adhesive wear for heterogeneous materials through atomistic simulations. Extreme Mechanics Letters, 2022, 57, 101913.	4.1	3
523	Cluster expansions of multicomponent ionic materials: Formalism and methodology. Physical Review B, 2022, $106$ , .	3.2	12
524	Two-temperature molecular dynamics simulations of crystal growth in a tungsten supercooled melt. Journal of Physics Condensed Matter, 0, , .	1.8	1
525	Ultrafast Laser-Induced Formation of Hollow Gold Nanorods and Their Optical Properties. ACS Omega, 2022, 7, 39287-39293.	3.5	1
526	Atomistic Simulations of Defects Production under Ion Irradiation in Epitaxial Graphene on SiC. Physica Status Solidi - Rapid Research Letters, 2023, 17, .	2.4	1
527	Molecular dynamics study on the thermal conductivity of a single polyethylene chain: Strain dependence and potential models' effect. AIP Advances, 2022, 12, 105223.	1.3	1
528	Accurate Modeling of Bromide and Iodide Hydration with Data-Driven Many-Body Potentials. Journal of Physical Chemistry B, 2022, 126, 8266-8278.	2.6	9
529	Simulating Polymerization by Boltzmann Inversion Force Field Approach and Dynamical Nonequilibrium Reactive Molecular Dynamics. Polymers, 2022, 14, 4529.	4.5	2
530	Active Refrigerators Powered by Inertia. Physical Review Letters, 2022, 129, .	7.8	6
531	Adhesion of Bis-Salphen-Based Coordination Polymers to Graphene: Insights from Free Energy Perturbation Study. Polymers, 2022, 14, 4525.	4.5	0
532	Revealing Atomistic Mechanisms of Gold-Catalyzed Germanium Growth Using Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2022, 126, 18867-18875.	3.1	1
533	Deposition of Horizontally Stacked Zn Crystals on Single Layer 1Tâ€VSe <sub>2</sub> for Dendriteâ€Free Zn Metal Anodes. Advanced Energy Materials, 2022, 12, .	19.5	11
534	Atomistic assessment of structural evolution for magnesium during hypervelocity nanoprojectile penetration. Journal of Molecular Modeling, 2022, 28, .	1.8	2
535	Bilayer Graphene Kirigami. Carbon Trends, 2022, , 100227.	3.0	0
536	Resolving the oddâ $\in$ "even oscillation of water dissociation at rutile TiO2(110)â $\in$ "water interface by machine learning accelerated molecular dynamics. Journal of Chemical Physics, 2022, 157, .	3.0	11
537	Modeling the Effect of Defects and Disorder in Amorphous Metal–Organic Frameworks. Chemistry of Materials, 2022, 34, 9042-9054.	6.7	15
538	Robust combined modeling of crystalline and amorphous silicon grain boundary conductance by machine learning. Npj Computational Materials, 2022, 8, .	8.7	2

#	Article	IF	CITATIONS
539	Molecular Dynamics Simulation of Nanoindentation of Nb-Zr Alloys with Different Zr Content. Metals, 2022, 12, 1820.	2.3	1
540	Isothermal and adiabatic elastic constants from virial fluctuations. Physical Review E, 2022, 106, .	2.1	0
541	Diffusion-Coefficient Power Laws and Defect-Driven Glassy Dynamics in Swap Acceleration. Physical Review Letters, 2022, 129, .	7.8	3
542	Explicit Polarization in Coarse-Grained Simulations of Ionomer Melts. Macromolecules, 2022, 55, 9980-9989.	4.8	3
543	Metal Affinity of Support Dictates Sintering of Gold Catalysts. Journal of the American Chemical Society, 2022, 144, 20601-20609.	13.7	26
544	Molecular dynamics simulation of the interaction of food proteins with small molecules. Food Chemistry, 2023, 405, 134824.	8.2	50
545	Comprehensive study on thermal decomposition mechanism and interaction of 3-Nitro-1,2,4-Triazol-5-One/Poly-3-nitromethyl-3-methyloxetane plastic bonded explosives. Journal of Analytical and Applied Pyrolysis, 2022, 168, 105753.	5.5	4
546	Hydration Structure of Na <sup>+</sup> and K <sup>+</sup> lons in Solution Predicted by Data-Driven Many-Body Potentials. Journal of Physical Chemistry B, 2022, 126, 9349-9360.	2.6	10
547	Plastic deformation of superionic water ices. Proceedings of the National Academy of Sciences of the United States of America, 2022, $119$ , .	7.1	4
548	A low-temperature prismatic slip instability in Mg understood using machine learning potentials. Acta Materialia, 2023, 243, 118490.	7.9	4
549	The Accuracy of Semi-Empirical Quantum Chemistry Methods on Soot Formation Simulation. International Journal of Molecular Sciences, 2022, 23, 13371.	4.1	1
550	Simulations of heat transport in single-molecule junctions: Investigations of the thermal diode effect. Journal of Chemical Physics, 2022, 157, .	3.0	5
551	Inter-channel conversion between population-/coherence-channel dictates thermal transport in MAPbI3 crystals. Materials Today Physics, 2022, 28, 100892.	6.0	6
552	Unravelling viral dynamics through molecular dynamics simulations - A brief overview. Biophysical Chemistry, 2022, 291, 106908.	2.8	7
553	An atomistic study of deformation mechanisms in metal matrix nanocomposite materials. Materials Today Communications, 2022, 33, 104658.	1.9	2
554	Ex-situ modification of lattice thermal transport through coherent and incoherent heat baths. Materials Today Physics, 2022, 29, 100884.	6.0	0
555	Size-dependent dissolution behavior of CaO in the CaO-SiO2-FeO slag system: A molecular dynamics study. Journal of Molecular Liquids, 2022, 367, 120488.	4.9	2
556	Distribution of the mechanical properties of Ti–Cu combinatorial thin film evaluated using nanoindentation experiments and molecular dynamics with a neural network potential. Materials Today Communications, 2022, 33, 104750.	1.9	1

#	Article	IF	CITATIONS
557	A Riemannian stochastic representation for quantifying model uncertainties in molecular dynamics simulations. Computer Methods in Applied Mechanics and Engineering, 2023, 403, 115702.	6.6	2
558	Molecular dynamics study of the effect of temperature on the shock response and plastic deformation mechanism of CoCrFeMnNi high-entropy alloys. Wuli Xuebao/Acta Physica Sinica, 2023, .	0.5	0
559	Generative multiscale analysis of de novo proteome-inspired molecular structures and nanomechanical optimization using a VoxelPerceiver transformer model. Journal of the Mechanics and Physics of Solids, 2023, 170, 105098.	4.8	8
560	Unexpected dynamic transformation from $\hat{l}\pm$ phase to $\hat{l}^2$ phase in zirconium alloy revealed by in-situ neutron diffraction during high temperature deformation. Acta Materialia, 2023, 242, 118427.	7.9	6
561	Mechanism of activator and pore surface adsorption in aluminum-based flameless ration heaters: A molecular dynamics study. Applied Surface Science, 2023, 609, 155343.	6.1	1
562	The nature and motion of deformation-induced dislocations in SrTiO3: Insights from atomistic simulations. Acta Materialia, 2023, 242, 118404.	7.9	4
563	The Z1+ package: Shortest multiple disconnected path for the analysis of entanglements in macromolecular systems. Computer Physics Communications, 2023, 283, 108567.	7.5	22
564	Controlling morphology in electrosprayed methylcellulose nanowires via nanoparticle addition: coarse-grained modeling and experiments. Nanoscale, 0, , .	5.6	0
565	Lithium ion battery electrode manufacturing model accounting for 3D realistic shapes of active material particles. Journal of Power Sources, 2023, 554, 232294.	7.8	11
566	An atomistic modeling framework for valence change memory cells. Solid-State Electronics, 2023, 199, 108506.	1.4	1
567	Predicting char yield of high-temperature resins. Carbon, 2023, 202, 336-347.	10.3	5
568	Computing the solid-liquid interfacial free energy and anisotropy of the Al-Mg system using a MEAM potential with atomistic simulations. Computational Materials Science, 2023, 217, 111901.	3.0	5
569	Helium bubbles diffusion in aluminum: Influence of gas pressure. Journal of Nuclear Materials, 2023, 573, 154123.	2.7	5
570	Helium bubble growth in tungsten nanotendrils. Journal of Nuclear Materials, 2023, 573, 154145.	2.7	0
571	Molecular geometry effect on gas transport through nanochannels: Beyond Knudsen theory. Applied Surface Science, 2023, 611, 155613.	6.1	5
572	Understanding mechanisms of pyridine oxidation with ozone addition via reactive force field molecular dynamics simulations. Chemical Engineering Science, 2023, 266, 118290.	3.8	6
573	On the reliability of using reverse Monte Carlo simulations to construct the atomic structure model of metallic glasses. Scripta Materialia, 2023, 225, 115159.	5.2	1
574	A granular energy-controlled boundary condition for discrete element simulations of granular flows on erodible surfaces. Computers and Geotechnics, 2023, 154, 105115.	4.7	5

#	Article	IF	CITATIONS
575	Removal of SiC at atomic and close-to-atomic scale by nanosecond ultraviolet laser. Optics and Laser Technology, 2023, 158, 108863.	4.6	10
576	Thermophysical properties of FLiBe using moment tensor potentials. Journal of Molecular Liquids, 2022, 368, 120803.	4.9	5
577	Influence of isotope effect on radiation resistance of monocrystalline silicon. AIP Advances, 2022, 12, 115215.	1.3	0
579	RadonPy: automated physical property calculation using all-atom classical molecular dynamics simulations for polymer informatics. Npj Computational Materials, 2022, 8, .	8.7	20
580	On the Choice of Different Water Model in Molecular Dynamics Simulations of Nanopore Transport Phenomena. Membranes, 2022, 12, 1109.	3.0	0
581	Modeling Method for Semicrystalline Polymers Controlling Aspects of the Morphology at the Molecular Scale for the Study of Mechanical and Physicochemical Properties. Journal of Physical Chemistry B, 2022, 126, 9673-9685.	2.6	2
582	Development of a ReaxFF potential for Au–Pd. Journal of Physics Condensed Matter, 2023, 35, 065901.	1.8	1
583	Graphene at Liquid Copper Catalysts: Atomicâ€Scale Agreement of Experimental and Firstâ€Principles Adsorption Height. Advanced Science, 2022, 9, .	11.2	7
584	Molecular dynamics simulation of bubble growth under surface of tungsten under helium irradiation. Journal of Nuclear Materials, 2023, 573, 154154.	2.7	0
585	High-Performance Ionanofluids from Subzipped Carbon Nanotube Networks. ACS Applied Materials & Lamp; Interfaces, 2022, 14, 50836-50848.	8.0	7
586	Perineuronal nets restrict transport near the neuron surface: A coarse-grained molecular dynamics study. Frontiers in Computational Neuroscience, $0,16,.$	2.1	2
587	<scp>FEMâ€DEM</scp> bridging coupling for the modeling of gouge. International Journal for Numerical Methods in Engineering, 0, , .	2.8	1
588	Predicted superconductivity and superionic state in the electride Li <sub>5</sub> N under high pressure. New Journal of Physics, 2022, 24, 113012.	2.9	8
589	Thermal and stress impacts on vacancy diffusion through atomistic simulations. International Journal of Mechanical Sciences, 2023, 240, 107944.	6.7	3
590	Challenges in Molecular Dynamics of Amorphous ZIFs Using Reactive Force Fields. Journal of Physical Chemistry C, 2022, 126, 19532-19541.	3.1	6
591	From the Design of Novel Tri- and Tetra-Epoxidized Ionic Liquid Monomers to the End-of-Life of Multifunctional Degradable Epoxy Thermosets. ACS Sustainable Chemistry and Engineering, 2022, 10, 15450-15466.	6.7	9
592	Neon-concentration dependent retarding effect on the recrystallization of irradiated tungsten: Experimental analysis and molecular dynamics simulation. Journal of Materials Science and Technology, 2023, 139, 245-259.	10.7	3
593	Libra: A modular software library for quantum nonadiabatic dynamics. Software Impacts, 2022, 14, 100445.	1.4	6

#	Article	IF	CITATIONS
594	Generating 3D architectured nature-inspired materials and granular media using diffusion models based on language cues. Oxford Open Materials Science, 2022, 2, .	1.8	5
595	Competing Effects of Cohesive Energy and Cross-Link Density on the Segmental Dynamics and Mechanical Properties of Cross-Linked Polymers. Macromolecules, 2022, 55, 9990-10004.	4.8	14
597	Optimization of parallel implementation of <scp>UNRES &lt; /scp&gt;package for coarseâ€grained simulations to treat large proteins. Journal of Computational Chemistry, 2023, 44, 602-625.</scp>	3.3	9
598	A generalizable, uncertainty-aware neural network potential for GeSbTe with Monte Carlo dropout. Solid-State Electronics, 2023, 199, 108508.	1.4	2
599	Extending and validating bubble nucleation rate predictions in a Lennard-Jones fluid with enhanced sampling methods and transition state theory. Journal of Chemical Physics, 2022, 157, .	3.0	5
600	Atomistic measurement and modeling of intrinsic fracture toughness of two-dimensional materials. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	8
601	Vapor Swelling of Polymer Brushes Compared to Nongrafted Films. Langmuir, 2022, 38, 13763-13770.	3.5	3
602	Theoretical Analysis of Physical and Chemical CO <sub>2</sub> Absorption by Tri- and Tetraepoxidized Imidazolium Ionic Liquids. Journal of Physical Chemistry B, 2022, 126, 9901-9910.	2.6	6
604	Molecular dynamics study of the growth of ZnO <i><sub>&lt;</sub></i> films. Journal of Applied Physics, 2022, 132, 185304.	2.5	2
605	Molecular progress of the corrosion of passivated Iron: The effects of structural strain.  Construction and Building Materials, 2022, 360, 129537.	7.2	1
606	Role of lattice resistance in the shock dynamics of fcc-structured high entropy alloy. Materials Today Communications, 2022, 33, 104884.	1.9	0
607	Comparison of molecular dynamics simulations of water with neutron and X-ray scattering experiments. EPJ Web of Conferences, 2022, 272, 01015.	0.3	1
608	Experimental absence of the non-perovskite ground state phases of MaPbl <sub>3</sub> explained by a Funnel Hopping Monte Carlo study based on a neural network potential. Materials Advances, 2023, 4, 184-194.	5.4	4
609	Atomistic simulations of dislocation plasticity in concentrated VCoNi medium entropy alloys: Effects of lattice distortion and short range order. Frontiers in Materials, 0, 9, .	2.4	4
610	Machine-learning-based prediction of first-principles XANES spectra for amorphous materials. Physical Review Materials, 2022, 6, .	2.4	1
611	Elucidating the Initial Oxidation of Pt(111) Using Large-Scale Atomistic Thermodynamics: A ReaxFF Study. Journal of Physical Chemistry C, 2022, 126, 20020-20027.	3.1	2
613	Molecular dynamic study on modulating the interfacial thermal conductivity of carbon fiber/epoxy interfaces. Computational Materials Science, 2023, 217, 111914.	3.0	8
614	Improved hydroxyl radical production by electric-field-induced catalysis in O3/H2O2 process: A reactive molecular dynamics perspective. Journal of Molecular Liquids, 2023, 369, 120966.	4.9	0

#	Article	IF	CITATIONS
615	Molecular dynamics study of temperature effects on shock response and plastic deformation mechanism of CoCrFeMnNi high-entropy alloys. Wuli Xuebao/Acta Physica Sinica, 2022, 71, 246101.	0.5	0
616	Development of coarse-grained models of liquid water by deep neural networks for simulating acoustic vibrations of nanostructures in aqueous environment. International Journal for Multiscale Computational Engineering, 2022, , .	1.2	0
617	Interface damage and fracture mechanisms of a ceramic/polymer interface based on atomic-scale simulations. Physical Chemistry Chemical Physics, 2022, 24, 29461-29470.	2.8	3
618	Root Causing MPI Workloads Imbalance Issues via Scalable MPI Critical Path Analysis. Lecture Notes in Computer Science, 2022, , 501-521.	1.3	O
619	Accelerating simulated annealing of glassy materials with data assimilation. Journal of Non-Crystalline Solids, 2023, 600, 122028.	3.1	2
620	Zn substituted hydroxide/oxyhydroxide heterostructure activates proton conduction. Energy Storage Materials, 2023, 55, 84-93.	18.0	9
621	Insights into interfacial thermal conductance in Bi2Te3-based systems for thermoelectrics. Materials Today Physics, 2023, 30, 100953.	6.0	7
622	Significant enhancement in hydrogen evolution rate of 2D bismuth oxychloride lamellar membrane photocatalyst with cellulose nanofibers. Chemical Engineering Journal, 2023, 456, 140933.	12.7	6
623	An in situ inhibition strategy: Forming a physical barrier around ionic crosslinkers to toughen double-network hydrogels. Materials and Design, 2023, 225, 111522.	7.0	1
624	On the microscopic origin of Soret coefficient minima in liquid mixtures. Physical Chemistry Chemical Physics, 2023, 25, 1606-1611.	2.8	4
625	Development of a nano-QSAR model for predicting the toxicity of nano-metal oxide mixtures to <i>Aliivibrio fischeri</i> . Environmental Science: Nano, 0, , .	4.3	2
626	Modeling of a two-stage polymerization considering glass fibre sizing using molecular dynamics. Nanoscale Advances, 2022, 5, 106-118.	4.6	O
627	Evaluation of ZIF-8 flexible force fields for structural and mechanical properties. Microporous and Mesoporous Materials, 2023, 348, 112406.	4.4	6
628	Experimentally informed structure optimization of amorphous TiO <sub>2</sub> films grown by atomic layer deposition. Nanoscale, 0, , .	5.6	1
629	Atomic-scale analysis of mechanical and wear characteristics of AlCoCrFeNi high entropy alloy coating on Ni substrate. Journal of Manufacturing Processes, 2023, 85, 1010-1023.	5.9	10
630	Rational design of cobaltocenium-containing polythioether type metallo-polyelectrolytes as HCl corrosion inhibitors for mild steel. Polymer Chemistry, 2023, 14, 330-342.	3.9	1
631	Understanding the role of quaternary ammonium cations on the interaction of bitumen with clay: A molecular modeling study. Construction and Building Materials, 2023, 364, 129970.	7.2	2
632	Frictionless nanohighways on crystalline surfaces. Nanoscale, 2023, 15, 1299-1316.	5.6	2

#	Article	IF	CITATIONS
633	Evaluating PAA/PVA thermal crosslinking process during the preparation of in-situ high-drug loading amorphous solid dispersions. Journal of Drug Delivery Science and Technology, 2023, 79, 104030.	3.0	3
634	Thermal decomposition mechanism investigation of hyperbranched polyglycerols by TGA-FTIR-GC/MS techniques and ReaxFF reactive molecular dynamics simulations. Biomass and Bioenergy, 2023, 168, 106675.	5.7	5
635	High-throughput computational screening of adsorbents and membrane materials for acetylene capture. Microporous and Mesoporous Materials, 2023, 348, 112396.	4.4	2
636	Deformation behavior of cell walls in an additively manufactured hybrid metallic foam. Additive Manufacturing, 2023, 61, 103365.	3.0	0
637	Grain boundary sliding and distortion on a nanosecond timescale induce trap states in CsPbBr <sub>3</sub> : <i>ab initio</i> investigation with machine learning force field. Nanoscale, 2022, 15, 285-293.	5.6	14
638	An atomistic study of the newly-developed single-phase refractory high entropy alloy of TiZrVMo: Defect accumulation and evolution under tensile deformation. Materials Letters, 2023, 333, 133664.	2.6	5
639	Behavior of the aqueous sodium chloride solutions from molecular simulations and theories. Journal of Molecular Liquids, 2023, 371, 121086.	4.9	1
640	Coupled effect of Cr and Al on interactions between a prismatic interstitial dislocation loop and an edge dislocation line in Fe-Cr-Al alloy. Acta Materialia, 2023, 245, 118651.	7.9	7
641	Characterization of graphene reinforced 3C-SiC composite as a metal-free friction material using molecular dynamics simulation. Computational Materials Science, 2023, 218, 111973.	3.0	1
642	Coupling between mechanical stresses and lithium penetration in a lithium ion battery. Mechanics of Materials, 2023, 177, 104532.	3.2	4
643	Molecular dynamics of electric-field driven ionic systems using a universal neural-network potential. Computational Materials Science, 2023, 218, 111955.	3.0	2
644	Temperature-dependent effect of cooling rate on the melt-quenching process of metallic glasses. Computational Materials Science, 2023, 218, 111930.	3.0	5
645	Ceramic nanoparticles enhancement of latent heat thermal energy storage properties for LiNO3/NaCl: Evaluation from material to system level. Applied Energy, 2023, 331, 120418.	10.1	9
646	Domain partitioning material point method for simulating shock in polycrystalline energetic materials. Computer Methods in Applied Mechanics and Engineering, 2023, 404, 115815.	6.6	3
647	Melting temperature, critical nucleus size, and interfacial free energy in single FCC metals — A Molecular Dynamics study of liquid–solid phase equilibria. Journal of Crystal Growth, 2023, 603, 126987.	1.5	1
648	Accurate Fe–He machine learning potential for studying He effects in BCC-Fe. Journal of Nuclear Materials, 2023, 574, 154183.	2.7	1
649	Atomistic simulations of nanoindentation on nanoglasses: Effects of grain size and gradient microstructure on the mechanical properties. Intermetallics, 2023, 153, 107782.	3.9	6
650	Applied-strain-promoted oxidation of Nickel: Insights from ReaxFF molecular dynamic simulation. Computational Materials Science, 2023, 218, 111992.	3.0	2

#	ARTICLE	IF	CITATIONS
651	Molecular insights into migration of heavy metal ion in calcium silicate hydrate (CSH) surface and intra-CSH (Ca/SiÂ=Â1.3). Construction and Building Materials, 2023, 365, 130097.	7.2	13
652	The significance and effectiveness of combining integrated photovoltaic systems and biomaterials to improve renewable energy utilization in the built environment via molecular dynamics method. Engineering Analysis With Boundary Elements, 2023, 148, 15-21.	3.7	3
653	Simulation of multi-shell fullerenes using Machine-Learning Gaussian Approximation Potential. Carbon Trends, 2023, 10, 100239.	3.0	8
654	Modeling experimental low energy ion scattering multi-angle maps with molecular dynamics FAN. Surface Science, 2023, 729, 122229.	1.9	0
655	Investigation of unified impact of Ti adatom and N doping on hydrogen gas adsorption capabilities of defected graphene sheets. Journal of Molecular Graphics and Modelling, 2023, 119, 108399.	2.4	5
656	Enhancing mechanism of CNT-CNT interface by metal nanoparticle and nanowire effect on the inside and outside of CNT. International Journal of Thermal Sciences, 2023, 185, 108094.	4.9	3
657	The viscosity of liquid ethene: Measurement and molecular dynamic simulation. Journal of Chemical Thermodynamics, 2023, 178, 106957.	2.0	5
658	Stability, reversibility, and recovery of radiation-induced phase transformations in nanowires under mechanical loads. Scripta Materialia, 2023, 226, 115226.	5.2	1
659	A molecular dynamics study of laser melting of densely packed stainless steel powders. International Journal of Mechanical Sciences, 2023, 243, 108034.	6.7	4
660	Part geometry-driven crystallographic texture control in a 3D-printed austenitic steel – a strategy for near-monocrystalline microstructure generation. Scripta Materialia, 2023, 226, 115255.	5.2	0
661	Variable thermal transport in black, blue, and violet phosphorene from extensive atomistic simulations with a neuroevolution potential. International Journal of Heat and Mass Transfer, 2023, 202, 123681.	4.8	5
662	Load versus displacement-controlled nanocompression: Insights from atomistic simulations. Scripta Materialia, 2023, 226, 115245.	5.2	2
663	Competing single-chain folding and multi-chain aggregation pathways control solution-phase aggregate morphology of organic semiconducting polymers. Nanoscale, 2022, 14, 18070-18086.	5.6	5
664	Interactive Virtual Reality Exploration of Large-Scale Datasets Using Omnidirectional Stereo Images. Lecture Notes in Computer Science, 2022, , 115-128.	1.3	0
665	State-of-the-Art Molecular Dynamics Packages forÂGPU Computations: Performance, Scalability andÂLimitations. Lecture Notes in Computer Science, 2022, , 342-355.	1.3	1
666	Towards OpenUCX andÂGPUDirect Technology Support forÂtheÂAngara Interconnect. Lecture Notes in Computer Science, 2022, , 591-603.	1.3	1
667	Harvesting osmotic energy from proton gradients enabled by two-dimensional Ti3C2Tx MXene membranes. , 2022, 2, 100046.		3
668	Enhancing pressure consistency and transferability of structure-based coarse-graining. Physical Chemistry Chemical Physics, 2023, 25, 2256-2264.	2.8	2

#	Article	IF	CITATIONS
669	Tribological gain enabled by the synergy of copper nanoparticles and friction induced <i>in situ</i> tribo-click reaction. Journal of Materials Chemistry A, 2022, 10, 25730-25739.	10.3	7
670	Reliable force field potential for modelling thermal transport in AlN. , 2022, , .		1
671	Guiding Hardware-Driven Turbo with Application Performance Awareness. , 2022, , .		2
672	Extending OpenKIM with an Uncertainty Quantification Toolkit for Molecular Modeling. , 2022, , .		0
673	Toward Bi-directional In Situ Visualization and Analysis of Blood Flow Simulations With Dynamic Deforming Walls. , 2022, , .		0
674	Convenient Way to Create an MD Model of a Hot Crystal with an Open Surface. , 2022, , .		2
675	Entropic Mixing of Ring/Linear Polymer Blends. ACS Polymers Au, 2023, 3, 209-216.	4.1	9
676	Amorphous Kane-Mele model in disordered hyperuniform two-dimensional networks. Physical Review B, 2022, 106, .	3.2	3
677	<i>Ab initio</i> construction of full phase diagram of MgO-CaO eutectic system using neural network interatomic potentials. Physical Review Materials, 2022, 6, .	2.4	3
678	DeepCV: A Deep Learning Framework for Blind Search of Collective Variables in Expanded Configurational Space. Journal of Chemical Information and Modeling, 2022, 62, 6352-6364.	5.4	9
679	The Challenges of Modeling Defect Behavior and Plasticity across Spatial and Temporal Scales: A Case Study of Metal Bilayer Impact. Metals, 2022, 12, 2036.	2.3	1
681	Examining the Long-Range Effect in Very Long Graphene Nanoribbons: A First-Principles Study. Journal of Physical Chemistry Letters, 2022, 13, 11223-11229.	4.6	0
682	Molecular Dynamics Study on Structure, Vibrational Properties, and Transport Coefficients of Liquid Alumina. Materials, 2022, 15, 8370.	2.9	1
683	Development of an insilico model of eccrine sweat using molecular modelling techniques. Scientific Reports, 2022, 12, .	3.3	2
684	Reactive Molecular Dynamics Simulation of the Structural Damages of the B-DNA Induced by the Oxidation/Nitration of Guanine. Journal of Physical Chemistry B, 2022, 126, 10347-10359.	2.6	0
685	Classical and machine learning interatomic potentials for BCC vanadium. Physical Review Materials, 2022, 6, .	2.4	3
686	Intelligent Transportation System: Need, Working, and Tools., 2023,, 201-228.		0
687	lce friction at the nanoscale. Proceedings of the National Academy of Sciences of the United States of America, 2022, $119$ , .	7.1	5

#	Article	IF	CITATIONS
688	Tunable Colloids with Dipolar and Depletion Interactions: Toward Field-Switchable Crystals and Gels. Physical Review X, 2022, 12, .	8.9	1
689	Molecular dynamics simulations of binary sphere mixtures. Physical Review E, 2022, 106, .	2.1	1
690	Circular Polycatenanes: Supramolecular Structures with Topologically Tunable Properties. Physical Review Letters, 2022, 129, .	7.8	11
691	The heterogeneous nature of mechanically accelerated grain growth. Journal of Materials Science, 2022, 57, 21743-21755.	3.7	1
692	Stochastic Resetting for Enhanced Sampling. Journal of Physical Chemistry Letters, 2022, 13, 11230-11236.	4.6	4
693	Highlight on H-Bond Interaction-Associated Multiple Ion Layer Formation of an Imidazolium-Based Ionic Liquid on a Potential-Bias Surface: Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2022, 126, 20644-20657.	3.1	0
694	Molecular Dynamics Simulation of the Thermal Diffusion Effect in <i>n</i> -Alkane Binary Mixtures. Journal of Physical Chemistry B, 2022, 126, 10164-10171.	2.6	0
695	Machine learning interatomic potential for simulations of carbon at extreme conditions. Physical Review B, 2022, 106, .	3.2	16
696	Engineering Single-Atom Sites into Pore-Confined Nanospaces of Porphyrinic Metal–Organic Frameworks for the Highly Efficient Photocatalytic Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2022, 144, 22747-22758.	13.7	53
697	Characterizing Molecular Dynamics Simulation on Commodity Platforms. , 2022, , .		2
698	Atomistic Insights into the Oxidation of Flat and Stepped Platinum Surfaces Using Large-Scale Machine Learning Potential-Based Grand-Canonical Monte Carlo. ACS Catalysis, 2022, 12, 14812-14824.	11.2	7
699	Toward a Mobility-Preserving Coarse-Grained Model: A Data-Driven Approach. Journal of Chemical Theory and Computation, 2022, 18, 7108-7120.	5.3	4
700	Hybrid simulation of plasma synthesis of linear-chain carbon on a semiconductor substrate., 0,,.		0
701	Study of the pressure effect on the thermodiffusion behavior in multicomponent n-alkane mixtures by using non-equilibrium molecular dynamics. Physica Scripta, 2023, 98, 015411.	2.5	1
702	Realistic simulation of thermoelectric characteristics of organic semiconductors based on electronic structure calculations. Applied Physics Express, 0, , .	2.4	0
703	Plasma Oxidation of Copper: Molecular Dynamics Study with Neural Network Potentials. ACS Nano, 2022, 16, 20680-20692.	14.6	4
704	Pressure Stabilized Lithium-Aluminum Compounds with Both Superconducting and Superionic Behaviors. Physical Review Letters, 2022, 129, .	7.8	13
705	Thermophysical properties of n-dodecane over a wide temperature and pressure range via molecular dynamics simulations with modification methods. Journal of Molecular Liquids, 2023, 371, 121102.	4.9	2

#	Article	IF	CITATIONS
706	Origin of the nucleation preference of coherent and semicoherent nanoprecipitates in Al–Cu alloys based on atomistically informed classical nucleation theory. Journal of Alloys and Compounds, 2022, , 168559.	5.5	0
707	PB <sup>3</sup> Opt: Profileâ€based biased Bayesian optimization to select computing clusters on the cloud. Concurrency Computation Practice and Experience, 0, , .	2.2	0
708	Plastic ridge formation in a compressed thin amorphous film. Physical Review Materials, 2022, 6, .	2.4	1
709	Effects of cracking on the deformation anisotropy of GaAs with different crystal orientations during scratching using molecular dynamics simulations. Tribology International, 2023, 179, 108200.	5.9	5
710	Tuning mechanical behavior of polymer materials via multi-arm crosslinked network architectures. Physical Review Materials, 2022, 6, .	2.4	0
711	Molecular Dynamics Simulation of Poly(Ether Ether Ketone) (PEEK) Polymer to Analyze Intermolecular Ordering by Low Wavenumber Raman Spectroscopy and X-ray Diffraction. Polymers, 2022, 14, 5406.	4.5	2
712	Capturing experimental properties in computationally efficient faceted titania nanoparticle models. International Journal of Quantum Chemistry, 0, , .	2.0	1
713	Mechanically Stable Ultrathin Layered Graphene Nanocomposites Alleviate Residual Interfacial Stresses: Implications for Nanoelectromechanical Systems. ACS Applied Nano Materials, 2022, 5, 17969-17976.	5.0	1
714	Understanding the Structure and Rheology of Galactomannan Solutions with Coarse-Grained Modeling. Macromolecules, 2023, 56, 177-187.	4.8	2
715	Fluctuations at Metal Halide Perovskite Grain Boundaries Create Transient Trap States: Machine Learning Assisted Ab Initio Analysis. ACS Applied Materials & Samp; Interfaces, 2022, 14, 55753-55761.	8.0	13
716	Cohesin and CTCF control the dynamics of chromosome folding. Nature Genetics, 2022, 54, 1907-1918.	21.4	76
717	Chirality-Dependent and Intrinsic Auxeticity for Single-Walled Carbon Nanotubes. Materials, 2022, 15, 8720.	2.9	3
718	Strong Coulomb coupling influences ion and neutral temperatures in atmospheric pressure plasmas. Plasma Sources Science and Technology, 2022, 31, 125005.	3.1	5
719	TADA: The Topology-Accommodating Direction Assignment Algorithm for Liquid Crystals. Journal of Chemical Theory and Computation, 0, , .	5.3	1
720	Structural Features and Nonlinear Rheology of Self-Assembled Networks of Cross-Linked Semiflexible Polymers. Journal of Physical Chemistry B, 2022, 126, 10741-10749.	2.6	2
721	ATESA: An Automated Aimless Shooting Workflow. Journal of Chemical Theory and Computation, 0, , .	5.3	1
722	Phase Behavior of Polymer-Grafted Nanoparticles in Homopolymer Blends from Simulations. Macromolecules, 2022, 55, 10245-10254.	4.8	2
723	A novel method for investigation of the impact of sterilization by gamma radiation on polycaprolactone scaffold. Frontiers in Physics, 0, $10$ , .	2.1	1

#	Article	IF	Citations
724	Detecting and quantifying liquid–liquid phase separation in living cells by model-free calibrated half-bleaching. Nature Communications, 2022, 13, .	12.8	31
725	Adsorption, Diffusion, and Transport of C <sub>1</sub> to C <sub>3</sub> Alkanes and Carbon Dioxide in Dual-Porosity Kerogens: Insights from Molecular Simulations. Energy & Ene	5.1	5
726	Investigation of point defect evolution and Voronoi cluster analysis for magnesium during nanoindentation. Journal of Magnesium and Alloys, 2023, 11, 1029-1042.	11.9	2
727	Multiscale equilibration of highly entangled isotropic model polymer melts. Journal of Chemical Physics, 2023, 158, .	3.0	4
728	Internal mechanical dissipation mechanisms in amorphous silicon. Physical Review Materials, 2022, 6, .	2.4	1
729	DNA Droplets: Intelligent, Dynamic Fluid. Advanced Biology, 2023, 7, .	2.5	11
730	Strengthening Modulus and Softening Strength of Nanoporous Gold in Multiaxial Tension: Insights from Molecular Dynamics. Nanomaterials, 2022, 12, 4381.	4.1	1
731	Microscopic Insights and Optimization of the CH <sub>4</sub> –CO <sub>2</sub> Replacement in Natural Gas Hydrates. ACS Omega, 2022, 7, 47239-47250.	3.5	3
732	Diffusion of a tracer in a dense mixture of soft particles connected to different thermostats. Physical Review E, 2022, 106, .	2.1	4
733	Molecular dynamics study on the mechanical properties of nanocrystalline Ni-W alloys with bimodal structure. Materials Research Express, 2022, 9, 125008.	1.6	0
734	Membrane formation by thermally induced phase separation: Materials, involved parameters, modeling, current efforts and future directions. Journal of Membrane Science, 2023, 669, 121303.	8.2	17
735	Single core and multicore aggregates from a polymer mixture: A dissipative particle dynamics study. Journal of Colloid and Interface Science, 2023, 635, 231-241.	9.4	8
736	Coarse-Grained Molecular Dynamics Simulation of Polycarbonate Deformation: Dependence of Mechanical Performance by the Effect of Spatial Distribution and Topological Constraints. Polymers, 2023, 15, 43.	4.5	2
737	Surface and size effects on the mechanical response of plates with a view to porous materials. European Journal of Mechanics, A/Solids, 2023, 98, 104903.	3.7	0
738	Atomic-Level Structure of Zinc-Modified Cementitious Calcium Silicate Hydrate. Journal of the American Chemical Society, 2022, 144, 22915-22924.	13.7	9
739	Influence of chemistry and structure on interfacial segregation in NbMoTaW with high-throughput atomistic simulations. Journal of Applied Physics, 2022, 132, .	2.5	5
740	Chemical order transitions within extended interfacial segregation zones in NbMoTaW. Journal of Applied Physics, 2022, 132, .	2.5	5
741	Molecular dynamics study of liquid–vapor transition in underwater electrical wire explosion. Physics of Plasmas, 2022, 29, .	1.9	2

#	Article	IF	CITATIONS
742	Entropy scaling of viscosity for molecular models of molten salts. Journal of Chemical Physics, 2023, 158, .	3.0	5
743	Buckling instability and compressive deformation of Ni-Co-Cr medium-entropy alloy nanotubes. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 015007.	2.0	3
744	The importance of localized modes spectral contribution to thermal conductivity in amorphous polymers. Communications Physics, 2022, 5, .	<b>5.</b> 3	4
745	Molecular dynamics simulations of austenite-martensite interface migration in NiTi alloy. Physical Review Materials, 2022, 6, .	2.4	2
746	Predicting molecule size distribution in hydrocarbon pyrolysis using random graph theory. Journal of Chemical Physics, 2023, 158, .	3.0	0
747	Adaptive Distributed Parallel Training Method for a Deep Learning Model Based on Dynamic Critical Paths of DAG. Mathematics, 2022, 10, 4788.	2.2	1
748	Computational Design of Antimicrobial Active Surfaces via Automated Bayesian Optimization. ACS Biomaterials Science and Engineering, 2023, 9, 269-279.	5.2	4
749	AutoMat: Automated materials discovery for electrochemical systems. MRS Bulletin, 0, , .	3.5	1
750	Wetting characteristics of ethane droplet – A molecular dynamics study. Journal of Molecular Liquids, 2023, 371, 121115.	4.9	6
751	Failure and Mechanical Properties of Glassy Diblock Copolymer Thin Films. Macromolecules, 2022, 55, 10880-10890.	4.8	2
752	Deformation Behavior of Crystalline Cr–Ni Multilayer Coatings by Using Molecular Dynamics Simulation. Lubricants, 2022, 10, 357.	2.9	1
753	Deformation behavior of single-crystal magnesium during Nano-ECAP simulation. Heliyon, 2022, 8, e11837.	3.2	1
754	The Role of the Extrafibrillar Volume on the Mechanical Properties of Molecular Models of Mineralized Bone Microfibrils. ACS Biomaterials Science and Engineering, 2023, 9, 230-245.	5.2	2
755	ReaxFF-based nonadiabatic dynamics method for azobenzene derivatives. Journal of Chemical Physics, 2022, 157, 244101.	3.0	0
756	Inclusion Polymerization of Pyrrole and Ethylenedioxythiophene in Assembled Triphenylamine <i>Bis</i> -Urea Macrocycles. Macromolecules, 2022, 55, 11013-11022.	4.8	4
757	AtomAl framework for deep learning analysis of image and spectroscopy data in electron and scanning probe microscopy. Nature Machine Intelligence, 2022, 4, 1101-1112.	16.0	23
758	Influence of Target-Substrate Distance on the Transport Process of Sputtered Atoms: MC-MD Multiscale Coupling Simulation. Materials, 2022, 15, 8904.	2.9	3
759	Emergence of layered nanoscale mesh networks through intrinsic molecular confinement self-assembly. Nature Nanotechnology, 2023, 18, 273-280.	31.5	16

#	Article	IF	CITATIONS
760	Development and Validation of Versatile Deep Atomistic Potentials for Metal Oxides. Journal of Physical Chemistry Letters, 2023, 14, 468-475.	4.6	8
761	A texture connection model of as-extruded magnesium alloy in semi-solid partial remelting process. Journal of Materials Science, 2023, 58, 1330-1344.	3.7	2
762	Free Energy Methods for the Description of Molecular Processes. Annual Review of Biophysics, 2023, 52, 113-138.	10.0	17
763	Building blocks of non-Euclidean ribbons: size-controlled self-assembly <i>via</i> discrete frustrated particles. Soft Matter, 2023, 19, 858-881.	2.7	4
764	Surface morphology and carbon structure effects on sputtering: Bridging scales between molecular dynamics simulations and experiments. Carbon, 2023, 205, 180-193.	10.3	6
765	A Mori–Zwanzig Dissipative Particle Dynamics Approach for Anisotropic Coarse Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2023, 19, 910-923.	5.3	3
766	HPC Hardware Design Reliability Benchmarking With HDFIT. IEEE Transactions on Parallel and Distributed Systems, 2023, 34, 995-1006.	5.6	3 Dyarloch 10 1
767		3.8	5
768	Detection of Toxic Gases. Physical Review Applied, 2023, 19,. Revisiting the Conformational Isomerism of Dihaloethanes: A Hybrid Computational and Experimental Laboratory for the Undergraduate Curriculum. ACS Physical Chemistry Au, 2023, 3, 157-166.	4.0	1
769	Conformations of polyolefins on platinum catalysts control product distribution in plastics recycling. Chemical Science, 2023, 14, 1966-1977.	7.4	7
770	Atomistic understanding towards twin boundary on the effect of crack propagation in FeNiCrCoCu high-entropy alloy and Ni. Materials Today Communications, 2023, 34, 105414.	1.9	1
771	Modulation of Structural, Electronic, and Optical Properties of Titanium Nitride Thin Films by Regulated In Situ Oxidation. ACS Applied Materials & Samp; Interfaces, 2023, 15, 4733-4742.	8.0	4
772	Molecular Dynamics Study on Hugoniot State and Mie–GrÃ⅓neisen Equation of State of 316 Stainless Steel for Hydrogen Storage Tank. Materials, 2023, 16, 628.	2.9	0
773	Formation of Amorphous Carbon Multiâ€Walled Nanotubes from Random Initial Configurations. Physica Status Solidi (B): Basic Research, 2023, 260, .	1.5	8
774	Disordered interfaces of alkaline aluminate salt hydrates provide glimpses of Al3+ coordination changes. Journal of Colloid and Interface Science, 2023, , .	9.4	0
775	Fibrin fiber deformation mechanisms: insights from phenomenological modeling to molecular details. Biomechanics and Modeling in Mechanobiology, 2023, 22, 851-869.	2.8	1
776	Giant Electrostriction Enabled by Defect-Induced Critical Phenomena in Relaxor Ferroelectric Polymers. Macromolecules, 2023, 56, 690-696.	4.8	8
777	Adsorption of water and organic solvents on the calcite <a href="millimg">millimg</a> : xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"> <mml:mrow><mml:moo><mml:moo><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mrow><mml:mrow><mml:mrow><mml:moo stretchv="false">Â-</mml:moo></mml:mrow></mml:mrow></mml:mrow></mml:mover></mml:moo></mml:moo></mml:mrow> <td>6.1</td> <td>2</td>	6.1	2

#	Article	IF	CITATIONS
778	Energy localization efficiency in 1,3,5-trinitro-2,4,6-triaminobenzene pore collapse mechanisms. Journal of Applied Physics, 2023, $133$ , .	2.5	9
779	Dispersion and orientation patterns in nanorod-infused polymer melts. Journal of Chemical Physics, 2023, 158, .	3.0	3
780	Learning pair potentials using differentiable simulations. Journal of Chemical Physics, 2023, 158, .	3.0	8
781	Decomposition mechanism of 1,3,5-trinitro-2,4,6-trinitroaminobenzene under thermal and shock stimuli using ReaxFF molecular dynamics simulations. Physical Chemistry Chemical Physics, 2023, 25, 3799-3805.	2.8	5
782	Computational Simulations of Fabrication of Aluminum-Based Josephson Junctions: Topological Aspects of the Barrier Structure. Entropy, 2023, 25, 182.	2.2	0
784	Model studies on motion of respiratory droplets driven through a face mask. Europhysics Letters, 2023, 141, 27001.	2.0	0
785	Thermal effects on removal mechanism of monocrystal SiC during micro-laser assisted nanogrinding process. Ceramics International, 2023, 49, 15349-15356.	4.8	4
786	TeraChem protocol buffers (TCPB): Accelerating QM and QM/MM simulations with a client–server model. Journal of Chemical Physics, 2023, 158, .	3.0	2
787	Tutorial: Systematic development of polynomial machine learning potentials for elemental and alloy systems. Journal of Applied Physics, 2023, 133, .	2.5	4
788	Predicting mechanical fields near cracks using a progressive transformer diffusion model and exploration of generalization capacity. Journal of Materials Research, 2023, 38, 1317-1331.	2.6	9
789	An interplay between a hydrogen atmosphere and dislocation characteristics in BCC Fe from time-averaged molecular dynamics. Physical Chemistry Chemical Physics, 2023, 25, 8369-8375.	2.8	3
790	Simulation of bulk and grain boundary diffusion phenomena in a high entropy CoCrFeMnNi alloy by molecular dynamics. Physica Scripta, 0, , .	2.5	1
791	How to accurately predict nanoscale flow: Theory of single-phase or two-phase?. Physics of Fluids, 2023, 35, .	4.0	9
792	Effects of 2D filler on rheology of additive manufacturing polymers: Simulation and experiment on polyetherketoneketone-mica composites. Polymer, 2023, 269, 125722.	3.8	3
793	Structure and Mechanical Properties of a Porous Polymer Material via Molecular Dynamics Simulations. Polymers, 2023, 15, 358.	4.5	0
794	Insight into pyrolysis behavior of silicone-phenolic hybrid aerogel through thermal kinetic analysis and ReaxFF MD simulations. Chemical Engineering Journal, 2023, 458, 141480.	12.7	14
795	Spatially resolved structural order in low-temperature liquid electrolyte. Science Advances, 2023, 9, .	10.3	12
796	Comparative studies of interatomic potentials for modeling point defects in wurtzite GaN. AIP Advances, 2023, 13, 015015.	1.3	1

#	Article	IF	CITATIONS
797	Atomic simulation study on the effect of Y atom and grain boundary on tensile deformation in polycrystalline magnesium alloy. Journal of Materials Research and Technology, 2023, 23, 931-942.	5.8	8
798	Machine Learning Techniques inÂReactive Atomistic Simulations. Lecture Notes in Energy, 2023, , 15-52.	0.3	0
799	Self-diffusion and shear viscosity for the TIP4P/Ice water model. Journal of Chemical Physics, 2023, 158,	3.0	5
800	Using molecular dynamics to simulate realistic structures of nitrocellulose of different nitration levels. Physical Chemistry Chemical Physics, 2023, 25, 3190-3198.	2.8	2
801	Effects of MOF linker rotation and functionalization on methane uptake and diffusion. Molecular Systems Design and Engineering, 2023, 8, 527-537.	3.4	1
802	Thermal transport across the CoSb <sub>3</sub> –graphene interface. Physical Chemistry Chemical Physics, 2023, 25, 2517-2522.	2.8	0
803	Molecular dynamics study of thermal transport across Ga2O3–diamond interfaces. Applied Physics Letters, 2023, 122, .	3.3	7
804	Predicting Structural Properties of Pure Silica Zeolites Using Deep Neural Network Potentials. Journal of Physical Chemistry C, 2023, 127, 1455-1463.	3.1	5
805	Penetration of Cell Surface Glycocalyx by Enveloped Viruses Is Aided by Weak Multivalent Adhesive Interaction. Journal of Physical Chemistry B, 2023, 127, 486-494.	2.6	0
806	Machine Learning Interatomic Potential to Investigate Fundamentals of Electrolytes for Li-ion Solid-State Batteries., 2023, 1, 83-91.		2
807	Fracture behavior of B2 phase matrix of Ti2AlNb-based alloy with microcracks of different orientations. Engineering Fracture Mechanics, 2023, 279, 109050.	4.3	2
808	Stretch-activated ionic currents through Ti3C2(OH)2 MXene nanopores. Electrochemistry Communications, 2023, 147, 107434.	4.7	1
809	The vibrational entropy spectra of grain boundary segregation in polycrystals. Acta Materialia, 2023, 245, 118630.	7.9	10
810	Molecular dynamics simulations of active entangled polymers reptating through a passive mesh. Polymer, 2023, 268, 125677.	3.8	4
811	Contact models for the multi-sphere discrete element method. Powder Technology, 2023, 416, 118209.	4.2	3
812	Effects of transverse compression on the structure and axial tensile properties of polyethylene: A molecular simulation study. Polymer, 2023, 267, 125660.	3.8	3
813	Atomistic investigation of the impact of phosphorus impurities on the tungsten grain boundary decohesion. Computational Materials Science, 2023, 219, 112017.	3.0	3
814	Biomimetic bone tissue structure: An ultrastrong thermal energy storage wood. Chemical Engineering Journal, 2023, 457, 141351.	12.7	10

#	Article	IF	CITATIONS
815	Deuterium retention in CVD diamond: Combined experimental and computational study. Fusion Engineering and Design, 2023, 188, 113403.	1.9	0
816	Design of functionally graded Ti–Al alloy with adjustable mechanical properties: a molecular dynamics insights. Journal of Materials Research and Technology, 2023, 23, 258-267.	5.8	3
817	Data-driven many-body potentials from density functional theory for aqueous phase chemistry. Chemical Physics Reviews, 2023, 4, .	5.7	4
818	Investigations on the damping of acoustic vibrations of single gold nanoparticles in water by continuum and atomistic simulations. Materials Today Communications, 2023, 34, 105314.	1.9	2
819	Mechanical properties of twisted CNT fibers: A molecular dynamic study. Materials Today Communications, 2023, 34, 105378.	1.9	1
820	Unravelling the dissolution dynamics of silicate minerals by deep learning molecular dynamics simulation: A case of dicalcium silicate. Cement and Concrete Research, 2023, 165, 107092.	11.0	6
821	Enabling molecular dynamics simulations of helium bubble formation in tritium-containing austenitic stainless steels: An Fe-Ni-Cr-H-He potential. Journal of Nuclear Materials, 2023, 575, 154232.	2.7	1
822	Molecular dynamics study of the effect of substrate temperature on the barrier behavior in aluminum oxide Josephson junctions. Applied Surface Science, 2023, 615, 156369.	6.1	0
823	Nonlinear elastic behavior of 2D materials using molecular statics and comparisons with first principles calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2023, 148, 115633.	2.7	2
824	Assessment of the impact of reactor residence time distribution on non-equilibrium product selectivity of polypropylene pyrolysis using reactive molecular dynamics simulations. Fuel, 2023, 338, 127328.	6.4	2
825	Influence of V addition on the mechanical properties of FeCo alloys: a molecular dynamics study. Materialia, 2023, 27, $101670$ .	2.7	1
826	Experimental and ReaxFF molecular dynamic study of NO emission during municipal sludge/coal co-combustion. Fuel, 2023, 338, 127342.	6.4	10
827	Cluster classification by chemi-topology. Computer Physics Communications, 2023, 286, 108659.	<b>7.</b> 5	1
828	Combustion simulations of AlH3 and ethanol nanofluid by ReaxFF. Fuel, 2023, 339, 127438.	6.4	2
829	The Impact of the Temperature Control Strategy in Steady-State Virtual Vacuum Simulation on the Spontaneous Evaporation Rate and Corresponding Evaporation Coefficient. Applied Sciences (Switzerland), 2023, 13, 256.	2.5	2
830	New findings related to carbothermal reduction of polysiloxane-derived ceramics. Ceramics International, 2023, 49, 10193-10197.	4.8	2
831	Expansion of Single Chains Released from a Spherical Cavity. Polymers, 2023, 15, 198.	4.5	1
832	Probing the Na <sup>+</sup> /Li <sup>+</sup> â€ions Insertion Mechanism in an Aqueous Mixedâ€ion Rechargeable Batteries with NASICONâ€NaTi <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> Anode and Olivineâ€LiFePO <sub>4</sub> Cathode. ChemElectroChem, 0, , .	3.4	0

#	Article	IF	CITATIONS
833	Optimally rejuvenated model binary glasses. Physical Review Materials, 2022, 6, .	2.4	0
834	A Guide to In Silico Drug Design. Pharmaceutics, 2023, 15, 49.	4.5	22
835	Molecular dynamics simulations of reactive neutral chemistry in an argonâ€methane plasma. Plasma Processes and Polymers, 2023, 20, .	3.0	3
836	Superfast Mass Transport of Na/K Via Mesochannels for Dendriteâ€Free Metal Batteries. Advanced Materials, 0, , 2210447.	21.0	8
837	Understanding Interfacial Block Copolymer Structure and Dynamics. Macromolecules, 2023, 56, 762-771.	4.8	4
838	Collective Variables for Conformational Polymorphism in Molecular Crystals. Journal of Physical Chemistry Letters, 2023, 14, 971-976.	4.6	5
839	Can graphene improve the thermal conductivity of copper nanofluids?. Physical Chemistry Chemical Physics, 2023, 25, 5489-5500.	2.8	2
840	Modeling of minimal systems based on ATP-Zn coordination for chemically fueled self-assembly. Physical Chemistry Chemical Physics, 2023, 25, 6102-6111.	2.8	2
841	Atomistic simulation of soft porous coordination polymers. Journal of Chemical Physics, 2023, 158, .	3.0	2
842	The application of QM/MM simulations in heterogeneous catalysis. Physical Chemistry Chemical Physics, 2023, 25, 6562-6585.	2.8	9
843	A coarse-grained molecular dynamics investigation of the role of mineral arrangement on the mechanical properties of mineralized collagen fibrils. Journal of the Royal Society Interface, 2023, 20, .	3.4	5
844	Response of Sulfonated Polystyrene Melts to Nonlinear Elongation Flows. Macromolecules, 2023, 56, 947-953.	4.8	3
845	Raman spectroscopy and molecular dynamics simulation studies of graphitic nanomaterials., 2023,, 363-399.		1
846	Plume-Material Interactions of Metallic Surfaces Bombarded by an [EMIM][BF <sub>4</sub> ] Electrospray Source., 2023,,.		1
847	Molecular study of core-shell ratio effect on thermophysical properties of SiO2@Au-water nanofluid. Journal of Enhanced Heat Transfer, 2023, , .	1.1	1
848	Unified graph neural network force-field for the periodic table: solid state applications. , 2023, 2, 346-355.		11
849	Inhibition of electric field on inception soot formation: A ReaxFF MD and DFT study. International Journal of Hydrogen Energy, 2023, 48, 15695-15708.	7.1	6
850	Current Trends and Changes in Use of Membrane Molecular Dynamics Simulations within Academia and the Pharmaceutical Industry. Membranes, 2023, 13, 148.	3.0	1

#	ARTICLE	IF	CITATIONS
851	Connecting Vibrational Spectroscopy to Atomic Structure via Supervised Manifold Learning: Beyond Peak Analysis. Chemistry of Materials, 2023, 35, 1186-1200.	6.7	2
852	Commensurate and incommensurate double moir $\tilde{A}$ $\tilde{\mathbb{Q}}$ interference in twisted trilayer graphene. Physical Review B, 2023, 107, .	3.2	5
853	Voronoi tessellation-based algorithm for determining rigorously defined classical and generalized geometric pore size distributions. Physical Review E, 2023, $107$ , .	2.1	2
854	Influencing Molecular Dynamics Simulations of Ion-Exchange Membranes by Considering Comonomer Propagation. Macromolecules, 2023, 56, 1263-1277.	4.8	1
855	Effect of the Graphitization Mechanism on the Friction and Wear Behavior of DLC Films Based on Molecular Dynamics Simulations. Langmuir, 2023, 39, 1905-1913.	3.5	8
856	2D Materials Guided Self-assembly of Polymer: Molecular Dynamics Simulation Study. , 2023, , .		2
857	Quantification of the Kinetic Energy Conversion to Temperature Increase in Metal-on-Metal Impacts up to Hypervelocity Conditions by Molecular Dynamics Simulation. Journal of Dynamic Behavior of Materials, 2023, 9, 240-246.	1.7	2
858	Molecular dynamics simulations of the monomer density profiles of knotted ring polymer chains confined in a slit of two parallel walls with one attractive and another repulsive surface Journal of Physics: Conference Series, 2023, 2436, 012031.	0.4	0
859	Impact of granular inclusions on the phase behavior of colloidal gels. Soft Matter, 2023, 19, 1342-1347.	2.7	1
860	Dynamic structure factor and excitation spectrum of the oneâ€component plasma: The case of weak to moderate magnetization. Contributions To Plasma Physics, 2023, 63, .	1.1	0
861	Investigation of H <sub>2</sub> S Diffusion in Transcritical and Supercritical Water: A Molecular Dynamics Simulation Study. Industrial & Engineering Chemistry Research, 2023, 62, 3026-3037.	3.7	1
862	From Molecular to Multiasperity Contacts: How Roughness Bridges the Friction Scale Gap. ACS Nano, 2023, 17, 2205-2211.	14.6	5
863	Molecular Dynamics Simulation Studies of Properties, Preparation, and Performance of Silicon Carbide Materials: A Review. Energies, 2023, 16, 1176.	3.1	8
864	Molecular Dynamics Approach to the Physical Mixture of In2O3 and ZrO2: Defect Formation and Ionic Diffusion. International Journal of Molecular Sciences, 2023, 24, 2426.	4.1	1
865	Titanium content and columnar particles effect on the deformation behaviors of nanocrystalline Ni–Ti alloy with GBAZ segregation. Applied Physics A: Materials Science and Processing, 2023, 129, .	2.3	2
866	Multiwall Carbon Nanotubes for Solid Lubrication of Highly Loaded Contacts. ACS Applied Nano Materials, 2023, 6, 1755-1769.	5.0	3
867	Thermal capillary waves on bounded nanoscale thin films. Physical Review E, 2023, 107, .	2.1	3
868	Probing the molecular-level energy absorption mechanism and strategic sequencing of graphene/Al composite laminates under high-velocity ballistic impact of nano-projectiles. Applied Surface Science, 2023, 629, 156502.	6.1	5

#	Article	IF	CITATIONS
869	Effects of Missing Linker Defects on the Elastic Properties and Mechanical Stability of the Metal–Organic Framework HKUST-1. Journal of Physical Chemistry C, 2023, 127, 2533-2543.	3.1	5
870	Learning local equivariant representations for large-scale atomistic dynamics. Nature Communications, 2023, $14$ , .	12.8	86
871	Physics-separating artificial neural networks for predicting initial stages of Al sputtering and thin film deposition in Ar plasma discharges. Journal Physics D: Applied Physics, 2023, 56, 084003.	2.8	5
872	LAVA 1.0: A general-purpose python toolkit for calculation of material properties with LAMMPS and VASP. Computer Physics Communications, 2023, 286, 108667.	7.5	4
873	Investigating the thermal behavior of phase change materials of ethylene glycol-filled SiO2 plates in the presence of solar radiation by molecular dynamics simulation. Engineering Analysis With Boundary Elements, 2023, 150, 1-6.	3.7	3
874	Water filling in carbon nanotubes with different wettability and implications on nanotube/water heat transfer via atomistic simulations. International Journal of Heat and Mass Transfer, 2023, 205, 123868.	4.8	4
875	Rigid Procedure to Calculate the Melting Point of Metal Using the Solid-Liquid Phase (Coexistence) Method. Jurnal Ilmu Fisika   Universitas Andalas, 2022, 14, 132-140.	0.2	0
876	Not All GPUs Are Created Equal: Characterizing Variability in Large-Scale, Accelerator-Rich Systems. , 2022, , .		3
877	Scaling Podman on Perlmutter: Embracing a community-supported container ecosystem., 2022,,.		0
878	Molecular Dynamics Simulations of a Cross-linked Epoxy-resin Sample. , 2022, , .		1
879	Structure of Hydrocarbon Fluid and Couette Flows in Slit Pores with Pyrophyllite Walls. Polymer Science - Series A, 2022, 64, 908-917.	1.0	1
880	Mechanical and thermal properties of graphyne-coated carbon nanotubes: a molecular dynamics simulation on one-dimensional all-carbon van der Waals heterostructures. Physical Chemistry Chemical Physics, 2023, 25, 8651-8663.	2.8	3
881	Molecular Dynamics Simulation of Ti Metal Cutting Using a TiN:Ag Self-Lubricating Coated Tool. Materials, 2023, 16, 1344.	2.9	2
882	A Review of the Mechanical Properties of Graphene Aerogel Materials: Experimental Measurements and Computer Simulations. Materials, 2023, 16, 1800.	2.9	3
883	Bottom-Up Informed and Iteratively Optimized Coarse-Grained Non-Markovian Water Models with Accurate Dynamics. Journal of Chemical Theory and Computation, 2023, 19, 1099-1110.	5.3	6
884	A Molecular Dynamics Study on the Local Structure of Al90Sm10 Marginal Metallic Glass and Liquid. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 0, , .	2.2	0
885	Molecular dynamics simulation of thermomechanical fatigue properties of Ni-based single crystal superalloys. International Journal of Fatigue, 2023, 173, 107667.	5.7	2
886	Research on pore closure behavior and microstructure evolution during hot isostatic pressing of Ti6Al4V alloy casting. Journal of Materials Research and Technology, 2023, 24, 3628-3642.	5.8	4

#	Article	IF	CITATIONS
887	Self-Ordering of Buckling, Bending, and Bumping Beams. Physical Review Letters, 2023, 130, .	7.8	5
888	Variation of Spring Stiffness, Monomeric Friction, and Brownian Intensity in the Simulation System of Unentangled Melt under Steady Flow. Macromolecules, 2023, 56, 2911-2929.	4.8	2
889	Modelling across Multiple Scales to Design Biopolymer Membranes for Sustainable Gas Separations: 1—Atomistic Approach. Polymers, 2023, 15, 1805.	4.5	2
890	Theoretical insight into the competitive effect of CO2 and additive H2O in coke gasification. Chemical Engineering Journal, 2023, 461, 142003.	12.7	3
891	Mechanistic insights into the deformation and degradation of a 2D metal organic framework. Npj 2D Materials and Applications, 2023, 7, .	7.9	1
892	How Regiochemistry Influences Aggregation Behavior and Charge Transport in Conjugated Organosulfur Polymer Cathodes for Lithium–Sulfur Batteries. ACS Nano, 2023, 17, 7889-7900.	14.6	8
893	Thermal conductivity across transition metal dichalcogenide bilayers. IScience, 2023, 26, 106447.	4.1	1
894	Fast proper orthogonal descriptors for many-body interatomic potentials. Physical Review B, 2023, 107,	3.2	1
895	Effects of oxidizers on the ignition and combustion characteristics of aluminum nanoparticles. Computational Materials Science, 2023, 223, 112116.	3.0	2
896	Effect of anisotropy on deformation and crack formation under the brittle removal of 6H-SiC during SPDT process. Journal of Advanced Research, 2024, 56, 103-112.	9.5	2
897	Tensile and Compressive Behavior of CHCâ€Reinforced Copper using Molecular Dynamics. Advanced Engineering Materials, 2023, 25, .	3.5	1
898	Interactions between Rigid Polyelectrolytes Mediated by Ordering and Orientation of Multivalent Nonspherical Ions in Salt Solutions. Physical Review Letters, 2023, 130, .	7.8	2
899	Soil amended with Algal Biochar Reduces Mobility of deicing salt contaminants in the environment: An atomistic insight. Chemosphere, 2023, 323, 138172.	8.2	6
900	Graph neural networks predict energetic and mechanical properties for models of solid solution metal alloy phases. Computational Materials Science, 2023, 224, 112141.	3.0	3
901	Block-movement-based calibration of a discrete element model for fine, cohesive powders. Powder Technology, 2023, 421, 118411.	4.2	1
902	Molecular dynamics simulation of the lubricant conformation changes and energy transfer of the confined thin lubricant film. Chemical Engineering Science, 2023, 270, 118541.	3.8	5
903	Solidification of the glass-forming Al86Ni2Co6Gd6 melt under high pressure. Materialia, 2023, 28, 101713.	2.7	0
904	Performance of supercapacitors containing graphene oxide and ionic liquids by molecular dynamics simulations. Carbon, 2023, 208, 102-110.	10.3	5

#	Article	IF	CITATIONS
905	Effect of crystalline phase on deformation behaviors of amorphous matrix in a metallic glass composite. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2023, 872, 144957.	5.6	1
906	A critical review on molecular dynamics applied to structure fracture and failure analysis. Engineering Analysis With Boundary Elements, 2023, 150, 413-422.	3.7	2
907	Multifunctional hyperbranched prepolymers with tailored degree of methylation and methacrylation. Polymer, 2023, 276, 125886.	3.8	2
908	A comprehensive atomistic investigation on the cascade induced helium bubble motion in bcc iron for neutron irradiated RAFM steels. Journal of Nuclear Materials, 2023, 578, 154373.	2.7	1
909	A novel strengthening mechanism in crystalline/amorphous dual-phase Mg alloys: A molecular dynamics study. Journal of Non-Crystalline Solids, 2023, 608, 122241.	3.1	4
910	Molecular dynamics study of grain boundary and radiation effects on tritium population and diffusion in zirconium. Journal of Nuclear Materials, 2023, 578, 154376.	2.7	3
911	Phonon thermal transport in two-dimensional PbTe monolayers via extensive molecular dynamics simulations with a neuroevolution potential. Materials Today Physics, 2023, 34, 101066.	6.0	2
912	Proper orthogonal descriptors for efficient and accurate interatomic potentials. Journal of Computational Physics, 2023, 480, 112030.	3.8	5
913	Monte Carlo simulations of ion channeling in the presence of dislocation loops: New development in the McChasy code. Nuclear Instruments & Methods in Physics Research B, 2023, 538, 198-204.	1.4	2
914	On the origins of backscattered solar wind energetic neutral hydrogen from the Moon and Mercury. Planetary and Space Science, 2023, 229, 105660.	1.7	5
915	Hydrogen distribution between the Earth's inner and outer core. Earth and Planetary Science Letters, 2023, 609, 118084.	4.4	4
916	Helium focused ion beam induced subsurface damage on Si and SiC substrates: experiments and generative deep neural network modeling via position-dependent input. Journal of Materials Research and Technology, 2023, 24, 3363-3382.	5.8	3
917	Two-dimensional borocarbonitrides nanosheets engineered sulfonated polyether sulfone microspheres as highly efficient and photothermally recyclable adsorbents for hemoperfusion. Chemical Engineering Journal, 2023, 463, 142365.	12.7	3
918	Atomic diffusion, segregation, and grain boundary migration in nickel-based alloys from molecular dynamics simulations. Materials Today Communications, 2023, 35, 105768.	1.9	5
919	Automated calculations of exchange magnetostriction. Computational Materials Science, 2023, 224, 112158.	3.0	1
920	Machine learning insight into h-BN growth on Pt(111) from atomic states. Applied Surface Science, 2023, 621, 156893.	6.1	4
921	Effect of natural zeolite on water distribution and migration in low water/binder cement-based composites (LW/B-CC) mixed with seawater: An experimental and computational investigation. Construction and Building Materials, 2023, 379, 131242.	7.2	2
922	Investigation of nanoparticles shape that influence the thermal conductivity and viscosity in argon-based nanofluids: A molecular dynamics simulation. International Journal of Heat and Mass Transfer, 2023, 207, 124031.	4.8	7

#	Article	IF	CITATIONS
923	Radiation-induced segregation at grain boundaries of alloy 800H: Experimentally-informed atomistic simulations. Journal of Nuclear Materials, 2023, 579, 154395.	2.7	0
924	Molecular dynamics investigation of the effect of ammonia on coal pyrolysis and the nitrogen transformation. Energy Conversion and Management, 2023, 285, 117006.	9.2	10
925	Thermo-physical characteristics of 3Câ€SiC structure subjected to microwave exposure: A molecular dynamics study. Materials Today Communications, 2023, 35, 105693.	1.9	3
926	Rheological analysis and molecular dynamics modeling of Ultra-High Performance Concrete for wet-mix spraying. Journal of Building Engineering, 2023, 68, 106167.	3.4	2
927	Subcontinuum scale analysis of diamond lattice films through spatial multi-level coarsening method. Thin-Walled Structures, 2023, 187, 110738.	5.3	3
928	Synergistic lubrication of organic friction modifiers in boundary lubrication regime by molecular dynamics simulations. Applied Surface Science, 2023, 623, 157087.	6.1	2
929	Thermomechanical characteristics of green nanofibers made from polylactic acid: An insight into tensile behavior via molecular dynamics simulation. Mechanics of Materials, 2023, 181, 104640.	3.2	3
930	Al-aided multiscale modeling of physiologically-significant blood clots. Computer Physics Communications, 2023, 287, 108718.	7.5	0
931	Development of an interatomic potential for mixed uranium-americium oxides and application to the determination of the structural and thermodynamic properties of (U,Am)O2 with americium contents below 50%. Journal of Nuclear Materials, 2023, 579, 154390.	2.7	2
932	Decoupling effects of C3H3/C4H5/i-C4H5/CN radicals on the formation and growth of aromatics: A ReaxFF molecular dynamics study. Journal of Aerosol Science, 2023, 171, 106185.	3.8	1
933	Molecular dynamics predictions of transport properties for carbon dioxide hydrates under pre-nucleation conditions using TIP4P/Ice water and EPM2, TraPPE, and Zhang carbon dioxide potentials. Journal of Molecular Liquids, 2023, 379, 121674.	4.9	4
934	Role of rejuvenator properties in determining the activation effects on aged asphalt based on molecular simulations. Journal of Cleaner Production, 2023, 405, 136970.	9.3	0
935	Atomistic insights into the inhomogeneous nature of solute segregation to grain boundaries in magnesium. Scripta Materialia, 2023, 230, 115432.	5.2	6
936	Theoretical and mechanistic insights into control factor-assisted CO2 mineralization with olivine. Journal of Industrial and Engineering Chemistry, 2023, 122, 241-250.	5.8	0
937	Structure, vibrations and electronic transport in silicon suboxides: Application to physical unclonable functions. Journal of Non-Crystalline Solids: X, 2023, 18, 100179.	1.2	1
938	Structural transformation and micro-phase separation of CaO-P2O5-SiO2 system under compression. Journal of Physics and Chemistry of Solids, 2023, 178, 111336.	4.0	0
939	Feasibility study on the use of single crystal silicon carbide as a tool material. Materials Today Communications, 2023, 35, 105824.	1.9	0
940	Molecular dynamics study on the role of hydrogen bonds and interfacial heat transfer between diverse silica surfaces and organic liquids. International Journal of Heat and Mass Transfer, 2023, 208, 124091.	4.8	7

#	Article	IF	CITATIONS
941	Nanoindentation and nanotribology behaviors of open-cell metallic glass nanofoams. International Journal of Mechanical Sciences, 2023, 249, 108254.	6.7	14
942	Self-ion irradiation effects on nanoindentation-induced plasticity of crystalline iron: A joint experimental and computational study. Nuclear Instruments & Methods in Physics Research B, 2023, 539, 55-61.	1.4	5
943	Investigation of the atomic-level microstructural evolution of quadruple-fused $\hat{l} \pm \hat{l}^2$ titanium particles during sintering. Journal of Molecular Liquids, 2023, 381, 121753.	4.9	0
944	Enhanced mechanical and thermal properties of two-dimensional SiC and GeC with temperature and size dependence. Chinese Physics B, 2023, 32, 076103.	1.4	4
945	Multiscale Acoustic Properties of Nanoporous Materials: From Microscopic Dynamics to Mechanics and Wave Propagation. Journal of Physical Chemistry C, O, , .	3.1	0
946	Ordered and amorphous phases of polyacrylonitrile: Effect of tensile deformation of structure on relaxation and glass transition. Polymer, 2023, 277, 125969.	3.8	1
947	Mechanisms of nucleation and defect growth in undercooled melt containing oxide clusters. Acta Materialia, 2023, 252, 118942.	7.9	0
948	Entrance loss of capillary flow in narrow slit nanochannels. Physics of Fluids, 2023, 35, .	4.0	7
949	Origin of metallic-like behavior in disordered carbon nano-onions. Carbon, 2023, 208, 303-310.	10.3	1
950	Effect of hydrogen on plasticity of <mml:math altimg="si15.svg" display="inline" id="d1e2764" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>î±</mml:mi></mml:math> -Fe: A multi-scale assessment. International Journal of Plasticity, 2023, 165, 103613.	8.8	4
951	<mml:math altimg="si178.svg" display="inline" id="d1e2925" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi> id="d1e2925"&gt;<mml:mi> id="d1e2925"&gt;<mml:mi> id="d1e2925"&gt;<mml:mi> id="d1e2925"&gt;<mml:math> id="d2e2925"&gt;<mml:math> id="d2e2925"&gt;&lt;</mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:math></mml:mi></mml:mi></mml:mi></mml:mi></mml:math>	3.0	7
952	Multiscale nanoindentation modelling of concentrated solid solutions: A continuum plasticity model. Mechanics of Materials, 2023, 181, 104644.	3.2	6
953	Exploring the effect of intra-chain rigidity on mixed-gas separation performance of a Triptycene-Tröger's base ladder polymer (PIM-Trip-TB) by atomistic simulations. Journal of Membrane Science, 2023, 677, 121614.	8.2	4
954	Strain driven anomalous anisotropic enhancement in the thermoelectric performance of monolayer MoS2. Applied Surface Science, 2023, 626, 157139.	6.1	12
955	New insights into the heat capacity enhancement of nano-SiO2 doped alkali metal chloride molten salt for thermal energy storage: A molecular dynamics study. Journal of Energy Storage, 2023, 63, 107015.	8.1	7
956	Evaluating the transferability of machine-learned force fields for material property modeling. Computer Physics Communications, 2023, 288, 108723.	7.5	1
957	Atomic investigation on optimal interfacial bonding for enhanced fracture properties in polymer nanocomposites. Engineering Fracture Mechanics, 2023, 281, 109078.	4.3	2
958	An atomistic study of fundamental bulk and defect properties in <mml:math altimg="si1.svg" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>1±</mml:mi></mml:math> -uranium. Journal of Nuclear Materials, 2023, 576, 154289.	2.7	1

#	Article	IF	CITATIONS
959	Strain-rate sensitivity of brittle deformation and removal mechanisms of monocrystalline 3C–SiC induced by nano cutting process. Journal of Materials Research and Technology, 2023, 23, 1397-1406.	5.8	4
960	The Physical Foundations of 3D-Printing Technology. Molecular Dynamics Simulation. Russian Physics Journal, 2022, 65, 1290-1298.	0.4	1
961	Nano and Sub-nano Scale Friction Behavior in Rotary Processing of 6H-SiC with Different Off-Axis Angles. Tribology Letters, 2023, 71, .	2.6	1
962	Effect of twins on scratching behavior of nanotwinned diamond: A molecular dynamics simulation. Applied Surface Science, 2023, 616, 156545.	6.1	6
963	Molecular dynamics simulation of reinforcement mechanism of graphene/aluminum composites and microstructure evolution. Journal of Materials Research and Technology, 2023, 23, 2147-2159.	5.8	10
964	Mechanism of polishing lutetium oxide single crystals with polyhedral diamond abrasive grains based on molecular dynamics simulation. Applied Surface Science, 2023, 616, 156549.	6.1	4
965	How Does Electronic Polarizability or Scaled-Charge Affect the Interfacial Properties of Room Temperature Ionic Liquids?. Journal of Physical Chemistry B, 2023, 127, 1264-1275.	2.6	6
966	A Practical Guide to Kinetics Calculation of Protein Conformational Change using Frequency Adaptive Metadynamics., 2023,, 1-16.		0
967	Nonequilibrium Thermodynamics of DNA Nanopore Unzipping. Physical Review Letters, 2023, 130, .	7.8	1
968	Origin of dynamical heterogeneities in borosilicate glass-forming systems. Journal of Non-Crystalline Solids, 2023, 605, 122138.	3.1	2
969	Round robin test on angle of repose: DEM simulation results collected from 16 groups around the world. Soils and Foundations, 2023, 63, 101272.	3.1	11
971	Conquering Noise With Hardware Counters on HPC Systems. , 2022, , .		0
972	A Methodology for Evaluating Tightly-integrated and Disaggregated Accelerated Architectures. , 2022, , .		0
973	Universality of moiré physics in collapsed chiral carbon nanotubes. Carbon, 2023, 205, 394-401.	10.3	5
974	KokkACC: Enhancing Kokkos with OpenACC. , 2022, , .		3
975	Effects of different incidence rates of carbon and silicon clusters on the surface properties of SiC films. Surfaces and Interfaces, 2023, 37, 102718.	3.0	1
976	A feedforward unitary equivariant neural network. Neural Networks, 2023, 161, 154-164.	5.9	0
977	One-dimensional harmonic chain model of vibration-mode matching in solid-liquid interfacial thermal transport. Physical Review E, 2023, 107, .	2.1	0

#	Article	IF	Citations
978	Molecular understanding of the Helmholtz capacitance difference between $Cu(100)$ and graphene electrodes. Journal of Chemical Physics, 2023, 158, .	3.0	8
979	Theory and molecular simulations of plasma sputtering, transport and deposition processes. European Physical Journal D, 2023, 77, .	1.3	4
980	Workflow for computational characterization of PDMS cross-linked systems. Frontiers in Built Environment, 0, 8, .	2.3	0
981	Size and Quality of Quantum Mechanical Data Set for Training Neural Network Force Fields for Liquid Water. Journal of Physical Chemistry B, 2023, 127, 1422-1428.	2.6	0
982	Evidence of Multiple Crystallization Pathways in Lithium Disilicate: A Metadynamics Investigation. Journal of Physical Chemistry Letters, 2023, 14, 1411-1417.	4.6	1
983	A "short blanket―dilemma for a state-of-the-art neural network potential for water: Reproducing experimental properties or the physics of the underlying many-body interactions?. Journal of Chemical Physics, 2023, 158, .	3.0	25
984	Effects of interfacial molecular mobility on thermal boundary conductance at solid–liquid interface. Journal of Chemical Physics, 2023, 158, .	3.0	1
985	Application Experiences on a GPU-Accelerated Arm-based HPC Testbed. , 2023, , .		2
986	Temperature-dependent elasticity of single crystalline graphite. Computational Materials Science, 2023, 220, 112045.	3.0	3
987	Calculation of dislocation binding to helium-vacancy defects in tungsten using hybrid ab initio-machine learning methods. Acta Materialia, 2023, 247, 118734.	7.9	10
988	Investigation of the Impact of High Concentration LiTFSI Electrolytes on Silicon Anodes with Reactive Force Field Simulations. Liquids, 2023, 3, 132-158.	2.5	1
989	Atomistic model of an oxide film in contact with a liquid metal coolant: Defects concentrations and chemical potentials of dissolved Fe–O. Computational Materials Science, 2023, 220, 112061.	3.0	7
990	One Step Closer to Converged Computing: Achieving Scalability with Cloud-Native HPC., 2022,,.		2
991	Molecular Dynamics Simulations ofÂtheÂThermal Evolution ofÂVoids inÂCu Bulk andÂGrain Boundaries. Minerals, Metals and Materials Series, 2023, , 1001-1010.	0.4	0
992	Interactions of cationic surfactant-fatty alcohol monolayers with natural human hair surface: Insights from dissipative particle dynamics. Journal of Molecular Liquids, 2023, 375, 121385.	4.9	3
993	Giant slip length at a supercooled liquid-solid interface. Physical Review E, 2023, 107, .	2.1	0
994	Strain-Driven Faceting of Graphene-Catalyst Interfaces. Nano Letters, 2023, 23, 1659-1665.	9.1	3
995	Simple Synthesis of Monodisperse Ultrasmall Au Icosahedral Nanoparticles. Journal of Physical Chemistry C, 2023, 127, 3047-3058.	3.1	4

#	Article	IF	CITATIONS
996	Melting conditions and entropies of superionic water ice: Free-energy calculations based on hybrid solid/liquid reference systems. Journal of Chemical Physics, 2023, 158, 064502.	3.0	0
997	Breakdown of Reye's theory in nanoscale wear. Journal of the Mechanics and Physics of Solids, 2023, 173, 105236.	4.8	4
998	Molecular dynamics simulation of illite: From particle associations to hydration properties. Applied Clay Science, 2023, 234, 106850.	5.2	1
999	Automated determination of grain boundary energy and potential-dependence using the OpenKIM framework. Computational Materials Science, 2023, 220, 112057.	3.0	4
1000	Classical density functional theory for interfacial properties of hydrogen, helium, deuterium, neon, and their mixtures. Journal of Chemical Physics, 2023, 158, .	3.0	4
1001	Fault Tolerance for Ensemble-based Molecular-Continuum Flow Simulations. , 2023, , .		1
1002	Universality of grain boundary phases in fcc metals: Case study on high-angle $[111]$ symmetric tilt grain boundaries. Physical Review B, 2023, 107, .	3.2	8
1003	Intercalation Chemistry of the Disordered Rocksalt Li <sub>3</sub> V <sub>2</sub> O <sub>5</sub> Anode from Cluster Expansions and Machine Learning Interatomic Potentials. Chemistry of Materials, 2023, 35, 1537-1546.	6.7	9
1004	Effects of Shape on Interaction Dynamics of Tetrahedral Nanoplastics and the Cell Membrane. Journal of Physical Chemistry B, 2023, 127, 1652-1663.	2.6	3
1005	Structural transformation of Ti-based alloys during tensile and compressive loading: An insight from molecular dynamics simulations. MRS Communications, 0, , .	1.8	1
1006	MDSuite: comprehensive post-processing tool for particle simulations. Journal of Cheminformatics, 2023, 15, .	6.1	0
1007	A variational approach to assess reaction coordinates for two-step crystallization. Journal of Chemical Physics, 2023, 158, .	3.0	5
1008	Study on surface thermal oxidation of silicon carbide irradiated by pulsed laser using reactive molecular dynamics. Journal of Chemical Physics, 2023, 158, .	3.0	3
1009	A Computational Study on the Role of Lubricants under Boundary Lubrication. Lubricants, 2023, 11, 80.	2.9	2
1010	Microstructural and phase changes in alpha uranium investigated via in-situ studies and molecular dynamics. Journal of Nuclear Materials, 2023, 577, 154341.	2.7	3
1011	The Sluggish Diffusion of Cations in CeO <sub>2</sub> Probed through Molecular Dynamics and Metadynamics Simulations. Advanced Engineering Materials, 2023, 25, .	3.5	О
1012	Atomistic simulation of Si-Al nanosponge structure features produced by laser printing method. Journal of Non-Crystalline Solids, 2023, 606, 122215.	3.1	0
1013	MoSDeF-GOMC: Python Software for the Creation of Scientific Workflows for the Monte Carlo Simulation Engine GOMC. Journal of Chemical Information and Modeling, 2023, 63, 1218-1228.	5.4	1

#	Article	IF	CITATIONS
1014	Frequency and field-dependent response of confined electrolytes from Brownian dynamics simulations. Journal of Chemical Physics, 2023, 158, .	3.0	3
1015	Machine learning mechanical properties of defect-engineered hexagonal boron nitride. Computational Materials Science, 2023, 220, 112030.	3.0	4
1016	Molecular Origin of Wetting Characteristics on Mineral Surfaces. Langmuir, 2023, 39, 2932-2942.	3.5	3
1017	Nanogel Degradation at Soft Interfaces and in Bulk: Tracking Shape Changes and Interfacial Spreading. Macromolecules, 2023, 56, 1289-1302.	4.8	6
1018	Solute trapping and solute drag during non-equilibrium solidification of Fe–Cr alloys. Acta Materialia, 2023, 248, 118769.	7.9	5
1019	Quantification of the atomic surfaces and volumes of a metal cluster based on the molecular surface model. Physica Scripta, 2023, 98, 045704.	2.5	O
1020	Non-polar ether-based electrolyte solutions for stable high-voltage non-aqueous lithium metal batteries. Nature Communications, 2023, $14$ , .	12.8	47
1021	Nano-deterioration of steel passivation film: chloride attack in material defects. Materials and Structures/Materiaux Et Constructions, 2023, 56, .	3.1	11
1022	Combining Machine Learning and Many-Body Calculations: Coverage-Dependent Adsorption of CO on Rh(111). Physical Review Letters, 2023, 130, .	7.8	11
1023	Stable Solid Molecular Hydrogen above 900ÂK from a Machine-Learned Potential Trained with Diffusion Quantum MonteÂCarlo. Physical Review Letters, 2023, 130, .	7.8	6
1025	Grain Boundary-Mediated Reduction of Radiation Defects in Different W-Based Alloys. Metals and Materials International, 2023, 29, 2648-2659.	3.4	1
1026	Influence of Grain Size on Mechanical Properties of a Refractory High Entropy Alloy under Uniaxial Tension. Crystals, 2023, 13, 357.	2.2	2
1027	Sensitivity of Dislocation-GB interactions to simulation setups in atomistic models. Computational Materials Science, 2023, 221, 112085.	3.0	2
1028	High-Performance and Scalable Agent-Based Simulation with BioDynaMo. , 2023, , .		1
1029	Molecular Dynamics of Nanodroplet Coalescence in Quasi-Saturated Vapor. Fluids, 2023, 8, 77.	1.7	2
1030	Comparison of Force Fields for the Prediction of Thermophysical Properties of Long Linear and Branched Alkanes. Journal of Physical Chemistry B, 2023, 127, 1789-1802.	2.6	19
1031	Elastogranular sheets. Matter, 2023, 6, 1217-1230.	10.0	2
1032	Deformation Driven Deswelling of Brush Gels. Macromolecules, 2023, 56, 2209-2216.	4.8	1

#	Article	IF	CITATIONS
1033	Mechanistic elucidation of shock response of bis(1,2,4-oxadiazole)bis(methylene) dinitrate (BOM): A ReaxFF molecular dynamics investigation. Journal of Applied Physics, 2023, 133, 085101.	2.5	0
1034	Anticorrosion Effect of Terephthalamide Core: Bis(2-hydroxybenzoic Acid) for Steel in Biogasoline. Energy & Ene	5.1	1
1035	Oxygen Vacancy Diffusion in Rutile TiO <sub>2</sub> : Insight from Deep Neural Network Potential Simulations. Journal of Physical Chemistry Letters, 2023, 14, 2208-2214.	4.6	2
1036	Templated Crystallization of Glycine Homopeptides: Experimental and Computational Developments. Chemical Engineering and Technology, 0, , .	1.5	1
1037	Electrostatic Fields Stimulate Absorption of Small Neutral Molecules in Gradient Polyelectrolyte Brushes. ChemPhysChem, 2023, 24, .	2.1	1
1038	A general expression for the statistical error in a diffusion coefficient obtained from a solidâ€state <scp>molecularâ€dynamics</scp> simulation. Journal of Computational Chemistry, 2023, 44, 1347-1359.	3.3	3
1039	Boron Nitride Nanotubes: Force Field Parameterization, Epoxy Interactions, and Comparison with Carbon Nanotubes for High-Performance Composite Materials. ACS Applied Nano Materials, 2023, 6, 3513-3524.	5.0	2
1040	Evolutionarily distinct and sperm-specific supersized chromatin loops are marked by Helitron transposons in Xenopus tropicalis. Cell Reports, 2023, 42, 112151.	6.4	1
1041	Toward Atomistic Understanding of Materials with the Conversion–Alloying Mechanism in Li-Ion Batteries. Chemistry of Materials, 2023, 35, 2835-2845.	6.7	2
1042	Aggregation and disaggregation processes in clusters of particles under flow: Simple numerical and theoretical insights. Physical Review Fluids, 2023, 8, .	2.5	0
1043	Effect of surfactants on SARS-CoV-2: Molecular dynamics simulations. Journal of Chemical Physics, 2023, 158, .	3.0	2
1044	Modeling and simulation of coverage and film properties in deposition process on large-scale pattern using statistical ensemble method. Japanese Journal of Applied Physics, 2023, 62, SI1006.	1.5	1
1045	Multiscale simulations of nanofluidics: Recent progress and perspective. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	3
1046	Polymer simulations guide the detection and quantification of chromatin loop extrusion by imaging. Nucleic Acids Research, 2023, 51, 2614-2632.	14.5	2
1047	Structural Spectrum of 2D Materials in Solution: Toward Establishing 2D Assemblies' Digital Factory. Advanced Materials Interfaces, 2023, 10, .	3.7	0
1048	Molecular simulation and experimental analysis on co-aging behaviors of SBS modifier and asphalt in SBS-modified asphalt. Molecular Simulation, 2023, 49, 629-642.	2.0	7
1049	Atomic study of the trapped and migration patterns of point defects around screw dislocation in tungsten. Nuclear Materials and Energy, 2023, 34, 101400.	1.3	0
1050	Network dynamics: a computational framework for the simulation of the glassy state. Molecular Systems Design and Engineering, 2023, 8, 1013-1029.	3.4	2

#	Article	IF	CITATIONS
1051	Molecular Dynamics Study on the Dependence of Size and Strain on Thermal Conductivity of GaN Nanofilms. Chinese Physics B, 0, , .	1.4	0
1052	Study on the Nano-Friction Behavior of Nickel-Based Ag Film Composites Based on Molecular Dynamics. Lubricants, 2023, 11, 110.	2.9	O
1053	Rocketâ€Released Neutral Clouds in the Ionosphere: Formation, Evolution, and Detection. Journal of Geophysical Research: Space Physics, 2023, 128, .	2.4	3
1054	Topological defects in silicene. Europhysics Letters, 2023, 141, 66001.	2.0	2
1055	Electrical noise in electrolytes: a theoretical perspective. Faraday Discussions, 0, , .	3.2	2
1056	Routine Molecular Dynamics Simulations Including Nuclear Quantum Effects: From Force Fields to Machine Learning Potentials. Journal of Chemical Theory and Computation, 2023, 19, 1432-1445.	<b>5.</b> 3	11
1057	Density dependence of elastic properties of graphynes. MRS Advances, 0, , .	0.9	0
1058	Nanoâ€Biotechnology and Challenges of Drug Delivery System in Cancer Treatment Pathway: Review Article. Chemistry and Biodiversity, 2023, 20, .	2.1	6
1059	Atomistic insights into the H2 adsorption and desorption behavior of novel Li-functionalized polycrystalline CNTs. Carbon, 2023, 207, 23-35.	10.3	8
1060	Physics-separating artificial neural networks for predicting sputtering and thin film deposition of AlN in Ar/N <sub>2</sub> discharges on experimental timescales. Journal Physics D: Applied Physics, 2023, 56, 194001.	2.8	2
1061	Lithium Ion Transport Environment by Molecular Vibrations in Ion onducting Glasses. Energy and Environmental Materials, 0, , .	12.8	2
1062	Experiment and multiscale molecular simulations on the Cu absorption by biochar-modified asphalt: An insight into removal capability and mechanism of heavy metals from stormwater runoff. Chemical Engineering Journal, 2023, 462, 142205.	12.7	12
1063	Composition-dependent fracture energy in metallic glasses. Physical Review Materials, 2023, 7, .	2.4	1
1064	<i>Ab Initio</i> Melting Temperatures of Bcc and Hcp Iron Under the Earth's Inner Core Condition. Geophysical Research Letters, 2023, 50, .	4.0	10
1065	Analyteâ€Driven Clustering of Bioâ€Conjugated Magnetic Nanoparticles. Advanced Theory and Simulations, 2023, 6, .	2.8	0
1066	Innate dynamics and identity crisis of a metal surface unveiled by machine learning of atomic environments. Journal of Chemical Physics, 2023, 158, .	3.0	6
1067	Molecular dynamics simulations of Carbyne/Carbon nanotube gigahertz oscillators. Computational Materials Science, 2023, 222, 112105.	3.0	2
1068	The characterization of plastic behavior and mechanical properties in the gradient nanostructured copper. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications, 2023, 237, 1910-1920.	1.1	5

#	Article	IF	CITATIONS
1069	Truncated atomic plane wave method for subband structure calculations of moir $\tilde{A}$ $\otimes$ systems. Physical Review B, 2023, 107, .	3.2	2
1070	On the challenge of sampling multiple nucleation pathways: A case study of heterogeneous ice nucleation on FCC (211) surface. Journal of Chemical Physics, 2023, 158, .	3.0	3
1071	Evolution of the Microstructure, Hybridization, and Internal Stress of Al-Doped Diamond-Like Carbon Coatings: A Molecular Dynamics Simulation. Langmuir, 2023, 39, 3895-3904.	3.5	3
1072	C–B–A Test of DNA Force Fields. ACS Omega, 2023, 8, 10253-10265.	3.5	5
1073	Crosslinking Rapidly Cured Epoxy Resin Thermosets: Experimental and Computational Modeling and Simulation Study. Polymers, 2023, 15, 1325.	4.5	0
1074	Effect of surfactants on the elasticity of the liquid–liquid interface. Journal of Chemical Physics, 2023, 158, 124901.	3.0	0
1075	Isolating Chemical Reaction Mechanism as a Variable with Reactive Coarse-Grained Molecular Dynamics: Step-Growth versus Chain-Growth Polymerization. Macromolecules, 2023, 56, 2225-2233.	4.8	3
1076	The Biological Qubit: Calcium Phosphate Dimers, Not Trimers. Journal of Physical Chemistry Letters, 2023, 14, 2518-2525.	4.6	2
1077	Modeling Catalyzed Reactions on Metal-Doped Amorphous Silicates: The Case of Niobium-Catalyzed Ethylene Epoxidation. Journal of Physical Chemistry C, 2023, 127, 4984-4997.	3.1	3
1078	A New Spinel Chloride Solid Electrolyte with High Ionic Conductivity and Stability for Na-Ion Batteries., 2023, 5, 1009-1017.		6
1079	lonic fluctuations in finite volumes: fractional noise and hyperuniformity. Faraday Discussions, 0, , .	3.2	3
1080	Atomistic Model of Wet Chemical Etching of Swift Heavy Ion Tracks. Journal of Physical Chemistry C, 2023, 127, 5090-5097.	3.1	2
1081	Anharmonic phonon behavior via irreducible derivatives: Self-consistent perturbation theory and molecular dynamics. Physical Review B, 2023, 107, .	3.2	1
1082	Quantum Informed Machine-Learning Potentials for Molecular Dynamics Simulations of CO <sub>2</sub> 's Chemisorption and Diffusion in Mg-MOF-74. ACS Nano, 2023, 17, 5579-5587.	14.6	13
1083	A Study on the Effect of Doping Metallic Nanoparticles on Fracture Properties of Polylactic Acid Nanofibres via Molecular Dynamics Simulation. Nanomaterials, 2023, 13, 989.	4.1	1
1084	Studying Crack Generation Mechanism in Single-Crystal Sapphire During Ultra-precision Machining by MD Simulation-Based Slip/Fracture Activation Model. International Journal of Precision Engineering and Manufacturing, 2023, 24, 715-727.	2.2	4
1085	Computing Viscosities of Mixtures of Ester-Based Lubricants at Different Temperatures. Journal of Physical Chemistry B, 2023, 127, 2587-2594.	2.6	1
1086	Damping of aluminum-matrix composite reinforced by carbon nanotube: Multiscale modeling and characteristics. Science China Technological Sciences, 2023, 66, 1062-1074.	4.0	3

#	Article	IF	CITATIONS
1087	Disassembly of Amphiphilic AB Block Copolymer Vesicles in Selective Solvents: A Molecular Dynamics Simulation Study. Macromolecules, 2023, 56, 2560-2567.	4.8	3
1088	SiCO Ceramics as Storage Materials for Alkali Metals/lons: Insights on Structure Moieties from Solidâ€State NMR and DFT Calculations. ChemSusChem, 2023, 16, .	6.8	О
1089	Strain-induced dark exciton generation in rippled monolayer MoS <sub>2</sub> . Physical Chemistry Chemical Physics, 2023, 25, 9894-9900.	2.8	1
1090	Understanding the solvation structures of glyme-based electrolytes by machine learning molecular dynamics., 2023, 42, 100061.		1
1091	Multi-scale modeling of gas solubility in semi-crystalline polymers: bridging Molecular Dynamics with Lattice Fluid Theory. Fluid Phase Equilibria, 2023, 570, 113798.	2.5	2
1092	Frictional Weakening of Vibrated Granular Flows. Physical Review Letters, 2023, 130, .	7.8	0
1093	Simulations of Subnanometer Scale Image Contrast in Atomic Force Microscopy of Self-Assembled Monolayers in Water. , 0, , .		0
1094	Frontiers, challenges, and solutions in modeling of swift heavy ion effects in materials. Journal of Applied Physics, 2023, 133, .	2.5	5
1095	Systematic atomic structure datasets for machine learning potentials: Application to defects in magnesium. Physical Review B, 2023, 107, .	3.2	6
1096	A 3D-Simulation and Experimental Study of the Fluid Flow Around a Nano-Step Structure Formed by UV-NIL. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2022, 35, 111-116.	0.3	0
1097	An Atomistic Insight into Moir $\tilde{A}$ © Reconstruction in Twisted Bilayer Graphene beyond the Magic Angle. , 2023, 1, 970-982.		5
1098	Continuum Modeling with Functional Lennard–Jones Parameters for DNAâ€Graphene Interactions. Advanced Theory and Simulations, 0, , 2200896.	2.8	0
1100	Wideâ∈Humidity Range Applicable, Antiâ∈Freezing, and Healable Zwitterionic Hydrogels for Ionâ∈Leakageâ∈Free Iontronic Sensors. Advanced Materials, 2023, 35, .	21.0	21
1101	The patterned assembly and stepwise Vps4-mediated disassembly of composite ESCRT-III polymers drives archaeal cell division. Science Advances, 2023, 9, .	10.3	5
1102	Do Machine-Learning Atomic Descriptors and Order Parameters Tell the Same Story? The Case of Liquid Water. Journal of Chemical Theory and Computation, 2023, 19, 4596-4605.	<b>5.</b> 3	3
1103	United atom and coarse grained models for crosslinked polydimethylsiloxane with applications to the rheology of silicone fluids. Physical Chemistry Chemical Physics, 2023, 25, 9669-9684.	2.8	3
1104	Machine learned interatomic potential for dispersion strengthened plasma facing components. Journal of Chemical Physics, 2023, 158, .	3.0	7
1105	Equation of State, Compressibility, and Vibrational Properties of Brucite over Wide Pressure and Temperature Ranges: Atomistic Computer Simulations with the Modified ClayFF Classical Force Field. Minerals (Basel, Switzerland), 2023, 13, 408.	2.0	4

#	Article	IF	CITATIONS
1106	Surface polarization enhances ionic transport and correlations in electrolyte solutions nanoconfined by conductors. Faraday Discussions, 0, 246, 576-591.	3.2	4
1107	Charge Transport in Water–NaCl Electrolytes with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2023, 127, 2729-2738.	2.6	5
1108	Concurrent Characterization of Surface Diffusion and Intermixing of Ge on Si: A Classical Molecular Dynamics Study. Advanced Theory and Simulations, 2023, 6, .	2.8	2
1109	Droplet-particle collision dynamics: A molecular dynamics simulation. Powder Technology, 2023, 422, 118456.	4.2	4
1110	Thermodiffusion of CO <sub>2</sub> in Water by Nonequilibrium Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2023, 127, 2749-2760.	2.6	2
1111	How surface roughness affects the interparticle interactions at a liquid interface. Journal of Colloid and Interface Science, 2023, 641, 492-498.	9.4	3
1112	Molecular Dynamics Simulation on Nanoindentation of M50 Bearing Steel. Materials, 2023, 16, 2386.	2.9	1
1113	Synthetic data enable experiments in atomistic machine learning. , 2023, 2, 651-662.		4
1114	Molecular Insights into the Effect of Crystal Planes on Droplet Wetting. Langmuir, 2023, 39, 4789-4798.	3.5	1
1115	Effects of h-BN additives on tensile mechanical behavior of Fe matrix: A molecular dynamics study. Computational Materials Science, 2023, 223, 112136.	3.0	3
1116	SchNetPack 2.0: A neural network toolbox for atomistic machine learning. Journal of Chemical Physics, 2023, 158, .	3.0	8
1117	On the exploration of the melting behavior of metallic compounds and solid solutions <i>via</i> multiple classical molecular dynamics approaches: application to Al-based systems. Physical Chemistry Chemical Physics, 2023, 25, 10866-10884.	2.8	1
1118	Dislocation plasticity in equiatomic NiCoCr alloys: Effect of short-range order. Physical Review B, 2023, 107, .	3.2	3
1120	Magnetization relaxation dynamics in polydisperse ferrofluids. Physical Review E, 2023, 107, .	2.1	0
1121	An Atomistic Model of Field-Induced Resistive Switching in Valence Change Memory. ACS Nano, 2023, 17, 8281-8292.	14.6	4
1122	How fast do defects migrate in halide perovskites: insights from on-the-fly machine-learned force fields. Chemical Communications, 2023, 59, 4660-4663.	4.1	6
1123	Investigation of Solid Formation Enthalpy and Molecular Mechanics Energies of Amino Acids via Force Field Approach. Bitlis Eren Üniversitesi Fen Bilimleri Dergisi, 2023, 12, 10-16.	0.5	0
1124	Nanoscale friction of biomimetic hair surfaces. Nanoscale, 2023, 15, 7086-7104.	5.6	2

#	Article	IF	CITATIONS
1125	A molecular dynamics study of water confined in between two graphene sheets under compression. Journal of Nanoparticle Research, 2023, 25, .	1.9	3
1126	A review on mechanical and material characterisation through molecular dynamics using large-scale atomic/molecular massively parallel simulator (LAMMPS). Functional Composites and Structures, 2023, 5, 012005.	3.4	5
1127	Ion Exchange Induced Efficient Nâ€Type Thermoelectrics in Solidâ€State. Advanced Functional Materials, 2023, 33, .	14.9	7
1128	Revisiting the Mechanisms of Charge Transport in Solutions of Redox-Active Molecules Using Computer Simulations: When and Why Do Analytical Theories Fail?. Journal of Physical Chemistry B, 2023, 127, 2968-2978.	2.6	3
1129	Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. Crystal Growth and Design, 2023, 23, 2155-2168.	3.0	4
1130	Temperature dependence of magnetic anisotropy and magnetoelasticity from classical spin-lattice calculations. Physical Review B, 2023, 107, .	3.2	2
1131	Theoretical and computational analysis of the electrophoretic polymer mobility inversion induced by charge correlations. Physical Review E, 2023, 107, .	2.1	1
1132	Theory of Cation Solvation and Ionic Association in Nonaqueous Solvent Mixtures. , 2023, 2, .		4
1133	Molecular Dynamics Simulations of Selected Amorphous Stilbenoids and Their Amorphous Solid Dispersions with Poly(Vinylpyrrolidone). Journal of Pharmaceutical Sciences, 2023, , .	3.3	0
1134	Fully atomistic molecular dynamics investigation of the simplest model of dry-draw fabrication of carbon nanotube fibers. MRS Advances, 0, , .	0.9	0
1135	Vapor-Like Water in the NU-1000 Zr-MOF: A Molecular Level Understanding of Balanced Hydrophobicity in Humid Conditions. Journal of Physical Chemistry C, 2023, 127, 6503-6514.	3.1	3
1136	Sequence-to-Sequence Change-Point Detection in Single-Particle Trajectories via Recurrent Neural Network for Measuring Self-Diffusion. Transport in Porous Media, 2023, 147, 679-701.	2.6	2
1137	Parametric crystalline characterization of Anatase/Rutile polymorphic ceramic. Applied Physics A: Materials Science and Processing, 2023, 129, .	2.3	0
1138	Diversity of platinum-sites at platinum/fullerene interface accelerates alkaline hydrogen evolution. Nature Communications, 2023, 14, .	12.8	30
1139	Evolution, Stability, and Applicability of Surfactant Aggregates in Targeted Delivery. Journal of Physical Chemistry B, 2023, 127, 3001-3009.	2.6	2
1140	Interplay Between Doping, Morphology, and Lattice Thermal Conductivity in PEDOT:PSS. Advanced Functional Materials, 2023, 33, .	14.9	7
1141	Molecular dynamics study on the structural properties and phase transformation of Cu-Au nanoparticles. Materials Research Express, 2023, 10, 045001.	1.6	0
1142	Tracking cubic ice at molecular resolution. Nature, 2023, 617, 86-91.	27.8	15

#	Article	IF	Citations
1143	Effect of Temperatures and Graphene on the Mechanical Properties of the Aluminum Matrix: A Molecular Dynamics Study. Materials, 2023, 16, 2722.	2.9	3
1144	Molecular simulation of confined ethalineâ€based deep eutectic solvents for separations of carbon dioxide from methane. AICHE Journal, 0, , .	3.6	O
1145	Noble gas (He, Ne, and Ar) solubilities in high-pressure silicate melts calculated based on deep-potential modeling. Geochimica Et Cosmochimica Acta, 2023, 350, 57-68.	3.9	0
1146	Nbæ·»åŠæ¥µä½Žç,ç´é‹¼æ¿ã«ãŠãʿã,‹å†·å»¶éŽç¨‹ã§ã®NbCã®æžå‡ºçŠ¶æ…‹å‰åŒ—. Tetsu-To-Hagane/Journal of t	:h <b>eol</b> ≄on an	d <b>6</b> teel Insti
1147	Coalescence and Break-Up Behaviors of Nanodroplets under AC Electric Field. Molecules, 2023, 28, 3064.	3.8	3
1148	Simulating dielectric spectra: A demonstration of the direct electric field method and a new model for the nonlinear dielectric response. Journal of Chemical Physics, 2023, 158, 124122.	3.0	O
1149	Carbon layers on Pt/TiO2 induced dramatic promotion of photocatalytic H2 production: a combined experimental and computation study. Materials Today Energy, 2023, 34, 101294.	4.7	2
1150	Comprehensive structural changes in nanoscale-deformed silicon modelled with an integrated atomic potential. Materialia, 2023, 28, 101761.	2.7	3
1151	Determination of thermal conductivity of eutectic Al–Cu compounds utilizing experiments, molecular dynamics simulations and machine learning. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 045001.	2.0	0
1152	Thermal Stability and CO Permeability of [C4C1Pyr][NTf2]/Pd(111) Model SCILLs: from UHV to Ambient Pressure. Topics in Catalysis, 2023, 66, 1202-1216.	2.8	2
1153	Microstructure evolution during sintering: discrete element method approach. Journal of the American Ceramic Society, 0, , .	3.8	2
1154	Insight into the Binding Mechanisms of Quartz-Selective Peptides: Toward Greener Flotation Processes. ACS Applied Materials & Samp; Interfaces, 2023, 15, 17922-17937.	8.0	2
1156	Periodic surface structure of 4H-SiC by 46.9â€nm laser. Optics Express, 2023, 31, 15438.	3.4	1
1157	Charge-optimized many-body interaction potential for AlN revisited to explore plasma–surface interactions. Scientific Reports, 2023, 13, .	3.3	1
1158	Hierarchical lath colonies induced by dislocation rearrangement improve thermal cyclic stability of NiTi shape memory alloy. Scripta Materialia, 2023, 231, 115469.	5.2	7
1159	A database of ultrastable MOFs reassembled from stable fragments with machine learning models. Matter, 2023, 6, 1585-1603.	10.0	12
1160	FitSNAP: Atomistic machine learning with LAMMPS. Journal of Open Source Software, 2023, 8, 5118.	4.6	10
1161	A Systematic Approach to Understanding and Optimizing the CO <sub>2</sub> Capture Performance of Triamine-Functionalized Mesoporous Silica with Amine Blends Using Molecular Simulations. Journal of Physical Chemistry C, 2023, 127, 7410-7424.	3.1	1

#	Article	IF	CITATIONS
1162	Improving the prediction of glassy dynamics by pinpointing the local cage. Journal of Chemical Physics, $2023,158,.$	3.0	6
1163	Electro-osmotic flow in different phosphorus nanochannels. Physics of Fluids, 2023, 35, .	4.0	6
1164	Dynamics Simulation and Light-Sheet Tomography of Multispecies Ion Coulomb Crystals. Journal of Physics: Conference Series, 2023, 2470, 012034.	0.4	0
1165	New Atomistic Insights on the Chemical Mechanical Polishing of Silica Glass with Ceria Nanoparticles. Langmuir, 2023, 39, 5527-5541.	3.5	7
1166	Promoting ion and heat transfer of solid polymer electrolytes by tuning polymer chain length and salt concentration. International Journal of Green Energy, 2024, 21, 512-520.	3.8	0
1167	Constraints on Knot Insertion, Not Internal Jamming, Control Polycatenane Translocation Dynamics through Crystalline Pores. Macromolecules, 0, , .	4.8	0
1168	Supercritical fluids behave as complex networks. Nature Communications, 2023, 14, .	12.8	4
1169	Peripherally "tertiary butyl ester―functionalized bipyridine cored dendrons: from synthesis and characterization to molecular dynamic simulation study. New Journal of Chemistry, 2023, 47, 8913-8924.	2.8	2
1170	Simple and efficient algorithms based on Volterra equations to compute memory kernels and projected cross-correlation functions from molecular dynamics. Journal of Chemical Physics, 2023, 158, .	3.0	5
1171	Molecular Dynamics Investigation of Nanoscale Hydrophobicity of Polymer Surfaces: What Makes Water Wet?. Journal of Physical Chemistry B, 2023, 127, 5115-5127.	2.6	2
1172	$ ilde{A}$ ngstrom-Depth Resolution with Chemical Specificity at the Liquid-Vapor Interface. Physical Review Letters, 2023, 130, .	7.8	2
1173	Parallel simulation via SPPARKS of on-lattice kinetic and Metropolis Monte Carlo models for materials processing. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 055001.	2.0	10
1174	Orientation order of a nonpolar molecular fluid compressed into a nanosmall space. Nanoscale, 0, , .	5.6	2
1175	Active learning strategies for atomic cluster expansion models. Physical Review Materials, 2023, 7, .	2.4	9
1176	Ring compaction as a mechanism of densification in amorphous silica. Physical Review B, 2023, 107, .	3.2	3
1177	Phase behaviour of mixtures of charged soft disks and spheres. Soft Matter, 2023, 19, 3311-3324.	2.7	1
1178	Crystal effects in the vibrational spectra of one-dimensional molecular spin crossover crystals using molecular dynamics simulations. Applied Physics A: Materials Science and Processing, 2023, 129, .	2.3	1
1179	Pressure-Controlled Layer-by-Layer to Continuous Oxidation of ZrS <sub>2</sub> (001) Surface. ACS Nano, 0, , .	14.6	O

#	ARTICLE	IF	CITATIONS
1180	Design and mechanical properties of SiC reinforced Gd2O3/6061Al neutron shielding composites. Ceramics International, 2023, 49, 27707-27715.	4.8	3
1181	An atomistic study of plastic deformation of SmCo5 by amorphous shear bands. Materials Today Communications, 2023, 35, 106002.	1.9	0
1182	Semi-hollow LTA zeolite membrane for water permeation in simulated CO2 hydrogenation to methanol. Journal of Membrane Science, 2023, 678, 121666.	8.2	7
1183	Constant Potential and Constrained Charge Ensembles for Simulations of Conductive Electrodes. Journal of Chemical Theory and Computation, 2023, 19, 2758-2768.	5.3	3
1184	Influence of Nonadditive Mixing on Colloidal Diamond Phase Formation from Patchy Particles. Journal of Physical Chemistry B, 2023, 127, 3746-3755.	2.6	3
1186	Transfer Learning Facilitates the Prediction of Polymer–Surface Adhesion Strength. Journal of Chemical Theory and Computation, 2023, 19, 4631-4640.	5.3	3
1187	Leadframe-Epoxy Moulding Compound Adhesion: a Micromechanics-driven Investigation. , 2023, , .		2
1188	Development of a coarse-grained model for surface-functionalized gold nanoparticles: towards an accurate description of their aggregation behavior. Soft Matter, 2023, 19, 3290-3300.	2.7	1
1189	Quantum mechanical and classical calculation of the transport and relaxation properties of Heâc CO sub>2 lsub> complex using a new PES. Physical Chemistry Chemical Physics, 2023, 25, 13521-13532.	2.8	1
1190	Unveiling deformation twin nucleation and growth mechanisms in BCC transition metals and alloys. Materials Today, 2023, 65, 90-99.	14.2	6
1191	Ab initio derived force field potential for the accurate simulation of thermal transport in AlN. , 2023, , .		0
1192	The three-dimensional elastodynamic solution for dislocation plasticity and its implementation in discrete dislocation dynamics simulations. Acta Materialia, 2023, 253, 118945.	7.9	3
1194	Evaluation of adsorption and mechanical strength of 13X zeolite mixtures with phyllosilicate binders using molecular dynamics simulation and positron annihilation spectroscopy. Chemical Engineering Science, 2023, 276, 118744.	3.8	1
1195	Aluminum nanotubes as an efficient catalyst for hydrogen production <i>via</i> thermochemical water splitting: a reactive molecular dynamics simulation. Physical Chemistry Chemical Physics, 2023, 25, 13487-13497.	2.8	5
1196	The critical role of the donor polymer in the stability of high-performance non-fullerene acceptor organic solar cells. Joule, 2023, 7, 810-829.	24.0	17
1197	Depolymerization of plastics by means of electrified spatiotemporal heating. Nature, 2023, 616, 488-494.	27.8	38
1198	Atomic-resolution observations of silver segregation in a $[111]$ tilt grain boundary in copper. Physical Review B, 2023, 107, .	3.2	2
1199	Impact of Ad Hoc Post-Processing Parameters on the Lubricant Viscosity Calculated with Equilibrium Molecular Dynamics Simulations. Lubricants, 2023, 11, 183.	2.9	1

#	Article	IF	CITATIONS
1200	Investigating the influence of pull-out speed on the interfacial properties and the pull-out behavior of CNT/polymer nanocomposites. Composite Structures, 2023, 316, 117049.	5.8	7
1201	App-Free Method for Visualization of Polymers in 3D and Augmented Reality. Journal of Chemical Education, 2023, 100, 2039-2044.	2.3	5
1202	Liquid–Crystal Structure Inheritance in Machine Learning Potentials for Network-Forming Systems. JETP Letters, 2023, 117, 370-376.	1.4	5
1203	Transition between a nano-sized prismatic dislocation loop and vacancy cluster in α-iron: An atomic scale study. Computational Materials Science, 2023, 225, 112195.	3.0	2
1204	Role of Strong Localized vs Weak Distributed Interactions in Disordered Protein Phase Separation. Journal of Physical Chemistry B, 2023, 127, 3829-3838.	2.6	15
1205	Ultraslow Settling Kinetics of Frictional Cohesive Powders. Physical Review Letters, 2023, 130, .	7.8	1
1206	Phase behavior and dynamics in a colloid-polymer mixture under spherical confinement. Soft Matter, 0, , .	2.7	2
1208	Field-driven cluster formation in two-dimensional colloidal binary mixtures. Physical Review E, 2023, 107, .	2.1	0
1209	Acidic Conditions Impact Hydrophobe Transfer across the Oil–Water Interface in Unusual Ways. Journal of Physical Chemistry B, 0, , .	2.6	0
1210	De Novo Evolution of an Antibodyâ€Mimicking Multivalent Aptamer via a DNA Framework. Small Methods, 2023, 7, .	8.6	1
1211	Fundamentals of Crystalline Evolution and Properties of Carbon Nanotube-Reinforced Polyether Ether Ketone Nanocomposites in Fused Filament Fabrication. ACS Applied Materials & Samp; Interfaces, 2023, 15, 22506-22523.	8.0	1
1212	Dissipative solitary waves in a two-dimensional complex plasma: Amorphous versus crystalline. Physical Review E, 2023, 107, .	2.1	1
1213	Roles of Hydrogen Bonds and Alignment in Oriented Attachment of Gibbsite Nanoparticles: Insights from Molecular Dynamics. Journal of Physical Chemistry C, 2023, 127, 8695-8703.	3.1	0
1214	Thermal Conductivities of Uniform and Random Sulfur Crosslinking in Polybutadiene by Molecular Dynamic Simulation. Polymers, 2023, 15, 2058.	4.5	5
1215	Polymers of intrinsic microporosity containing aryl-phthalimide moieties: synthesis, modeling, and membrane gas transport properties. Polymer Chemistry, 2023, 14, 2363-2373.	3.9	1
1216	Mechanisms for mechanical responses of asphalt under uniaxial tension with computational simulation. Construction and Building Materials, 2023, 385, 131497.	7.2	2
1217	$\tilde{A}     net\text{-PyTorch}$ : A GPU-supported implementation for machine learning atomic potentials training. Journal of Chemical Physics, 2023, 158, .	3.0	6
1218	An Approach for Quantitative EHD Friction Prediction Based on Rheological Experiments and Molecular Dynamics Simulations. Tribology Letters, 2023, 71, .	2.6	3

#	Article	IF	CITATIONS
1219	Molecular Dynamics Simulations of Ionic Liquid Crystals., 2024,, 723-761.		1
1220	Catalytic performance and mechanism of PTFE modified NiCo2O4 in high-salt organic wastewater treatment during wet air oxidation at ambient pressure. Applied Catalysis B: Environmental, 2023, 334, 122786.	20.2	2
1221	Deformation and failure processes of Na-montmorillonite under uniaxial compressive strain condition via molecular dynamic method. Materials Today Communications, 2023, 35, 106132.	1.9	0
1222	Thermal Expansion and Thermal Conductivity of Ni/Graphene Composite: Molecular Dynamics Simulation. Materials, 2023, 16, 3747.	2.9	1
1223	Pyro-layered heterostructured nanosheet membrane for hydrogen separation. Nature Communications, 2023, 14, .	12.8	6
1224	Structure and thermodynamics of water adsorption in NU-1500-Cr. Communications Chemistry, 2023, 6, .	4.5	8
1225	Tuning the potential drop at graphene/protic ionic liquid interface by molecular structure engineering. Electrochimica Acta, 2023, 458, 142344.	5.2	2
1226	Structure and dynamics of dynamic covalent cross-linked PEOs and PEO/LiPF <sub>6</sub> electrolytes: a coarse-grained simulation study. Physical Chemistry Chemical Physics, 2023, 25, 14530-14537.	2.8	0
1227	Imaging the strain evolution of a platinum nanoparticle under electrochemical control. Nature Materials, 2023, 22, 754-761.	27.5	12
1228	Optimization of the wetting-drying characteristics of hydrophobic metal organic frameworks via crystallite size: The role of hydrogen bonding between intruded and bulk liquid. Journal of Colloid and Interface Science, 2023, 645, 775-783.	9.4	8
1229	A Maxwell relation for dynamical timescales with application to the pressure and temperature dependence of water self-diffusion and shear viscosity. Physical Chemistry Chemical Physics, 2023, 25, 12820-12832.	2.8	0
1230	A layout-dependent formula for the critical separation size of parallelogram-type deterministic lateral displacement arrays. Physics of Fluids, 2023, 35, .	4.0	0
1231	Insights into solvent and surface charge effects on Volmer step kinetics on Pt (111). Nature Communications, 2023, 14, .	12.8	3
1232	Subclass Effects on Self-Association and Viscosity of Monoclonal Antibodies at High Concentrations. Molecular Pharmaceutics, 2023, 20, 2991-3008.	4.6	5
1233	Reunderstanding aqueous Zn electrochemistry from interfacial specific adsorption of solvation structures. Energy and Environmental Science, 2023, 16, 2910-2923.	30.8	25
1234	Uniaxial deformation of nanowires in 16 refractory multi-principal element alloys. Journal of Alloys and Compounds, 2023, 959, 170556.	5.5	1
1235	Using Raman Spectroscopy and Molecular Dynamics to Study Conformation Changes of Sodium Lauryl Ether Sulfate Molecules. Journal of Physical Chemistry B, 2023, 127, 4676-4686.	2.6	2
1236	Pursuing colloidal diamond. Nanoscale, 0, , .	5.6	0

#	Article	IF	CITATIONS
1237	Uncovering stress fields and defects distributions in graphene using deep neural networks. International Journal of Fracture, 2023, 242, 107-127.	2.2	3
1238	A Regulation Method of the Wettability of Solid Surfaces: Oil–Water Wettability Alteration by Replacing Adsorbed Polar Molecules via Salt Ions. Industrial & Engineering Chemistry Research, 0,	3.7	1
1239	Revisiting the stable structures of gold clusters: Au $\langle sub \rangle n \langle sub \rangle$ (n = $16\hat{a} \in 25$ ) by artificial neural network potential. Journal Physics D: Applied Physics, 2023, 56, 375302.	2.8	1
1240	A computational building block approach towards multiscale architected materials analysis and design with application to hierarchical metal metamaterials. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 054001.	2.0	10
1241	Nonadditive Interactions Unlock Small-Particle Mobility in Binary Colloidal Monolayers. ACS Nano, 2023, 17, 8303-8314.	14.6	0
1242	Nanoindentation of tungsten: From interatomic potentials to dislocation plasticity mechanisms. Physical Review Materials, 2023, 7, .	2.4	4
1243	Size–Pore-Dependent Methanol Sequestration from Water–Methanol Mixtures by an Embedded Graphene Slit. Molecules, 2023, 28, 3697.	3.8	1
1244	On the Friction Behavior of SiO <sub>2</sub> Tip Sliding on the Au(111) Surface: How Does an Amorphous SiO <sub>2</sub> Tip Produce Regular Stick–Slip Friction and Friction Duality?. Langmuir, 2023, 39, 6425-6432.	3.5	1
1245	Atomistic simulation of tribology behaviors of Ti-based FeCoNiTi high entropy alloy coating during nanoscratching. Vacuum, 2023, 213, 112124.	3.5	1
1246	Site-Averaged <i>Ab Initio</i> Kinetics: Importance Learning for Multistep Reactions on Amorphous Supports. Journal of Chemical Theory and Computation, 2023, 19, 2873-2886.	<b>5.</b> 3	1
1247	Atomistic Simulations of the Crystalline-to-Amorphous Transformation of Î <sup>3</sup> -Al <sub>2</sub> O <sub>3</sub> Nanoparticles: Delicate Interplay between Lattice Distortions, Stresses, and Space Charges. Langmuir, 2023, 39, 6301-6315.	3.5	3
1248	Revisiting particle dynamics in the NPT ensemble under the extended Lagrangian approach. Molecular Simulation, 2023, 49, 855-866.	2.0	2
1249	Investigating the microplastic behavior of hierarchical polycrystalline <mml:math altimg="si2.svg" display="inline" id="d1e124" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">γ</mml:mi></mml:math> -TiAl microstructures. Computational Materials Science, 2023, 226, 112197.	3.0	O
1250	Symmetrized Drude Oscillator Force Fields Improve Numerical Performance of Polarizable Molecular Dynamics. Journal of Chemical Theory and Computation, 2023, 19, 2906-2917.	5.3	2
1251	Unsupervised learning of representative local atomic arrangements in molecular dynamics data. Physical Chemistry Chemical Physics, 2023, 25, 13741-13754.	2.8	3
1252	Ionic Conductivity of Lithium Phosphides. Crystals, 2023, 13, 756.	2.2	2
1253	Molecular Weight Segregation and Thermal Conductivity of Polydisperse Wax–Graphene Nanocomposites. Polymers, 2023, 15, 2175.	4.5	1
1254	Discrete element simulation of Pebble Bed Reactors on graphics processing units. Annals of Nuclear Energy, 2023, 190, 109896.	1.8	5

#	Article	IF	CITATIONS
1255	Modelling the impact of configurational entropy on the stability of amorphous SiO2. Scripta Materialia, 2023, 233, 115507.	5.2	1
1256	Predicting partner fitness based on spatial structuring in a light-driven microbial community. PLoS Computational Biology, 2023, 19, e1011045.	3.2	0
1257	Molecular dynamics simulation of the nano-cutting mechanism of a high-phosphorus NiP coating. Journal of Materials Research and Technology, 2023, 24, 8109-8120.	5.8	3
1258	Origin of the elastic anisotropy of silica particles: Insights from first-principles calculations and nanoindentation molecular dynamic simulations. Computers and Geotechnics, 2023, 159, 105489.	4.7	3
1259	Selective Reduction of CO <sub>2</sub> to Methanol via Hydrosilylation Boosted by a Porphyrinic Metal–Organic Framework. ACS Catalysis, 2023, 13, 6837-6845.	11.2	5
1260	Acceleration of generalized replica exchange with solute tempering simulations of large biological systems on massively parallel supercomputer. Journal of Computational Chemistry, 2023, 44, 1740-1749.	3.3	1
1261	Structure and Thermodynamics of Linear, Ring, and Catenane Polymers in Solutions and at Liquid–Liquid Interfaces. Langmuir, 2023, 39, 7154-7166.	3.5	2
1262	Irradiation performance of concentrated solid-solution alloys: Insight into defect behaviors. Journal of Nuclear Materials, 2023, 583, 154510.	2.7	2
1264	Lightweight and effective tensor sensitivity for atomistic neural networks. Journal of Chemical Physics, 2023, 158, .	3.0	5
1265	Entropic Origin of Ionic Interactions in Polar Solvents. Journal of Physical Chemistry B, 2023, 127, 4328-4337.	2.6	3
1266	Computation of Finite Temperature Mechanical Properties of Zeolitic Imidazolate Framework Glasses by Molecular Dynamics. Chemistry of Materials, 2023, 35, 4038-4047.	6.7	4
1267	Development of thermodynamically consistent machine-learning equations of state: Application to the Mie fluid. Journal of Chemical Physics, 2023, 158, .	3.0	4
1268	Mechanical behavior of monolayer MoS2 films with arrayed dislocation defects. Results in Physics, 2023, 49, 106514.	4.1	0
1269	Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases. Physical Review Materials, 2023, 7, .	2.4	O
1270	Structural Signatures of Ultrastability in a Deposited Glassformer. Physical Review Letters, 2023, 130, .	7.8	1
1271	Synergism Effect between Nanofibrillation and Interface Tuning on the Stiffness–Toughness Balance of Rubber-Toughened Polymer Nanocomposites: A Multiscale Analysis. ACS Applied Materials & Samp; Interfaces, 2023, 15, 24948-24967.	8.0	3
1272	Computer simulation of phosphate-silicate and calcium phosphate-silicate systems. Physica Scripta, 2023, 98, 065704.	2.5	0
1273	Influence of Pore Surface Structure and Contents on Shock-Induced Collapse and Energy Localization. Journal of Physical Chemistry C, 2023, 127, 9887-9895.	3.1	2

#	Article	IF	CITATIONS
1274	Adsorption behavior of long-chain perfluoroalkyl substances on hydrophobic surface: A combined molecular characterization and simulation study. Water Research, 2023, 239, 120074.	11.3	9
1275	On surface pre-melting of metallic nanoparticles: molecular dynamics study. Journal of Nanoparticle Research, 2023, 25, .	1.9	0
1276	Asymmetry in core structure and mobility of basal dislocations in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Ti</mml:mi><td>r<b>o2v4</b>-<mm< td=""><td>เ<b>l:เด</b>ิก&gt;3</td></mm<></td></mml:mrow></mml:msub></mml:math>	r <b>o2v4</b> - <mm< td=""><td>เ<b>l:เด</b>ิก&gt;3</td></mm<>	เ <b>l:เด</b> ิก>3
1277	Horizontally Asymmetric Nanochannels of Graphene Oxide Membranes for Efficient Osmotic Energy Harvesting. ACS Nano, 2023, 17, 10000-10009.	14.6	7
1278	Degradation of fiber/matrix interface under various environmental and loading conditions: Insights from molecular simulations. Construction and Building Materials, 2023, 390, 131101.	7.2	4
1279	mdapy: A flexible and efficient analysis software for molecular dynamics simulations. Computer Physics Communications, 2023, 290, 108764.	7.5	6
1280	Reactive molecular dynamics simulations of lysozyme desorption under Ar cluster impact. Applied Surface Science, 2023, 631, 157487.	6.1	3
1281	Classical Molecular Dynamics Simulation of Molecular Crystals and Materials: Old Lessons and New Perspectives. , 2024, , 777-803.		1
1282	Metal–Organic Frameworks for Water Harvesting: Machine Learning-Based Prediction and Rapid Screening. ACS Sustainable Chemistry and Engineering, 2023, 11, 8148-8160.	6.7	4
1283	Development of a neuroevolution machine learning potential of Pd-Cu-Ni-P alloys. Materials and Design, 2023, 231, 112012.	7.0	3
1284	Molecular dynamics simulation of dislocation network formation and tensile properties of graphene/TiAl-layered composites. Surfaces and Interfaces, 2023, 39, 102983.	3.0	1
1285	Grain-size effects of TiC on mechanical properties in diamond/TiC combinations: A molecular dynamics exploration. Diamond and Related Materials, 2023, $136$ , $110051$ .	3.9	0
1286	Finite-size excess-entropy scaling for simple liquids. Journal of Chemical Physics, 2023, 158, .	3.0	0
1287	Experimental and simulation study of the effects of multi-walled carbon nanotubes in clayey soils. Applied Nanoscience (Switzerland), 2023, 13, 6249-6257.	3.1	1
1288	Thermal conductivity tensor of $\langle i \rangle \hat{l}^2 \langle i \rangle \hat{a} \in HMX$ as a function of pressure and temperature from equilibrium molecular dynamics simulations. Propellants, Explosives, Pyrotechnics, 0, , .	1.6	0
1289	Deciphering the Anomalous Acidic Tendency of Terminal Water at Rutile(110)–Water Interfaces. Journal of Physical Chemistry C, 2023, 127, 10532-10540.	3.1	2
1290	A fully quantum-mechanical treatment for kaolinite. Journal of Chemical Physics, 2023, 158, .	3.0	0
1291	Machine learning quantum-chemical bond scission in thermosets under extreme deformation. Applied Physics Letters, 2023, 122, .	3.3	1

#	ARTICLE	IF	CITATIONS
1292	Molecular dynamics simulations of flavour molecules in Scotch whisky. Journal of Molecular Liquids, 2023, 383, 122152.	4.9	0
1293	Scaling Perspective on Dynamics of Nanoparticles in Polymers: Length- and Time-Scale Dependent Nanoparticle–Polymer Coupling. Macromolecules, 2023, 56, 3809-3837.	4.8	8
1294	Investigating percolation and clustering effects on aquivion and nafion membranes at the molecular scale. International Journal of Hydrogen Energy, 2023, 48, 33283-33296.	7.1	2
1295	Electrons Surf Phason Waves in Moiré Bilayers. Nano Letters, 2023, 23, 4870-4875.	9.1	O
1296	An interpretable deep learning approach for designing nanoporous silicon nitride membranes with tunable mechanical properties. Npj Computational Materials, 2023, 9, .	8.7	5
1297	Enabling selective zinc-ion intercalation by a eutectic electrolyte for practical anodeless zinc batteries. Nature Communications, $2023,14,.$	12.8	38
1298	Addressing the Folding of Intermolecular Springs in Particle Simulations: Fixed Image Convention. Computation, 2023, 11, 106.	2.0	0
1299	Clustering of caffeine in water and its adsorption in activated carbon: Molecular simulations and experiments. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 673, 131645.	4.7	3
1300	Cluster-size distribution of ions in concentrated aqueous NaCl solutions: Molecular dynamics simulations. Chemical Physics Letters, 2023, 825, 140627.	2.6	1
1301	Influence of Sputtering Pressure on the Micro-Topography of Sputtered Cu/Si Films: Integrated Multiscale Simulation. Processes, 2023, 11, 1649.	2.8	2
1302	Anisotropic orientation dependent shock wave responses of monocrystalline molybdenum. Journal of Materials Research and Technology, 2023, 25, 285-296.	5.8	4
1303	Investigating structure and dynamics of unentangled poly(dimethyl- <i>co</i> diphenyl)siloxane <i>via</i> molecular dynamics simulation. Soft Matter, 2023, 19, 4265-4276.	2.7	0
1304	Atomic strain and catalytic properties of formate oxidation and dehydrogenation in AgPd nanoalloys. Nanoscale, 0, , .	5.6	0
1305	Effect of aluminum nanoparticle size on phase transitions: a molecular dynamics study. Indian Journal of Physics, 0, , .	1.8	O
1306	Shape optimization of a meniscus-adherent nanotip. Nanoscale, 2023, 15, 11099-11106.	5.6	3
1307	Fieldâ€programmable gate array acceleration of the Tersoff potential in LAMMPS. Engineering Reports, 0, , .	1.7	O
1308	Understanding the Correlation Between Structure and Entangled Photon Pair Properties with Metal–Organic Frameworks. Journal of Physical Chemistry C, 2023, 127, 10987-10996.	3.1	0
1309	Yielding under compression and the polyamorphic transition in silicon. Physical Review Materials, 2023, 7, .	2.4	2

#	Article	IF	CITATIONS
1310	Molecular Dynamics Simulation of Pore-Size Effects on Gas Adsorption Kinetics in Zeolites. Clays and Clay Minerals, 2023, 71, 54-73.	1.3	0
1311	Janus Ligand-Tethered Nanoparticles at Liquid–Liquid Interfaces. Journal of Physical Chemistry B, 2023, 127, 5150-5161.	2.6	2
1312	MB-pol(2023): Sub-chemical Accuracy for Water Simulations from the Gas to the Liquid Phase. Journal of Chemical Theory and Computation, 2023, 19, 3551-3566.	5.3	9
1313	Study of the shear-band evolution across the interface between different spatial scales. Computational Particle Mechanics, 2024, 11, 73-88.	3.0	0
1314	Dynamics of Associative Polymers with High Density of Reversible Bonds. Physical Review Letters, 2023, 130, .	7.8	6
1315	Unwrapping NPT Simulations to Calculate Diffusion Coefficients. Journal of Chemical Theory and Computation, 2023, 19, 3406-3417.	5.3	3
1316	Structural impact of niobium oxide on lithium silicate glasses: Results from advanced interaction-selective solid-state nuclear magnetic resonance and Raman spectroscopy. Acta Materialia, 2023, 255, 119061.	7.9	1
1318	Antoine Equation Coefficients for Novichok Agents (A230, A232, and A234) via Molecular Dynamics Simulations. Physchem, 2023, 3, 244-258.	1.1	2
1319	Highly cross-linked carbon tube aerogels with enhanced elasticity and fatigue resistance. Nature Communications, 2023, 14, .	12.8	11
1320	Electric field modulation effect and mechanism on n-alkanes fuel pyrolysis: A ReaxFF MD and DFT study. Fuel, 2023, 350, 128759.	6.4	2
1321	Molecular dynamics simulation of cathode crater formation in the cathode spot of vacuum arcs. Journal Physics D: Applied Physics, 2023, 56, 375203.	2.8	3
1322	An interatomic potential for ternary NiTiHf shape memory alloys based on modified embedded atom method. Computational Materials Science, 2023, 227, 112278.	3.0	4
1323	High-Temperature Pyrolysis of <i>N</i> -Tetracosane Based on ReaxFF Molecular Dynamics Simulation. ACS Omega, 2023, 8, 20823-20833.	3.5	1
1324	On the role of history-dependent adsorbate distribution and metastable states in switchable mesoporous metal-organic frameworks. Nature Communications, 2023, 14, .	12.8	3
1325	Reversible densification and cooperative atomic movement induced "compaction―in vitreous silica: a new sight from deep neural network interatomic potentials. Journal of Materials Science, 2023, 58, 9515-9532.	3.7	3
1326	Effect of Interfacial Regions and Surface Functional Groups on Chemical Transport in Polymer–Particle Composites. Journal of Physical Chemistry C, 2023, 127, 11231-11239.	3.1	0
1327	Deep-learning-assisted theoretical insights into the compatibility of environment friendly insulation medium with metal surface of power equipment. Journal of Colloid and Interface Science, 2023, 648, 317-326.	9.4	4
1328	Investigation on liquid thermal conductivity of ethylene glycol (EG)/water mixtures: A comparative experimental and molecular dynamics simulation study. Journal of Molecular Liquids, 2023, 384, 122268.	4.9	2

#	Article	IF	CITATIONS
1329	Computational study of native defects and oxygen diffusion in the YTiO3 $\hat{A}\pm\hat{I}$ as cathode materials in SOFCs. Journal of Solid State Chemistry, 2023, 325, 124142.	2.9	1
1330	Structure-based virtual screening. , 2023, , 239-262.		0
1331	Sequence Patterning, Morphology, and Dispersity in Single-Chain Nanoparticles: Insights from Simulation and Machine Learning. ACS Polymers Au, 2023, 3, 284-294.	4.1	6
1332	Tools and software for computer-aided drug design and discovery. , 2023, , 637-661.		1
1333	Mechanical properties and deformation behavior of equiatomic CoCrFeMnNi high-entropy alloy foam: A molecular dynamics study. Solid State Communications, 2023, 371, 115236.	1.9	2
1334	Improvement of desalination performance by adjusting the arrangement of lamellar MXene membrane. Separation and Purification Technology, 2023, 322, 124265.	7.9	4
1335	Impact of nanodroplets on cone-textured surfaces. Physical Review E, 2023, 107, .	2.1	0
1336	On the surface chemisorption of oxidizing fine iron particles: Insights gained from molecular dynamics simulations. Combustion and Flame, 2023, 254, 112871.	5.2	4
1337	Probing radiation resistance in simulated metallic core–shell nanoparticles. Computational Materials Science, 2023, 227, 112304.	3.0	3
1338	Data-driven models for predicting intrinsically disordered protein polymer physics directly from composition or sequence. Molecular Systems Design and Engineering, 2023, 8, 1146-1155.	3.4	2
1339	Mechanics of tunable adhesion with surface wrinkles. Journal of Applied Mechanics, Transactions ASME, 0, , 1-22.	2.2	0
1341	Reliable machine learning potentials based on artificial neural network for graphene. Computational Materials Science, 2023, 227, 112272.	3.0	5
1342	Coarse-grained molecular dynamic model for metallic materials. Computational Materials Science, 2023, 228, 112306.	3.0	5
1343	Morse potential parameters of dissipative particle dynamics force fields for non-polarizable water models. Journal of Molecular Liquids, 2023, 384, 122246.	4.9	0
1344	Stress corrosion phenomenon of BeO at room temperature and its mechanism: Experimental and molecular dynamics study. Materials Today Communications, 2023, 35, 106385.	1.9	0
1345	Structure Formation in an Ionic Liquid Wetting Layer: A Combined STM, IRAS, DFT and MD Study of [C <sub>2</sub> C <sub>1</sub> Im][OTf] on Au(111). Chemistry - A European Journal, 2023, 29, .	3.3	2
1346	Evidence of twinning-induced plasticity (TWIP) and ultrahigh hardness in additively-manufactured near-eutectic Ni–Nb. Journal of Materials Science, 2023, 58, 9723-9736.	3.7	0
1347	The Fe addition as an effective treatment for improving the radiation resistance of fcc NixFe1-x single-crystal alloys. Journal of Nuclear Materials, 2023, 584, 154565.	2.7	1

#	Article	IF	CITATIONS
1348	Thermally activated nature of synchro-Shockley dislocations in Laves phases. Scripta Materialia, 2023, 235, 115588.	5.2	3
1350	Mussel-Inspired Polydopamine Composite Mesoporous Bioactive Glass Nanoparticles: An Exploration of Potential Metal-Ion Loading Platform and In Vitro Bioactivity. ACS Applied Materials & Discrete Services, 2023, 15, 29550-29560.	8.0	1
1351	Failure to reproduce the results of "A new transferable interatomic potential for molecular dynamics simulations of borosilicate glasses― Journal of Non-Crystalline Solids, 2023, 615, 122423.	3.1	1
1352	Formation of nanoribbons by carbon atoms confined in a single-walled carbon nanotube—A molecular dynamics study. Journal of Chemical Physics, 2023, 158, .	3.0	1
1353	Effect of solvation shell structure on thermopower of liquid redox pairs. EcoMat, 2023, 5, .	11.9	10
1354	Coarse-grained modeling of polymers with end-on and side-on liquid crystal moieties: Effect of architecture. Journal of Chemical Physics, 2023, 158, .	3.0	3
1355	Realistic phase diagram of water from "first principles―data-driven quantum simulations. Nature Communications, 2023, 14, .	12.8	13
1356	Poly(A)-binding protein is an ataxin-2 chaperone that regulates biomolecular condensates. Molecular Cell, 2023, 83, 2020-2034.e6.	9.7	1
1358	Determining Ion Activity Coefficients in Ion-Exchange Membranes with Machine Learning and Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2023, 62, 9533-9548.	3.7	2
1359	Interplay of multiple clusters and initial interface positioning for forward flux sampling simulations of crystal nucleation. Journal of Chemical Physics, 2023, 158, .	3.0	1
1360	Getting over the hump with KAMEL-LOBE: Kernel-averaging method to eliminate length-of-bin effects in radial distribution functions. Journal of Chemical Physics, 2023, 158, .	3.0	0
1361	Accelerating Non-Empirical Structure Determination of Ziegler–Natta Catalysts with a High-Dimensional Neural Network Potential. Journal of Physical Chemistry C, 2023, 127, 11683-11691.	3.1	1
1362	Poisoning of Copper Chabazite Catalyst by Biodiesel Metal Contaminants: Effect of Alkali and Alkaline Earth Metals. Journal of Physical Chemistry C, 2023, 127, 11490-11505.	3.1	0
1363	Atomic Oxygen-Induced Surface Erosion Behavior and Mechanical Degradation of Polyether Ether Ketone via Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2023, 127, 5509-5520.	2.6	1
1364	Evaluation of Machine Learning Interatomic Potentials for Gold Nanoparticlesâ€"Transferability towards Bulk. Nanomaterials, 2023, 13, 1832.	4.1	2
1365	Predicting Dynamic Heterogeneity in Glass-Forming Liquids by Physics-Inspired Machine Learning. Physical Review Letters, 2023, 130, .	7.8	13
1366	ESPResSo, a Versatile Open-Source Software Package for Simulating Soft Matter Systems. , 2024, , 578-601.		1
1367	Extending a generic and fast coarse-grained molecular dynamics model to examine the mechanical behavior of grafted polymer nanocomposites. Forces in Mechanics, 2023, 12, 100207.	2.8	1

#	Article	IF	CITATIONS
1368	Influence of surface burnishing process with single strain path and reciprocating strain path on copper wear behavior. Wear, 2023, 530-531, 205022.	3.1	2
1369	Atomistic determination of Peierls barriers of dislocation glide in nickel. Journal of the Mechanics and Physics of Solids, 2023, 178, 105359.	4.8	2
1370	Solvation Structure of Conjugated Organosulfur Polymers for Lithium–Sulfur Battery Cathodes. ACS Applied Polymer Materials, 0, , .	4.4	0
1371	Investigation of different nanoparticles properties on the thermal conductivity and viscosity of nanofluids by molecular dynamics simulation. Nanotechnology Reviews, 2023, 12, .	5.8	1
1372	Ultra-Fast Heating Process of Cu-Pd Bimetallic Nanoparticles Unraveled by Molecular Dynamics Simulation. Coatings, 2023, 13, 1078.	2.6	0
1373	Machine learning predictions of diffusion in bulk and confined ionic liquids using simple descriptors. Molecular Systems Design and Engineering, 2023, 8, 1257-1274.	3.4	1
1374	Equation of state for He bubbles in W and model of He bubble growth and bursting near W $\{100\}$ surfaces derived from molecular dynamics simulations. Scientific Reports, 2023, 13, .	3.3	2
1375	Elastic properties of diamane. Letters on Materials, 2023, 13, 171-176.	0.7	3
1376	Pair distribution function analysis for oxide defect identification through feature extraction and supervised learning. , 2023, $1$ , .		1
1377	Unusual Aspects of Charge Regulation in Flexible Weak Polyelectrolytes. Polymers, 2023, 15, 2680.	4.5	2
1378	Microtubule-binding-induced allostery triggers LIS1 dissociation from dynein prior to cargo transport. Nature Structural and Molecular Biology, 2023, 30, 1365-1379.	8.2	5
1379	A combined SPH-DEM approach for extremely deformed granular packings: validation and compression tests. Computational Particle Mechanics, 2024, 11, 185-196.	3.0	O
1380	Stability of binary precipitates in Cu-Ni-Si-Cr alloys investigated through active learning. Materials Chemistry and Physics, 2023, 306, 128053.	4.0	1
1381	Objective molecular dynamics study of cross slip under high-rate deformation. Journal of the Mechanics and Physics of Solids, 2023, 179, 105361.	4.8	0
1382	Filler-induced heterogeneous nucleation of polymer crystals investigated by molecular dynamics simulations. Polymer, 2023, 281, 126113.	3.8	1
1383	Porosity effect on the thermal and mechanical properties of U-50Zr alloy: A molecular dynamics study. Journal of Nuclear Materials, 2023, 584, 154578.	2.7	0
1384	Self-Assembly and the Properties of Micro-Mesoporous Carbon. Journal of Chemical Theory and Computation, 2024, 20, 1753-1762.	5 <b>.</b> 3	2
1385	Mechanical, Electronic, and Optical Properties of 8-16-4 Graphyne: A 2D Carbon Allotrope with Dirac Cones. Journal of Physical Chemistry C, 2023, 127, 12226-12234.	3.1	6

#	Article	IF	CITATIONS
1386	Encapsulation of catechin derivatives in single-walled carbon nanotubes. Computational and Theoretical Chemistry, 2023, 1226, 114206.	2.5	0
1387	The key role of interfacial non-bonding interactions in regulating lubricant viscosity using nanoparticles. Tribology International, 2023, 187, 108716.	5.9	0
1388	Influence of water penetration on glass fiber-epoxy resin interface under electric field: A DFT and molecular dynamics study. Journal of Molecular Liquids, 2023, 385, 122346.	4.9	1
1389	Effect of crystal orientation on the nanoindentation deformation behavior of TiN coating based on molecular dynamics. Surface and Coatings Technology, 2023, 467, 129721.	4.8	2
1390	Molecular dynamics simulation of argon pool boiling: A comparative study of employing nanoparticles and creating tree-root type nanostructures. International Communications in Heat and Mass Transfer, 2023, 146, 106890.	5.6	3
1391	Molecular dynamic study of oxygen ion diffusion and grain boundary in SrSc0.1Co0.9O3-δ perovskite solid oxide membrane. Solid State Ionics, 2023, 399, 116291.	2.7	0
1392	Quantifying low-energy nitrogen ion channeling in $\hat{l}$ ±-titanium by molecular dynamics simulations. Materials Chemistry and Physics, 2023, 306, 128098.	4.0	0
1393	Dynamical scattering in ice-embedded proteins in conventional and scanning transmission electron microscopy. IUCrJ, 2023, 10, 475-486.	2.2	1
1394	Plastic deformations of ceria nanocubes under compression: An atomistic simulations study. Materialia, 2023, 30, 101824.	2.7	0
1395	Unveiling the phonon frequency-dependent mechanism of heat transport across stacking fault in silicon carbide. Chinese Physics B, O, , .	1.4	0
1396	Molecular dynamics simulation of the mechanical and thermal properties of phagraphene nanosheets and nanotubes: a review. Journal of Materials Science, 2023, 58, 10222-10260.	3.7	0
1397	Computational Discovery of Stable Metal–Organic Frameworks for Methane-to-Methanol Catalysis. Journal of the American Chemical Society, 2023, 145, 14365-14378.	13.7	8
1398	Molecular Dynamics Simulation of Acetylene Pyrolysis into Fullerenes. Acta Chimica Sinica, 2023, 81, 502.	1.4	0
1399	Coalescence of surfactant-laden droplets. Physics of Fluids, 2023, 35, .	4.0	6
1400	A computational view on nanomaterial intrinsic and extrinsic features for nanosafety and sustainability. Materials Today, 2023, 67, 344-370.	14.2	1
1401	3Dâ€Printed Inherently Porous Structures with Tetrahedral Lattice Architecture: Experimental and Computational Study of Their Mechanical Behavior. Macromolecular Materials and Engineering, 0, , .	3.6	0
1402	Updates to the DScribe library: New descriptors and derivatives. Journal of Chemical Physics, 2023, 158,	3.0	6
1403	Prediction of Temperature-Dependent Mechanical Properties for SWCNT/Cu Nanocomposite Metamaterials: A Molecular Dynamics Study. Nanomaterials, 2023, 13, 1885.	4.1	1

#	Article	IF	CITATIONS
1404	Segregation of fluids with polymer additives at domain interfaces: a dissipative particle dynamics study. Soft Matter, 2023, 19, 6433-6445.	2.7	3
1405	Molecular dynamics study of the irradiation damage accumulation in beryllium oxide at different temperatures. Materialia, 2023, 30, 101830.	2.7	0
1406	Automated extraction of interfacial dislocations and disconnections from atomistic data. Acta Materialia, $2023$ , , $119096$ .	7.9	0
1407	Atomic Cluster Expansion for Quantum-Accurate Large-Scale Simulations of Carbon. Journal of Chemical Theory and Computation, 2023, 19, 5151-5167.	<b>5.</b> 3	14
1408	Investigations of void collapse in nanoporous Cu by molecular dynamics simulations. AIP Advances, 2023, 13, .	1.3	1
1409	Structure and ion transport in super-concentrated water-in-salt electrolytes: Insights from molecular dynamics simulations. Electrochimica Acta, 2023, 462, 142772.	<b>5.2</b>	0
1410	The limit of macroscopic homogeneous ice nucleation at the nanoscale. Faraday Discussions, 0, 249, 210-228.	3.2	0
1411	Atomistic model of the anisotropic response of <i>ortho</i> -Mo2C to indentation. AIP Advances, 2023, 13, .	1.3	0
1412	Anisotropic and Finite Effects on Intermolecular Vibration and Relaxation Dynamics: Low-Frequency Raman Spectroscopy of Water Film and Droplet on Graphene by Molecular Dynamics Simulations. Journal of Physical Chemistry B, O, , .	2.6	0
1413	Light-driven self-assembly of spiropyran-functionalized covalent organic framework. Nature Communications, 2023, 14, .	12.8	12
1414	Scaling of nanoscale elastic and tensile failure properties of cementitious calcium-silicate-hydrate materials at cryogenic temperatures: A molecular simulation study. Cement and Concrete Research, 2023, 172, 107242.	11.0	5
1415	A first-principles machine-learning force field for heterogeneous ice nucleation on microcline feldspar. Faraday Discussions, 0, 249, 98-113.	3.2	4
1416	Development of pebble-based extruded carbon rods for extreme plasma heat flux environments. Journal of Applied Physics, 2023, 133, .	2.5	0
1417	Toward new liquid crystal phases of DNA mesogens. APL Materials, 2023, 11, .	5.1	1
1418	Dynamic interaction between dislocations and obstacles in bcc iron based on atomic potentials derived using neural networks. Physical Review Materials, 2023, 7, .	2.4	1
1419	Molecular simulations of sliding on SDS surfactant films. Journal of Chemical Physics, 2023, 158, .	3.0	0
1420	Physicsâ€Informed Multistage Machine Learning Strategy for the Nanomachiningâ€Induced Plastic Deformation Behavior. Advanced Engineering Materials, 2023, 25, .	3 <b>.</b> 5	0
1421	Stacking and thickness effects on cross-plane thermal conductivity of hexagonal boron nitride. Computational Materials Science, 2023, 228, 112345.	3.0	O

#	Article	IF	CITATIONS
1422	A deep learning approach to the measurement of long-lived memory kernels from generalized Langevin dynamics. Journal of Chemical Physics, $2023$ , $158$ , .	3.0	3
1423	Scalable Empirical Dynamic Modeling With Parallel Computing and Approximate k-NN Search. IEEE Access, 2023, 11, 68171-68183.	4.2	2
1424	The Riddle of Dark LLZO: Cobalt Diffusion in Garnet Separators of Solidâ€State Lithium Batteries. Advanced Functional Materials, 2023, 33, .	14.9	4
1425	Multi-scale simulations aiming to advance heavy ion beam cancer therapy. AIP Conference Proceedings, 2023, , .	0.4	0
1426	Predicting Electronic Structure of Realistic Amorphous Surfaces. Advanced Theory and Simulations, 2023, 6, .	2.8	0
1427	Reaction Network of Ammonium Perchlorate (AP) Decomposition: The Missing Piece from Atomic Simulations. Journal of Physical Chemistry C, 2023, 127, 12976-12982.	3.1	1
1428	Atomistic to Mesoscopic Modelling of Thermophysical Properties of Graphene-Reinforced Epoxy Nanocomposites. Nanomaterials, 2023, 13, 1960.	4.1	3
1429	Shadow Molecular Dynamics and Atomic Cluster Expansions for Flexible Charge Models. Journal of Chemical Theory and Computation, 2023, 19, 4255-4272.	5.3	1
1430	Atom Sampling method for mesoscale molecular dynamics and its application to graphene assemblies. Physical Chemistry Chemical Physics, 0, , .	2.8	0
1431	Toward a 3D physical model of diffusive polymer chains. Frontiers in Physics, $0,11,.$	2.1	0
1433	Toward Data-Driven Many-Body Simulations of Biomolecules in Solution: <i>N</i> -Methyl Acetamide as a Proxy for the Protein Backbone. Journal of Chemical Theory and Computation, 2023, 19, 4308-4321.	5.3	1
1434	Ordered and disordered microstructures of nanoconfined conducting polymers. Soft Matter, 2023, 19, 5641-5650.	2.7	2
1435	Montmorillonite swelling properties with various surfactants based on molecular simulation. Journal of Dispersion Science and Technology, $0$ , , $1$ - $10$ .	2.4	0
1436	Compact aerosol aggregate model (CA <sup>2</sup> M): A fast tool to estimate the aerosol properties of fractal-like aggregates. Aerosol Science and Technology, 2023, 57, 797-809.	3.1	3
1437	Enabling large-scale quantum path integral molecular dynamics simulations through the integration of D <scp>cdftbmd</scp> and i-PI codes. Journal of Chemical Physics, 2023, 158, .	3.0	0
1438	GPU-Based Molecular Dynamics ofÂTurbulent Liquid Flows withÂOpenMM. Lecture Notes in Computer Science, 2023, , 346-358.	1.3	1
1439	Atomic Understanding of the Plastic Deformation Mechanism of 4H-SiC Under Different Grain Depth-of-cut During Nano-Grinding. Journal of Electronic Materials, 2023, 52, 4865-4877.	2.2	2
1440	Deep potential molecular dynamics on the microstructure and thermodynamic properties of FLiNaK–ThF <sub>4</sub> . Scientia Sinica Chimica, 2023, 53, 1008-1019.	0.4	1

#	Article	IF	Citations
1441	Roadmap on measurement technologies for next generation structural health monitoring systems. Measurement Science and Technology, 2023, 34, 093001.	2.6	13
1442	Inferring electrospray emission characteristics from molecular dynamics and simulated retarding potential analysis. Journal of Applied Physics, 2023, 133, .	2.5	2
1443	On the Application of Non-Gaussian Noise in Stochastic Langevin Simulations. Journal of Statistical Physics, 2023, 190, .	1.2	1
1444	Derivation of parameter sets for the ReaxFF+ method for modeling an electrochemical machining process. Procedia CIRP, 2023, 117, 231-236.	1.9	1
1445	Size-tunable graphitized carbon spheres for water defluoridation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 670, 131582.	4.7	0
1446	Code modernization strategies for short-range non-bonded molecular dynamics simulations. Computer Physics Communications, 2023, 290, 108760.	<b>7.</b> 5	1
1447	Analytic bond order potential for indium gallium zinc oxide. Journal of Materials Chemistry C, 2023, 11, 7595-7602.	5 <b>.</b> 5	0
1448	Atomistic Insights into the Deposition of Corrosion Products on the Surfaces of Steels and Passivation Films. Langmuir, 2023, 39, 6812-6822.	3.5	2
1449	Nonlinear multiscale model for interstitial structures of densely ordered multi-walled carbon nanotube bundles. Carbon, 2023, 210, 118091.	10.3	3
1450	GNN-assisted phase space integration with application to atomistics. Mechanics of Materials, 2023, 182, 104681.	3.2	1
1451	Molecular-Dynamics Simulation of Silicon Irradiation with 2–8 keV C60 Fullerene Ions. Journal of Surface Investigation, 2023, 17, 66-71.	0.5	3
1452	Coacervation-Induced Remodeling of Nanovesicles. Journal of Physical Chemistry Letters, 2023, 14, 4532-4540.	4.6	1
1453	Detection of Water Vapor by Chemiluminescence. Chemosensors, 2023, 11, 284.	3.6	0
1454	Molecular Dynamics Simulations on Epoxy/Silica Interfaces Using Stable Atomic Models of Silica Surfaces. Langmuir, 2023, 39, 7063-7078.	3.5	4
1455	Comparing transferability in neural network approaches and linear models for machine-learning interaction potentials. Physical Review B, 2023, 107, .	3.2	1
1456	The influence of oxygen content on the crystallization mechanism of aluminum oxide: Molecular dynamics study. AIP Conference Proceedings, 2023, , .	0.4	0
1457	The morphology of dryout nanofluid droplet and underlying mechanisms based on coarse-grained molecular dynamic simulations. Journal of Molecular Liquids, 2023, 383, 122064.	4.9	1
1458	Intergranular Hotspots: A Molecular Dynamics Study on the Influence of Compressive and Shear Work. Journal of Physical Chemistry C, 2023, 127, 9858-9870.	3.1	3

#	Article	IF	CITATIONS
1460	Early Stage Growth Process of Dinaphtho[2,3â€b:2',3'â€f]thieno[3,2â€b]thiophene (DNTT) Thin Film. Physica Status Solidi (A) Applications and Materials Science, 2023, 220, .	1.8	0
1461	A general strategy for synthesizing biomacromolecular ionogel membranes via solvent-induced self-assembly., 2023, 2, 864-872.		16
1462	Plastic behavior of a nanoporous high-entropy alloy under compression. Computational Materials Science, 2023, 226, 112241.	3.0	0
1463	Thermomechanical Properties of Nontoxic Plasticizers for Polyvinyl Chloride Predicted from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2023, 15, 24858-24867.	8.0	4
1465	Determination of cooperatively rearranging regions in a binary glass former. Journal of Physics Condensed Matter, 2023, 35, 334003.	1.8	0
1466	Diffusion of knots in nanochannel-confined DNA molecules. Journal of Chemical Physics, 2023, 158, .	3.0	1
1467	Surface modification of silicon carbide at atomic and close-to-atomic scale by femtosecond laser. , 2022, , .		0
1468	On the equivalence of the hybrid particle–field and Gaussian core models. Journal of Chemical Physics, 2023, 158, .	3.0	0
1469	Formation, Diffusion, and Growth of Gas Bubbles in Î <sup>3</sup> -Uranium with the Excess of Interstitial Atoms: Relation between Molecular Dynamics and Kinetics. Journal of Experimental and Theoretical Physics, 2023, 136, 174-184.	0.9	2
1470	High energy vibrational excitations of nitromethane in liquid water. Journal of Chemical Physics, 2023, 158, .	3.0	1
1471	An improved grand-potential phase-field model of solid-state sintering for many particles. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 055006.	2.0	4
1472	Colloidal gelation with non-sticky particles. Nature Communications, 2023, 14, .	12.8	3
1473	Disclose effect and mechanism of external electric field on RP-1 fuel pyrolysis. Fuel, 2023, 349, 128567.	6.4	1
1474	Nitric oxide-mediated S-nitrosylation of IAA17 protein in intrinsically disordered region represses auxin signaling. Journal of Genetics and Genomics, 2023, 50, 473-485.	3.9	4
1475	Molecular Dynamics Simulation of the Influence of External Electric Fields on the Glass Transition Temperature of the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide. Journal of Physical Chemistry B, 2023, 127, 4623-4632.	2.6	2
1476	Machine Learning Predictions of Simulated Self-Diffusion Coefficients for Bulk and Confined Pure Liquids. Journal of Chemical Theory and Computation, 2023, 19, 3054-3062.	5.3	2
1477	Molecular dynamics study of primary damage in the near-surface region in nickel. Journal of Nuclear Materials, 2023, 583, 154514.	2.7	0
1478	Effect of surface wettability on specific heat capacity of nano-confined liquid. Journal of Molecular Liquids, 2023, 383, 122115.	4.9	1

#	Article	IF	CITATIONS
1479	Modelling of dislocations, twins and crack-tips in HCP and BCC Ti. International Journal of Plasticity, 2023, 166, 103644.	8.8	4
1480	Structural rationale for boson peak in metallic glass informed by an interpretable neural network model. Physical Review Research, 2023, 5, .	3.6	3
1481	Data-driven prediction of complex crystal structures of dense lithium. Nature Communications, 2023, 14, .	12.8	4
1482	The Local Electronic Structure of Supercritical CO <sub>2</sub> from X-ray Raman Spectroscopy and Atomistic-Scale Modeling. Journal of Physical Chemistry Letters, 2023, 14, 4955-4961.	4.6	O
1483	A combined experimental and molecular dynamic studies of curing of shape memory lignin-liquid crystalline elastomeric composites. Composites Science and Technology, 2023, 240, 110099.	7.8	1
1484	Importance of surface morphology on secondary electron emission: a case study of Cu covered with carbon, carbon pairs, or graphitic-like layers. Scientific Reports, 2023, 13, .	3.3	0
1485	Effect of salinity, mineralogy, and organic materials in hydrogen wetting and its implications for underground hydrogen storage (UHS). International Journal of Hydrogen Energy, 2023, 48, 32839-32848.	7.1	2
1486	Molecular Dynamics Simulation of Cu-Cu Solid-State Bonding under Various Bonding Parameters. , 2023, , .		0
1487	Molecular dynamics study on the transport of water molecules and chloride ions in graphene oxide-modified cement composites. Composite Interfaces, 2023, 30, 1343-1361.	2.3	2
1489	Multi-scale simulation study on the evolution of stress waves and dislocations in Ti alloy during laser shock peening processing. Optics and Laser Technology, 2023, 165, 109629.	4.6	2
1490	Atomistic simulation of αâ€Al <sub>2</sub> O <sub>3</sub> nanoparticle plastic anisotropy under compression. Journal of the American Ceramic Society, 2023, 106, 5986-5999.	3.8	0
1491	Development of a Reactive Force Field for Simulating Photoinitiated Acrylate Polymerization. Journal of Physical Chemistry B, 2023, 127, 5094-5101.	2.6	0
1492	Universality in conformations and transverse fluctuations of a semi-flexible polymer in a crowded environment. Journal of Chemical Physics, 2023, 158, .	3.0	1
1493	Model for Humidity-Mediated Diffusion on Aluminum Surfaces and Its Role in Accelerating Atmospheric Aluminum Corrosion. ACS Applied Materials & Samp; Interfaces, 2023, 15, 28716-28730.	8.0	0
1494	MultiSOM: Multi-layer Self Organizing Maps for local structure identification in crystalline structures. Computational Materials Science, 2023, 227, 112263.	3.0	3
1495	InPc-modified gel electrolyte based on in situ polymerization in practical high-loading lithium-sulfur batteries. Chemical Engineering Journal, 2023, 469, 143714.	12.7	3
1496	Exploring pressure-dependent inelastic deformation and failure in bonded granular composites: An energetic materials perspective. Mechanics of Materials, 2023, 184, 104693.	3.2	6
1497	Accurate prediction of heat conductivity of water by a neuroevolution potential. Journal of Chemical Physics, 2023, 158, .	3.0	6

#	ARTICLE	IF	CITATIONS
1498	Shock Wave–Induced Dynamic Mechanical Behavior of Calcium Silicate Aluminate Hydrate at the Molecular Scale. Journal of Materials in Civil Engineering, 2023, 35, .	2.9	3
1499	An artificial neural network potential for uranium metal at low pressures. Chinese Physics B, 2023, 32, 098401.	1.4	1
1500	Atomistic simulation of local chemical order in NbTiZrMoV high entropy alloy based on a newly-developed interatomic potential. Computational Materials Science, 2023, 227, 112269.	3.0	1
1501	Mechanism of structural colors in binary mixtures of nanoparticle-based supraballs. Science Advances, 2023, 9, .	10.3	6
1502	Reactive Force Field Molecular Dynamics Study of the Effects of Gaseous Species on the Composition and Crystallinity of Silicon–Germanium Thin Films. Crystal Growth and Design, 2023, 23, 4990-5000.	3.0	0
1503	<i>Time</i> SOAP: Tracking high-dimensional fluctuations in complex molecular systems via time variations of SOAP spectra. Journal of Chemical Physics, 2023, 158, .	3.0	4
1504	Bayesian optimization of metastable nickel formation during the spontaneous crystallization under extreme conditions. Journal of Applied Physics, 2023, 133, .	2.5	0
1505	A composite calcium silicate hydrate model of molecular dynamics simulations for mechanical properties. Chemical Physics Letters, 2023, 825, 140632.	2.6	0
1506	Study of Speciation and Transport Properties for Different Compositions of Carbonates in Li <sub>2</sub> CO <sub>3</sub> <i>â€"</i> Na <sub>2</sub> CO <sub>3</sub> and Li <sub>2</sub> CO <sub>3</sub> Binary Systems at High Temperature in Molten State. Journal of Physical Chemistry C, 2023, 127, 11186-11194.	3.1	1
1507	Microstructural evolution of periclase under irradiation by molecular dynamics simulations. Journal of Applied Physics, 2023, 133, .	2.5	0
1508	Water-aluminum reaction by MD simulations and its interpretation defect formation. Computational Materials Science, 2023, 227, 112301.	3.0	1
1509	Revisiting thermal transport in single-layer graphene: On the applicability of thermal snapshot interatomic force constant extraction methodology for layered materials. Journal of Applied Physics, 2023, 133, .	2.5	2
1510	Leaflet Tensions Control the Spatio-Temporal Remodeling of Lipid Bilayers and Nanovesicles. Biomolecules, 2023, 13, 926.	4.0	7
1511	Autonomous alignment and healing in multilayer soft electronics using immiscible dynamic polymers. Science, 2023, 380, 935-941.	12.6	31
1512	A method for coarse graining fluctuation velocities in granular flows. Granular Matter, 2023, 25, .	2.2	0
1513	Rapid Prediction of a Liquid Structure from a Single Molecular Configuration Using Deep Learning. Journal of Chemical Information and Modeling, 2023, 63, 3742-3750.	5.4	1
1514	A ReaxFF-based molecular dynamics study of the destruction of PFAS due to ultrasound. Environmental Pollution, 2023, 333, 122026.	7.5	5
1515	From microemulsion phase diagrams to hydrophilicity and hydration controlled adsorption: a dissipative particle dynamics modelling study of phospholipid assembly in bio oils. Soft Matter, 2023, 19, 5538-5550.	2.7	2

#	Article	IF	CITATIONS
1516	Influence of rhenium-decorated dislocation loops on edge dislocation gliding in tungsten. Scripta Materialia, 2023, 235, 115624.	5.2	1
1517	Molecular dynamics simulations study on structure and properties of CaO–MgO–B2O3–Al2O3–SiO2 glasses with different B2O3/MgO. Journal of Non-Crystalline Solids, 2023, 616, 122458.	3.1	3
1518	Adiabatic limit collapse and local interaction effects in non-linear active microrheology molecular simulations of two-dimensional fluids. Soft Matter, 2023, 19, 5288-5299.	2.7	0
1519	Artificial Intelligence Enhanced Molecular Simulations. Journal of Chemical Theory and Computation, 2023, 19, 4338-4350.	5.3	9
1520	Surface properties of alkali silicate glasses: Influence of the modifiers. Journal of Chemical Physics, 2023, 158, .	3.0	0
1521	Modeling the Interaction and Uptake of Cdâ^'As(V) Mixture to Wheat Roots Affected by Humic Acids, in Terms of root cell Membrane Surface Potential (Î^O). Bulletin of Environmental Contamination and Toxicology, 2023, 111, .	2.7	0
1522	Evaluating approaches for on-the-fly machine learning interatomic potentials for activated mechanisms sampling with the activation-relaxation technique nouveau. Journal of Chemical Physics, 2023, 158, .	3.0	0
1523	Recent advances and challenges of carbon nano onions (CNOs) for application in supercapacitor devices (SCDs). Journal of Energy Storage, 2023, 71, 107928.	8.1	5
1524	Polydots, soft nanoparticles, at membrane interfaces. RSC Advances, 2023, 13, 19227-19234.	3.6	0
1525	Molecular Simulation of Argon Adsorption and Diffusion in a Microporous Carbon with Poroelastic Couplings. Langmuir, 2023, 39, 9384-9395.	3.5	1
1526	Evaluating HPC Job Run Time Predictions Using Application Input Parameters. , 2023, , .		0
1527	Locality of contacts determines the subdiffusion exponents in polymeric models of chromatin. Physical Review E, 2023, 107, .	2.1	0
1528	Molecular Dynamics Simulation of High Temperature Mechanical Properties of Nano-Polycrystalline Beryllium Oxide and Relevant Experimental Verification. Energies, 2023, 16, 4927.	3.1	2
1529	Anomalous Pressure-Resilient Thermal Conductivity in Hybrid Perovskites with Strong Lattice Anharmonicity and Small Bulk Modulus. Chemistry of Materials, 2023, 35, 5185-5192.	6.7	2
1530	Computational study of Na diffusion and conduction in P2- and O3-Na2x[NixTi1-x]O2 materials with machine-learning interatomic potentials. Solid State Ionics, 2023, 399, 116298.	2.7	0
1531	Predicting electronic structures at any length scale with machine learning. Npj Computational Materials, 2023, 9, .	8.7	10
1532	Novel study of perovskite materials and the use of biomaterials to further solar cell application in the built environment: A molecular dynamic study. Engineering Analysis With Boundary Elements, 2023, 155, 425-431.	3.7	13
1533	Molecularly imprinted polymers-isolated AuNP-enhanced CdTe QD fluorescence sensor for selective and sensitive oxytetracycline detection in real water samples. Journal of Hazardous Materials, 2023, 458, 131941.	12.4	8

#	Article	IF	CITATIONS
1534	Dislocation patterning in the TiZrVTa refractory high-entropy alloy under tribological loading. Tribology International, 2023, 187, 108740.	5.9	0
1535	Computer Simulation Insight into the Adsorption and Diffusion of Polyelectrolytes on Oppositely Charged Surface. Polymers, 2023, 15, 2845.	4.5	0
1536	Combining particle and field-theoretic polymer models with multi-representation simulations. Journal of Chemical Physics, 2023, $158$ , .	3.0	4
1537	<scp>CO<sub>2</sub></scp> â€Induced Modulation of <scp>Si–O</scp> Bonds for Low Temperature Plastic Deformation of Amorphous Silica Nanoparticles with Enhanced Photoluminescence. Energy and Environmental Materials, 0, , .	12.8	0
1538	Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113.		1
1539	Reactivity of Single-Atom Alloy Nanoparticles: Modeling the Dehydrogenation of Propane. Journal of the American Chemical Society, 2023, 145, 14894-14902.	13.7	9
1540	Disentangling the effects of non-adiabatic interactions upon ion self-diffusion within warm dense hydrogen. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2023, 381, .	3.4	1
1541	On the low cycle fatigue behaviour of an Al-Zn-Mg-Cu alloy processed via non-isothermal ageing. Journal of Materials Science and Technology, 2024, 168, 227-238.	10.7	3
1542	Does the Sign of Charge Affect the Surface Affinity of Simple Ions?. Journal of Physical Chemistry B, 2023, 127, 6205-6216.	2.6	1
1544	Strength and Electrical Properties of Cementitious Composite with Integrated Carbon Nanotubes. Materials, 2023, 16, 4771.	2.9	0
1545	Efficient generation of stable linear machine-learning force fields with uncertainty-aware active learning. Machine Learning: Science and Technology, 2023, 4, 035005.	5.0	0
1546	TribChem: A Software for the First-Principles, High-Throughput Study of Solid Interfaces and Their Tribological Properties. Journal of Chemical Theory and Computation, 0, , .	5.3	0
1547	Changing of the Interfacial Contacts and Shear Behaviors between a-C Films Caused by Si Doping. Langmuir, 2023, 39, 9725-9733.	3 <b>.</b> 5	0
1549	Accurate force-field methodology capturing atomic reconstructions in transition metal dichalcogenide moiré system. Physical Review B, 2023, 108, .	3.2	1
1550	Development of an automated reliable method to compute transport properties from DPD equilibrium simulations: Application to simple fluids. Computer Physics Communications, 2023, 291, 108843.	7.5	3
1551	MATILDA.FT: A mesoscale simulation package for inhomogeneous soft matter. Journal of Chemical Physics, 2023, 159, .	3.0	1
1552	Real-Time In Situ Observation of CsPbBr <sub>3</sub> Perovskite Nanoplatelets Transforming into Nanosheets. ACS Nano, 2023, 17, 13648-13658.	14.6	5
1553	Atomistic study of the impact response of bicontinuous nanoporous gold as a protection medium: Effect of porous-nonporous interface on failure evolution. Computational Materials Science, 2023, 228, 112363.	3.0	O

#	Article	IF	CITATIONS
1554	High rejection stacked single-layer graphene membranes for water treatment. 2D Materials, 2023, 10, 045002.	4.4	0
1555	Revisiting the effect of shear stress on the $\hat{I}^3\hat{a}^{\dagger}\hat{I}^{\pm}$ phase transition of cerium under shock loading. Mechanics of Materials, 2023, 184, 104743.	3.2	0
1556	Machine learning of atomic dynamics and statistical surface identities in gold nanoparticles. Communications Chemistry, 2023, 6, .	4.5	3
1557	Water molecules mute the dependence of the double-layer potential profile on ionic strength. Faraday Discussions, 0, 249, 267-288.	3.2	0
1558	Electric-field frictional effects in confined zwitterionic molecules. Physical Chemistry Chemical Physics, 2023, 25, 19037-19045.	2.8	1
1559	Simulations of Glass Transition and Mechanical Behavior of Off-Stoichiometric Crosslinked Polymers. Macromolecules, 2023, 56, 5268-5277.	4.8	0
1560	Thermal conductivity of hydrogenated h-BN nanosheets: a reactive force field study. Soft Materials, 2023, 21, 271-279.	1.7	1
1561	The atomic structure evolution and strengthening mechanism in three-dimensional network graphene enhanced Cu: A molecular dynamics simulation. Journal of Alloys and Compounds, 2023, 963, 171293.	5.5	3
1562	An Atomistic Study of the Tensile Deformation of Carbon Nanotube–Polymethylmethacrylate Composites. Polymers, 2023, 15, 2956.	4.5	4
1563	Plasticity in cyclic indentation of a Cu-Zr-based bulk metallic glass after tensile loading: An experimental and molecular dynamics simulation study. Journal of Non-Crystalline Solids, 2023, 617, 122486.	3.1	2
1565	Increase in Charge and Density Improves the Strength and Toughness of Mussel Foot Protein 5 Inspired Protein Materials. ACS Biomaterials Science and Engineering, 2023, 9, 4662-4672.	5.2	1
1566	Mobility percolation as a source of Johari-Goldstein relaxation in glasses. Physical Review B, 2023, 108,	3.2	2
1567	Icosahedron-dominated tension–compression asymmetry and brittle–ductile transition of metallic glass. Journal of Materials Research, 2023, 38, 3901-3912.	2.6	1
1568	Anharmonicity and the emergence of diffusive behavior in a lattice-solute model solid-state electrolyte. Computational Materials Science, 2023, 228, 112359.	3.0	0
1569	Enhanced Pulley Effect for Translocation: The Interplay of Electrostatic and Hydrodynamic Forces. Biomacromolecules, 0, , .	5.4	0
1570	PXLink: A simulation program of polymer crosslinking to study of polyamide membrane. Computer Physics Communications, 2023, 291, 108840.	<b>7.</b> 5	2
1572	Atomistic Study of the Bandgap Engineering of Two-Dimensional Silicon Carbide by Hydrogenation. ACS Omega, 2023, 8, 25424-25431.	3.5	1
1573	Shock-induced deformation and spallation in CoCrFeMnNi high-entropy alloys at high strain-rates. International Journal of Plasticity, 2023, 168, 103691.	8.8	11

#	Article	IF	Citations
1574	A spall and diffraction study of nanosecond pressure release across the iron $\hat{l}\mu$ - $\hat{l}\pm$ phase boundary. Acta Materialia, 2023, 257, 119148.	7.9	3
1575	A dynamic load balancing algorithm for CFD–DEM simulation with CPU–GPU heterogeneous computing. Powder Technology, 2023, 428, 118782.	4.2	2
1576	Dynamics of fluid bilayer vesicles: Soft meshes and robust curvature energy discretization. Physical Review E, 2023, 108, .	2.1	0
1577	Enhancing the Whole Migration Kinetics of Na <sup>+</sup> in the Anode Side for Advanced Ultralow Temperature Sodiumâ€lon Hybrid Capacitor. Advanced Energy Materials, 2023, 13, .	19.5	8
1578	Equilibrium molecular dynamics evaluation of the solid–liquid friction coefficient: Role of timescales. Journal of Chemical Physics, 2023, 159, .	3.0	0
1579	Omnidirectional Energy Harvesting Fleeces. ACS Applied Materials & Samp; Interfaces, 2023, 15, 36688-36697.	8.0	4
1580	Effects of solvents on Li+Âdistribution and dynamics in PVDF/LiFSI solid polymer electrolytes: An all-atom molecular dynamics simulation study. Solid State Ionics, 2023, 399, 116304.	2.7	2
1581	Underexcitation prevents crystallization of granular assemblies subjected to high-frequency vibration. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	O
1582	STRUCTURAL PROPERTIES OF AMORPHOUS GEO2: A MOLECULAR DYNAMICS SIMULATION STUDIES. FUDMA Journal of Sciences, 2023, 7, 251-256.	0.2	0
1583	altimg="si12.svg" display="inline" id="d1e958"> <mml:mo>&lt;110<mml:math altimg="si13.svg" display="inline" id="d1e963" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>&gt;</mml:mo></mml:math>{001} dislocations and {110} prismatic loops in uranium dioxide: Implications for strain-hardening under irradiation. International lournal of</mml:mo>	8.8	5
1584	Plasticity, 2023, 168, 103702.  Development of novel natural gas hydrate inhibitor and the synergistic inhibition mechanism with NaCl: Experiments and molecular dynamics simulation. Fuel, 2023, 353, 129162.	6.4	2
1585	A combined ensemble-volume average homogenization method for lattice structures with defects under dynamic and static loading. Computational Materials Science, 2023, 228, 112357.	3.0	0
1586	Temperature-pressure phase diagram of confined monolayer water/ice at first-principles accuracy with a machine-learning force field. Nature Communications, 2023, 14, .	12.8	4
1587	Zeolite Encapsulation of Indole as an Antibacterial with Controllable Release Property. Langmuir, 2023, 39, 10122-10132.	3.5	0
1588	Reinforcement learning based hybrid bond-order coarse-grained interatomic potentials for exploring mesoscale aggregation in liquid–liquid mixtures. Journal of Chemical Physics, 2023, 159, .	3.0	1
1589	Selective Carbon Dioxide Binding on Carbon Quantum Dots. Journal of Physical Chemistry C, 2023, 127, 13639-13650.	3.1	0
1590	Cross-platform hyperparameter optimization for machine learning interatomic potentials. Journal of Chemical Physics, 2023, 159, .	3.0	0
1591	Interfaces in reinforced epoxy resins: from molecular scale understanding towards mechanical properties. Journal of Molecular Modeling, 2023, 29, .	1.8	0

#	Article	IF	CITATIONS
1592	Regulation of chromatin microphase separation by binding of protein complexes. ELife, 0, 12, .	6.0	2
1593	A deep learning interatomic potential suitable for simulating radiation damage in bulk tungsten. Tungsten, 0, , .	4.8	O
1594	An Empirical Study of High Performance Computing (HPC) Performance Bugs. , 2023, , .		0
1595	La ley penal de 1845 en Cuba: procesos de negociaci $\tilde{A}^3$ n, propuestas, contrapropuestas y resultado. Anuario De Estudios Americanos, 2023, 80, 285-309.	0.1	O
1596	Structural and Dynamical Properties of H <sub>2</sub> O and D <sub>2</sub> O under Confinement. Journal of Physical Chemistry B, 2023, 127, 6532-6542.	2.6	3
1597	Application of machine-learning algorithms to predict the transport properties of Mie fluids. Journal of Chemical Physics, 2023, 159, .	3.0	1
1598	Atomic simulation study on the effect of nanotwin on the compression behavior of Mg–Y alloys. Journal of Materials Research and Technology, 2023, 25, 6369-6379.	5.8	1
1599	Mixed modifier effects on structural, mechanical, chemical, and mechanochemical properties of sodium calcium aluminosilicate glass. Journal of the American Ceramic Society, 0, , .	3.8	O
1600	Numerical flows studies in a hyperbolic microchannel for biomedical applications. , 2023, , .		0
1601	Nucleation of helium in pure liquid lithium. Journal of Chemical Physics, 2023, 159, .	3.0	1
1602	Elucidating the Molecular Mechanism of CO <sub>2</sub> Capture by Amino Acid Ionic Liquids. Journal of the American Chemical Society, 2023, 145, 15663-15667.	13.7	4
1603	Molecular dynamics study on structural characteristics and mechanical properties of sodium aluminosilicate hydrate with immobilized radioactive Cs and Sr ions. Applied Clay Science, 2023, 243, 107042.	5.2	1
1604	Athermal swelling and creep of heavily irradiated iron under uniaxial stress. Physical Review Materials, 2023, 7, .	2.4	0
1605	Fitting the charged-optimized many-body potential for the Al-O-Se-Zn system. Computational Materials Science, 2023, 228, 112371.	3.0	O
1606	Drag, lift, and buoyancy forces on a single large particle in dense granular flows. Physical Review Fluids, 2023, 8, .	2.5	1
1607	Puzzles of Surface Segregation in Binary Pt–Pd Nanoparticles: Molecular Dynamics and Thermodynamic Simulations. Metals, 2023, 13, 1269.	2.3	2
1608	Ultra-long-range interactions between active regulatory elements. Genome Research, 2023, 33, 1269-1283.	5.5	6
1610	Reactive molecular dynamics simulations on the pyrolysis of SF <sub>6</sub> . Journal Physics D: Applied Physics, 2023, 56, 445503.	2.8	1

#	Article	IF	CITATIONS
1611	Deciphering the scope of inÂsilico screening of novel natural lead molecules against putative molecular targets of multidrug-resistant bacterial pathogens., 2024,, 269-284.		0
1612	Exploring the structural acrobatics of fold-switching proteins using simplified structure-based models. Biophysical Reviews, 0, , .	3.2	1
1613	Design of nanoporous materials for trace removal of benzene through high throughput screening. Separation and Purification Technology, 2023, 324, 124558.	7.9	0
1614	Elastic constants of nano-scale hydrated cement paste composites using reactive molecular dynamics simulations to homogenization of hardened cement paste mechanical properties. Materials Today Communications, 2023, 36, 106671.	1.9	0
1615	Effect of periodic image interactions on kink pair activation of screw dislocation. Computational Materials Science, 2023, 228, 112369.	3.0	0
1616	Degrees of freedom of atoms in a rigid molecule for local temperature calculation in molecular dynamics simulation. Molecular Simulation, 0, , 1-8.	2.0	0
1617	CoFeNiTi and CrFeNiTi high entropy alloy thin films microstructure formation. Acta Materialia, 2023, 257, 119163.	7.9	2
1618	A microcracking-based model for the dynamic failure of carbon/carbon composites. International Journal of Mechanical Sciences, 2023, 260, 108625.	6.7	1
1619	Solubility of NaCl under anisotropic stress state. Journal of Chemical Physics, 2023, 159, .	3.0	0
1620	Transport coefficients for ion and solvent coupling. The case of the lithium-ion battery electrolyte. Journal of Chemical Physics, 2023, 159, .	3.0	2
1621	Investigation of Kinetics of Formation of MethaneÂ+ Propane Hydrates by Molecular Dynamics Method in the Presence of Hydrate Seed and Sea Salt. Journal of Engineering Thermophysics, 2023, 32, 312-320.	1.4	0
1622	Interaction of Nitrite Ions with Hydrated Portlandite Surfaces: Atomistic Computer Simulation Study. Materials, 2023, 16, 5026.	2.9	0
1623	Grain Size-Dependent Thermal Expansion of Nanocrystalline Metals. Materials, 2023, 16, 5032.	2.9	0
1624	Machine learning-assisted MD simulation of melting in superheated AlCu validates the Classical Nucleation Theory. Journal of Molecular Liquids, 2023, 387, 122606.	4.9	3
1625	Enhanced hydrogen-gas permeation through rippled graphene. Physical Review B, 2023, 108, .	3.2	2
1626	Chemistry of zipping reactions in mesoporous carbon consisting of minimally stacked graphene layers. Chemical Science, 2023, 14, 8448-8457.	7.4	7
1627	Kinetics of radiation-induced DNA double-strand breaks through coarse-grained simulations. Biophysical Journal, 2023, , .	0.5	0
1628	Multi-reward reinforcement learning based development of inter-atomic potential models for silica. Npj Computational Materials, 2023, 9, .	8.7	1

#	Article	IF	CITATIONS
1629	Influence of temperature on the microstructural evolution of SIMP and T91 steels in liquid lead-bismuth eutectic: Experiments and molecular dynamics simulations. Corrosion Science, 2023, 222, 111411.	6.6	4
1630	Temperature dependence of O solubility in liquid Na by atomistic simulation of Na(l)–Na <sub>2</sub> O(s) interfaces using corrected machine learning potential: a step towards simulating Na combustion. Physical Chemistry Chemical Physics, O, , .	2.8	O
1631	Habit plane of $\hat{l}$ -hydride in $\hat{l}$ ±-zirconium: Atomistic simulations. Journal of Nuclear Materials, 2023, 585, 154626.	2.7	0
1632	Atomistic modeling of metal–nonmetal interphase boundary diffusion. Acta Materialia, 2023, 257, 119172.	7.9	2
1633	Dependence of simulated radiation damage on crystal structure and atomic misfit in metals. Journal of Nuclear Materials, 2023, 585, 154633.	2.7	1
1634	Detecting dynamic domains and local fluctuations in complex molecular systems via timelapse neighbors shuffling. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	5
1635	Shear Thinning from Bond Orientation in Model Unentangled Bottlebrush Polymer Melts. Macromolecules, 2023, 56, 5708-5717.	4.8	1
1636	Transition dynamics and metastable states during premelting and freezing of ice surfaces. Physical Review B, 2023, 108, .	3.2	2
1637	Elastocaloric Effect in Graphene Kirigami. Nano Letters, 2023, 23, 8801-8807.	9.1	3
1638	Influence of nanofiller agglomeration on fracture properties of polymer nanocomposite: Insights from atomistic simulation. Engineering Fracture Mechanics, 2023, 290, 109503.	4.3	2
1639	Investigating surface effect on stress concentration in amorphous carbon materials with nano-scale pores: A molecular dynamics study. Mechanics of Materials, 2023, , 104750.	3.2	0
1640	Atomistic simulation of hardening in bcc iron-based alloys caused by nanoprecipitates. Computational Materials Science, 2023, 229, 112383.	3.0	1
1641	Sub-Micrometer Phonon Mean Free Paths in Metal–Organic Frameworks Revealed by Machine Learning Molecular Dynamics Simulations. ACS Applied Materials & Samp; Interfaces, 2023, 15, 36412-36422.	8.0	9
1642	Uncovering metallic glasses hidden vacancy-like motifs using machine learning. Materials and Design, 2023, , 112185.	7.0	1
1643	Charge equilibration model with shielded long-range Coulomb for reactive molecular dynamics simulations. Journal of Chemical Physics, 2023, 159, .	3.0	2
1644	Electrolytes with moderate lithium polysulfide solubility for high-performance long-calendar-life lithium–sulfur batteries. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	9
1645	Surface Heterogeneity Affects Adsorption Selectivity for CO <sub>2</sub> Over CH <sub>4</sub> in Bare Mesostructured Silica with 2D Hexagonal Symmetry and Different Pore Size. Advanced Materials Interfaces, 2023, 10, .	3.7	0
1646	Application of molecular dynamics simulation in the field of food enzymes: improving the thermal-stability and catalytic ability. Critical Reviews in Food Science and Nutrition, $0$ , $1-13$ .	10.3	O

#	Article	IF	CITATIONS
1647	Structural Characterization and Molecular Model Construction of High-Ash Coal from Northern China. Molecules, 2023, 28, 5593.	3.8	3
1648	Many-body mechanochemistry: Intramolecular strain in condensed matter chemistry. Physical Review Materials, 2023, 7, .	2.4	2
1649	Defect formation mechanisms in metal nanowire under cyclic loading: a molecular dynamics study. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 065020.	2.0	2
1650	Investigation of mechanical properties and structural integrity of graphene aerogels via molecular dynamics simulations. Physical Chemistry Chemical Physics, 0, , .	2.8	1
1651	Coarse-Grained Molecular Simulation of Bolapolyphiles with a Multident Lateral Chain: Formation and Structural Analysis of Cubic Network Phases. Journal of Chemical Theory and Computation, 2024, 20, 1519-1537.	5.3	1
1652	Mixed precision support in HPC applications: What about reliability?. Journal of Parallel and Distributed Computing, 2023, 181, 104746.	4.1	0
1653	Dislocation generation in diamond under extreme loading. Matter, 2023, 6, 3040-3056.	10.0	2
1654	Liquid state theory study of the phase behavior and macromolecular scale structure of model biomolecular condensates. Journal of Chemical Physics, 2023, 159, .	3.0	3
1655	AlphaMat: a material informatics hub connecting data, features, models and applications. Npj Computational Materials, 2023, 9, .	8.7	3
1656	Understanding the role of polymers on the nucleating behavior of water in dilute supercooled solutions. Journal of Chemical Physics, 2023, 159, .	3.0	2
1657	Molecular dynamics simulations of electrified interfaces including the metal polarisation. Physical Chemistry Chemical Physics, 2023, 25, 22619-22625.	2.8	1
1658	Interplay of shell evolution and oxidation depth on the ignition and combustion behavior of aluminum nanoparticles. Fuel, 2023, 353, 129260.	6.4	1
1659	Simulation of surface sputtering of fused quartz by clusters of different gases. AIP Conference Proceedings, 2023, , .	0.4	0
1660	Molecular Insight into the Effects of Clustering on the Dynamics of Ionomers in Solutions. ACS Macro Letters, 2023, 12, 1118-1124.	4.8	2
1661	Role of stacking fault energy in confined layer slip in nanolaminated Cu. Journal of Materials Science, 2024, 59, 4775-4787.	3.7	2
1662	Atomistic modeling of Mg-Al-Zn solid–liquid interfacial free energy. Computational Materials Science, 2023, 229, 112398.	3.0	0
1663	Machine-learned acceleration for molecular dynamics in CASTEP. Journal of Chemical Physics, 2023, 159, .	3.0	2
1664	Multi-aspect simulation insight on thermolysis mechanism and interaction of NTO/HMX-based plastic-bonded explosives: a new conception of the mixed explosive model. Physical Chemistry Chemical Physics, 2023, 25, 20951-20968.	2.8	2

#	Article	IF	CITATIONS
1665	Unconventional colloidal aggregation in chiral bacterial baths. Nature Physics, 2023, 19, 1680-1688.	16.7	2
1666	Mechanical properties and pore network connectivity of sodium montmorillonite as predicted by a coarse-grained molecular model. Applied Clay Science, 2023, 243, 107077.	5.2	1
1667	What do far-infrared spectra of solitary water in "water-in-solvent―systems reveal about water's solvation and dynamics?. Journal of Chemical Physics, 2023, 159, .	3.0	0
1668	Saddle point search with dynamic active volume. Computational Materials Science, 2023, 228, 112354.	3.0	O
1669	Study of ageing and size effects in Nickel–Titanium shape memory alloy using molecular dynamics simulations. Phase Transitions, 2023, 96, 596-606.	1.3	0
1670	SOURSOP: A Python Package for the Analysis of Simulations of Intrinsically Disordered Proteins. Journal of Chemical Theory and Computation, 2023, 19, 5609-5620.	5.3	3
1672	Open-Source Machine Learning in Computational Chemistry. Journal of Chemical Information and Modeling, 2023, 63, 4505-4532.	5 <b>.</b> 4	3
1673	PyL3dMD: Python LAMMPS 3D molecular descriptors package. Journal of Cheminformatics, 2023, 15, .	6.1	1
1674	Nanoscale modeling of shock response of polyurea., 2023,, 273-302.		0
1675	Identifying crack tip position and stress intensity factors from displacement data. International Journal of Fracture, 0, , .	2.2	0
1676	Structural morphology and surface recrystallization properties of GaN nanoparticles with different sizes during sintering. Ceramics International, 2023, 49, 32292-32300.	4.8	0
1677	Partial proton ordering during phase transition in Friedel's salt. Applied Clay Science, 2023, 243, 107072.	5.2	0
1678	Molecular simulation and machine learning tools to predict bioglass modulus of elasticity. Journal of Non-Crystalline Solids, 2023, 618, 122507.	3.1	1
1679	Thermal Conductivity of 3C/4H-SiC Nanowires by Molecular Dynamics Simulation. Nanomaterials, 2023, 13, 2196.	4.1	2
1680	High Mechanical Energy Storage Capacity of Ultranarrow Carbon Nanowires Bundles by Machine Learning Driving Predictions. Advanced Energy and Sustainability Research, 2023, 4, .	5.8	3
1682	Impact of flexibility on the aggregation of polymeric macromolecules. European Physical Journal E, 2023, 46, .	1.6	0
1683	Electronegativity Force Field for Prediction of Elastic Moduli. Journal of Physical Chemistry A, 2023, 127, 6628-6634.	2,5	0
1684	Influence characteristics of water penetration on fibreâ€reinforced polymer/rigid polyurethane foam interface of the composite crossâ€arm considering natural ageing. High Voltage, 2024, 9, 81-93.	4.7	1

#	ARTICLE	IF	CITATIONS
1685	Atomic Local Ordering and Alloying Effects on the Mg <sub>3</sub> (Sb <sub>1â€"<i>x</i></sub> Bi <sub><i>x</i></sub> ) <sub>2</sub> Thermoelectric Material. ACS Applied Materials & Description of the Mg (Sb <sub) (s<="" (sb<sub)="" action="" td=""><td>8.0</td><td>3</td></sub)>	8.0	3
1687	Acid Radical Tolerance of Silane Coatings on Calcium Silicate Hydrate Surfaces in Aggressive Environments: The Role of Nitrate/Sulfate Ratio. Langmuir, 2023, 39, 11304-11316.	3.5	5
1688	Catalytic effect of graphene on the inversion of corannulene using a continuum approach with the Lennard-Jones potential. Nanoscale Advances, 2023, 5, 4571-4578.	4.6	2
1689	Energetic contributions to deformation twinning in magnesium. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 075002.	2.0	1
1690	Exploring the 3D Conformation of Hard ore Soft‧hell Particles Adsorbed at a Fluid Interface. Advanced Science, 2023, 10, .	11.2	2
1691	In-Depth Evaluation of a Lower-Level Direct-Verbs API on InfiniBand-based Clusters: Early Experiences. , 2023, , .		0
1692	Enhanced thermal conductivity in Ag-H2O nanofluids by nanoparticles of different shapes: Insights from molecular dynamics simulation. Journal of Molecular Liquids, 2023, 388, 122750.	4.9	1
1693	A Task Based Approach for Co-Scheduling Ensemble Workloads on Heterogeneous Nodes. , 2023, , .		0
1694	Insights from molecular dynamics into the chemistry-structure relationships of calcium aluminosilicate glasses. Journal of Non-Crystalline Solids, 2023, 618, 122545.	3.1	1
1695	Controlling surface cation segregation in a double perovskite for oxygen anion transport in high temperature energy conversion devices. Physical Chemistry Chemical Physics, 2023, 25, 22022-22031.	2.8	2
1696	Coarse-Graining of Molecular Dynamics Using Neural Ordinary Differential Equations. , 2023, , .		1
1697	Proton transport through interfaces in nanophase-separation of hydrated aquivion membrane: Molecular dynamics simulation approach. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 676, 132187.	4.7	0
1699	Effect of five typical vacancy defects on the tribological behaviors of MoS2 sheet: A molecular dynamics study. Applied Surface Science, 2023, 639, 158175.	6.1	1
1700	Volatile Organic Compounds Adsorption Capacities of Zeolite/Activated Carbon Composites Formed by Flectrostatic Self-Assembly, ACS Applied Materials & Samp; Interfaces, 2023, 15, 38781-38794. Bridging adsorption behavior of confined CH mml.math	8.0	1
1701	xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si259.svg" display="inline" id="d1e1527"> <mml:msub><mml:mrow></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub> -CO <mml:math <="" altimg="si260.svg" display="inline" td="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>6.4</td><td>2</td></mml:math>	6.4	2
1702	id="d1e1535"> < mml:msub> < mml:mrow / mml:msub> < lambda / mml:msub> <	0.9	0
1703	Tuning the reactivity of Ni/MoS2 membrane for efficient methane pyrolysis and hydrogen production: A multi-scale study. Energy Conversion and Management, 2023, 293, 117476.	9.2	2
1704	Local structure, thermodynamics, and melting of boron phosphide at high pressures by deep learning-driven <i>abÂinitio</i> simulations. Journal of Chemical Physics, 2023, 159, .	3.0	2

#	Article	IF	CITATIONS
1705	Semi-supervised generative approach to chemical disorder: application to point-defect formation in uranium–plutonium mixed oxides. Physical Chemistry Chemical Physics, 2023, 25, 23069-23080.	2.8	0
1706	Recent advances in Accelerated Molecular Dynamics Methods: Theory and Applications. , 2024, , 360-383.		0
1707	Deformation insensitive thermal conductance of the designed Si metamaterial. Applied Physics Letters, 2023, 123, .	3.3	0
1708	Roadmap on electronic structure codes in the exascale era. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 063301.	2.0	8
1709	Graph neural networks classify molecular geometry and design novel order parameters of crystal and liquid. Journal of Chemical Physics, 2023, 159, .	3.0	3
1710	Effects of surfactant adsorption on the wettability and friction of biomimetic surfaces. Physical Chemistry Chemical Physics, 2023, 25, 21916-21934.	2.8	0
1711	Phase Behavior and Liquid Crystalline Ordering of [2]Catenated Molecular Systems. Macromolecules, 2023, 56, 6189-6198.	4.8	0
1712	Dynamics of Motility-Induced Clusters: Coarsening beyond Ostwald Ripening. Physical Review Letters, 2023, 131, .	7.8	2
1713	Modulating grain boundary-mediated plasticity of high-entropy alloys via chemo-mechanical coupling. Acta Materialia, 2023, 258, 119228.	7.9	1
1714	Effect of Frenkel pairs on the tensile and shock compression strength of multi-elemental alloys. Physica Scripta, 2023, 98, 095939.	2.5	1
1715	Athermal evolution of nanocrystalline tungsten driven by irradiation. Journal of Nuclear Materials, 2023, 586, 154662.	2.7	0
1716	Dynamics of chromosome organization in a minimal bacterial cell. Frontiers in Cell and Developmental Biology, 0, $11$ , .	3.7	2
1718	Dynamic magnetic properties of magnetosomes. Smart Materials and Structures, 2023, 32, 095030.	3.5	1
1719	Molecular dynamics modeling of thermodiffusion in solids with charged defects using uranium dioxide as the case study. Chemical Engineering Science, 2023, 281, 119141.	3.8	0
1721	Over- and Undercoordinated Atoms as a Source of Electron and Hole Traps in Amorphous Silicon Nitride (a-Si3N4). Nanomaterials, 2023, 13, 2286.	4.1	2
1722	xmins:mmi="http://www.w3.org/1998/Math/MathML" altimg="si52.svg" display="inline" id="d1e425"> <mml:msub><mml:mrow></mml:mrow><mml:mrow></mml:mrow></mml:msub> O <mml:math altimg="si53.svg" display="inline" in="" inline"="" tab<="" table="" td="" the="" to="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>7.9</td><td>2</td></mml:math>	7.9	2
1723	Molecular dynamics approach for the calculation of the surface loss probabilities of neutral species in argon–methane plasma. Plasma Processes and Polymers, 2024, 21, .	3.0	1
1724	Viscosity mechanism of perfluorosulfonic acid-based materials and their application in proton exchange membrane fuel cells. Applied Materials Today, 2023, 34, 101896.	4.3	1

#	Article	IF	CITATIONS
1725	Modular Functionalization of Metalâ€Organic Frameworks for Nitrogen Recovery from Fresh Urine**. Angewandte Chemie, 2023, 135, .	2.0	0
1726	Computational study of graphene flakes for carbon capture. Chemical Physics, 2023, 574, 112046.	1.9	0
1727	Tribochemistry and frictional properties of octene molecules confined between iron oxide surfaces. Tribology International, 2023, 188, 108865.	5.9	0
1728	Using limited neural networks to assess relative mechanistic influence on shock heating in granular solids. Physical Review Materials, 2023, 7, .	2.4	1
1729	Methane hydrate nucleation path and structure evolution revealed by Markov modelling. Fuel, 2024, 355, 129504.	6.4	0
1730	Developing machine-learned potentials to simultaneously capture the dynamics of excess protons and hydroxide ions in classical and path integral simulations. Journal of Chemical Physics, 2023, 159, .	3.0	1
1731	Probing the elastic response of lipid bilayers and nanovesicles to leaflet tensions via volume per lipid. Soft Matter, 0, , .	2.7	0
1732	Molecular Dynamic Simulation and Experiment Validation on the Diffusion Behavior of Diffusion Welded Fe-Ti by Hot Isostatic Pressing Process. Materials, 2023, 16, 5626.	2.9	0
1733	High-Accuracy Machine-Learned Interatomic Potentials for the Phase Change Material Ge <sub>3</sub> Sb <sub>6</sub> Te <sub>5</sub> . Chemistry of Materials, 0, , .	6.7	0
1734	A molecular dynamics study of the effects of velocity and diameter on the impact behavior of zinc oxide nanoparticles. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 075008.	2.0	1
1735	Lifetime Optimization of Amorphous Silicon Thin-Film Anodes for Lithium-Ion Batteries. ACS Applied Energy Materials, 2023, 6, 8388-8396.	5.1	3
1736	Discovery of enhanced lattice dynamics in a single-layered hybrid perovskite. Science Advances, 2023, 9,	10.3	3
1737	Molecular Dynamics Simulation Study on Self-Assembly of Polymer-Grafted Nanocrystals: From Isotropic Cores to Anisotropic Cores. Journal of Chemical Theory and Computation, 2024, 20, 1625-1635.	5.3	0
1738	Stress-dependent activation entropy in thermally activated cross-slip of dislocations. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	3
1739	Molecular simulations of transport properties of polar hydrofluoroethers: Force field development, fractional Stokes-Einstein and free volume relations. Journal of Molecular Liquids, 2023, 389, 122847.	4.9	1
1740	A temperature-dependent length-scale for transferable local density potentials. Journal of Chemical Physics, 2023, 159, .	3.0	2
1741	Modeling the 4D discharge of lithium-ion batteries with a multiscale time-dependent deep learning framework. Energy Storage Materials, 2023, 63, 102927.	18.0	2
1742	DNA-protamine condensates under low salt conditions: molecular dynamics simulation with a simple coarse-grained model focusing on electrostatic interactions. Nanoscale Advances, 0, , .	4.6	1

#	Article	IF	CITATIONS
1743	Multi-component delocalized nonlinear vibrational modes in nickel. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 075009.	2.0	1
1744	DMFF: An Open-Source Automatic Differentiable Platform for Molecular Force Field Development and Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2023, 19, 5897-5909.	5.3	1
1745	Thermoporoelastic Moduli from Molecular Fluctuations and Application to Moisture Effect on Amorphous Cellulose. Journal of Engineering Mechanics - ASCE, 2023, 149, .	2.9	0
1746	Temperature, strain rate, and point vacancy dependent anisotropic mechanical behaviors of titanium carbide (Ti3C2) MXene: A molecular dynamics study. Materials Today Communications, 2023, 37, 106898.	1.9	0
1747	A hybrid off-lattice kinetic Monte Carlo/molecular dynamics method for amorphous thin film growth. Computational Materials Science, 2023, 229, 112421.	3.0	1
1748	Local Rearrangement in Adsorption Layers of Nanoconfined Ethane. Journal of Physical Chemistry C, 2023, 127, 17290-17297.	3.1	0
1749	Spatial localization of high-frequency particle oscillations in a complex plasma monolayer. Journal Physics D: Applied Physics, 2023, 56, 485203.	2.8	1
1750	Janus magnetoelastic membrane swimmers. Soft Matter, 0, , .	2.7	0
1751	Understanding Rapid PET Degradation via Reactive Molecular Dynamics Simulation and Kinetic Modeling. Journal of Physical Chemistry A, O, , .	2.5	0
1752	Self–ion irradiation of high purity iron: Unveiling plasticity mechanisms through nanoindentation experiments and large-scale atomistic simulations. Journal of Nuclear Materials, 2023, 586, 154690.	2.7	6
1753	A Molecular Dynamics Study of Nucleation and Grain Growth of Novel Al-15Mg <sub>2</sub> Si-4.5Si Composite during Rapid Cooling Based Semi Solid Slurry Preparation. Solid State Phenomena, 0, 347, 197-203.	0.3	1
1754	Modified embedded atom method interatomic potential for FCC $\hat{I}^3$ -cerium. Computational Materials Science, 2023, 230, 112454.	3.0	0
1755	Nanoscale friction behavior and deformation during copper chemical mechanical polishing process. Journal of Molecular Modeling, 2023, 29, .	1.8	0
1756	Cracking polymer coatings of paper-like surfaces: Control via block co-polymer structure and system composition. Applied Surface Science, 2023, 640, 158324.	6.1	1
1757	Resonance with surface waves induces forbidden velocity bands in dislocation glide. Journal of the Mechanics and Physics of Solids, 2023, 180, 105422.	4.8	2
1759	Tuning structural and thermal conductivity of carbon nanotubes under strain effects. Chinese Journal of Physics, 2023, 86, 24-38.	3.9	1
1760	Clustering of fluoride and phosphate ions in bioactive glass from computer simulation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2023, 381, .	3.4	1
1761	Investigation of N Migration during Municipal Sludge/Coal Co-Pyrolysis via ReaxFF Molecular Dynamics. Energy & Dynamics.	5.1	1

#	Article	IF	CITATIONS
1762	Reactant-induced dynamics of lithium imide surfaces during the ammonia decomposition process. Nature Catalysis, 2023, 6, 829-836.	34.4	9
1763	Nanoscale phenomena during wetting of copper on nickel-based superalloy: A molecular dynamics study. Computational Materials Science, 2023, 230, 112453.	3.0	0
1764	Atomistic analysis of temperature-dependent dislocation dynamics in Ni3Al-based intermetallic alloys. Materials Today Communications, 2023, 37, 106987.	1.9	0
1765	Unraveling Anisotropy in Crystalline Orientation under Shock-Induced Dynamic Responses in High-Entropy Alloy Co25Ni25Fe25Al7.5Cu17.5. Nanomaterials, 2023, 13, 2446.	4.1	0
1766	Probabilistic Approach to Low Strain Rate Atomistic Simulations of Ultimate Tensile Strength of Polymer Crystals. Journal of Chemical Theory and Computation, 0, , .	5.3	0
1767	Complex coupling between surface charge and thermo-osmotic phenomena. Physical Chemistry Chemical Physics, 2023, 25, 24321-24331.	2.8	1
1768	Steric effects in induced-charge electro-osmosis for strong electric fields. Physical Review Fluids, 2023, 8, .	2.5	0
1769	Effect of Flexibility in Molecular Simulations of Carbon Dioxide Adsorption and Diffusion in a Cuprous Triazolate Framework. Journal of Physical Chemistry C, 0, , .	3.1	0
1770	Methodology for Calculation of Elastic Constants of Diamane by Molecular Dynamics. , 2023, , .		0
1771	Implementation of a ternary lattice Boltzmann model in LAMMPS. Computer Physics Communications, 2024, 294, 108898.	7.5	0
1772	Atomistic modeling of extreme near-field heat transport across nanogaps between two polar dielectric materials. Physical Review B, 2023, 108, .	3.2	1
1773	Simulated surface diffusion in nanoporous gold and its dependence on surface curvature. Computational Materials Science, 2023, 230, 112430.	3.0	0
1774	PANNA 2.0: Efficient neural network interatomic potentials and new architectures. Journal of Chemical Physics, 2023, 159, .	3.0	3
1775	An approach using molecular dynamics to connect biomaterials with solar systems to increase the amount of renewable energy: Application in built environments. Engineering Analysis With Boundary Elements, 2023, 156, 467-474.	3.7	0
1776	Structure of the Hexadecane Rotator Phase: Combination of X-ray Spectra and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2023, 127, 7772-7784.	2.6	2
1777	An atomistic-continuum concurrent statistical coupling technique for amorphous materials using anchor points. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 075012.	2.0	0
1778	Shear stress-induced delamination method for the mass production of Ti3C2T MXene nanosheets. Journal of Materiomics, 2023, 9, 1151-1159.	5.7	1
1779	Comparing interatomic potentials in calculating basic structural parameters and Peierls stress in tungsten-based random binary alloys. Physica Scripta, 2023, 98, 105923.	2.5	1

#	Article	IF	CITATIONS
1780	Xe Recovery from Nuclear Power Plants Off-Gas Streams: Molecular Simulations of Gas Permeation through DD3R Zeolite Membrane. Membranes, 2023, 13, 768.	3.0	0
1781	Spin-lattice-dynamics analysis of magnetic properties of iron under compression. Scientific Reports, 2023, 13, .	3.3	0
1782	Structural Dynamics Descriptors for Metal Halide Perovskites. Journal of Physical Chemistry C, 2023, 127, 19141-19151.	3.1	4
1783	Functionalized Carbon Honeycomb Membranes for Reverse Osmosis Water Desalination. Advanced Materials Interfaces, 2023, 10, .	3.7	0
1784	Molecular dynamics simulation-based study of single-crystal 3C-SiC nano-indentation with water film. Applied Physics A: Materials Science and Processing, 2023, 129, .	2.3	1
1785	Study of In-Plane and Interlayer Interactions During Aluminum Fluoride Intercalation in Graphite: Implications for the Development of Rechargeable Batteries. ACS Applied Nano Materials, 2023, 6, 16977-16985.	5.0	1
1786	Universal and interpretable classification of atomistic structural transitions via unsupervised graph learning. Applied Physics Letters, 2023, 123, .	3.3	0
1787	ChecMatE: A workflow package to automatically generate machine learning potentials and phase diagrams for semiconductor alloys. Journal of Chemical Physics, 2023, 159, .	3.0	1
1788	High-throughput screening of amorphous polymers with high intrinsic thermal conductivity <i>via</i> automated physical feature engineering. Journal of Materials Chemistry A, 2023, 11, 20539-20548.	10.3	2
1789	Microscopic insight into the shaping of MOFs and its impact on CO <sub>2</sub> capture performance. Chemical Science, 2023, 14, 10435-10445.	7.4	3
1790	Structure and energetics of hydrogen bonding networks in dilute HOD/H <sub>2</sub> O solutions confined in silica nanopores. Environmental Science: Nano, 0, , .	4.3	0
1791	Hyperactive learning for data-driven interatomic potentials. Npj Computational Materials, 2023, 9, .	8.7	12
1792	Modeling the relationship between mechanical yield stress and material geometry using convolutional neural networks. Applied Physics Letters, 2023, 123, .	3.3	0
1793	Mass dipole contribution to the isotopic Soret effect in molecular mixtures. Journal of Chemical Physics, 2023, 159, .	3.0	0
1794	Molecular dynamics study on nanoscale scratch characteristics of FeNiCrCoAl high-entropy alloy. AIP Advances, 2023, 13, .	1.3	0
1795	Giant Atomic Swirl in Graphene Bilayers with Biaxial Heterostrain. Advanced Materials, 2023, 35, .	21.0	3
1796	OpenABC enables flexible, simplified, and efficient GPU accelerated simulations of biomolecular condensates. PLoS Computational Biology, 2023, 19, e1011442.	3.2	1
1797	Methane adsorption of nanocomposite shale in the presence of water: Insights from molecular simulations. Chemical Engineering Journal, 2023, 475, 146196.	12.7	3

#	Article	IF	CITATIONS
1798	kMCpy: A python package to simulate transport properties in solids with kinetic Monte Carlo. Computational Materials Science, 2023, 229, 112394.	3.0	1
1799	Atomistic simulation of carbide formation in ferrite. Computational Materials Science, 2023, 230, 112455.	3.0	1
1802	Mechanical properties of Sb <sub>2</sub> Te <sub>3</sub> nanostructures under tensile loading. Japanese Journal of Applied Physics, 2023, 62, SN1009.	1.5	0
1803	Effect of shock-induced plastic deformation on mesoscale criticality of 1,3,5-trinitro-1,3,5-triazinane (RDX). Journal of Applied Physics, 2023, 134, 105901.	2.5	O
1804	Understanding continuous wave laser-induced chemical reactions at micro- and nano-diamond-glass interface under infrared excitation. Materials Research Express, 2023, 10, 095601.	1.6	0
1805	Molecular dynamics exploration of helium bubble nucleation and growth mechanisms in Fe <sub>70</sub> Ni <sub>11</sub> Cr <sub>19</sub> austenitic stainless steel. RSC Advances, 2023, 13, 23236-23243.	3.6	0
1806	Computational approach for structure generation of anisotropic particles (CASGAP) with targeted distributions of particle design and orientational order. Nanoscale, 2023, 15, 14958-14970.	5.6	1
1807	Performance Evaluation of Graphene Nanofluid to Mitigate the Wear of a Diamond Tool in Micro-Machining of Ti6Al4V Alloy. Journal of Manufacturing and Materials Processing, 2023, 7, 131.	2.2	1
1808	Structure and self-diffusivity of alkali-halide electrolytes in neutral and charged graphene nanochannels. Physical Chemistry Chemical Physics, 2023, 25, 21579-21594.	2.8	2
1809	The impact of binding energies on the necessary conditions in aerosol deposition. Proceedings in Applied Mathematics and Mechanics, 2023, 23, .	0.2	0
1810	Shock compression of semiflexible polymers. Soft Matter, 2023, 19, 6131-6139.	2.7	0
1811	Anelasticity to plasticity transition in a model two-dimensional amorphous solid. Chinese Physics B, O,	1.4	0
1812	Dynamic formation of preferentially lattice oriented, self trapped hydrogen clusters. Materials Research Express, 2023, 10, 106513.	1.6	0
1813	Does freezing induce self-assembly of polymers? A molecular dynamics study. Soft Matter, 2023, 19, 7570-7579.	2.7	0
1814	Effects of Stress State, Crack—γ/γ′ Phase Interface Relative Locations and Orientations on the Deformation and Crack Propagation Behaviors of the Ni-Based Superalloy—A Molecular Dynamics Study. Crystals, 2023, 13, 1446.	2.2	0
1815	Simulation of Crystal Nuclei at the Liquid-Air Interface toward Morphology Control via Surface Tension. Journal of Physical Chemistry C, 2023, 127, 17231-17238.	3.1	0
1816	Revisiting the pseudo-supercritical path method: An improved formulation for the alchemical calculation of solid–liquid coexistence. Journal of Chemical Physics, 2023, 159, .	3.0	0
1818	Ab Initio-Derived Force Field for Amorphous Silica Interfaces for Use in Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2023, 127, 16567-16578.	3.1	О

#	Article	IF	CITATIONS
1819	Study of the Structural Changes and Internal Activator Transport Behavior after Activation of Aluminum-Based Flameless Ration Heaters: Experimental and Molecular Dynamics Simulations. ACS Omega, 2023, 8, 30929-30938.	3.5	0
1820	Modular Functionalization of Metalâ€Organic Frameworks for Nitrogen Recovery from Fresh Urine**. Angewandte Chemie - International Edition, 2023, 62, .	13.8	1
1821	Structure and Properties of Water in a New Model of the 10-Ã Phase: Classical and Ab Initio Atomistic Computational Modeling. Minerals (Basel, Switzerland), 2023, 13, 1018. athmic altimg="si14.svg"	2.0	2
1822	id="d1e1144"> <mml:mrow><mml:mo>ã€^</mml:mo><mml:mi>a</mml:mi><mml:mo>〉</mml:mo>prismatic screw dislocations with the <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">altimg="si167.svg" display="inline" id="d1e1154"&gt;<mml:mrow><mml:mi>α</mml:mi><mml:mo< td=""><td>ow&gt;7.9</td><td>:math&gt; O</td></mml:mo<></mml:mrow></mml:math></mml:mrow>	ow>7.9	:math> O
1823	Designing phosphazene-derivative electrolyte matrices to enable high-voltage lithium metal batteries for extreme working conditions. Nature Energy, 2023, 8, 1023-1033.	39.5	12
1824	Shared metadata for data-centric materials science. Scientific Data, 2023, 10, .	<b>5.</b> 3	3
1825	Deep learning modeling in microscopy imaging: A review of materials science applications. Progress in Materials Science, 2023, 138, 101165.	32.8	1
1826	Molecular dynamics study on the uniaxial tensile behavior of mono-layer MoTe2 film defected by mirror twin boundary. Computational Materials Science, 2023, 230, 112481.	3.0	1
1827	Ultra-fast interpretable machine-learning potentials. Npj Computational Materials, 2023, 9, .	8.7	3
1828	Unravelling densification during sintering by multiscale modelling of grain motion. Journal of Materials Science, 2023, 58, 14051-14071.	3.7	1
1829	Shock-induced melting and crystallization in titanium irradiated by ultrashort laser pulse. Physics of Fluids, 2023, 35, .	4.0	5
1830	Thermal mass transport mechanism of an adatom on a crystalline surface. Physical Review B, 2023, 108,	3.2	O
1831	Effects of copper on BCC-FCC phase transition of tungsten under compression and shear deformation. Physica B: Condensed Matter, 2023, 670, 415352.	2.7	1
1832	Tailoring the Selectivity of 1,3-Butadiene versus 1-Butene Adsorption on $Pt(111)$ by Ultrathin Ionic Liquid Films. ACS Catalysis, 2023, 13, 10866-10877.	11.2	O
1833	Influence of Chain Stiffness on the Segmental Dynamics and Mechanical Properties of Cross-Linked Polymers. Macromolecules, 2023, 56, 7636-7650.	4.8	2
1834	Sorption-Deformation Interplay in Hierarchical Porous Polymeric Structures Composed of a Slit Pore in an Amorphous Matrix. Langmuir, 2023, 39, 11345-11356.	3.5	1
1835	Effects of bismuth nanoparticles on the nano-cutting properties of single-crystal iron materials: a molecular dynamics study. Applied Physics A: Materials Science and Processing, 2023, 129, .	2.3	2
1836	Chemical Modifications on Cellulose Nanocrystals for Composites: Surface Chemistry to Tailored Compatibility and Mechanical Enhancement. Macromolecules, 2023, 56, 7505-7519.	4.8	2

#	Article	IF	CITATIONS
1837	Order–Disorder Phase Transition and Ionic Conductivity in a Li <sub>2</sub> B <sub>12</sub> H <sub>12</sub> Solid Electrolyte. ACS Applied Materials & Discrete Subsubsets (1998) According to the conductivity in a Li <sub>1000 Solid Electrolyte. ACS Applied Materials &amp; Discrete Subsubsets (1998) According to the conductivity in a Li  Interfaces, 2023, 15, 42511-42519.</sub>	8.0	0
1838	Inorganic glass electrolytes with polymer-like viscoelasticity. Nature Energy, 2023, 8, 1221-1228.	39.5	9
1839	Influence of Temperature-Guided SAM Growth on Wetting and Its Mass Transfer Models. Journal of Physical Chemistry B, 2023, 127, 8208-8215.	2.6	0
1840	Machine-Learning Accelerated First-Principles Accurate Modeling of the Solid–Liquid Phase Transition in MgO under Mantle Conditions. Journal of Physical Chemistry Letters, 2023, 14, 8741-8748.	4.6	1
1841	Molecular Dynamics Simulation of the Influence of Temperature and Salt on the Dynamic Hydration Layer in a Model Polyzwitterionic Polymer PAEDAPS. Journal of Physical Chemistry B, 2023, 127, 8185-8198.	2.6	O
1842	An Updated Review on Developing Small Molecule Kinase Inhibitors Using Computer-Aided Drug Design Approaches. International Journal of Molecular Sciences, 2023, 24, 13953.	4.1	5
1843	Multiscale Investigation of Carbon Fiber Oxidation Kinetics: Bridging Atomistic Simulation and a Finite-Rate Reaction Model. Journal of Physical Chemistry C, 2023, 127, 19947-19962.	3.1	0
1844	MBX: A many-body energy and force calculator for data-driven many-body simulations. Journal of Chemical Physics, 2023, 159, .	3.0	8
1845	Multiscale Reactive Model for 1,3,5-Triamino-2,4,6-trinitrobenzene Inferred by Reactive MD Simulations and Unsupervised Learning. Journal of Physical Chemistry C, 2023, 127, 15556-15572.	3.1	4
1846	Coarse-Grained Simulation of PEO/LiTFSI Electrolytes with Assistance of Bayesian Optimization. Macromolecules, 2023, 56, 6609-6617.	4.8	O
1847	Dioctyl sodium sulfosuccinate surfactant self-assembly dependency of solvent hydrophilicity: a modelling study. Physical Chemistry Chemical Physics, 2023, 25, 27250-27263.	2.8	0
1848	Atomistic simulations of calcium aluminosilicate interfaced with liquid water. Journal of Chemical Physics, 2023, 159, .	3.0	1
1849	Unraveling pyrolysis mechanisms of lignin dimer model compounds: Neural network-based molecular dynamics simulation investigations. Fuel, 2024, 357, 129909.	6.4	1
1850	Effect of gas cluster species on crater formation for fused silica. Journal of Non-Crystalline Solids, 2023, 619, 122590.	3.1	O
1851	Ultralow-energy amorphization of contaminated silicon samples investigated by molecular dynamics. Beilstein Journal of Nanotechnology, 0, 14, 834-849.	2.8	0
1852	Geometrically frustrated interactions drive structural complexity in amorphous calcium carbonate. Nature Chemistry, 2024, 16, 36-41.	13.6	2
1853	Graphyne-based membrane as a promising candidate for Li-Battery electrodes protection: Insight from atomistic simulations. Journal of Power Sources, 2023, 581, 233482.	7.8	1
1854	Cationic-group-functionalized electrocatalysts enable stable acidic CO2 electrolysis. Nature Catalysis, 2023, 6, 763-772.	34.4	23

#	Article	IF	CITATIONS
1855	Velocity effect in swift heavy ion irradiation: how the low- and high-energy track formation thresholds meet. Journal of Materials Science, 2023, 58, 14072-14079.	3.7	0
1856	Structural and Electromagnetic Signatures of Anatase and Rutile NTs and Sheets in Three Different Water Models under Different Temperature Conditions. International Journal of Molecular Sciences, 2023, 24, 14878.	4.1	O
1857	Nanoindentation Study of Calcium-Silicate-Hydrate Gel via Molecular Dynamics Simulations. Nanomaterials, 2023, 13, 2578.	4.1	2
1858	Molecular Dynamics Studies of the Ho(III) Aqua-tris(dibenzoylmethane) Complex: Role of Water Dynamics. Inorganic Chemistry, 2023, 62, 11897-11909.	4.0	1
1859	DeePMD-kit v2: A software package for deep potential models. Journal of Chemical Physics, 2023, 159, .	3.0	39
1860	Single-Layer and Double-Layer Filtration Materials Based on Polyvinylidene Fluoride-Co-hexafluoropropylene Nanofibers Coated on Melamine Microfibers. ACS Applied Nano Materials, 2023, 6, 15807-15819.	5.0	1
1861	Compression and Ordering of Hollow Microgels in Monolayers Formed at Liquid–Liquid Interfaces. Langmuir, 2023, 39, 12420-12429.	3.5	0
1862	Logarithmic aging via instability cascades in disordered systems. Nature Physics, 2023, 19, 1890-1895.	16.7	2
1863	Laser-Induced MXene-Functionalized Graphene Nanoarchitectonics-Based Microsupercapacitor for Health Monitoring Application. ACS Nano, 2023, 17, 20537-20550.	14.6	4
1864	Crystal nucleation in a vapor deposited Lennard-Jones mixture. Journal of Molecular Liquids, 2023, 391, 123178.	4.9	0
1865	An investigation of the density of nano-confined subcritical/supercritical water. Energy, 2023, 284, 129185.	8.8	0
1866	Molecular Signatures of Asphaltene Precipitation in a Depressurization Process. Energy & Depress. Energy & Depressurization Process. Energy & Depressurization Process. Energy & Depression Process. Energy & Depression Process. Energy & Depress. Energy & Depression Process. Energy	5.1	0
1867	An atomistic model of aged asphalt guided by the oxidation chemistry of benzylic carbon with application to asphalt rejuvenated with a triglyceride. Construction and Building Materials, 2023, 400, 132743.	7.2	1
1868	Effects of temperature on microstructures of MSA-type electroplating solution: a coarse-grained molecular dynamics simulation. Physical Chemistry Chemical Physics, 2023, 25, 28272-28281.	2.8	0
1869	Accurate Calculation of Solvation Properties of Lithium Ions in Nonaqueous Solutions. Journal of Physical Chemistry B, 2023, 127, 8002-8008.	2.6	0
1870	Dynamical coarse-grained models of molecular liquids and their ideal and non-ideal mixtures. Journal of Chemical Physics, 2023, 159, .	3.0	1
1871	The Back Door to the Surface Hydrated Electron. Journal of Physical Chemistry Letters, 2023, 14, 8221-8226.	4.6	0
1872	Predicting elastic and plastic properties of small iron polycrystals by machine learning. Scientific Reports, 2023, 13, .	3.3	1

#	Article	IF	CITATIONS
1873	Dislocation-mediated migration of the $\hat{l}\pm/\hat{l}^2$ interfaces in titanium. Acta Materialia, 2023, 261, 119364.	7.9	1
1874	Working mechanism of MXene as the anode protection layer of aqueous zinc-ion batteries. Journal of Colloid and Interface Science, 2024, 654, 289-299.	9.4	3
1875	Insights into Interfacial Thermal Resistance in Bi <sub>2</sub> Te <sub>3</sub> /Graphene Composites for Thermoelectric Applications. Journal of Physical Chemistry C, 2023, 127, 19796-19804.	3.1	1
1876	Tribological behaviors of amorphous carbon under water lubrication through a bottom-up coarse-grained method. Tribology International, 2023, 189, 109022.	5.9	O
1877	Mechano-Chemical Properties and Tribological Performance of Thin Perfluoropolyether (PFPE) Lubricant Film under Environmental Contaminants. Lubricants, 2023, 11, 306.	2.9	0
1878	Adhesion Performance of Rubber Modified Asphalt in Chip Seal: A Molecular Dynamic Study. Materials, 2023, 16, 6324.	2.9	O
1879	Nonfluorinated Antisolvents for Ultrastable Potassium-Ion Batteries. ACS Nano, 2023, 17, 16135-16146.	14.6	5
1880	The effects of composition and microstructure on compressive strength of Ag-Au nanoparticles. Acta Materialia, 2023, 261, 119417.	7.9	1
1881	Force Field Parameters for Ammonium Perchlorate Validated Using Surface Energies and Applied to Interactions with Polymer Binder. Journal of Physical Chemistry C, 2023, 127, 18598-18608.	3.1	0
1882	Exploring the Structural, Dynamic, and Functional Properties of Metalâ€Organic Frameworks through Molecular Modeling. Advanced Functional Materials, 0, , .	14.9	3
1883	Thermal Conductivity of Water at Extreme Conditions. Journal of Physical Chemistry B, 2023, 127, 7011-7017.	2.6	1
1884	Molecular dynamics study of diffusionless phase transformations in HMX: $\langle i \rangle \hat{l}^2 \langle  i \rangle$ -HMX twinning and $\langle i \rangle \hat{l}^2 \langle  i \rangle$ - $\langle i \rangle \hat{E} \rangle \langle  i \rangle$ phase transition. Journal of Applied Physics, 2023, 134, .	2.5	2
1885	Crystallographic and temperature effects in low-energy collisions for plasma–material interactions. Materialia, 2023, 32, 101886.	2.7	0
1886	Origins of Charge Mobility Decreasing from Stretching–Releasing Cycles in Polymer Semiconductors. Macromolecules, 2023, 56, 7078-7085.	4.8	1
1887	Advancing Accurate and Efficient Surface Behavior Modeling of Al Clusters with Machine Learning Potential. Journal of Physical Chemistry C, 2023, 127, 19115-19126.	3.1	0
1888	Data Driven Discovery of MOFs for Hydrogen Gas Adsorption. Journal of Chemical Theory and Computation, 2023, 19, 6686-6703.	5.3	4
1889	Accurate energy barriers for catalytic reaction pathways: an automatic training protocol for machine learning force fields. Npj Computational Materials, 2023, 9, .	8.7	4
1890	Insights into the auxetic behavior of graphene: A study on the temperature dependence of Poisson's ratio and in-plane moduli. Carbon, 2023, 215, 118416.	10.3	O

#	Article	IF	CITATIONS
1891	Interfacial engineering for enhanced mechanical performance: High-entropy alloy/graphene nanocomposites. Materials Today Physics, 2023, 38, 101220.	6.0	3
1892	Deformation response of highly stretchable and ductile graphene kirigami under uniaxial and biaxial tension. Physical Review B, 2023, 108, .	3.2	6
1893	Effect of Characteristics of Polymer Microgel Catalysts on the Efficiency of Interfacial Catalysis. Polymer Science - Series C, 0, , .	1.7	0
1894	Transient of flow regimes and slip boundary analysis of water and gas in nano clay pores. Molecular Simulation, 2023, 49, 1519-1530.	2.0	0
1895	Structural organization of phase-separated bioactive glasses and the clustering of Si, P, B, Na and F atoms investigated by solid-state NMR and Monte Carlo simulations. Acta Materialia, 2023, 259, 119203.	7.9	0
1896	Discrepancies and error evaluation metrics for machine learning interatomic potentials. Npj Computational Materials, 2023, 9, .	8.7	3
1897	Mechanism of thermally-activated prismatic slip in Mg. Acta Materialia, 2024, 262, 119402.	7.9	1
1898	High damping and modulus of aluminum matrix composites reinforced with carbon nanotube skeleton inspired by diamond lattice. Composite Structures, 2023, 323, 117451.	5.8	1
1899	Microstructural mechanisms of hysteresis and transformation width in NiTi alloy from molecular dynamics simulations. Journal of Physics Condensed Matter, 2023, 35, 495404.	1.8	0
1900	Insights of the Ultralow Wear and Low Friction of Carbon Fiber Reinforced PTFE in Inert Trace Moisture Environment. Tribology Letters, 2023, 71, .	2.6	4
1901	Unraveling the pressure-viscosity behavior and shear thinning in glycerol using atomic scale molecular dynamics simulations. Journal of Molecular Liquids, 2023, 390, 122990.	4.9	0
1902	Atomic-Level and Surface Structure of Calcium Silicate Hydrate Nanofoils. Journal of Physical Chemistry C, 2023, 127, 18652-18661.	3.1	3
1903	Deciphering the Atomistic Mechanism of Si(111)-7 $\tilde{A}$ — 7 Surface Reconstruction Using a Machine-Learning Force Field. Journal of the American Chemical Society, 2023, 145, 20511-20520.	13.7	0
1904	Agglomeration Drives the Reversed Fractionation of Aqueous Carbonate and Bicarbonate at the Air–Water Interface. Journal of the American Chemical Society, 2023, 145, 22384-22393.	13.7	0
1905	Enhancing ion transport in nanofluidic systems through counter-charged nanochannels. Physics of Fluids, 2023, 35, .	4.0	2
1906	Bending the rules: Strain accommodation in layered crystalline solids through nanoscale buckling over dislocations. Journal of the Mechanics and Physics of Solids, 2023, , 105450.	4.8	O
1907	Reactive molecular dynamics simulation and chemical kinetic modeling of ammonia/methane co-combustion. Fuel, 2023, 354, 129341.	6.4	4
1908	Exceeding the hydrogen gravimetric capacity targets in cubic bundles of Li doped carbon nanotubes. Carbon, 2023, 215, 118388.	10.3	O

#	ARTICLE	IF	CITATIONS
1909	Quadratic scaling bosonic path integral molecular dynamics. Journal of Chemical Physics, 2023, 159, .	3.0	1
1910	Polyelectrolyte Gels: Swelling and Deswelling upon Nonlinear Deformations. Macromolecules, 2023, 56, 6543-6551.	4.8	1
1912	Atomistic insights into the effect of temperature on capillary transport of water molecules in epoxy-modified calcium silicate hydrate nanopore: diffusion, kinetics, and mechanism. Journal of Materials Science, 2023, 58, 14773-14787.	3.7	5
1913	From molecular sieving to gas effusion through nanoporous 2D graphenes: Comparison between analytical predictions and molecular simulations. Journal of Chemical Physics, 2023, 159, .	3.0	1
1914	Global structure optimization following imaginary phonon modes accelerated by machine learning potentials in Cu, Ag, and Au. Journal of the Ceramic Society of Japan, 2023, 131, 746-750.	1.1	0
1915	Reshaping Covalent Nanowires by Exploiting an Unexpected Plasticity Mediated by Deformation Twinning. Small, 2024, 20, .	10.0	0
1916	Developments and further applications of ephemeral data derived potentials. Journal of Chemical Physics, $2023, 159, .$	3.0	0
1917	Fracture toughness and destructive mechanism of ductile nanoporous metallic glass and its crystal-impregnated nanocomposite. Science China Technological Sciences, 2023, 66, 3328-3342.	4.0	1
1918	Explicit solvent machine-learned coarse-grained model of sodium polystyrene sulfonate to capture polymer structure and dynamics. European Physical Journal E, 2023, 46, .	1.6	1
1919	Automated characterization of spatial and dynamical heterogeneity in supercooled liquids via implementation of machine learning. Journal of Physics Condensed Matter, 2023, 35, 465401.	1.8	0
1920	Unveiling the Interactions between Water Molecule Clusters and Conical Structures via Molecular Dynamics Simulations. Langmuir, 2023, 39, 13028-13037.	3.5	0
1921	Self-Assembling of Nonadditive Mixtures Containing Patchy Particles with Tunable Interactions. Journal of Physical Chemistry B, 2023, 127, 8982-8992.	2.6	0
1922	Dynamics of molecular collisions in air and its mean free path. Physics of Fluids, 2023, 35, .	4.0	1
1924	Controllable ion transport in bilayer graphene with charged nanopores. Materials Today Chemistry, 2023, 34, 101767.	3.5	0
1925	First-principles spectroscopy of aqueous interfaces using machine-learned electronic and quantum nuclear effects. Faraday Discussions, 0, 249, 50-68.	3.2	2
1926	Random Batch Sum-of-Gaussians Method for Molecular Dynamics Simulations of Particle Systems. SIAM Journal of Scientific Computing, 2023, 45, B591-B617.	2.8	1
1927	Hydrogen passivation accelerated conversion of cotton to graphene. Sustainable Materials and Technologies, 2023, 38, e00736.	3.3	0
1928	Accelerated Design of Ultra-High-Performance Aramid Copolymers via a High-Throughput Screening Approach. ACS Applied Materials & Samp; Interfaces, 2023, 15, 40877-40886.	8.0	0

#	Article	IF	Citations
1929	Elucidating the Competitive Adsorption of H <sub>2</sub> O and CO <sub>2</sub> in CALF-20: New Insights for Enhanced Carbon Capture Metal–Organic Frameworks. ACS Applied Materials & Lamp; Interfaces, 2023, 15, 48287-48295.	8.0	4
1930	Spontaneously Generated Stress Waves inside Nanoparticles during Rapid Heating in Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2023, 127, 20477-20483.	3.1	0
1931	Probing the mechanical and deformation behaviour of CNT-reinforced AlCoCrFeNi high-entropy alloy – a molecular dynamics approach. Molecular Simulation, 2023, 49, 1726-1741.	2.0	1
1932	Exploring model complexity in machine learned potentials for simulated properties. Journal of Materials Research, 0, , .	2.6	1
1933	Role of Crystal Orientation, Temperature, and Strain Rate on the Mechanical Characterization of Nickel: An Atomistic-scale investigation. Journal of Micromanufacturing, 0, , .	1.1	4
1934	Writing Into Water. Small, 2023, 19, .	10.0	0
1936	Molecular dynamics simulation of water droplets interacting on a conical surface. MRS Communications, 0, , .	1.8	0
1937	Rapid screening of gas solubility in ionic liquids using biased particle insertions with pre-sampled liquid trajectories. Molecular Simulation, 2024, 50, 26-42.	2.0	0
1938	Droplet slipperiness despite surface heterogeneity at molecular scale. Nature Chemistry, 0, , .	13.6	0
1939	A nanoscale view of the origin of boiling and its dynamics. Nature Communications, 2023, 14, .	12.8	1
1941	Molecular Simulation of Water Structure in Narrow Slitlike Pores. Colloid Journal, 2023, 85, 605-628.	1.3	0
1942	Atomic mechanisms of long-term pyrolysis and gas production in cellulose-oil composite for transformer insulation. Applied Energy, 2023, 350, 121695.	10.1	1
1943	Assessment and Ranking of Difluoromethane (R32) and Pentafluoroethane (R125) Interatomic Potentials Using Several Thermophysical and Transport Properties Across Multiple State Points. Journal of Chemical & December 1981 (1988) Journal of Chemical & December 1981 (1988) Journal of Chemical & December 1981 (1988) Properties Across Multiple State Points. Journal of Chemical & December 1981 (1988) Properties Properties Across Multiple State Points. Journal of Chemical & December 1981 (1988) Properties Pro	1.9	0
1944	Coarse-grained molecular dynamics simulation on strain-hardening and fracture behaviors of polycarbonate: Effect of polydispersity and spatial distribution. Journal of Polymer Research, 2023, 30, .	2.4	0
1945	Dynamic Local Structure in Caesium Lead Iodide: Spatial Correlation and Transient Domains. Small, 2024, 20, .	10.0	5
1946	Mechanism-informed constitutive modeling of molecular crystal cyclotetramethylene tetranitramine ( $\hat{l}^2$ -HMX). International Journal of Plasticity, 2023, 169, 103722.	8.8	1
1947	High tensile strength glass fiber with different ratios of Na2O and SiO2 prepared by chemical strengthening method. Journal of Non-Crystalline Solids, 2023, 621, 122621.	3.1	0
1948	Fast and accurate calculation on CO2/CH4 competitive adsorption in shale nanopores: From molecular kinetic theory to machine learning model. Chemical Engineering Journal, 2023, 474, 145562.	12.7	2

#	Article	IF	CITATIONS
1949	Interplay of Mechanochemistry and Material Processes in the Graphite to Diamond Phase Transformation. Journal of Physical Chemistry Letters, 2023, 14, 8584-8589.	4.6	1
1950	Mechanical Responses of a Single Myelin Layer: A Molecular Simulation Study. Biomolecules, 2023, 13, 1525.	4.0	0
1951	Modeling the effects of salt concentration on aqueous and organic electrolytes. Npj Computational Materials, 2023, 9, .	8.7	0
1952	Coil–Helix Block Copolymers Can Exhibit Divergent Thermodynamics in the Disordered Phase. Journal of Chemical Theory and Computation, 2024, 20, 1547-1558.	5.3	0
1953	Numerical Study of Metachronal Waveâ€Modulated Locomotion in Magnetic Cilia Carpets. Advanced Intelligent Systems, 2023, 5, .	6.1	2
1954	Solvent Dependency of Catalystâ€Substrate Aggregation Through ⟨i⟩Ï€⟨ i⟩â€∢i⟩Ï€⟨ i⟩ Stacking in Photoredox Catalysis. ChemPhysChem, 2023, 24, .	2.1	3
1955	Comparison of Friction Parametrization from Dynamics and Material Properties for a Coarse-Grained Polymer Melt. Journal of Physical Chemistry B, 2023, 127, 7054-7069.	2.6	3
1956	Distinct nucleation and propagation of prismatic dislocation loop arrays in Ni and medium-entropy CrCoNi alloy: Insights from molecular dynamics simulations. Materials Today Communications, 2023, 36, 106791.	1.9	0
1957	Atomic-scale insights into the tribochemical wear of diamond on quartz surfaces. Applied Surface Science, 2023, 639, 158152.	6.1	2
1960	Molecular Dynamics Study of Gas–Surface Interactions on β-Cristobalite Surface. Journal of Spacecraft and Rockets, 0, , 1-7.	1.9	2
1961	Melting curves of ice polymorphs in the vicinity of the liquid–liquid critical point. Journal of Chemical Physics, 2023, 159, .	3.0	1
1962	Insights into factors that affect non-Arrhenius migration of a simulated incoherent Σ3 grain boundary. Acta Materialia, 2023, 258, 119210.	7.9	6
1963	Predicted viscosity of liquid HMX up to 40 GPa. Propellants, Explosives, Pyrotechnics, 2023, 48, .	1.6	0
1964	Micro-structural Behavior and Macro-experimental Analysis of Asphalt Mixture Cracking at Low Temperature Based on Molecular Simulation. International Journal of Pavement Research and Technology, 0, , .	2.6	0
1965	On cyclic plasticity of nanostructured dual-phase CoCrFeNiAl high-entropy alloy: An atomistic study. Journal of Applied Physics, 2022, 132, .	2.5	0
1966	Collisional-energy-cascade model for nonthermal velocity distributions of neutral atoms in plasmas. Physical Review E, 2023, 108, .	2.1	0
1967	Effect of Pyramidal Plane II Twinning in Tensile Deformation on Tensile–Compression Yield Asymmetry in Three Orthogonal Directions of Mg Alloy. Journal of Materials Engineering and Performance, 0, , .	2.5	0
1968	Flexible fluid-based encapsulation platform for water-sensitive materials. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	2

#	Article	IF	CITATIONS
1969	Review of effects of zero-carbon fuel ammonia addition on soot formation in combustion. Renewable and Sustainable Energy Reviews, 2023, 185, 113640.	16.4	6
1970	Strain enhances the activity of molecular electrocatalysts via carbon nanotube supports. Nature Catalysis, 2023, 6, 818-828.	34.4	51
1971	Exploiting grain boundary diffusion to minimize dendrite formation in lithium metal-solid state batteries. Journal of Materials Chemistry A, 2023, 11, 23288-23299.	10.3	1
1972	Atom-centered machine-learning force field package. Computer Physics Communications, 2023, 292, 108883.	7.5	2
1973	Bending stiffness collapse, buckling, topological bands of freestanding twisted bilayer graphene. Physical Review B, 2023, 108, .	3.2	1
1974	Multiscale modeling of particle-induced damage in AA7075 aluminum sheet at large plastic strains. International Journal of Plasticity, 2023, 169, 103741.	8.8	2
1975	Strong and ductile nanoscale Ti-1Fe dual-phase alloy via deformation twinning. Scripta Materialia, 2023, 237, 115720.	5.2	0
1976	Confinement-Induced Diffusive Sound Transport in Nanoscale Fluidic Channels. Physical Review Letters, 2023, 131, .	7.8	1
1977	Viewpoint: Can symmetric tilt grain boundaries represent polycrystals?. Scripta Materialia, 2023, 237, 115716.	5.2	8
1978	Atomic cluster expansion for Pt–Rh catalysts: From ab initio to the simulation of nanoclusters in few steps. Journal of Materials Research, 0, , .	2.6	3
1979	Twin-boundary and precipitate interaction in Mg–Al alloy: an MD study. Modelling and Simulation in Materials Science and Engineering, 2023, 31, 075007.	2.0	0
1980	Water–Aluminum Interaction as Driving Force of Linde Type A Aluminophosphate Hydration. Nanomaterials, 2023, 13, 2387.	4.1	O
1981	Mechanical characteristics and deformation behavior of Al polycrystal reinforced with SiC particles. Journal of Physics and Chemistry of Solids, 2023, 183, 111617.	4.0	1
1982	Atomistic study of hydrogen diffusion in presence of defects in bcc and fcc iron. Computational Materials Science, 2023, 230, 112433.	3.0	1
1984	Emergence of rigidity percolation in flowing granular systems. Science Advances, 2023, 9, .	10.3	0
1985	Hybrid ceramic nanofiltration membranes prepared by impregnation and solid-state grafting of organo-phosphonic acids. Journal of Membrane Science, 2023, 687, 122041.	8.2	O
1986	Magnetic Colloidal Currents Guided on Selfâ€Assembled Colloidal Tracks. Advanced Functional Materials, 2023, 33, .	14.9	1
1988	Role of microscopic degrees of freedom in mechanical response of bicrystal nanopillars. Materials Research Letters, 2023, 11, 872-878.	8.7	O

#	Article	IF	CITATIONS
1989	Carbon-doped metal oxide interfacial nanofilms for ultrafast and precise separation of molecules. Science, 2023, 381, 1098-1104.	12.6	8
1990	Modified embedded atom method interatomic potentials for the Fe-Al, Fe-Cu, Fe-Nb, Fe-W, and Co-Nb binary alloys. Computational Materials Science, 2023, 230, 112488.	3.0	1
1991	Molecular dynamics simulations of displacement damage in SiGe alloys induced by single and binary primary knock-on atoms under different temperatures. Radiation Effects and Defects in Solids, 2023, 178, 1384-1403.	1,2	1
1992	Mechanical Slowing Down of Network-Forming Phase Separation of Polymer Solutions. ACS Nano, 2023, 17, 18025-18036.	14.6	2
1993	Measuring Thread Timing to Assess the Feasibility of Early-bird Message Delivery. , 2023, , .		2
1994	Deposition freezing, pore condensation freezing and adsorption: three processes, one description?. Atmospheric Chemistry and Physics, 2023, 23, 10057-10074.	4.9	1
1995	Effect of an oxide layer on high velocity impact of tantalum particles characterized using molecular dynamics. Applied Surface Science, 2023, 640, 158394.	6.1	1
1996	Spall characteristics of three-dimensional graphene networks with embedded copper: A molecular dynamics study. Mechanics of Materials, 2023, 186, 104803.	3.2	0
1997	Semi-Automatic Hybrid Software Deployment Workflow in a Research Computing Center., 2023,,.		0
1998	Evolution of residual stress and interface coherency and their impact on deformation mechanisms in Al/Ti multilayers. Journal of Materials Science, 0, , .	3.7	0
1999	Synthesis of Clean Hydrogen Gas from Waste Plastic at Zero Net Cost. Advanced Materials, 2023, 35, .	21.0	3
2000	Inner energy relaxation and growth of nanosize particles. Physical Review A, 2023, 108, .	2.5	0
2001	Rogue nanowaves: A route to film rupture. Physical Review Fluids, 2023, 8, .	2.5	2
2002	Universal behavior in fragmenting brittle, isotropic solids across material properties. Physical Review E, 2023, 108, .	2.1	2
2003	Construction and analysis of surface phase diagrams to describe segregation and dissolution behavior of Al and Ca in Mg alloys. Physical Review Materials, 2023, 7, .	2.4	1
2004	Machine learning molecular dynamics simulation of CO-driven formation of Cu clusters on the Cu(111) surface. Journal of Physics Condensed Matter, 2023, 35, 495001.	1.8	0
2005	Structure search method for atomic clusters based on the dividing rectangles algorithm. Physical Review E, 2023, 108, .	2.1	0
2006	Performance-Aware Energy-Efficient GPU Frequency Selection using DNN-based Models. , 2023, , .		2

#	Article	IF	CITATIONS
2007	ORAQL â€" Optimistic Responses to Alias Queries in LLVM. , 2023, , .		0
2008	The resistance of amorphous metals to thermal effects. Molecular dynamics modeling. AIP Conference Proceedings, 2023, , .	0.4	0
2009	Identifying a machine-learning structural descriptor linked to the creep behavior of Kob-Andersen glasses. Frontiers in Materials, $0,10,10$	2.4	0
2010	Suntulip: New Tool to Simulate Solar Cells. IEEE Access, 2023, 11, 102140-102148.	4.2	0
2011	Hierarchical bubble size distributions in coarsening wet liquid foams. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	0
2012	MLMOD: Machine Learning Methods for Data-Driven Modeling in LAMMPS. Journal of Open Source Software, 2023, 8, 5620.	4.6	0
2013	Coarse-grained molecular dynamics simulations of microstructure evolution and debonding in water-based cathode electrode drying. Journal of Materials Processing Technology, 2023, 321, 118154.	6.3	0
2014	Collective behavior of active molecules: Dynamic clusters, holes, and active fractalytes. Physical Review Research, 2023, 5, .	3.6	0
2015	Enhanced spall strength of single crystal aluminum by temperature rise mitigation and structural phase transition under shock pulse. Mechanics of Materials, 2023, 186, 104809.	3.2	1
2016	Computational Model for Predicting Particle Fracture During Electrode Calendering. Batteries and Supercaps, 2023, 6, .	4.7	2
2018	Atomic Scale Diffusion Study in Quaternary and Quinary Alloys of Co–Cr–Fe–Mn–Ni System. Metals and Materials International, 0, , .	3.4	0
2019	Exploring the impact of cooling rates and pressure on fragility and structural transformations in iron monatomic metallic glasses: Insights from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2023, 621, 122623.	3.1	6
2020	Challenges of high-fidelity virtual reactor for exascale computing and research progress of China Virtual Reactor. Nuclear Engineering and Design, 2023, 413, 112566.	1.7	1
2021	Unsupervised learning for structure detection in plastically deformed crystals. Computational Materials Science, 2023, 230, 112459.	3.0	0
2023	Parametrization of embedded-atom method potential for liquid lithium and lead-lithium eutectic alloy. Journal of Nuclear Materials, 2023, 587, 154735.	2.7	0
2024	Enhancing the interfacial thermal conductance of Si/PVDF by strengthening atomic couplings. Nanoscale, 2023, 15, 16472-16479.	5.6	2
2025	Modeling water transport properties in carbon nanotubes: Interplay between force-field flexibility and geometrical parameters. Physical Review E, 2023, 108, .	2.1	1
2026	Simulating the isotropic Raman spectra of O–H stretching mode in liquid H <sub>2</sub> O based on a machine learning potential: the influence of vibrational couplings. Physical Chemistry Chemical Physics, 2023, 25, 28180-28188.	2.8	1

#	Article	IF	CITATIONS
2028	Anisotropic diffusion of radiation-induced self-interstitial clusters in HCP zirconium: A molecular dynamics and rate-theory assessment. Scripta Materialia, 2024, 238, 115755.	5.2	0
2030	Study on Plasticity of Cu–Ni Alloy at Atomic Scale: Insight from Molecular Dynamics Simulation. Lecture Notes in Mechanical Engineering, 2023, , 639-647.	0.4	0
2031	Development of an interatomic potential for the W–Ta system. Computational Materials Science, 2023, 230, 112486.	3.0	2
2032	Rapid design of top-performing metal-organic frameworks with qualitative representations of building blocks. Npj Computational Materials, 2023, 9, .	8.7	6
2033	Evaluating the elastic behaviour of boron nitride nanotube (BNNT) reinforced phenolic nanocomposites. Engineering Research Express, 2023, 5, 045003.	1.6	0
2034	Molecular simulation and object-orientation. , 2024, , 405-525.		0
2035	Structural effect on the dielectric constant of hydrocarbon liquids: A molecular dynamics study using the Drude polarizable force field. Bulletin of the Chemical Society of Japan, 0, , .	3.2	0
2037	Fluid-fluid interfacial properties during low salinity waterflooding. Journal of Molecular Liquids, 2023, 390, 123142.	4.9	0
2039	Investigation on wear-resistance of nanocrystalline Pt-Au by molecular dynamics simulations. Tribology International, 2023, 189, 108966.	5.9	0
2040	Device-scale atomistic modelling of phase-change memory materials. Nature Electronics, 2023, 6, 746-754.	26.0	10
2041	Asymmetric Domain Nucleation from Dislocation Core in Barium Titanate: Molecular Dynamics Simulation Using Machineâ€Learning Potential through Active Learning. Physica Status Solidi - Rapid Research Letters, 0, , .	2.4	0
2042	Computation of Dielectric Constant of Cross-linked Epoxy resin through Molecular Dynamics. , 2023, , .		0
2043	Interpretation of dynamic compression experiments using simulated X-ray diffraction and machine learning. AIP Conference Proceedings, 2023, , .	0.4	0
2044	Origin of Deformation Twinning in bcc Tungsten and Molybdenum. Physical Review Letters, 2023, 131, .	7.8	1
2045	Shock-ramp of SiO2 melt. AIP Conference Proceedings, 2023, , .	0.4	0
2046	Nuclear induction lineshape modeling via hybrid SDE and MD approach. Journal of Chemical Physics, 2023, 159, .	3.0	1
2047	Space-resolved line shape model for sputtered atoms of finite-size targets. Physica Scripta, 2023, 98, 115603.	2.5	0
2049	Modeling hard–soft block copolymers as a liquid crystalline polymer. Polymer, 2023, 287, 126389.	3.8	0

#	Article	IF	CITATIONS
2050	X-ray and molecular dynamics study of the temperature-dependent structure of FLiNaK. Nuclear Materials and Energy, 2023, 37, 101530.	1.3	0
2051	Molecular insights of condensate trapping mechanism in shale oil reservoirs and its implications on lean gas enhanced oil recovery. Chemical Engineering Journal, 2023, 476, 146366.	12.7	1
2052	Robust crystal structure identification at extreme conditions using a density-independent spectral descriptor and supervised learning. Computational Materials Science, 2023, 230, 112534.	3.0	0
2053	A guideline for searching for stable grain boundary structure by utilizing crystallographic information: A method based on non-identical termination. Journal of the Ceramic Society of Japan, 2023, 131, 738-745.	1.1	O
2054	Mapping microstructure to shock-induced temperature fields using deep learning. Npj Computational Materials, 2023, 9, .	8.7	0
2055	Machine-Learning for Static andÂDynamic Electronic StructureÂTheory. Challenges and Advances in Computational Chemistry and Physics, 2023, , 113-160.	0.6	0
2056	Enhanced radiation resistance of W-based HEA under helium-ion irradiation conditions. Journal of Nuclear Materials, 2024, 588, 154761.	2.7	0
2057	Effects of seawater on the formation and mechanical properties of Friedel's salt associated with tricalcium aluminate. Cement and Concrete Research, 2023, 174, 107340.	11.0	2
2058	Molecular dynamics simulation of the coalescence of surfactant-laden droplets. Soft Matter, 2023, 19, 8070-8080.	2.7	1
2059	Anticancer Potential of Dendritic Poly(aryl ether)-Substituted Polypyridyl Ligand-Based Ruthenium(II) Coordination Entities. ACS Applied Bio Materials, 2023, 6, 4226-4239.	4.6	0
2060	Evolution of Glassy Carbon Derived from Pyrolysis of Furan Resin., 2023, 1, 2555-2566.		1
2061	Local surface dynamics in the adsorbed film of pentane isomers on graphite. Chemical Engineering Science, 2023, 282, 119359.	3.8	0
2063	Order–Disorder Transition of Two-Dimensional Molecular Networks through a Stoichiometric Design. ACS Nano, 2023, 17, 20194-20202.	14.6	0
2064	Bulk metallic glass Al <sub>2</sub> Ca from a biomedical application viewpoint: A molecular dynamics study. IOP Conference Series: Materials Science and Engineering, 2023, 1291, 012026.	0.6	0
2065	Redesign and Accelerate the AIREBO Bond-Order Potential on the New Sunway Supercomputer. IEEE Transactions on Parallel and Distributed Systems, 2023, 34, 3117-3132.	5.6	0
2066	Molecular dynamics simulations of droplet coalescence and impact dynamics on the modified surfaces: A review. Computational Materials Science, 2023, 230, 112547.	3.0	2
2068	On the missing single collision peak in low energy heavy ion scattering. Nuclear Instruments & Methods in Physics Research B, 2023, 544, 165123.	1.4	2
2069	Data-Driven Approach to Coarse-Graining Simple Liquids in Confinement. Journal of Chemical Theory and Computation, 2023, 19, 7358-7370.	5.3	0

#	Article	IF	CITATIONS
2070	Disordering complexion transition of grain boundaries in bcc metals: Insights from atomistic simulations. Acta Materialia, 2023, 261, 119399.	7.9	0
2071	Going against the Grain: Atomistic Modeling of Grain Boundaries in Solid Electrolytes for Solid-State Batteries. ACS Materials Au, 0, , .	6.0	2
2072	Coarse-grained explicit-solvent molecular dynamics simulations of semidilute unentangled polyelectrolyte solutions. European Physical Journal E, 2023, 46, .	1.6	3
2073	An atomistic study on grain-size and temperature effects on mechanical properties of polycrystal CoCrFeNi high-entropy alloys. Materials Today Communications, 2023, 37, 107264.	1.9	o
2074	Effect of loading rate on the dislocation emission from crack-tip under hydrogen environment. Materials Today Communications, 2023, 37, 107269.	1.9	0
2076	Nonmonotonic magnetic field dependence of magnetization of self-assembled magnetite nanoparticles. Applied Physics Letters, 2023, 123, .	3.3	O
2078	Molecular simulations of premelted films between C-S-H and ice: Implication for cryo-suction in cement-based materials. Cement and Concrete Research, 2023, 174, 107341.	11.0	2
2079	Craze Extension Ratio of Semiflexible Polymer Glasses. Macromolecules, 2023, 56, 8369-8375.	4.8	o
2080	Virtual Volumetric Additive Manufacturing (VirtualVAM). Advanced Materials Technologies, 2023, 8, .	5.8	0
2081	The Influence of Large Pendent Groups on Chain Anisotropy and Electrical Energy Loss of Polyimides at High Frequency through Allâ Atomic Molecular Simulation. ChemPhysChem, 2023, 24, . investigation of lattice thermal conductivity of Ammillmeth	2.1	O
2082	altimg="si2.svg"> <mml:msup><mml:mrow><mml:mi>α</mml:mi></mml:mrow><mml:mo>′</mml:mo><td>:msup&gt; 2.1 :msup&gt; <td>nml:math&gt; O nml:math&gt;</td></td></mml:msup>	:msup> 2.1 :msup> <td>nml:math&gt; O nml:math&gt;</td>	nml:math> O nml:math>
2083	borophene using reverse nonequilibrium molecular dynamics simulation. Physics Letters, Section A: livestigation of the Multimechanism Laser Cleaning Dynamics for Rough Fused Silica Surfaces with Organic Contaminants: A Computational Simulation and Atomic Analysis. Langmuir, 2023, 39, 15095-15106.	3.5	О
2084	Mechanistic Insights into Water Autoionization through Metadynamics Simulation Enhanced by Machine Learning. Physical Review Letters, 2023, 131, .	7.8	0
2085	Machine learning predicts the glass transition of two-dimensional colloids besides medium-range crystalline order. Physical Review E, 2023, 108, .	2.1	О
2086	Concretized structural evolution supported assembly-controlled film-forming kinetics in slot-die coated organic photovoltaics. Nature Communications, 2023, 14, .	12.8	2
2089	The role of carbon monoxide in the catalytic synthesis of endohedral carbyne. Journal of Applied Physics, 2023, 134, .	2.5	О
2090	Coalescence of Al0.3CoCrFeNi polycrystalline high-entropy alloy in hot-pressed sintering: a molecular dynamics and phase-field study. Npj Computational Materials, 2023, 9, .	8.7	5
2091	Multiscale simulation of nanodrop over surfaces with varying hydrophilicity. Computer Physics Communications, 2024, 294, 108963.	7.5	1

#	ARTICLE	IF	CITATIONS
2092	Water flow in a polymeric nanoslit channel with graphene and hexagonal boron nitride wall coatings: An atomistic study. Physics of Fluids, 2023, 35, .	4.0	2
2093	Scalable simulation of coupled adsorption and transport of methane in confined complex porous media with density preconditioning., 2023, 119, 205131.		0
2094	Effect of temperature on the creep properties of polycrystalline Cu-Ni alloy: insight from molecular dynamics simulation. Journal of Physics: Conference Series, 2023, 2596, 012010.	0.4	0
2095	MatGPT: A Vane of Materials Informatics from Past, Present, to Future. Advanced Materials, 2024, 36, .	21.0	1
2096	Mechanical energy absorption of architecturally interlocked petal-schwarzites. Carbon Trends, 2023, 13, 100299.	3.0	0
2097	Enhancing interfacial thermal conductance of an amorphous interface by optimizing the interfacial mass distribution. Physical Review B, 2023, 108, .	3.2	1
2098	Unraveling the Molecular Dynamics of Glucose Oxidase Desorption Induced by Argon Cluster Collision. Journal of Physical Chemistry B, O, , .	2.6	0
2099	Investigating the Chemical Stability of Electrospray Plumes During Particle Collisions. Journal of Propulsion and Power, 2024, 40, 247-256.	2.2	2
2100	Simultaneously enhancing the tensile strength and ductility of high entropy alloys by nanoscale precipitates/fillers. APL Materials, 2023, $11$ , .	5.1	1
2101	High speed impact and solid-state deposition of alumina particles: A molecular dynamics study. Journal of the European Ceramic Society, 2024, 44, 1733-1747.	5.7	0
2102	Asymmetric nanoparticle oxidation observed in-situ by the evolution of diffraction contrast. JPhys Materials, 2023, 6, 045013.	4.2	0
2103	On the strain rate sensitivity of mechanical properties of nanoporous gold: Temperature effect. Materials Today Communications, 2023, 37, 107321.	1.9	1
2104	Seebeck Coefficient of Liquid Water from Equilibrium Molecular Dynamics. Journal of Chemical Theory and Computation, 0, , .	5.3	1
2105	Computational Chemistry as Applied in Environmental Research: Opportunities and Challenges. ACS ES&T Engineering, 0, , .	7.6	1
2106	Machine-learned potentials for eucryptite: A systematic comparison. Journal of Materials Research, 0, ,	2.6	1
2107	Investigating the Effect of Structural Modifications on Mechanical Properties of Carbon Nanotubes under Tensile Loading Using Molecular Dynamics Simulations. Key Engineering Materials, 0, 962, 45-52.	0.4	O
2108	Assessing Li accommodation at amorphous ZrO2 grain boundaries. Journal of Nuclear Materials, 2024, 588, 154780.	2.7	1
2109	All-Atom Molecular Dynamics Simulations of Poly(ethylene glycol) Networks in Water for Evaluating Negative Energetic Elasticity. Macromolecules, 2023, 56, 8095-8105.	4.8	0

#	ARTICLE  Machine learning moment tensor potential for modeling dislocation and fracture in <mml:math< th=""><th>IF</th><th>CITATIONS</th></mml:math<>	IF	CITATIONS
2110	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mrow><mml:mi>L1</mml:mi>TiAl and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>D0</mml:mi></mml:mrow></mml:msub></mml:math></mml:mrow></mml:msub>	2.4	0
2111	Physical Review Materials, 2023, 7, .  Dislocation breakaway from nanoparticle array linear complexions: Plasticity mechanisms and strength scaling laws. Materialia, 2023, 32, 101929.	2.7	0
2112	Feasibility analysis towards the simulation of hysteresis with spin-lattice dynamics. Physical Review B, 2023, 108, .	3.2	0
2113	Atomic-Level Insights into Hollow Silica-Based Materials for Drug Delivery: Effects of Wettability and Porosity. ACS Biomaterials Science and Engineering, 0, , .	5.2	O
2114	Cathode atomic structures and their electrolyte interfaces in lithium sulfur batteries. Batteries and Supercaps, $0$ , , .	4.7	0
2115	An insight into sintering mechanisms of silicon carbide nanoparticles with additives using MD simulation. Powder Technology, 2024, 431, 119053.	4.2	1
2116	Reversible and irreversible photon-absorption in amorphous SiO2 revealed by deep potential. Journal of Non-Crystalline Solids, 2023, 622, 122682.	3.1	0
2117	Imaging of atomic stress at grain boundaries based on machine learning. Journal of the Mechanics and Physics of Solids, 2023, 181, 105455.	4.8	3
2118	Molecular insights into the role of tetrafluoromethane in mitigating the boiling crisis suffered by liquid nitrogen in superconducting apparatus. International Journal of Heat and Mass Transfer, 2024, 218, 124804.	4.8	0
2120	Solution-processable polytriazoles from spirocyclic monomers for membrane-based hydrocarbon separations. Nature Materials, 2023, 22, 1540-1547.	27.5	2
2121	Indentation Depthâ€Dependent Hardness of Metalâ€Organic Framework Crystals: The Effect of Local Amorphization Induced by Indentation. ChemPhysChem, 2024, 25, .	2.1	0
2122	Understanding the Anomalous Diffusion of Water in Aqueous Electrolytes Using Machine Learned Potentials. Journal of Physical Chemistry Letters, 2023, 14, 9500-9507.	4.6	1
2123	Molecular dynamics study on surface effect in ultrasonic vibration assisted upsetting of monocrystalline copper. Journal of Materials Processing Technology, 2023, 322, 118189.	6.3	1
2124	Data-driven Whitney forms for structure-preserving control volume analysis. Journal of Computational Physics, 2024, 496, 112520.	3.8	0
2125	Development of charge-transfer interatomic potential for O-Fe-P-Zn systems and its application to tribochemical reactions between ZnDTP-derived tribofilm and iron oxide. Computational Materials Science, 2024, 231, 112550.	3.0	2
2126	Polymorphic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>âŒ@</mml:mo><mml:mi>a<mml:mi>α</mml:mi></mml:mi></mml:mrow></mml:math> -Ti. Physical	l:mi> <mm 2.4</mm 	nl:mo>〉 <mark>√</mark> O
2127	Multiscale simulations reveal TDP-43 molecular-level interactions driving condensation. Biophysical Journal, 2023, 122, 4370-4381.	0.5	4
2128	Uncertainties in the transport properties of helium gas at cryogenic temperatures determined using molecular dynamics simulation. Fluid Phase Equilibria, 2024, 577, 113979.	2.5	0

#	Article	IF	CITATIONS
2129	Effect of sliding velocity on the nanoscale friction behaviour of articular cartilage contact interface: insights from all-atom molecular dynamics investigation. Molecular Simulation, 2023, 49, 1667-1683.	2.0	0
2130	Coupled ion transport in concentrated PEO–LiTFSI polymer electrolytes. New Journal of Chemistry, 2023, 47, 20344-20357.	2.8	1
2131	Molecular dynamics simulation of deposition of amorphous carbon films on sapphire surfaces. Diamond and Related Materials, 2023, 140, 110514.	3.9	0
2133	Decoding the nanoscale porosity in serpentinites from multidimensional electron microscopy and discrete element modelling. Contributions To Mineralogy and Petrology, 2023, 178, .	3.1	0
2134	Combining machine-learned and empirical force fields with the parareal algorithm: application to the diffusion of atomistic defects. Comptes Rendus - Mecanique, 2023, 351, 1-25.	0.7	1
2135	Recent progress in the JARVIS infrastructure for next-generation data-driven materials design. Applied Physics Reviews, 2023, 10, .	11.3	0
2136	Electron Dynamics in Open Quantum Systems: The Driven Liouville-von Neumann Methodology within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 0, , .	5.3	0
2137	Atomic insights into hydrogen peroxide decomposition on the surface of pure and pre-treated silver: A reactive molecular dynamics simulation study. Applied Surface Science, 2023, , 158701.	6.1	0
2138	Fluid-phase helium: Shock-compression experiments, quantum molecular dynamics simulations, and development of an equationÂof state. Physical Review B, 2023, 108, .	3.2	0
2139	Molecular simulation of the confined crystallization of ice in cement nanopore. Journal of Chemical Physics, 2023, 159, .	3.0	0
2140	pARTn: A plugin implementation of the Activation Relaxation Technique nouveau that takes over the FIRE minimisation algorithm. Computer Physics Communications, 2024, 295, 108961.	<b>7.</b> 5	0
2141	Effects of nanotwins and stacking faults on the mechanical properties of CrCoNi medium-entropy alloys. Journal of Materials Research and Technology, 2023, 27, 3447-3458.	5.8	1
2142	A continuum particle model for micro-scratch simulations of crystalline silicon. Journal of the Mechanics and Physics of Solids, 2024, 182, 105469.	4.8	0
2143	Effect of cation size of binary cation ionic liquid mixtures on capacitive energy storage. Journal of Molecular Liquids, 2023, 391, 123369.	4.9	0
2144	Fractal dimensions of jammed packings with power-law particle size distributions in two and three dimensions. Physical Review E, 2023, $108$ , .	2.1	1
2145	New understanding of one-dimensional thermal glide of a nano-sized prismatic dislocation loop in bcc iron: an atomic scale study. Materials Today Communications, 2023, , 107387.	1.9	0
2146	Ballistic phonon lensing by the non-planar interfaces of embedded nanoparticles. New Journal of Physics, 2023, 25, 103038.	2.9	1
2147	ColabFit exchange: Open-access datasets for data-driven interatomic potentials. Journal of Chemical Physics, 2023, 159, .	3.0	1

#	Article	IF	CITATIONS
2148	Statistical model of synchronized cooperative motion in glass-forming liquids. Physica A: Statistical Mechanics and Its Applications, 2023, 632, 129310.	2.6	0
2149	Effects of aging and diabetes on the deformation mechanisms and molecular structural characteristics of collagen fibrils under daily activity. International Journal of Biological Macromolecules, 2024, 254, 127603.	7.5	0
2150	Molecular dynamics study of the influence of water molecular phase state on the replacement of CO2–CH4 hydrate in porous media. Journal of Molecular Liquids, 2023, 391, 123401.	4.9	0
2151	Accelerating Solvent Dynamics with Replica Exchange for Improved Free Energy Sampling. Journal of Chemical Theory and Computation, 0, , .	5.3	0
2152	Mechanical properties of heterogeneous metallic glasses: Insights from brick-and-mortar designs. Thin-Walled Structures, 2023, 193, 111298.	5.3	0
2153	Development of machine learning and empirical interatomic potentials for the binary Zr-Sn system. Journal of Nuclear Materials, 2024, 588, 154794.	2.7	0
2154	Atomistic insights into the influence of hydrogen on crack propagation in tungsten. Fusion Engineering and Design, 2023, 197, 114030.	1.9	0
2155	Uniform, Strainâ€Free, Largeâ€Scale Graphene and hâ€BN Monolayers Enabled by Hydrogel Substrates. Small, 2024, 20, .	10.0	0
2156	ACEpotentials.jl: A Julia implementation of the atomic cluster expansion. Journal of Chemical Physics, 2023, 159, .	3.0	2
2157	Colloidal Adsorption in Planar Polymeric Brushes. Nanoscale Advances, 0, , .	4.6	0
2158	An Enhanced Sampling Approach for Computing the Free Energy of Solid Surface and Solid–Liquid Interface. Advanced Theory and Simulations, 2024, 7, .	2.8	0
2159	Shock compression of semicrystalline polymers. Physical Review Materials, 2023, 7, .	2.4	0
2160	Exploring optimal graphene slit-pore width for the physical separation of water-methanol mixture. Journal of Molecular Liquids, 2023, 391, 123356.	4.9	0
2161	Special glass structures for first principles studies of bulk metallic glasses. Acta Materialia, 2023, , 119456.	7.9	0
2162	Atomistic insight into dendrite growth orientation transition in Al-Cu alloy. Materials Today Communications, 2023, 37, 107404.	1.9	0
2163	Water diffusion mechanisms in bitumen studied through molecular dynamics simulations. Construction and Building Materials, 2023, 409, 133828.	7.2	4
2164	Quantum mechanics based non-bonded force field functions for use in molecular dynamics simulations of materials and systems: The nitrogen and oxygen columns. Journal of Chemical Physics, 2023, 159, .	3.0	0
2165	Virtual lattice method for efficient Monte Carlo transport simulation of dispersion nuclear fuels. Computer Physics Communications, 2024, 295, 108985.	7.5	1

#	Article	IF	CITATIONS
2167	Modeling Exchange Reactions in Covalent Adaptable Networks with Machine Learning Force Fields. Macromolecules, $0, \dots$	4.8	0
2168	Machine Learning Nucleation Collective Variables with Graph Neural Networks. Journal of Chemical Theory and Computation, 2024, 20, 1600-1611.	5.3	2
2169	Conformational Behavior of a Single Dipolar Chain under Stretching Force. Macromolecules, 2023, 56, 8461-8473.	4.8	1
2170	Chiral Recognition Mechanism of Two-Dimensional Self-Assembly Formed by [7]Thiaheterohelicene. Journal of Physical Chemistry C, 2023, 127, 21305-21312.	3.1	1
2171	Insights on grain boundary effects on crack formation and propagation in Nb3Sn coatings at low temperature and high strain rates: a molecular dynamics simulation study. Superconductor Science and Technology, 0, , .	3.5	O
2172	Effect of defects on mechanical properties of $\hat{\Gamma}$ -graphene nanotubes via molecular dynamics simulations. Physica B: Condensed Matter, 2024, 674, 415461.	2.7	0
2173	Effect of ethane on condensation characteristics of methane heterogeneous nucleation: A molecular dynamics study. Fuel, 2024, 358, 130182.	6.4	1
2174	Finding Bottlenecks in Message Passing Interface Programs by Scalable Critical Path Analysis. Algorithms, 2023, 16, 505.	2.1	0
2175	High Energy Absorption Nacreâ€Like Calcium Silicate Hydrate (Câ€Sâ€H) Composite Toward Elastic Cementitious Materials. Advanced Functional Materials, 2024, 34, .	14.9	0
2176	Unveiling the impact of temperature on magnon diffuse scattering detection in the transmission electron microscope. Physical Review B, 2023, 108, .	3.2	0
2177	Dynamics of Cu–Zr metallic glass devitrification under ultrafast laser excitation revealed by atomistic modeling. Acta Materialia, 2024, 263, 119487.	7.9	0
2178	Ion Partition in Polyelectrolyte Gels and Nanogels. Gels, 2023, 9, 881.	4.5	0
2179	Molecular dynamics calculations of the enthalpy of vaporization for different water models. Journal of Molecular Liquids, 2024, 393, 123455.	4.9	0
2180	A multiscale approach to uncover the self-assembly of ligand-covered palladium nanocubes. Soft Matter, 2023, 19, 8625-8634.	2.7	0
2181	Valley-polarized excitonic Mott insulator in WS2/WSe2 moiré superlattice. Nature Physics, 2024, 20, 34-39.	16.7	3
2182	Development of mechanically-consistent coarse-grained molecular dynamics model: case study of mechanics of spider silk. Scientific Reports, 2023, 13, .	3.3	0
2183	Elucidating the impact of microstructure on mechanical properties of phase-segregated polyurea: Finite element modeling of molecular dynamics derived microstructures. Mechanics of Materials, 2024, 188, 104863.	3.2	1
2184	Superlubricity and Stress-Shielding of Graphene Enables Ultra Scratch-Resistant Glasses. ACS Applied Materials & Samp; Interfaces, 2023, 15, 51905-51914.	8.0	0

#	Article	IF	CITATIONS
2186	Surface atom migration-involved two-dimensional nucleation and growth of nanotwinned copper in DC electrodeposition. Acta Materialia, 2024, 262, 119468.	7.9	1
2187	Enhancing the hemocompatibility of polyethersulfone (PES) hemodialysis membranes using synthesized pseudo zwittronic polymers with various orientations. Results in Surfaces and Interfaces, 2023, 13, 100159.	2.4	O
2188	Molecular dynamics simulations for interfacial structure and affinity between carboxylic acid-modified Al2O3 and polymer melts. Journal of Chemical Physics, 2023, 159, .	3.0	1
2189	Mechanisms of Shock Dissipation in Semicrystalline Polyethylene. Polymers, 2023, 15, 4262.	4.5	0
2190	Artificial Neural Networks for Predicting Mechanical Properties of Crystalline Polyamide12 via Molecular Dynamics Simulations. Polymers, 2023, 15, 4254.	4.5	1
2191	Multiscale Mechanochemical Modeling of Spiropyran–Merocyanine Isomerization in Linear PMMA Polymers. Macromolecules, 2023, 56, 8438-8447.	4.8	O
2192	High-Dimensional Neural Network Potentials for Accurate Prediction of Equation of State: A Case Study of Methane. Journal of Chemical Theory and Computation, 2023, 19, 7825-7832.	<b>5.</b> 3	0
2193	Insight of temperature and density-driven transition of sawtooth penta-silicene nanoribbons via molecular dynamics study. Materials Today Communications, 2023, 37, 107490.	1.9	O
2194	Effects of Airless Bodies' Regolith Structures and of the Solar Wind's Properties on the Backscattered Energetic Neutral Atoms Flux. Planetary Science Journal, 2023, 4, 197.	3.6	1
2195	Atomistic Modeling Approach for Predicting Association of Photoacid Generators in Extreme Ultraviolet Polymeric Photoresists. Chemistry of Materials, 2023, 35, 9050-9063.	6.7	0
2196	Core atoms escape from the shell: reverse segregation of Pb–Al core–shell nanoclusters via nanoscale melting. , 2023, 18, .		0
2197	A ReaxFF and DFT study of effect and mechanism of an electric field on JP-10 fuel pyrolysis. Journal of the Energy Institute, 2023, 111, 101445.	5.3	0
2198	Molecular Dynamics Simulations of Amylose- and Cellulose-Based Selectors and Related Enantioseparations in Liquid Phase Chromatography. Molecules, 2023, 28, 7419.	3.8	2
2199	Reactive force field potential with shielded long-range Coulomb interaction: Application to graphene–water capacitors. Journal of Applied Physics, 2023, 134, .	2.5	1
2200	DNA supercoiling in bacteria: state of play and challenges from a viewpoint of physics based modeling. Frontiers in Microbiology, 0, 14, .	3.5	2
2201	Cavity formation at metal–water interfaces. Journal of Chemical Physics, 2023, 159, .	3.0	0
2202	Different glassy characteristics are related to either caging or dynamical heterogeneity. Journal of Chemical Physics, 2023, 159, .	3.0	2
2203	Molecular-level insights to structure and hydrogen bonds network of 1,4-dioxane aqueous solution. Journal of Molecular Liquids, 2024, 393, 123523.	4.9	O

#	Article	IF	CITATIONS
2204	Grain size dependence of grain rotation under high pressure and high temperature. Journal of Applied Physics, $2023,134,.$	2.5	0
2205	Mechanisms of dissolution from gibbsite step edges elucidated by ab initio molecular dynamics with enhanced sampling. Geochimica Et Cosmochimica Acta, 2023, , .	3.9	0
2206	Bending behavior of diamane and twisted bilayer graphene: Insights from four-point bending deformation. Thin-Walled Structures, 2024, 195, 111415.	5.3	0
2207	Competing mechanisms govern the thermal rectification behavior in semi-stochastic polycrystalline graphene with graded grain-size distribution. Carbon, 2024, 218, 118638.	10.3	O
2208	Generation of Amorphous Silica Surfaces with Controlled Roughness. Journal of Physical Chemistry A, 2023, 127, 9831-9841.	2.5	0
2209	Connecting micro- and macroscopic variables in the design of a granular stirrer using simulations. , $0, 3, .$		O
2210	Intrinsic Charge Trapping and Reversible Charge Induced Structural Modifications in $a\hat{a}\in S$ is $S$ in		1
2211	Simulation studies of water adsorption on MIL-101(Cr) revealing the role of inhomogeneous potential field composed of open metal sites and organic linkers. , 0, , .		O
2212	Understanding the pore structure evolution of polyethylene separator with dissipative particle dynamics simulation. Polymer Engineering and Science, 2024, 64, 518-533.	3.1	0
2213	Pipelines for automating compliance-based elimination and extension (PACE <sup>2</sup> ): a systematic framework for high-throughput biomolecular materials simulation workflows. JPhys Materials, 2024, 7, 015006.	4.2	O
2214	Simulation of two nanoparticle melting to understand the conductivity drop of 3D-printed silver nanowires. Materials and Design, 2023, 236, 112502.	7.0	0
2215	Ring-originated anisotropy of local structural ordering in amorphous and crystalline silicon dioxide. Communications Materials, 2023, 4, .	6.9	O
2216	Dynamical control enables the formation of demixed biomolecular condensates. Nature Communications, 2023, $14$ , .	12.8	3
2217	Mechanochemistry in Block Copolymers: New Scission Site due to Dynamic Phase Separation. Angewandte Chemie - International Edition, 2023, 62, .	13.8	1
2218	Mechanochemistry in Block Copolymers: New Scission Site due to Dynamic Phase Separation. Angewandte Chemie, 2023, 135, .	2.0	0
2219	Folding kinetics of an entangled protein. PLoS Computational Biology, 2023, 19, e1011107.	3.2	O
2220	Molecular insights on optimizing nanoporous carbon-based supercapacitors with various electrolytes. Electrochimica Acta, 2024, 474, 143500.	5.2	0
2221	Fabrication of beryllium oxide based fully ceramic microencapsulated nuclear fuels with dispersed TRISO particles by pressureless sintering method. Journal of Nuclear Materials, 2024, 588, 154798.	2.7	O

#	Article	IF	CITATIONS
2222	Development of a Transferable Force Field between Metal–Organic Framework and Its Polymorph. ACS Omega, 2023, 8, 44328-44337.	3 <b>.</b> 5	0
2224	Modeling interlayer interactions and phonon thermal transport in silicene bilayers. Physical Review B, 2023, 108, .	3.2	1
2225	Corrosion-resistant cobalt phosphide electrocatalysts for salinity tolerance hydrogen evolution. Nature Communications, 2023, 14, .	12.8	3
2226	Elucidating microcystin-LR adsorption on pyrolyzed hydrochars via experiments and molecular simulations. Journal of Analytical and Applied Pyrolysis, 2023, 176, 106243.	5.5	0
2227	Inducing stratification of colloidal mixtures with a mixed binary solvent. Soft Matter, 2023, 19, 9195-9205.	2.7	0
2228	Accurate estimation of transport coefficients using time correlation functions without fitting any analytic forms in equilibrium simulations. Polymer, 2024, 290, 126519.	3.8	0
2229	A Comparative Study of Gallium-, Xenon-, and Helium-Focused Ion Beams for the Milling of GaN. Nanomaterials, 2023, 13, 2898.	4.1	0
2230	Effect of confinement and topology: 2-TIPS <i>vs.</i> MIPS. Soft Matter, 2023, 19, 8561-8576.	2.7	2
2231	Kinetic mechanisms of methane hydrate replacement and carbon dioxide hydrate reorganization. Chemical Engineering Journal, 2023, 477, 146973.	12.7	9
2232	Structure, Dynamics, and Hydrogen Transport in Amorphous Polymers: An Analysis of the Interplay between Free Volume Element Distribution and Local Segmental Dynamics from Molecular Dynamics Simulations. Macromolecules, 2023, 56, 9042-9053.	4.8	1
2233	Molecular dynamics analysis for the effect of the wettability and the slip on the solid wall surface on bubble growth. Transactions of the JSME (in Japanese), 2023, 89, 22-00320-22-00320.	0.2	0
2234	Single-layer soil-water coupled SPH method and its application to sinkhole simulation. Acta Geotechnica, 0, , .	5.7	0
2235	Interfacial Interaction between the Ruthenium(IV) Oxide Cluster and Graphitic Carbon Nitride Governing the Photocatalytic Activity. Journal of Physical Chemistry C, 2023, 127, 22076-22084.	3.1	0
2236	3D Printing of Sustainable Coal Polymer Composites: Study of Processing, Mechanical Performance, and Atomistic Matrix–Filler Interaction. ACS Applied Polymer Materials, 2023, 5, 9286-9296.	4.4	1
2237	Molecular dynamics simulations of magnesium aluminosilicate glass structure: Highâ€coordinated alumina and oxygen tricluster formation. Journal of the American Ceramic Society, 2024, 107, 2155-2171.	3.8	0
2238	Lattice thermal conductivity of embedded nanoparticle composites: the role of particle size distribution. Nanotechnology, 2024, 35, 055701.	2.6	0
2239	Bead–Spring Simulation of Ionomer Melts—Studying the Effects of Chain-Length and Associating Group Fraction on Equilibrium Structure and Extensional Flow Behavior. Polymers, 2023, 15, 4560.	4.5	0
2240	Strength and Deformation Behavior of Graphene Aerogel of Different Morphologies. Materials, 2023, 16, 7388.	2.9	0

#	Article	IF	CITATIONS
2241	Extension of the <i>MolMod</i> Database to Transferable Force Fields. Journal of Chemical Information and Modeling, 2023, 63, 7148-7158.	5.4	0
2242	Theta Temperature Depression of Mechanically Interlocked Polymers: [2]catenane as a Model Polymer. Macromolecules, 2023, 56, 9164-9174.	4.8	1
2243	An Investigation of the Growth of Fatigue Cracks in Single Crystal Superelastic NiTi Under High Strain Level Using Molecular Dynamics Simulations. Arabian Journal for Science and Engineering, 0, , .	3.0	1
2244	Advancing Understanding of the Influence of Drained Cyclic Loading on Sand Behavior Using DEM. Journal of Engineering Mechanics - ASCE, 2024, 150, .	2.9	0
2245	Efficient Assessment of â€~Instantaneous <i>pK'</i> Values from Molecular Dynamics Simulations. ChemPhysChem, 2024, 25, .	2.1	1
2246	Toward Metal Extraction from Regolith: Theoretical Investigation of the Solvation Structure and Dynamics of Metal Ions in Ionic Liquids. Journal of Physical Chemistry B, 2023, 127, 9985-9996.	2.6	0
2247	Age-hardening behavior of the extruded Al 7075/Mg EW75 composite. Materials Today Communications, 2023, 37, 107443.	1.9	0
2248	Atomistic simulations reveal strength reductions due to short-range order in alloys. Acta Materialia, 2024, 263, 119471.	7.9	0
2249	Thermodynamic and molecular simulation analysis of molecular interactions between methyl 2â€"hydroxyisobutyrateÂ+Âwater or nâ€"alkanol (C1â€"C2) mixtures. Journal of Molecular Liquids, 2023, 392, 123461.	4.9	1
2250	Evaluation and Analysis of Thermosetting Phenolic Resins Using Multiscale Modeling that Combine Quantum Chemical Calculations and Molecular Reaction Simulations. Journal of the Japan Society for Composite Materials, 2022, 48, 217-222.	0.2	0
2251	Nanoscale Insights into the Protection of Calcium Silicate Hydrate by Polydimethylsiloxane Coatings in Sulfate Environments: Different Degrees of Polymerization. Coatings, 2023, 13, 2004.	2.6	1
2252	Molecular dynamics models to investigate the diffusion behavior of emulsified asphalt. Construction and Building Materials, 2023, 409, 134061.	7.2	1
2253	Analysis and Augmentation of Guest–Host Interaction Energy Models as CHA and AEI Zeolite Crystallization Phase Predictors. Journal of Physical Chemistry C, 2023, 127, 22740-22751.	3.1	0
2254	Molecular dynamics study of carbon dioxide and nitrogen selectivity through poly[bis((methoxyethoxy)ethoxy)phosphazene] (MEEP) membrane. Chemical Engineering Science, 2024, 284, 119480.	3.8	0
2255	A Unified Empirical Equation for Determining the Mechanical Properties of Porous NiTi Alloy: From Nanoporosity to Microporosity. Crystals, 2023, 13, 1656.	2.2	0
2256	Interface regulation of diamond-doped GalnSn composites. Diamond and Related Materials, 2024, 141, 110655.	3.9	1
2257	Influence of Temperature and Incidence Angle on the Irradiation Cascade Effect of 6H-SiC: Molecular Dynamics Simulations. Micromachines, 2023, 14, 2126.	2.9	0
2258	Conformation-Induced stiffening effect of crosslinked polymer thin films. Communications Physics, 2023, 6, .	5.3	1

#	Article	IF	CITATIONS
2259	Effects of graphene oxide on shearing performance of C–S–H composites: a molecular dynamics study. Journal of Materials Science, 2023, 58, 16972-16987.	3.7	0
2262	Multi-step nucleation pathway of C-S-H during cement hydration from atomistic simulations. Nature Communications, 2023, 14, .	12.8	5
2263	Host-guest dynamics in porous trimesic acid supramolecular network on graphene. Outstanding stability of the coronene guest. Carbon, 2024, 217, 118643.	10.3	0
2264	Tuning and optimization of two-phase absorbents (DEEA/AEEA/H2O) with hybrid phase splitter (n-butanol/DEEA) for several properties: Carbon capture, phase separation, physical properties. Energy, 2024, 288, 129802.	8.8	1
2265	Heat conductivity from energy-density fluctuations. Journal of Chemical Physics, 2023, 159, .	3.0	1
2266	Configuration sampling in multi-component multi-sublattice systems enabled by ab Initio Configuration Sampling Toolkit (abICS). Science and Technology of Advanced Materials Methods, 2023, 3, .	1.3	0
2267	Unveiling the radiation-induced defect production and damage evolution in tungsten using multi-energy Rutherford backscattering spectroscopy in channeling configuration. Acta Materialia, 2024, 263, 119499.	7.9	1
2268	Molecular dynamics simulation of coalescence behavior of carbon nanoparticle. Chemical Engineering Research and Design, 2024, 201, 209-217.	5.6	O
2269	Flow regime transition of multicomponent oil in shale nanopores. Fuel, 2024, 359, 130431.	6.4	1
2270	Modulation of ionic conduction using polarizable surfaces. Physical Review Research, 2023, 5, .	3.6	1
2271	Reinforcing or weakening? Determined by the interfacial nanostructures in graphene reinforced copper matrix composites. Diamond and Related Materials, 2024, 141, 110664.	3.9	0
2272	Reactive molecular dynamics simulations of plastics pyrolysis with additives: Comparison of ReaxFF branches and experimental results. Journal of Analytical and Applied Pyrolysis, 2024, 177, 106266.	5.5	1
2273	A colloidal viewpoint on the sausage catastrophe and the finite sphere packing problem. Nature Communications, 2023, 14, .	12.8	3
2275	Effect of regulating the interfacial structure of multiple non-covalent bonding on improving thermal management capability. Journal of Materials Chemistry A, 0, , .	10.3	0
2276	Adsorption of CO <sub>2</sub> on Gold Surfaces: Adsorbate Density Assumption Investigated Using Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2023, 62, 19884-19892.	3.7	1
2277	Influence of strong Coulomb coupling on diffusion in atmospheric pressure plasmas. Plasma Sources Science and Technology, 2023, 32, 115004.	3.1	1
2278	Evolution of free volume elements in amorphous polymers undergoing uniaxial deformation: a molecular dynamics simulations study. Molecular Systems Design and Engineering, 2024, 9, 214-225.	3.4	0
2279	Studying the mechanical behavior of a generic thermoplastic by means of a fast coarse-grained molecular dynamics model. Polymers and Polymer Composites, 2023, 31, .	1.9	O

#	Article	IF	CITATIONS
2280	Integrated colloidal deformation to advanced polymer network design through polymer-nanoparticle alternating hybrids. Giant, 2023, , 100218.	5.1	0
2281	Facile spinning of tough and conductive eutectogel fibers via Li+-induced dense hydrogen-bond networks. Chemical Engineering Journal, 2023, 478, 147405.	12.7	0
2283	Hydrogen embrittlement of iron nanowires: investigating size and orientation dependence on loading behaviour. Molecular Simulation, 2024, 50, 129-136.	2.0	0
2284	The boson peak in silicate glasses: insight from molecular dynamics. Physical Chemistry Chemical Physics, 2023, 25, 31270-31280.	2.8	0
2285	Effects of surface chemistry on the mechanochemical decomposition of tricresyl phosphate. Physical Chemistry Chemical Physics, 2023, 26, 278-292.	2.8	1
2286	A cloud platform for sharing and automated analysis of raw data from high throughput polymer MD simulations. , 2023, $1$ , .		1
2287	Multi-aspect and comprehensive atomic insight: the whole process of thermolysis of HMX/Poly-NIMMO–based plastic bonded explosive. Journal of Molecular Modeling, 2023, 29, .	1.8	1
2288	Mechanism of elemental segregation around extended defects in high-entropy alloys and its effect on mechanical properties. Acta Materialia, 2024, 264, 119537.	7.9	1
2289	Molecular Characterization of Mesoporous Silica (Un)loading by Gemcitabine and Ibuprofen – An Interplay of Salt-Bridges and Hydrogen Bonds. Journal of Pharmaceutical Sciences, 2024, 113, 785-790.	3.3	0
2290	Trilayer Moir $\tilde{A}$ © Superlattices of MoS <sub>2</sub> as a Simulator for the Ionic Hubbard Model on Honeycomb Lattice. Advanced Functional Materials, 0, , .	14.9	0
2291	Phase stability and nucleation kinetics of salts in confinement. Journal of Molecular Liquids, 2024, 394, 123698.	4.9	0
2292	Durable high-entropy non-noble metal anodes for neutral seawater electrolysis. Chemical Engineering Journal, 2024, 479, 147862.	12.7	0
2293	Enhancing Structure–Property Relationships in Porous Materials through Transfer Learning and Cross-Material Few-Shot Learning. ACS Applied Materials & Samp; Interfaces, 2023, 15, 56375-56385.	8.0	1
2294	Evaluating the Influence of Waste Cooking Oil Molecular Structure on Aged Asphalt Modification. Construction Materials, 2023, 3, 543-557.	0.9	O
2295	Response of ionizable block copolymer assemblies to solvent dielectrics: A molecular dynamics study. Journal of Chemical Physics, 2023, 159, .	3.0	0
2296	Atomic-scale insights into damage produced by swift heavy ions in polyethylene. Journal of Materials Science, 2023, 58, 17275-17291.	3.7	1
2297	Deep learning interatomic potential for thermal and defect behaviour of aluminum nitride with quantum accuracy. Computational Materials Science, 2024, 232, 112656.	3.0	0
2298	Kinetic nature of electrochemical plasticization. International Journal of Plasticity, 2023, 171, 103820.	8.8	0

#	Article	IF	CITATIONS
2299	Impact of deposited Pt particles on water channel connectivity and proton conductivity in proton exchange membranes: A molecular dynamics study. International Journal of Hydrogen Energy, 2024, 55, 1456-1464.	7.1	0
2300	Multiscale Molecular Dynamics Simulations of Ice-Binding Proteins. Methods in Molecular Biology, 2024, , 185-202.	0.9	0
2301	Molecular kinetic modelling of non-equilibrium transport of confined van der Waals fluids. Journal of Fluid Mechanics, 2023, 976, .	3.4	0
2302	Machine-learned interatomic potentials: Recent developments and prospective applications. Journal of Materials Research, 2023, 38, 5079-5094.	2.6	2
2303	Machine-learning-accelerated simulations to enable automatic surface reconstruction. Nature Computational Science, 2023, 3, 1034-1044.	8.0	2
2304	Effects of heat-dry curing temperature on porous silicate cement membranes fabricated by the coupling process of freeze casting and heat-dry curing. Ceramics International, 2024, 50, 5411-5423.	4.8	0
2305	Water-CO2 wettability on sandstone surface with asphaltene adsorption: Molecular dynamics simulation. Fuel, 2024, 360, 130558.	6.4	0
2306	CO <sub>2</sub> -philicity to CO <sub>2</sub> -phobicity Transition on Smooth and Stochastic Rough Cu-like Substrate Surfaces. Langmuir, 2023, 39, 17818-17829.	3.5	O
2307	Coarse-Grained Many-Body Potentials of Ligand-Stabilized Nanoparticles from Machine-Learned Mean Forces. ACS Nano, 2023, 17, 23391-23404.	14.6	0
2308	Kinetic Mechanism of Surfactant-Based Molecular Recognition: Selective Permeability across an Oil–Water Interface Regulated by Supramolecular Aggregates. Journal of Physical Chemistry B, 2023, 127, 10201-10214.	2.6	O
2309	Can a coarse-grained water model capture the key physical features of the hydrophobic effect?. Journal of Chemical Physics, 2023, 159, .	3.0	0
2310	The effect of nanopores on the mechanism of martensitic transformation in pure iron during the heating-cooling cycle: A molecular dynamics study. Materials Today Communications, 2023, 37, 107481.	1.9	0
2311	Model Amphiphilic Polymer Conetworks in the Bulk: Dissipative Particle Dynamics Simulations of Their Self-Assembly and Mechanical Properties. Macromolecules, 2023, 56, 9299-9311.	4.8	0
2312	Structural optimization strategies for improving the maximum strength of gradient nanotwinned metals. Mechanics of Materials, 2024, 189, 104876.	3.2	0
2313	What dictates soft clay-like lithium superionic conductor formation from rigid salts mixture. Nature Communications, 2023, $14$ , .	12.8	0
2314	Effect of film thickness and temperature on condensation and momentum accommodation at the liquid–vapor methane interphase in contact with a quartz substrate. International Journal of Thermal Sciences, 2024, 196, 108739.	4.9	O
2315	FASDA: An FPGA-Aided, Scalable and Distributed Accelerator for Range-Limited Molecular Dynamics. , 2023, , .		0
2316	Unveiling a medium-range structural commonality of amorphous alloys. Journal of Non-Crystalline Solids, 2024, 624, 122696.	3.1	O

#	Article	IF	CITATIONS
2318	Enzymatic metabolons dramatically enhance metabolic fluxes of low-efficiency biochemical reactions. Biophysical Journal, 2023, 122, 4555-4566.	0.5	1
2319	Multiferroic skyrmions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BiFeO</mml:mi><mi .<="" 2023,="" 5,="" physical="" research,="" review="" td=""><td>ท<b>l:ma</b>&gt;3<!--</td--><td>m<b>o</b>l:mn&gt;</td></td></mi></mml:msub></mml:mrow></mml:math>	ท <b>l:ma</b> >3 </td <td>m<b>o</b>l:mn&gt;</td>	m <b>o</b> l:mn>
2320	Unusual energy–structure–property relation in a metallic glass coupled with temperature-dependent relaxation memories. Intermetallics, 2024, 164, 108101.	3.9	0
2321	Pair-distribution function of active Brownian spheres in three spatial dimensions: simulation results and analytical representation. Soft Matter, 0, , .	2.7	2
2322	Computational modeling of grain boundary segregation: A review. Computational Materials Science, 2024, 232, 112596.	3.0	1
2323	Correlation between grain size and dynamic response of NiTi alloy during intense shock-induced multi-spallation. Materials Today Communications, 2023, 37, 107515.	1.9	0
2324	Investigation of interfacial matching between 3C-SiC substrate crystals and its surface layer deposited Cu elements using molecular dynamics simulations. Surfaces and Interfaces, 2023, 43, 103600.	3.0	0
2325	Molecular Dynamics Study on Adding Tungstenâ€Carbide Grains to 304 Stainless Steel Polycrystals. Physica Status Solidi (B): Basic Research, 2024, 261, .	1.5	0
2326	MolSieve: A Progressive Visual Analytics System for Molecular Dynamics Simulations. IEEE Transactions on Visualization and Computer Graphics, 2023, , 1-11.	4.4	0
2327	Theoretical Study of Formation of Hydrates from High-Concentration Metastable Solution of Carbon Dioxide in Water at Various Gas Concentrations. Journal of Engineering Thermophysics, 2023, 32, 502-507.	1.4	2
2328	Competing Effects of Molecular Additives and Cross-Link Density on the Segmental Dynamics and Mechanical Properties of Cross-Linked Polymers. ACS Engineering Au, 2023, 3, 512-526.	5.1	1
2329	Modelling of partial basal dislocation dipoles in bilayer graphene and graphite. Carbon, 2024, 217, 118613.	10.3	0
2330	GrIOt: Graph-based Modeling of HPC Application I/O Call Stacks for Predictive Prefetch., 2023,,.		0
2331	Trigger Smart Data Saving Applied to CO2 Capture in Metal-Organic Frameworks. , 2023, , .		0
2332	Experiences Detecting Defective Hardware in Exascale Supercomputers. , 2023, , .		0
2333	Implementation-Oblivious Transparent Checkpoint-Restart for MPI. , 2023, , .		0
2334	Benchmarking a portable lattice quantum chromodynamics kernel written in Kokkos and MPI., 2023, , .		0
2335	Enabling Performant Thermal Conductivity Modeling with DeePMD and LAMMPS on CPUs., 2023,,.		0

#	Article	IF	CITATIONS
2336	Unravelling the mechanisms of copper precipitation-induced strengthening in austenitic stainless steels: An atomistic approach. Materialia, 2023, 32, 101962.	2.7	0
2337	Comparing Power Signatures of HPC Workloads: Machine Learning vs Simulation. , 2023, , .		0
2338	Atomic level simulation of amorphous/nanocrystalline transition behavior in the Fe based amorphous alloys. Journal of Non-Crystalline Solids, 2024, 624, 122726.	3.1	0
2339	A molecular dynamics study on the Mie-Gr $\tilde{A}^{1}$ /4neisen equation-of-state and high strain-rate behavior of equiatomic CoCrFeMnNi. Materials Research Letters, 2023, 11, 1055-1062.	8.7	0
2341	Modelling electrified microporous carbon/electrolyte electrochemical interface and unraveling charge storage mechanism by machine learning accelerated molecular dynamics. Energy Storage Materials, 2023, 63, 103069.	18.0	0
2342	Frontier: Exploring Exascale. , 2023, , .		1
2343	Radiative heat exchange driven by acoustic vibration modes between two solids at the atomic scale. Physical Review B, 2023, 108, .	3.2	0
2344	Hermes-3: Multi-component plasma simulations with BOUT++. Computer Physics Communications, 2024, 296, 108991.	7.5	2
2345	Lightweight Extendable Stacking Framework for Structure Classification in Atomistic Simulations. Journal of Chemical Theory and Computation, 2023, 19, 8332-8339.	5.3	0
2346	Effect of Salinity on CO <sub>2</sub> Thermodiffusion in Aqueous Mixtures by Molecular Dynamics Simulations. ACS Sustainable Chemistry and Engineering, 2023, 11, 17086-17097.	6.7	1
2347	<i>AbÂlnitio</i> Phase Diagram of Gold in Extreme Conditions. Physical Review Letters, 2023, 131, .	7.8	1
2348	Scaling the Leading Accuracy of Deep Equivariant Models to Biomolecular Simulations of Realistic Size. , 2023, , .		0
2349	Direct Numerical Simulation ofÂScalar Transport Across theÂInterface Between aÂPorous Medium andÂaÂTurbulent Flow. ERCOFTAC Series, 2024, , 374-379.	0.1	0
2350	Effects of length, diameter, and doping on the thermal transport in carbon nanotubes: a molecular dynamics study. Applied Nanoscience (Switzerland), 2024, 14, 339-351.	3.1	0
2351	Efficient Molecular Dynamics Simulations of Deep Eutectic Solvents with First-Principles Accuracy Using Machine Learning Interatomic Potentials. Journal of Chemical Theory and Computation, 2023, 19, 8732-8742.	5.3	1
2352	Surface tension and evaporation behavior of liquid fuel droplets at transcritical conditions: Towards bridging the gap between molecular dynamics and continuum simulations. Fuel, 2024, 358, 130187.	6.4	1
2353	Atomic cluster expansion for a general-purpose interatomic potential of magnesium. Physical Review Materials, 2023, 7, .	2.4	1
2354	Ligament rotation-dominated creep in stochastic bicontinuous nanoporous metallic glass. Materials and Design, 2023, 236, 112480.	7.0	0

#	Article	IF	CITATIONS
2355	Unraveling the motion and deformation characteristics of red blood cells in a deterministic lateral displacement device. Computers in Biology and Medicine, 2024, 168, 107712.	7.0	0
2356	Atomic scale melting/solidification behavior and structural evolutions of AlCoCrFeNi high-entropy alloy in selective laser melting process. Journal of Materials Research and Technology, 2023, 27, 6811-6821.	5.8	2
2357	Temperature- and internal structural size-dependent strength of nanotwinned face-centered cubic metals. Journal of Materials Research and Technology, 2023, 27, 7159-7166.	5.8	0
2358	The Way to Analyse MD Simulation Results of Cluster Ion Bombardment., 2023,,.  Active learning prediction and experimental confirmation of atomic structure and thermophysical		O
2359	properties for liquid <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Hf</mml:mi><mml:m width="0.16em"></mml:m><mml:msub><mml:mi mathvariant="normal">W</mml:mi><mml:mn>24</mml:mn></mml:msub></mml:msub></mml:mrow></mml:math>	n>762.1	nl:mn>
2360	refractory alloy. Physical Review E, 2023, 108, . The effect of collisions on the chemomechanics of ice-covered silica slabs: a molecular dynamics study. Physical Chemistry Chemical Physics, 2023, 25, 32208-32215.	2.8	0
2361	Alâ $\in$ Driven Design System for Fabrication of Inhalable Nanocatchers for Virus Capture and Neutralization. Advanced Healthcare Materials, 2024, 13, .	7.6	0
2362	Facilitation of Hydrate Dissociation and Structural Evolution by Major Marine Anions under Static Electric Fields. Journal of Physical Chemistry B, 2023, 127, 10447-10457.	2.6	1
2363	Damage mechanism and mechanical properties of carbon nanotubes induced by He2+ ion irradiation: Molecular dynamics simulations and experiments. Diamond and Related Materials, 2024, 141, 110652.	3.9	0
2364	Enhanced machinability of aluminium-based silicon carbide by non-resonant vibration-assisted magnetorheological finishing. Journal of Materials Processing Technology, 2024, 324, 118223.	6.3	3
2365	Can endohedral transition metals enhance hydrogen storage in carbon nanotubes?. International Journal of Hydrogen Energy, 2024, 55, 604-610.	7.1	1
2366	Underlying mechanisms of enhanced plasticity in Ti/Al laminates at elevated temperatures: A molecular dynamics study. Journal of Materials Research and Technology, 2024, 28, 31-42.	5.8	2
2367	Machine learning of microscopic structure-dynamics relationships in complex molecular systems. Machine Learning: Science and Technology, 2023, 4, 045044.	5.0	0
2369	Deep machine learning, molecular dynamics and experimental studies of liquid Al-Cu-Co alloys. Journal of Molecular Liquids, 2024, 393, 123659.	4.9	0
2371	Unraveling the Interplay between Quantum Transport and Geometrical Conformations in Monocyclic Hydrocarbons' Molecular Junctions. Journal of Physical Chemistry C, 2023, 127, 23303-23311.	3.1	0
2372	Understanding Deformation Behavior in Sintered Fe36Ni Alloy Through Nanoindentation Experiments and Molecular Dynamics Simulation. Advanced Engineering Materials, 0, , .	3.5	0
2373	VIAMD: a Software for Visual Interactive Analysis of Molecular Dynamics. Journal of Chemical Information and Modeling, 2023, 63, 7382-7391.	5.4	2
2376	Accuracy of classical force fields for polyethylene structures away from equilibrium. MRS Communications, 2024, 14, 1-7.	1.8	0

#	Article	IF	CITATIONS
2377	Glassy phases of the Gaussian core model. Soft Matter, 0, , .	2.7	0
2378	The influence of various factors on the transition of the fluorinated graphene wettability from superhydrophilicity to high hydrophobicity. Surfaces and Interfaces, 2024, 44, 103686.	3.0	1
2379	Unveiling the anatomy of mode-coupling theory. SciPost Physics, 2023, 15, .	4.9	0
2380	Unlocking the mysterious polytypic features within vaterite CaCO3. Nature Communications, 2023, 14, .	12.8	0
2381	Computer simulation of carbonization and graphitization of coal. Nanotechnology, 2024, 35, 095703.	2.6	1
2383	Electrorheological Effect of Suspensions of Polyaniline Nanoparticles with Different Morphologies. Polymers, 2023, 15, 4568.	4.5	0
2384	Multiscale Simulation of Fluids: Coupling Molecular and Continuum. Physical Chemistry Chemical Physics, 0, , .	2.8	0
2385	A simulation study of linker vacancy distribution and its effect on UiO-66 stability. Microporous and Mesoporous Materials, 2024, 366, 112922.	4.4	1
2386	Ligandâ€Mediated Interaction of Nanoparticles with Lipid Membranes. Macromolecular Theory and Simulations, 2024, 33, .	1.4	0
2387	Coarse-Graining with Equivariant Neural Networks: A Path Toward Accurate and Data-Efficient Models. Journal of Physical Chemistry B, 2023, 127, 10564-10572.	2.6	3
2388	Thawed matrix method for computing local mechanical properties of amorphous solids. Journal of Chemical Physics, 2023, 159, .	3.0	1
2389	A quantitative insight into strain hardening behavior of typical Hadfield steel under dynamic load. Journal of Materials Research and Technology, 2023, 27, 8050-8061.	5.8	0
2390	Reduction of Interlayer Interaction in Multilayer Stacking Graphene with Carbon Nanotube Insertion: Insights from Experiment and Simulation. Journal of Physical Chemistry C, 0, , .	3.1	0
2391	The effects of grain size and fractal porosity on thermal conductivity of nano-grained graphite: A molecular dynamics study. International Journal of Heat and Mass Transfer, 2024, 220, 125030.	4.8	0
2393	Effects of π–π Stacking on Shale Gas Adsorption and Transport in Nanopores. ACS Omega, 2023, 8, 46577-46588.	3.5	0
2394	Investigation of edge dislocation mobility in Ni-Co solid solutions by molecular dynamics simulation. Materials Today Communications, 2024, 38, 107779.	1.9	0
2395	Molecular Dynamics Simulations of Displacement Cascades in BCC-Fe: Effects of Dislocation, Dislocation Loop and Grain Boundary. Materials, 2023, 16, 7497.	2.9	1
2396	Registry-dependent potential energy and lattice corrugation of twisted bilayer graphene from quantum Monte Carlo. Physical Review B, 2023, 108, .	3.2	0

#	Article	IF	CITATIONS
2397	Comparing theoretical predictions of radiation-free velocities of edge dislocations to molecular dynamics simulations. Physical Review B, 2023, 108, .	3.2	0
2398	Nanoscale Meniscus Dynamics in Evaporating Thin Films: Insights from Molecular Dynamics Simulations. Langmuir, 0, , .	3.5	0
2399	Prediction of the binding energy of self interstitial atoms in alpha iron by a graph neural network. Materialia, 2024, 33, 101977.	2.7	0
2400	Impact of Molecular-level Structural Disruption on Relaxation Dynamics of Polymers with End-on and Side-on Liquid Crystal Moieties. ACS Nano, 2023, 17, 24790-24801.	14.6	2
2401	Atomistic simulation of rolling contact fatigue behavior of a faceâ€centered cubic material (nickel). Fatigue and Fracture of Engineering Materials and Structures, 0, , .	3.4	0
2402	The effect of atomic hydrogen on the behavior of a single dislocation of ã€^111〉{112} in bcc tungsten: Atomistic study. Journal of Nuclear Materials, 2024, 589, 154842.	2.7	0
2403	Oxidation-induced superelasticity in metallic glass nanotubes. Nature Materials, 0, , .	27.5	0
2404	SEM2: Introducing mechanics in cell and tissue modeling using coarse-grained homogeneous particle dynamics. APL Bioengineering, 2023, 7, .	6.2	0
2406	Molecular dynamics study on the effect of grain size on the plastic deformation of Fe-Cr-Ni alloy nanopolycrystals. Materials Today Communications, 2024, 38, 107770.	1.9	0
2407	Incommensurate grain-boundary atomic structure. Nature Communications, 2023, 14, .	12.8	0
2408	Heterogeneous-elasticity theory of instantaneous normal modes in liquids. Scientific Reports, 2023, 13, .	3.3	0
2410	Diffusion and Coalescence of Phosphorene Monovacancies Studied Using High-Dimensional Neural Network Potentials. Journal of Physical Chemistry C, 0, , .	3.1	0
2411	Bottom-Up Transient Time Models in Coarse-Graining Molecular Systems. Multiscale Modeling and Simulation, 2023, 21, 1746-1774.	1.6	0
2412	Validating continuum theory for Cottrell atmosphere solute drag by molecular dynamics simulations. Journal of the Mechanics and Physics of Solids, 2024, 183, 105514.	4.8	1
2413	Study of the positional and orientational contributions to the Helmholtz free energy of a finite hard-disk system. A molecular dynamics analysis of its hexatic transition. Molecular Physics, 0, , .	1.7	0
2414	Mesoscopic Modeling and Experimental Validation of Thermal and Mechanical Properties of Polypropylene Nanocomposites Reinforced By Graphene-Based Fillers. Macromolecules, 0, , .	4.8	1
2415	Influence of Atomic Relaxations on the Moir $\tilde{A}$ © Flat Band Wave Functions in Antiparallel Twisted Bilayer WS <sub>2</sub> . Nano Letters, 0, , .	9.1	0
2416	Fundamentals of freeze desalination: Critical review of ion inclusion and rejection studies from molecular dynamics perspective. Desalination, 2024, 573, 117216.	8.2	O

#	Article	IF	Citations
2417	Nanoprecipitate and stacking fault-induced high strength and ductility in a multiscale heterostructured high-entropy alloy. International Journal of Plasticity, 2024, 172, 103853.	8.8	0
2418	Unravelling the atomistic-scale insights into tensile response of equiatomic cupronickel alloy with pre-existing faceted grain boundary interface. Results in Surfaces and Interfaces, 2024, 14, 100172.	2.4	0
2419	Investigation into the mechanism of surface atom emission from an individual cathode spot using Molecular Dynamics simulation. Journal Physics D: Applied Physics, O, , .	2.8	0
2420	Machine learning is funny but physics makes the money: How machine-learning potentials can advance computer-aided materials design in metallurgy. Computational Materials Science, 2024, 233, 112715.	3.0	0
2421	Impact of diamond nanothread on the viscosity of asphalt binder: Insights from atomistic simulations. Journal of Cleaner Production, 2024, 434, 139945.	9.3	0
2422	Automatic Potential Energy Surface Exploration by Accelerated Reactive Molecular Dynamics Simulations: From Pyrolysis to Oxidation Chemistry. Journal of Physical Chemistry A, 0, , .	2.5	O
2423	A performance evaluation of the Kunpeng 920 cluster in benchmarks and HPC applications. , 2023, , .		0
2424	Coarse-grained molecular dynamics study on submicron structuring of calcium silicate hydrate with enhanced tensile modulus and strength. Journal of Building Engineering, 2024, 82, 108271.	3.4	0
2425	Precise major compounds in Barringtonia acutangula flower $\hat{a}\in$ water extract for mitigating carbon steel corrosion. Journal of the Taiwan Institute of Chemical Engineers, 2024, 155, 105251.	<b>5.</b> 3	3
2426	Unveiling the crystallization mechanism of cadmium selenide via molecular dynamics simulation with machine-learning-based deep potential. Journal of Materials Science and Technology, 2024, 185, 23-31.	10.7	O
2427	Atomistic fracture in bcc iron revealed by active learning of Gaussian approximation potential. Npj Computational Materials, 2023, 9, .	8.7	1
2429	MAD MAcce: Supporting Multiply-Add Operations for Democratizing Matrix-Multiplication Accelerators., 2023,,.		0
2431	Development of machine learning interatomic potential for zinc. Computational Materials Science, 2024, 233, 112723.	3.0	0
2432	Nucleation of threading dislocations in atomistic simulations of strained layer epitaxy of III-nitrides. Acta Materialia, 2024, 264, 119570.	7.9	0
2433	Enhancing the impact property of high-entropy alloys with graphene layers: a molecular dynamics study. Journal of Materials Science, 2023, 58, 18105-18119.	3.7	1
2434	GPU-based molecular dynamics of fluid flows: Reaching for turbulence. International Journal of High Performance Computing Applications, 0, , .	3.7	2
2435	Anisotropy of field-controlled shear viscosity of dipolar fluids. Journal of Statistical Mechanics: Theory and Experiment, 2023, 2023, 123204.	2.3	0
2436	Thermodynamics of Water and Ice from a Fast and Scalable First-Principles Neuroevolution Potential. Journal of Chemical & Engineering Data, 0, , .	1.9	O

#	Article	IF	CITATIONS
2438	Multi-scale analysis of corrosion-induced fracture failure mechanisms of high-strength steel wire. Applications in Engineering Science, 2024, 17, 100172.	0.8	0
2439	Ultralow Lattice Thermal Transport and Considerable Wave-like Phonon Tunneling in Chalcogenide Perovskite BaZrS <sub>3</sub> . Journal of Physical Chemistry Letters, 0, , 11465-11473.	4.6	0
2440	Computational approach for investigating nanoscale interfacial ice adhesion trends. RSC Advances, 2023, 13, 36088-36097.	3.6	0
2441	Structural criticality manifested by a polarized ionic layer on a MWCNT yarn surface under mechanical loading. Carbon, 2024, 218, 118707.	10.3	0
2442	Investigation of the influence of nano-sized particles on the entanglement distribution of a generic polymer nanocomposite using molecular dynamics. Mathematics and Mechanics of Solids, 2024, 29, 596-611.	2.4	2
2443	Effect of Fe–O ReaxFF on Liquid Iron Oxide Properties Derived from Reactive Molecular Dynamics. Journal of Physical Chemistry A, 2023, 127, 10339-10355.	2.5	0
2444	Ballistic properties of highly stretchable graphene kirigami pyramid. Computational Materials Science, 2024, 232, 112558.	3.0	0
2445	Molecular simulation for food protein–ligand interactions: A comprehensive review on principles, current applications, and emerging trends. Comprehensive Reviews in Food Science and Food Safety, 2024, 23, .	11.7	2
2446	Electrochemical Degradation of Pt <sub>3</sub> Co Nanoparticles Investigated by Off-Lattice Kinetic Monte Carlo Simulations with Machine-Learned Potentials. ACS Catalysis, 2023, 13, 16078-16087.	11.2	0
2447	Shear banding in monodisperse polymer melt. Journal of Chemical Physics, 2023, 159, .	3.0	0
2448	Hierarchy of hydrogen bonding among constitutional isomers of hexanol. Journal of Molecular Liquids, 2024, 394, 123804.	4.9	0
2449	Electrostatic interactions dominate thermal conductivity and anisotropy in three-dimensional hydrogen-bonded organic frameworks. International Journal of Heat and Mass Transfer, 2024, 221, 125071.	4.8	1
2450	Hydrophobically gated memristive nanopores for neuromorphic applications. Nature Communications, 2023, 14, .	12.8	3
2451	Effect of heat treatment paths on the aging and rejuvenation of metallic glasses. Physical Review Materials, 2023, 7, .	2.4	0
2452	Enhance the Strong Scaling of LAMMPS on Fugaku. , 2023, , .		0
2453	Developing an Implicit Solvation Machine Learning Model for Molecular Simulations of Ionic Media. Journal of Chemical Theory and Computation, 0, , .	5.3	0
2454	Electric-field-induced ion evaporation from the ionic liquid–vacuum interface. Physics of Fluids, 2023, 35, .	4.0	0
2455	Probing Reactivity with External Forces: The Case of Nitroacetamides in Water. Molecules, 2024, 29, 9.	3.8	0

#	Article	IF	CITATIONS
2456	New insights into the hydrothermal carbonization process of sewage sludge: A reactive molecular dynamics study. Fuel, 2024, 361, 130692.	6.4	0
2458	Molecular dynamics study of Al implantation in 4H-SiC. , 2023, , .		0
2459	Intrinsic Electron Trapping in Amorphous Silicon Nitride (a-Si <sub>3</sub> N <sub>4</sub> :H)., 2023,,.		1
2460	Self-assembly of colloids with competing interactions confined in spheres. Soft Matter, 0, , .	2.7	0
2461	Enhanced diffusion of tracer particles in nonreciprocal mixtures. Physical Review E, 2023, 108, .	2.1	0
2462	Green–Kubo expressions for transport coefficients from dissipative particle dynamics simulations revisited. Physical Chemistry Chemical Physics, 0, , .	2.8	0
2463	Electrolytes and cathode designs for next generation of siliconâ€based batteries ―Comprehensive experimental and computational considerations. Batteries and Supercaps, 0, , .	4.7	0
2464	Molecular Dynamics Study of Stress Relaxation During Ge Deposition on Si(100) \$2imes 1\$ Substrates., 2023,,.		0
2465	Tracing the Influence of Large Language Models across the Most Impactful Scientific Works. Electronics (Switzerland), 2023, 12, 4957.	3.1	1
2466	Integrated Quantum-Classical Protocol for the Realistic Description of Solvated Multinuclear Mixed-Valence Transition-Metal Complexes and Their Solvatochromic Properties. Journal of Chemical Theory and Computation, 2024, 20, 1306-1323.	5.3	0
2467	Phase Behaviour and Dynamics of Three-Dimensional Active Dumbbell Systems. Soft Matter, 0, , .	2.7	0
2468	Data Efficient and Stability Indicated Sampling for Developing Reactive Machine Learning Potential to Achieve Ultralong Simulation in Lithium-Metal Batteries. Journal of Physical Chemistry C, 2023, 127, 24106-24117.	3.1	0
2469	Mechanical and fracture behaviour of pristine and defective single/bi-crystal graphene/Ti nanocomposites using molecular dynamics simulations. Computational Materials Science, 2024, 233, 112726.	3.0	0
2470	Microscopic deformation mechanism and residual plastic accumulation in cross-connection area in nano-grooving process of Zr-based metallic glass. Materials Today Communications, 2024, 38, 107860.	1.9	0
2471	Molecular Dynamics Study of the Structural and Diffusion Properties of Dehydrated Layered Double Aluminum and Lithium Hydroxide. JETP Letters, 2023, 118, 597-602.	1.4	0
2472	On the mechanical response of graphene-capped copper nanoparticles. Physical Chemistry Chemical Physics, 2024, 26, 2260-2268.	2.8	0
2473	Thermal-gated polyanionic hydrogel films for stable and smart aqueous batteries. Energy Storage Materials, 2024, 65, 103136.	18.0	1
2474	Solute influence in transitions from non-Arrhenius to stick-slip Arrhenius grain boundary migration. Acta Materialia, 2024, 265, 119605.	7.9	2

#	Article	IF	CITATIONS
2475	Mesoscale material modeling with memoryless isotropic point particles. Journal of Computational Science, 2024, 75, 102198.	2.9	0
2476	An elastomer with ultrahigh strain-induced crystallization. Science Advances, 2023, 9, .	10.3	0
2477	Thermal stability of equiatomic FePt nanoclusters of different habitus with ordered and disordered structure. E3S Web of Conferences, 2023, 460, 10040.	0.5	0
2479	Using Metadynamics to Reveal Extractant Conformational Free Energy Landscapes. Journal of Physical Chemistry B, O, , .	2.6	0
2480	Generation of viable nanocrystalline structures using the melt-cool method: the influence of force field selection. Philosophical Magazine, 2024, 104, 205-238.	1.6	0
2481	Evaluating shock sensitivity and decomposition of energetic materials by ReaxFF molecular dynamics. Journal of Materials Science, 0, , .	3.7	0
2482	Mode-coupling theory of lattice dynamics for classical and quantum crystals. Journal of Chemical Physics, 2023, 159, .	3.0	2
2483	Anomalous Concentration Dependence of Viscosity: Hidden Role of Cross-Correlations in Aqueous Electrolyte Solutions. Journal of Physical Chemistry B, 0, , .	2.6	2
2484	FlowerMD: Flexible Library of Organic Workflows and Extensible Recipes for Molecular Dynamics. Journal of Open Source Software, 2023, 8, 5989.	4.6	0
2485	Synthetic pre-training for neural-network interatomic potentials. Machine Learning: Science and Technology, 0, , .	5.0	1
2486	Effect of CaO on the ionic microstructure and properties in dephosphorization slag by molecular dynamics simulation. Journal of Molecular Liquids, 2024, 395, 123799.	4.9	0
2487	Atomistic study on the origins of the anisotropic lithiation behaviors of the silicon anode using the reactive force field based molecular dynamics simulations. Acta Materialia, 2024, 265, 119610.	7.9	0
2488	Synthesis and Characterization of the New Li <sub>1+<i>x</i></sub> 1+ <i>x</i> 1ê€" <i>x</i> 0 <sub>4</sub> ( <i>x</i> =) Tj ET	-Q <b>q</b> @000 r	g&T /Overloo
2489	Kibble–Zurek scaling of nonequilibrium phase transition in barium titanate. Applied Physics Letters, 2023, 123, .	3.3	0
2490	Mechanical performance of CNT-reinforced aluminum matrix composite fabricated via flake powder metallurgy: Experimental modeling and molecular dynamics study. Diamond and Related Materials, 2024, 142, 110742.	3.9	0
2491	Predicting Ion Diffusion from the Shape of Potential Energy Landscapes. Journal of Chemical Theory and Computation, 0, , .	5.3	O
2492	Effect of chemical short-range ordering on thermodynamics, structure, and dynamics of ZrCu-based metallic glass-forming liquids. Journal of Applied Physics, 2023, 134, .	2.5	0
2493	Computational Prediction of Coiled–Coil Protein Gelation Dynamics and Structure. Biomacromolecules, 0, , .	5.4	O

#	Article	IF	CITATIONS
2494	Computational Nanotoxicology and its Applications. , 2023, , 183-213.		0
2495	Deep Charge: Deep learning model of electron density from a one-shot density functional theory calculation. Physical Review B, 2023, 108, .	3.2	0
2496	Nanofibrous Membranes from Catalytic Arene–Norbornene Annulation (CANAL)-Based Polymers for Scavenging Organic Micropollutants. ACS Applied Polymer Materials, 0, , .	4.4	0
2497	Precision machining performance and mechanism of Ni/Ni3Al alloy under cryogenic temperature. Materials Today Communications, 2024, 38, 107915.	1.9	0
2499	Predicting the Raman Spectra of Liquid Water with a Monomer-Field Model. Journal of Physical Chemistry Letters, 2023, 14, 11742-11749.	4.6	1
2500	Experimental and simulation study of self-assembly and adsorption of glycerol monooleate in $\langle i \rangle n <  i \rangle$ -dodecane with varying water content onto iron oxide. Nanoscale, 0, , .	5.6	0
2501	Microstructure and magnetization evolution in bcc iron via direct first-principles predictions of radiation effects. Physical Review Materials, 2023, $7$ , .	2.4	0
2502	Development of NaCl–MgCl <sub>2</sub> –CaCl <sub>2</sub> Ternary Salt for High-Temperature Thermal Energy Storage Using Machine Learning. ACS Applied Materials & Development of NaCl–MgCl <sub>2</sub>	8.0	0
2503	<i>Ab initio</i> based study on atomic ordering in (Ba, Sr)TiO <sub>3</sub> . Physica Status Solidi - Rapid Research Letters, 0, , .	2.4	0
2504	Analyzing the Li–Al–O Interphase of Atomic Layer-Deposited Al <sub>2</sub> O <sub>3</sub> Films on Layered Oxide Cathodes Using Atomistic Simulations. ACS Applied Materials & Diterfaces, 0, , .	8.0	0
2505	Effects of Nanoparticle Size on the Thermal Decomposition Mechanisms of 3,5-Diamino-6-hydroxy-2-oxide-4-nitropyrimidone through ReaxFF Large-Scale Molecular Dynamics Simulations. Molecules, 2024, 29, 56.	3.8	0
2506	Effect of Hf and Al on Self-Diffusion in Amorphous Silica Using Molecular Dynamics. Jom, 0, , .	1.9	0
2507	Topological analysis and control of post-synthetic metalation sites in Zr-based metal–organic frameworks. Journal of Materials Chemistry C, 2024, 12, 2359-2369.	5.5	0
2508	Exploring ablation of GaAs at atomic and close-to-atomic scale by pulsed laser and 3D TTM–MD simulations. Optics and Laser Technology, 2024, 171, 110427.	4.6	0
2509	Studying the effects of Nb on high-temperature deformation in TiAl alloys using atomistic simulations. Materials and Design, 2024, 237, 112596.	7.0	1
2510	Plasticity in diamond nanoparticles: dislocations and amorphization during loading and dislocation multiplication during unloading. Journal of Materials Science, 0, , .	3.7	0
2511	Chemistry of the interaction between Imidazole derivatives as corrosion inhibitors molecules and copper/brass/zinc surfaces: A DFT, reactive and classical molecular force fields study. Surfaces and Interfaces, 2024, 44, 103799.	3.0	1
2512	The effects of transferred heat and wall material on thermal behavior of a nano-grooved micro-heat pipe, molecular dynamics simulation. Engineering Analysis With Boundary Elements, 2024, 160, 1-13.	3.7	0

#	Article	IF	CITATIONS
2513	Angular-dependent interatomic potential for large-scale atomistic simulation of W-Mo-Nb ternary alloys. Computational Materials Science, 2024, 233, 112734.	3.0	0
2514	Influence of surface roughness on interfacial adsorption and laser ablation mechanisms of organic contaminants on fused silica. , 2023, , .		0
2515	Unveiling optimal wetting additives for extinguishing wood fires: Insights from molecular simulation and experimental investigations. Surfaces and Interfaces, 2024, 44, 103805.	3.0	0
2516	Effect of interface layer on the enhancement of thermal conductivity of SiC-Water nanofluids: Molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2024, 127, 108696.	2.4	0
2518	Nucleation of Nano-sized Prismatic Dislocation Loop from Spherical Vacancy Clusters in <i>î±</i> -iron: An Atomic-scale Study. ISIJ International, 2024, 64, 765-771.	1.4	0
2519	Prediction of crack initiation in single-crystal sapphire during ultra-precision machining using MD simulation-based slip/fracture activation model. Precision Engineering, 2024, 86, 265-275.	3.4	0
2520	Molecular design of polyimide films for combating atomic oxygen erosion through combing experiments with simulations: A state-of-the-art review. Polymer Degradation and Stability, 2024, 220, 110645.	5.8	0
2521	TOPCon Solar Cell Degradation via Pinhole Nucleation. , 2023, , .		0
2522	Implicit multiscale finite element analysis of polymer physics-based multiscale constitutive model for elastomers. Mechanics of Materials, 2024, 189, 104904.	3.2	0
2523	Computer Simulation of a Biphasic Catalytic Process in the Presence of Polymer Microgels. Doklady Physical Chemistry, 2023, 512, 141-147.	0.9	0
2524	First-principles study for orientation dependence of band alignments at 4H-SiC/SiO <sub>2</sub> interface. Japanese Journal of Applied Physics, 0, , .	1.5	0
2525	Experiences readying applications for Exascale. , 2023, , .		0
2526	NOVEL APPROACH FOR IDENTIFYING EVAPORATING AND CONDENSING ATOMS AT THE ARGON LIQUID SURFACE IN MOLECULAR DYNAMICS SIMULATIONS. , 2023, , .		0
2527	Structural Properties of Cyclic Polyelectrolytes in a Dilute Good Solvent. Macromolecules, 0, , .	4.8	O
2528	Role of crystallographic orientation in material behaviour under nanoindentation: Molecular Dynamics study. Materials Science-Poland, 2023, 41, 18-26.	1.0	0
2529	Effect of temperature on tensile and vibration properties of bilayer boron nitride. International Journal of Mechanical System Dynamics, 2023, 3, 397-405.	2.8	0
2530	Roadmap for focused ion beam technologies. Applied Physics Reviews, 2023, 10, .	11.3	4
2531	A simulation study of magnetic nanoparticle clustering in a fluid flow. Journal of Physics: Conference Series, 2023, 2653, 012041.	0.4	O

#	Article	IF	CITATIONS
2532	Two-phase imbibition of water-oil displacement in silica nanochannels. International Journal of Multiphase Flow, 2024, 172, 104710.	3.4	0
2533	Modeling single-molecule stretching experiments using statistical thermodynamics. Physical Review E, 2023, 108, .	2.1	0
2534	Hydrophilic and Apolar Hydration in Densely Grafted Cationic Brushes and Counterions with Large Mobilities. Journal of Physical Chemistry B, 2024, 128, 381-392.	2.6	2
2535	Molecular Design of Functional Polymers for Silica Scale Inhibition. Environmental Science & Eamp; Technology, 0, , .	10.0	0
2536	Self-Assembly of Star-Polyelectrolytes in Various Solution Conditions. Macromolecules, 0, , .	4.8	0
2537	Freezing of water confined between calcium-silicate-hydrate layers: a coarse-grained molecular dynamics study. Journal of Sustainable Cement-Based Materials, $0$ , , $1$ - $16$ .	3.1	0
2538	Correlated Hybrid DNA Structures Explored by the oxDNA Model. Langmuir, 0, , .	3.5	0
2539	Impact of crystalline orientation on Cu–Cu solid-state bonding behavior by molecular dynamics simulations. Scientific Reports, 2023, 13, .	3.3	0
2540	Nonthermal effects in solids after swift heavy ion impact. Nuclear Instruments & Methods in Physics Research B, 2024, 547, 165218.	1.4	0
2541	Molecular Simulation of Lithium Carbonate Reactive Vapor–Liquid Equilibria Using a Deep Potential Model. Journal of Chemical & Engineering Data, 2024, 69, 204-214.	1.9	0
2542	Direct Visualization of Aluminum Particle Wetting on Carbon Using In Situ Laser Heating TEM. Journal of Physical Chemistry C, 0, , .	3.1	0
2543	Unveiling the Influence of Ionic Liquid on the Interfacial Structure and Capacitive Performance of Water-in-Salt Electrolytes at Graphite Electrodes. Journal of Physical Chemistry C, 0, , .	3.1	0
2544	Henry's constant of helium in liquid alkali metals. Journal of Molecular Liquids, 2024, 395, 123853.	4.9	0
2546	pSPICA Force Field Extended for Proteins and Peptides. Journal of Chemical Information and Modeling, 0, , .	5.4	0
2547	Direct measurement of the structural change associated with amorphous solidification using static scattering of coherent radiation. Journal of Chemical Physics, 2023, 159, .	3.0	0
2548	Analysis of phase stability and chemical segregation in the Mo-V alloys using a generalized embedded atom method potential. Computational Materials Science, 2024, 233, 112732.	3.0	0
2549	MD Simulation of Water Using a Rigid Body Description Requires a Small Time Step to Ensure Equipartition. Journal of Chemical Theory and Computation, 0, , .	5.3	0
2550	Kinetically Stable and Highly Ordered Two-Dimensional CN <sub>2</sub> Crystal Structures. Journal of Physical Chemistry C, 0, , .	3.1	O

#	Article	IF	CITATIONS
2551	Higher Hydrogen Fractions in Dielectric Polymers Boost Self-Healing in Electrical Capacitors. Physical Chemistry Chemical Physics, 0, , .	2.8	0
2552	The Tunable Rhenium Effect on the Creep Properties of a Nickel-Based Superalloy. Materials, 2024, 17, 191.	2.9	0
2553	Simulation and study of the milling parameters on CuFeTaTiW multicomponent alloy. Nuclear Materials and Energy, 2024, 38, 101568.	1.3	0
2554	Neighbor List Artifacts in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2023, 19, 8919-8929.	<b>5.</b> 3	1
2555	Accelerating training of MLIPs through small-cell training. Journal of Materials Research, 2023, 38, 5095-5105.	2.6	3
2556	Performance of Reinforcement Learning in Molecular Dynamics Simulations: A Case Study of Hydrocarbon Dynamics. Lecture Notes in Mechanical Engineering, 2024, , 61-73.	0.4	0
2557	Nuclear quantum effects in the acetylene:ammonia plastic co-crystal. Journal of Chemical Physics, 2024, 160, .	3.0	0
2558	Coupling at the molecular scale between the graphene nanosheet and water and its effect on the thermal conductivity of the nanofluid. Physical Chemistry Chemical Physics, 2024, 26, 2402-2413.	2.8	0
2559	Comparing the Tribological Performance of Water-Based and Oil-Based Drilling Fluids in Diamond–Rock Contacts. Tribology Letters, 2024, 72, .	2.6	0
2560	Effect of hydrogen on the chemical state, stoichiometry and density of amorphous Al <sub>0<sub>3</sub> films grown by thermal atomic layer deposition. Surface and Interface Analysis, 2024, 56, 293-304.</sub>	1.8	0
2561	Active learning of the thermodynamics-dynamics trade-off in protein condensates. Science Advances, 2024, 10, .	10.3	0
2562	Nonmonotonic electrophoretic mobility of rodlike polyelectrolytes by multivalent coions in added salt. Physical Review E, 2024, 109, .	2.1	0
2563	Enhancing ReaxFF for molecular dynamics simulations of lithium-ion batteries: an interactive reparameterization protocol. Scientific Reports, 2024, 14, .	3.3	0
2564	Machine learning interatomic potentials for amorphous zeolitic imidazolate frameworks., 2024, 3, 355-368.		1
2565	Rapid and accurate predictions of perfect and defective material properties in atomistic simulation using the power of 3D CNN-based trained artificial neural networks. Scientific Reports, 2024, 14, .	3.3	0
2566	Active machine learning model for the dynamic simulation and growth mechanisms of carbon on metal surface. Nature Communications, 2024, 15, .	12.8	0
2567	Elevated temperature effects (TÂ>Â100°C) on the interfacial water and microstructure swelling of Na-montmorillonite. Chemical Engineering Journal, 2024, 481, 148647.	12.7	0
2568	Deciphering the ultra-high plasticity in metal monochalcogenides. Nature Materials, 2024, 23, 196-204.	27.5	O

#	Article	IF	CITATIONS
2569	Simulation and Data-Driven Modeling of the Transport Properties of the Mie Fluid. Journal of Physical Chemistry B, 2024, 128, 551-566.	2.6	1
2570	Hygroscopic Growth of Adsorbed Water Films on Smectite Clay Particles. Environmental Science & Environmental &	10.0	0
2571	Exploring the Unusual Reactivity of the Hydrated Electron with CO <sub>2</sub> . Journal of Physical Chemistry B, 2024, 128, 567-575.	2.6	0
2572	Multisource Energy Harvester on Textile and Plants for Clean Energy Generation from Wind and Rainwater Droplets. ACS Sustainable Chemistry and Engineering, 2024, 12, 695-705.	6.7	0
2573	Solubilizer reconstructs the influences of the hydrogen-bond network of nonaqueous biphasic solvent on the absorption, phase splitting and desorption. Separation and Purification Technology, 2024, 338, 126324.	7.9	0
2574	Machine learned force-fields for an Ab-initio quality description of metal-organic frameworks. Npj Computational Materials, 2024, 10, .	8.7	1
2575	Rich proton dynamics and phase behaviours of nanoconfined ices. Nature Physics, 2024, 20, 456-464.	16.7	0
2576	Surface stratification determines the interfacial water structure of simple electrolyte solutions. Nature Chemistry, 2024, 16, 644-650.	13.6	1
2577	Practical classical molecular dynamics simulations for low-temperature plasma processing: a review. Reviews of Modern Plasma Physics, 2024, 8, .	4.1	0
2578	SIMULATION OF WETTABILITY OF NANOTEXTURED SURFACES BY MOLECULAR DYNAMICS. Journal of Applied Mechanics and Technical Physics, 2023, 64, 814-820.	0.5	0
2579	Vesicle condensation induced by synapsin: condensate size, geometry, and vesicle shape deformations. European Physical Journal E, 2024, 47, .	1.6	0
2580	An atomistic study on the HELP mechanism of hydrogen embrittlement in pure metal Fe. International Journal of Hydrogen Energy, 2024, 57, 60-68.	7.1	0
2581	Computing equilibrium free energies through a nonequilibrium quench. Journal of Chemical Physics, 2024, 160, .	3.0	0
2582	Mesoscale simulation of biomembranes with FreeDTS. Nature Communications, 2024, 15, .	12.8	2
2583	On De Gennes narrowing of fluids confined at the molecular scale in nanoporous materials. Journal of Chemical Physics, 2024, $160$ , .	3.0	0
2584	Effect of Adsorbed Carboxylates on the Dissolution of Boehmite Nanoplates in Highly Alkaline Solutions. Environmental Science & Environmental Science	10.0	1
2585	Coaxially printed biomimetic BSPC with high strength and toughness. Materials and Design, 2024, 238, 112648.	7.0	0
2586	Microscopic mechanism of thermal amorphization of ZIF-4 and melting of ZIF-zni revealed <i>via</i> molecular dynamics and machine learning techniques. Journal of Materials Chemistry A, 2024, 12, 4572-4582.	10.3	O

#	Article	IF	CITATIONS
2587	Study of field ion emission from ionic liquids using molecular dynamics simulations. Physics of Fluids, 2024, $36$ , .	4.0	0
2588	Elucidating Morphologyâ€Mobility Relationships of Organic Thin Films Through Transfer Learningâ€Assisted Multiscale Simulation. Advanced Functional Materials, 0, , .	14.9	O
2589	Deformation twins as a probe for tribologically induced stress states. Communications Materials, 2024, 5, .	6.9	0
2590	Investigation of dislocation and twinning behavior in HMX under high-velocity impact employing molecular dynamics simulations. Journal of Molecular Modeling, 2024, 30, .	1.8	0
2591	Combining stochastic resetting with Metadynamics to speed-up molecular dynamics simulations. Nature Communications, 2024, 15, .	12.8	1
2593	Replica exchange molecular dynamics for Li-intercalation in graphite: a new solution for an old problem. Chemical Science, 2024, 15, 2745-2754.	7.4	O
2594	Depletion-induced crystallization of anisotropic triblock colloids. Nanoscale, 2024, 16, 4724-4736.	5.6	0
2595	Study of vacancy ordering and the boson peak in metastable cubic Ge-Sb-Te using machine learning potentials. Physical Review Materials, 2024, 8, .	2.4	0
2596	GAFF-Based Polarizable Force Field Development and Validation for Ionic Liquids. Journal of Physical Chemistry B, 2024, 128, 871-881.	2.6	0
2597	Gain reversal in the translocation dynamics of a semiflexible polymer through a flickering pore. Journal of Physics Condensed Matter, 2024, 36, 185101.	1.8	0
2598	Predicted tenfold increase of hydrogen solubility in water under pore confinement. Environmental Chemistry Letters, 2024, 22, 945-951.	16.2	0
2599	An Overview of Mechanical Properties of Diamond-like Phases under Tension. Nanomaterials, 2024, 14, 129.	4.1	O
2600	A complex network of interdomain interactions underlies the conformational ensemble of monomeric <scp>TDP</scp> â€43 and modulates its phase behavior. Protein Science, 2024, 33, .	7.6	3
2602	Anomalous temperature dependence of elastic limit in metallic glasses. Nature Communications, 2024, 15, .	12.8	O
2604	Atomic-Scale Insights Into Graphene/Fullerene Tribological Mechanisms and Machine Learning Prediction of Properties. Journal of Tribology, 2024, 146, .	1.9	0
2605	Pressure-induced flat bands in one-dimensional moir $\tilde{A}$ $\!$	3.2	0
2606	The Study on Fatigue Crack Growth Rate of 4130X Material under Different Hydrogen Corrosion Conditions. Materials, 2024, 17, 257.	2.9	0
2607	Recent Advancements and Developments of Molecular Dynamics Simulations in the Discovery of Antiâ€protozoal Agents. ChemistrySelect, 2024, 9, .	1.5	O

#	ARTICLE	IF	CITATIONS
2608	On the Key Influence of Amino Acid Ionic Liquid Anions on CO $<$ sub $>$ 2 $<$ /sub $>$ Capture. Journal of the American Chemical Society, 2024, 146, 1612-1618.	13.7	0
2609	Molecular Dynamics Simulations of Displacement Cascade in Ni-Based Concentrated Solid Solution Alloys. Acta Mechanica Solida Sinica, 2024, 37, 82-89.	1.9	1
2610	Prediction of mechanical properties of phagraphene nanosheets and nanotubes: A molecular dynamics study. Computational Materials Science, 2024, 233, 112770.	3.0	0
2611	Silicene growth mechanisms on $Au(111)$ and $Au(110)$ substrates. Nanotechnology, 2024, 35, 165602.	2.6	0
2612	MDProcessing.jl: Julia Programming Language Application forÂMolecular Dynamics Trajectory Processing. Lecture Notes in Computer Science, 2023, , 209-222.	1.3	0
2613	Assessment of the classical theory validity through Cu50Zr50 nucleation and growth molecular dynamics simulations. Journal of Non-Crystalline Solids, 2024, 627, 122786.	3.1	0
2614	Influence of thermostat on droplet spreading in molecular dynamics simulations. Journal of Molecular Liquids, 2024, 396, 123936.	4.9	0
2615	Nanoscale Ion Transport Enhances Conductivity in Solid Polymer-Ceramic Lithium Electrolytes. ACS Nano, 2024, 18, 2750-2762.	14.6	0
2616	Probing the thermal resistance of solid–liquid interfaces in nanofluids with molecular dynamics. Journal of Chemical Physics, 2024, 160, .	3.0	0
2617	Active learning with moment tensor potentials to predict material properties: Ti0.5Al0.5N at elevated temperature. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2024, 42, .	2.1	0
2618	SPIRAL: An efficient algorithm for the integration of the equation of rotational motion. Computer Physics Communications, 2024, 297, 109077.	7.5	0
2619	A story of two transitions: From adhesive to abrasive wear and from ductile to brittle regime. Journal of Chemical Physics, 2024, 160, .	3.0	0
2620	Pair potential description on phase stability variations in close-packed polytypism. MRS Advances, 0, , .	0.9	0
2621	Polishing-induced material attrition in surface-texturing AlN using a nanoscale polishing tool: An atomic-scale understanding. Tribology International, 2024, 192, 109254.	5.9	1
2622	Comparison of hydrostatic and non-hydrostatic compression of glassy carbon to 80 GPa. Carbon, 2024, 219, 118763.	10.3	0
2623	Molecular dynamics simulation of microstructure and thermophysical properties of LiCl–CaCl <sub>2</sub> eutectic molten salt. International Journal of Chemical Reactor Engineering, 2024, 22, 337-348.	1.1	0
2624	A deep-neural network potential to study transformation-induced plasticity in zirconia. Journal of the European Ceramic Society, 2024, 44, 4243-4254.	5.7	0
2625	Discrete gradients in short-range molecular dynamics simulations. Numerical Algorithms, 0, , .	1.9	O

#	Article	IF	CITATIONS
2626	Topology of anisotropic glasses from persistent homology analysis. Journal of Non-Crystalline Solids, 2024, 627, 122801.	3.1	1
2629	PES and transport properties of the Heâc-HBr complex from kinetic theory and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2024, 26, 4724-4735.	2.8	0
2630	NVIDIA Grace Superchip Early Evaluation for HPC Applications. , 2024, , .		0
2631	Evaluating Stresses in SiO2 Thin Films Using Molecular Dynamics Simulations. , 0, , .		0
2632	Learning the stable and metastable phase diagram to accelerate the discovery of metastable phases of boron. , 2024, 2, .		1
2633	Existence state of Ti in diamond-like carbon coatings and its effects on hybrid structure and residual stress: Molecular dynamics simulations. Computational Materials Science, 2024, 234, 112790.	3.0	0
2634	Dislocation-mediated plasticity in the intermetallic SmCo5 phase. Acta Materialia, 2024, 266, 119669.	7.9	0
2635	A priori procedure to establish spinodal decomposition in alloys. Acta Materialia, 2024, 266, 119667.	7.9	0
2636	Nuclear induction line shape: Non-Markovian diffusion with boundaries. Journal of Chemical Physics, 2024, 160, .	3.0	0
2637	Electrochemical rewiring through quantum conductance effects in single metallic memristive nanowires. Nanoscale Horizons, 2024, 9, 416-426.	8.0	0
2638	Self-interstitial atom properties in Nb–Mo–Ta–W alloys. Computational Materials Science, 2024, 234, 112765.	3.0	0
2639	Formation Onset of Flat-Perylene Prenucleation Clusters in Vacuum. Chemical Physics, 2024, 579, 112191.	1.9	O
2640	Bottom-to-top modeling of epoxy resins: From atomic models to mesoscale fracture mechanisms. Journal of Chemical Physics, 2024, 160, .	3.0	0
2641	Defect-guided self-tearing in graphene. Nanotechnology, 2024, 35, 155602.	2.6	0
2642	Electrodeposition of nanocrystalline cobalt from sulfate baths containing butynediol ethoxylate. Materials Chemistry and Physics, 2024, 314, 128927.	4.0	0
2643	PMC-IZ: A Simple Algorithm for the Electrostatics Calculation in Slab Geometric Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2024, 20, 832-841.	<b>5.</b> 3	O
2644	Screw dislocation core interaction with C or Nb in <mml:math altimg="si27.svg" display="inline" id="d1e1320" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>γ</mml:mi></mml:math> -TiAl: A multiscale study. Acta Materialia, 2024, 266, 119647.	7.9	0
2645	Efficient characterization of double-cross-linked networks in hydrogels using data-inspired coarse-grained molecular dynamics model. Journal of Chemical Physics, 2024, 160, .	3.0	O

#	Article	IF	CITATIONS
2646	Molecular Dynamics Study of the Diffusion of Helium in High-Density Polyethylene Composites Reinforced with Monocrystalline and Bicrystalline Hexagonal Boron Nitride Nanosheets: Implications for Helium Storage. ACS Applied Nano Materials, 2024, 7, 1978-1985.	5.0	0
2647	Modeling Chemical Exfoliation of Non-van der Waals Chromium Sulfides by Machine Learning Interatomic Potentials and Monte Carlo Simulations. Journal of Physical Chemistry C, 2024, 128, 1267-1283.	3.1	0
2648	Compressive reactive molecular dynamics on mechanical and structural behaviors of geopolymers: Imposing lateral constraints and varied temperatures. Applied Clay Science, 2024, 249, 107257.	5.2	0
2649	Enabling Bitwise Reproducibility for the Unstructured Computational Motif. Applied Sciences (Switzerland), 2024, 14, 639.	2.5	0
2650	Thermodynamically Optimized Machine-Learned Reaction Coordinates for Hydrophobic Ligand Dissociation. Journal of Physical Chemistry B, 2024, 128, 755-767.	2.6	0
2651	The investigation of the carbon on irradiation hardening and defect clustering in RPV model alloy using ion irradiation and OKMC simulation. Nuclear Engineering and Technology, 2024, , .	2.3	0
2652	Development of Heteroatomic Constant Potential Method with Application to MXene-Based Supercapacitors. Journal of Chemical Theory and Computation, 2024, 20, 651-664.	<b>5.</b> 3	0
2653	Hydrogen-bond regulation in organic/aqueous hybrid electrolyte for safe and high-voltage K-ion batteries. Energy and Environmental Science, 2024, 17, 1255-1265.	30.8	3
2654	Pool boiling simulation using molecular dynamics approach: Comparing the effectiveness of adding nanoparticles versus creating porous nanostructures. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 0, , .	2.1	0
2655	Quantifying defects in graphene oxide structures. Carbon Trends, 2024, 14, 100323.	3.0	0
2656	Helium bubble evolution under cascade in bcc iron relevant to fusion conditions investigated by a novel coupling MD-OKMC method. Journal of Nuclear Materials, 2024, 591, 154908.	2.7	0
2657	The sensitive aspects of modelling polymer–ceramic composite solid-state electrolytes using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2024, 26, 6216-6227.	2.8	0
2658	Accurate and Transferable Machine Learning Potential for Molecular Dynamics Simulation of Sodium Silicate Glasses. Journal of Chemical Theory and Computation, 2024, 20, 1358-1370.	<b>5.</b> 3	0
2659	Tensile behavior and microstructural evolution of TiMoZrV HEAs: a molecular dynamics study. Applied Physics A: Materials Science and Processing, 2024, 130, .	2.3	0
2660	Machine-Learning Based Multi-Scale Simulation for Polymer Melt Spinning Process. Nihon Reoroji Gakkaishi, 2023, 51, 281-294.	1.0	0
2661	Deformation and boundary motion analysis of a faceted twin grain boundary. International Journal of Mechanical Sciences, 2024, 269, 109044.	6.7	1
2662	Rejuvenating oxidized paving asphalts – When softeners meet asphaltene dispersants. Fuel, 2024, 363, 130948.	6.4	0
2664	Energy stable scheme for random batch molecular dynamics. Journal of Chemical Physics, 2024, 160, .	3.0	0

#	Article	IF	CITATIONS
2665	First principles and molecular dynamics simulations of effect of dopants on properties of high strength steel for hydrogen storage vessels. Wuli Xuebao/Acta Physica Sinica, 2024, 73, 067101.	0.5	0
2666	Understanding neural network tuned Langevin thermostat effect on predicting thermal conductivity of graphene-coated copper using nonequilibrium molecular dynamics simulations. Modelling and Simulation in Materials Science and Engineering, 2024, 32, 025008.	2.0	O
2667	Time–temperature correlations of amorphous thermoplastics at large strains based on molecular dynamics simulations. Mechanics of Materials, 2024, 190, 104926.	3.2	0
2668	Unravelling abnormal in-plane stretchability of two-dimensional metal–organic frameworks by machine learning potential molecular dynamics. Nanoscale, 2024, 16, 3438-3447.	5.6	0
2669	Modeling the Coupled Massâ€Heat Transport in Lennard–Jonesâ€Like Binary Mixtures by Approachâ€toâ€Equilibrium Molecular Dynamics. Advanced Theory and Simulations, 2024, 7, .	2.8	1
2670	The role of randomly packed particles on macroscopic elastic bonded grain properties. Computational Particle Mechanics, 0, , .	3.0	0
2671	Contact Stiffness and Damping in Atomic-Scale Friction: An Approximate Estimation from Molecular Dynamics Simulations. Tribology Letters, 2024, 72, .	2.6	0
2672	The effect of boron carbide doping content on the mechanical properties of polyethylene. Journal of Nuclear Science and Technology, 0, , 1-8.	1.3	0
2673	Understanding the dielectric relaxation of liquid water using neural network potential and classical pairwise potential. Journal of Molecular Liquids, 2024, 397, 124054.	4.9	0
2674	A-site cation controlled localization of dipole correlations in a relaxor material. Physical Review Materials, 2024, 8, .	2.4	0
2675	Designing the composition and optimizing the mechanical properties of non-equiatomic FeCoNiTi high-entropy alloys. Journal of Materials Research and Technology, 2024, 29, 376-385.	5.8	0
2676	Mobility of screw dislocations absorbed in <110> symmetric tilt grain boundaries in Al. Philosophical Magazine, 2024, 104, 343-363.	1.6	0
2677	A simple efficient algorithm for molecular simulations of constant potential electrodes. Journal of Chemical Physics, 2024, $160$ , .	3.0	1
2678	Particle-resolved study of the onset of turbulence. Physical Review Research, 2024, 6, .	3.6	0
2679	Control of segregation by non-uniform aeration in a fluidized bed spray granulator. Powder Technology, 2024, 435, 119348.	4.2	0
2680	Deep Learning on Atomistic Physical Fields of Graphene for Strain and Defect Engineering. Advanced Intelligent Systems, 2024, 6, .	6.1	0
2681	Atomistic Computer Simulations of Uranyl Adsorption on Hydrated Illite and Smectite Surfaces. Minerals (Basel, Switzerland), 2024, 14, 109.	2.0	0
2682	Study of α″-phase Fe16X2â^'nYn (X,Y = N, C) alloys by molecular dynamics modeling. AIP Advances, 2024, 14, .	1.3	0

#	Article	IF	CITATIONS
2683	Universal properties of repulsive self-propelled particles and attractive driven particles. Physical Review Research, 2024, 6, .	3.6	0
2684	Role of metal passivator on production of hydrogen gas in insulating oil and oil-impregnated insulation paper. Energy Reports, 2024, 11, 1544-1550.	5.1	0
2685	Effects of radiation damage on the yielding and fracture of nanowires. Nanoscale, 2024, 16, 3071-3080.	5.6	0
2686	Effects of extreme hydrostatic pressure on the molecular structure and properties of the elastomeric material for soft robots. Materials and Design, 2024, 238, 112686.	7.0	0
2687	Concurring effect of doping and composition on the thermodynamic properties of amorphous GexSe1-x alloys. Acta Materialia, 2024, 266, 119676.	7.9	0
2688	New insights into the degradation mechanism of TNT in supercritical water: Combining density functional theory with the reactive force field. Journal of Molecular Liquids, 2024, 396, 124040.	4.9	0
2689	A 3D metallic porous sulfurized carbon anode identified by global structure search for Na-ion batteries with fast diffusion kinetics. Journal of Energy Storage, 2024, 82, 110587.	8.1	0
2690	Revisiting bitumen-clay interaction using molecular dynamics: The role of surfactants. Journal of Molecular Liquids, 2024, 396, 124066.	4.9	0
2691	Possible approaches for simulating the formation of fuzz structure on tungsten surface under helium irradiation. Computational Materials Science, 2024, 235, 112807.	3.0	0
2692	Etching mechanism of amorphous hydrogenated silicon nitride by hydrogen fluoride. Applied Surface Science, 2024, 654, 159414.	6.1	0
2693	Experimental study and modeling of the wettability of fluorine graphene. Corrosion behavior of the fluorine graphene layer on a copper substrate. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2024, 685, 133269.	4.7	0
2694	Revealing the effect of inverse dislocation pileups on the mechanical properties of multi-principal element alloys. Journal of Materials Science and Technology, 2024, 190, 155-171.	10.7	0
2695	Liquid-like thermal conductivity in solid materials: Dynamic behavior of silver ions in argyrodites. Nano Energy, 2024, 122, 109324.	16.0	0
2696	Molecular dynamics simulations of tensile and creep-ratcheting behaviour of CNT reinforced columnar nanocrystalline Al nanocomposites. Diamond and Related Materials, 2024, 142, 110850.	3.9	O
2697	Mechanism of initial activation of carbon–oxygen bonds for deoxidation of acetic acid. Chemical Engineering Science, 2024, 287, 119804.	3.8	0
2698	Confined Layer Slip Process in Nanolaminated Ag and Two Ag/Cu Nanolaminates. Materials, 2024, 17, 501.	2.9	1
2699	Investigations into penetration depth profiles of hydrogenic species in beryllium plasma-facing components via molecular dynamics simulations. Plasma Physics and Controlled Fusion, 2024, 66, 045005.	2.1	0
2700	Atomic erosion behavior and influence mechanism during erosion impact of TiC coatings with different crystal faces in oil production environment: A molecular dynamics simulation. Tribology International, 2024, 193, 109320.	5.9	0

#	Article	IF	CITATIONS
2701	Theoretical mechanism behind the higher efficiency of O than OH radicals in polypropylene surface modification: a molecular dynamics study. Plasma Sources Science and Technology, 2024, 33, 025009.	3.1	0
2702	Simulation of proton-induced primary displacement damage in GaAs under different ambient temperatures. AIP Advances, 2024, 14, .	1.3	0
2703	The Dynamics of Per- and Polyfluoroalkyl Substances (PFAS) at Interfaces in Porous Media: A Computational Roadmap from Nanoscale Molecular Dynamics Simulation to Macroscale Modeling. ACS Omega, 2024, 9, 5193-5202.	3.5	1
2704	Exploring the Heat of Water Intrusion into a Metal–Organic Framework by Experiment and Simulation. ACS Applied Materials & Simulation. Simulation. ACS Applied Materials & Simulation. Simulation. ACS Applied Materials & Simulation.	8.0	0
2705	Dependence between glass transition and plasticity in amorphous aluminum oxide: A molecular dynamics study. Journal of Non-Crystalline Solids, 2024, 628, 122840.	3.1	1
2706	PDMATLAB2D: A Peridynamics MATLAB Two-dimensional Code. Journal of Peridynamics and Nonlocal Modeling, 2024, 6, 149-205.	2.9	1
2707	Molecular simulation on CO2 adsorption heterogeneity in montmorillonite nanopores with different surface charges in presence of water. Chemical Engineering Journal, 2024, 482, 148958.	12.7	0
2708	Accuracy of TIP4P/2005 and SPC/Fw Water Models. Journal of Physical Chemistry B, 2024, 128, 1091-1097.	2.6	0
2709	Molecular Dynamics Study on Mechanical Properties of Calcium–Silicate–Hydrate Considering Model and Parameter Effects. Mechanisms and Machine Science, 2024, , 885-903.	0.5	0
2710	Coarse-Grained Molecular Dynamics Simulations of Organic Friction Modifier Adsorption on Rough Surfaces under Shear. Lubricants, 2024, 12, 30.	2.9	0
2711	Dependence of Critical Stress Intensity Factor on Crack Depth From the Loading Boundary of Crystalline Silicon. Journal of Applied Mechanics, Transactions ASME, 2024, 91, .	2.2	0
2712	Atomistic investigation of surface modification effect on interfacial properties of CNTs reinforced AAS geopolymer. Journal of Building Engineering, 2024, 84, 108630.	3.4	0
2713	Combined Experimental and Computational Insight into the Role of Substrate in the Synthesis of Two-Dimensional WSe <sub>2</sub> . ACS Applied Materials & Interfaces, 2024, 16, 6644-6652.	8.0	0
2714	Hidden phonon highways promote photoinduced interlayer energy transfer in twisted transition metal dichalcogenide heterostructures. Science Advances, 2024, 10, .	10.3	0
2715	Insight into the Density-Dependence of Pair Potentials for Predictive Coarse-Grained Models. Journal of Physical Chemistry B, 2024, 128, 1298-1316.	2.6	0
2718	Instantaneous normal modes of glass-forming liquids during the athermal relaxation process of the steepest descent algorithm. Soft Matter, 2024, 20, 1583-1602.	2.7	0
2719	Templating Effect of MoSe <sub>2</sub> on Crystallization of Polyethylene: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2024, 128, 2147-2162.	3.1	0
2720	â€~Heat engine' mechanism of latent heat release during the recalescence stage in supercooled heterogeneous icing. International Journal of Heat and Mass Transfer, 2024, 223, 125214.	4.8	0

#	Article	IF	CITATIONS
2721	Charging and discharging a supercapacitor in molecular simulations. Journal of Chemical Physics, $2024, 160, .$	3.0	0
2722	Threading Subunits for Polymers to Predict the Equilibrium Ensemble of Solid Polymer Electrolytes. Journal of Physical Chemistry Letters, 2024, 15, 1227-1233.	4.6	O
2723	Investigating thermal conductivity and mechanical properties of a hybrid material based on cellulose nanofibers and boron nitride nanotubes using molecular dynamics simulations. Journal Physics D: Applied Physics, 2024, 57, 185302.	2.8	0
2724	Computation of X-ray and Neutron Scattering Patterns to Benchmark Atomistic Simulations against Experiments. International Journal of Molecular Sciences, 2024, 25, 1547.	4.1	0
2725	Accelerating Elastic Property Prediction in Fe-C Alloys through Coupling of Molecular Dynamics and Machine Learning. Materials, 2024, 17, 601.	2.9	0
2726	Atomic irradiation defects induced hardening model in irradiated tungsten based on molecular dynamics and CPFEM. International Journal of Plasticity, 2024, 174, 103895.	8.8	1
2727	Electrochemical corrosion behavior variation of WC-10Co4Cr coating subjected to different magnetic treatments and its mechanism. Corrosion Science, 2024, 229, 111883.	6.6	0
2728	Revealing microstructure evolution and strengthening behavior of high-temperature laser shock peened copper. Materials Characterization, 2024, 209, 113706.	4.4	O
2729	Interfacial Thermal Transport and Electrical Performances of Supercapacitors with Graphene/Carbon Nanotube Composite Electrodes. Journal of Physical Chemistry C, 2024, 128, 2190-2204.	3.1	0
2730	matscipy: materials science at the atomic scale with Python. Journal of Open Source Software, 2024, 9, 5668.	4.6	2
2731	Quasi-classical Trajectory Calculation of Rate Constants Using Ab-initio Trained Machine Learning Force Field (aML-MD). , 2024, , .		0
2732	A soft departure from jamming: the compaction of deformable granular matter under high pressures. Soft Matter, 2024, 20, 1702-1718.	2.7	1
2733	Emergence of compact disordered phase in a polymer Potts model. Physical Review E, 2024, 109, .	2.1	0
2734	Sound waves, diffusive transport, and wall slip in nanoconfined compressible fluids. Physical Review Fluids, 2024, 9, .	2.5	0
2735	Protocol-dependent frictional granular jamming simulations: cyclical, compression, and expansion. , 0, 3, .		0
2736	Effects of Pressure and Electric Field Strength on the Emission Rate for a Molecular Dynamics Model of [EMIM-BF <sub>4</sub> ] Ionic Liquid., 2024,,.		0
2737	Characterization of Propellant-Surface Collision Byproducts Using MD Simulations and RGA Measurements. , 2024, , .		0
2738	The stress in static granular media under gravity. Journal of Fluid Mechanics, 2024, 980, .	3.4	O

#	Article	IF	CITATIONS
2739	Enhanced Radiation Damage Tolerance of Amorphous Interphase and Grain Boundary Complexions in Cu-Ta. Jom, $0,  ,  .$	1.9	0
2741	The formation mechanism of Sc-based metallofullerenes: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2024, 26, 5499-5507.	2.8	1
2742	Product Characteristics of Cellulose Initial Pyrolysis by Reactive Molecular Dynamics Simulation. Nihon Enerugi Gakkaishi/Journal of the Japan Institute of Energy, 2024, 103, 1-10.	0.2	0
2743	The interplay of field-tunable strongly correlated states in a multi-orbital moiré system. Nature Physics, 2024, 20, 589-596.	16.7	0
2744	Harmonic transition state theory applied to vacancy diffusion pre-exponential factors in a concentrated solid-solution alloy. Physical Review Materials, 2024, 8, .	2.4	0
2745	Al-Based Nano-Scale Material Property Prediction for Li-Ion Batteries. Batteries, 2024, 10, 51.	4.5	0
2746	Glass Transition Temperatures and Thermal Conductivities of Polybutadiene Crosslinked with Randomly Distributed Sulfur Chains Using Molecular Dynamic Simulation. Polymers, 2024, 16, 384.	4.5	1
2747	Computational Analysis of Secondary Droplet Breakup at Transcritical Conditions with Surface Tension Effects. , 2024, , .		0
2748	Effect of electric fields on tungsten distribution in Na <sub>2</sub> WO <sub>4</sub> –WO <sub>3</sub> molten salt. Physical Chemistry Chemical Physics, 2024, 26, 6590-6599.	2.8	0
2749	Solute-enhanced twin boundary migration in CuAg alloy. Journal of Applied Physics, 2024, 135, .	2.5	0
2750	Direct prediction of intrinsically disordered protein conformational properties from sequence. Nature Methods, 2024, 21, 465-476.	19.0	4
2751	Isothermal Titration Calorimetry Reveals Entropy-Driven Bisphenol A Epoxy Resin Adhesion to Metal Oxide Surfaces. Macromolecules, 2024, 57, 2130-2141.	4.8	0
2752	Conformation and dynamics of partially active linear polymers. Soft Matter, 2024, 20, 1892-1904.	2.7	0
2753	Structure and polymerization of liquid sulfur across the λ-transition. Chemical Science, 2024, 15, 3382-3392.	7.4	0
2754	Molecular dynamics study on desublimation and crystal nucleation of carbon dioxide on a low temperature surface. Energy, 2024, 292, 130546.	8.8	0
2755	Superlubricity of Silicon-Based Ceramics Sliding against Hydrogenated Amorphous Carbon in Ultrahigh Vacuum: Mechanisms of Transfer Film Formation. ACS Applied Materials & Eamp; Interfaces, 2024, 16, 8032-8044.	8.0	1
2756	All-Atom Molecular Dynamics Simulations of Uncharged Linear Polymer Bottlebrushes: Effect of the Brush Sizes and the Number of Side-Chain Monomers. Langmuir, 2024, 40, 2946-2956.	3.5	0
2757	Uniaxial Strain-Induced Stacking Order Change in Trilayer Graphene. ACS Applied Materials & Samp; Interfaces, 2024, 16, 8169-8183.	8.0	0

#	Article	IF	CITATIONS
2758	Study of grain-patterned and highly ordered L10-FePt HAMR media using reactive molecular dynamics method. AIP Advances, 2024, $14$ , .	1.3	0
2759	Simulation of mechanical effects of hydrogen in bicrystalline Cu using DFT and bond order potentials. Procedia Structural Integrity, 2024, 52, 356-365.	0.8	0
2760	Salt Effects on the Mechanical Properties of Ionic Conductive Polymer: A Molecular Dynamics Study. ACS Materials Au, 0, , .	6.0	0
2761	The effect of mixed wettability on flow characteristics in porous media of ultra-deep gas reservoirs: Molecular dynamics simulations and numerical simulations. Applied Surface Science, 2024, 654, 159541.	6.1	0
2762	Impact of edge dislocation and grain boundaries on mechanical properties in CoCrCuFeNi high entropy alloy. Journal of Applied Physics, 2024, 135, .	2.5	1
2763	Effect of polycaprolactone percentage on thermal and mechanical behavior of polyurethane/polycaprolactone/graphene oxide nanocomposite utilizing molecular dynamics simulation. Engineering Analysis With Boundary Elements, 2024, 161, 179-187.	3.7	0
2764	Exploring thermal properties of PbSnTeSe and PbSnTeS high entropy alloys with machine-learned potentials. Modelling and Simulation in Materials Science and Engineering, 2024, 32, 035008.	2.0	0
2765	Molecular Dynamics Simulation Research on Fe Atom Precipitation Behaviour of Cu-Fe Alloys during the Rapid Solidification Processes. Materials, 2024, 17, 719.	2.9	O
2766	Delocalized nonlinear vibrational modes in Ni <mml:math altimg="si1.svg" display="inline" id="d1e665" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow></mml:mrow><mml:mrow></mml:mrow></mml:msub></mml:math> Al. Communications in Nonlinear Science and Numerical Simulation, 2024, 132, 107890.	3.3	О
2767	Modeling Properties and Phenomena at High Temperatures: Atomistic and Phase-Field Approaches., 2024, , 201-273.		O
2768	Structure of diclofenac in an aqueous medium and its adsorption onto carbons: Molecular insights through simulation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2024, 686, 133373.	4.7	0
2769	Gas-surface interaction features under effects of gas-gas molecules interaction in high-speed flows. Chinese Journal of Aeronautics, 2024, , .	<b>5.</b> 3	O
2770	Boundary slip and lubrication mechanisms of organic friction modifiers with effect of surface moisture. Friction, 0, , .	6.4	0
2771	Molecular dynamic study to investigate the system size effects on tetrahedral materials in supercooled region. Materials Today: Proceedings, 2024, , .	1.8	0
2772	Study on the atomic removal behavior and damage formation mechanism of nano cutting copper–nickel alloy with diamond tool. Modelling and Simulation in Materials Science and Engineering, 2024, 32, 035011.	2.0	0
2773	Disorder-induced heating as a mechanism for fast neutral gas heating in atmospheric pressure plasmas. Plasma Sources Science and Technology, 2024, 33, 02LT02.	3.1	0
2774	Artificial neural network for deciphering the structural transformation of condensed ZnO by extended x-ray absorption fine structure spectroscopy. Journal of Physics Condensed Matter, 2024, 36, 195402.	1.8	0
2775	Magic Momenta and Three-Dimensional Landau Levels from a Three-Dimensional Graphite Moir $\tilde{A}$ Superlattice. Physical Review Letters, 2024, 132, .	7.8	0

#	Article	IF	CITATIONS
2776	A strain density function to analyze particle size effects during high velocity impacts of yttria. Journal of the American Ceramic Society, 2024, 107, 3925-3944.	3.8	0
2777	Capturing CO2 using novel nonaqueous biphasic solvent TMEDA/MEA/DMSO: Absorption and phase splitting mechanism. Chemical Engineering Journal, 2024, 484, 149293.	12.7	0
2778	New Insights into Phenolic Resin Decomposition under Oxidative Conditions of High Temperature. Industrial & Engineering Chemistry Research, 2024, 63, 2642-2656.	3.7	0
2779	Electrical percolation networks of MWCNT/Graphene/Polyaniline nanocomposites with enhanced electromagnetic interference shielding efficiency. Applied Surface Science, 2024, 655, 159613.	6.1	O
2780	How close are the classical two-body potentials to <i>abÂinitio</i> calculations? Insights from linear machine learning based force matching. Journal of Chemical Physics, 2024, 160, .	3.0	0
2781	On the thermodynamics of plasticity during quasi-isentropic compression of metallic glass. Matter and Radiation at Extremes, 2024, 9, .	3.9	0
2782	Molecular dynamics simulation study of water structure and dynamics on the gold electrode surface with adsorbed 4-mercaptobenzonitrile. Journal of Chemical Physics, 2024, 160, .	3.0	0
2783	Experimental and Simulation Insights into the Thermophysical Properties of Dibutyl Ether Mixed with n-Heptane and n-Octane. Korean Journal of Chemical Engineering, 2024, 41, 1197-1208.	2.7	0
2784	Molecular dynamics study on the effect of surface ionization on the interfacial heat transfer between silica and water. Applied Thermal Engineering, 2024, 244, 122762.	6.0	0
2785	High-strong-ductile magnesium alloys by interactions of nanoscale quasi-long period stacking order unit with twin. Journal of Magnesium and Alloys, 2024, , .	11.9	O
2786	Impact of Li, Na and Zn metal cation concentration in EMIM–TFSI ionic liquids on ion clustering, structure and dynamics. Physical Chemistry Chemical Physics, 2024, 26, 7049-7059.	2.8	0
2787	Safe electrolyte for long-cycling alkali-ion batteries. Nature Sustainability, 2024, 7, 326-337.	23.7	2
2788	Formalizing Coarse-Grained Representations of Anisotropic Interactions at Multimeric Protein Interfaces Using Virtual Sites. Journal of Physical Chemistry B, 2024, 128, 1394-1406.	2.6	0
2789	Atomic scale study of the impact of metallic glass nanoparticles at high velocities. Journal of Non-Crystalline Solids, 2024, 628, 122866.	3.1	0
2790	Upper storage-capacity limit and multiple occupancy phenomena in H <sub>2</sub> <b>-</b> hydroquinone clathrates using Monte Carlo and DFT simulations. Physical Chemistry Chemical Physics, 2024, 26, 6939-6948.	2.8	0
2791	Influence of variation in grain boundary parameters on the evolution of atomic structure and properties of [111] tilt boundaries in aluminum. Acta Materialia, 2024, 268, 119732.	7.9	O
2792	Mechanism of RGD-conjugated nanodevice binding to its target protein integrin $\hat{l}\pm < \text{sub} > \hat{l}^2 < \text{sub} > 3 < / \text{sub} > by atomistic molecular dynamics and machine learning. Nanoscale, 2024, 16, 4063-4081.}$	5.6	0
2793	Mechanism of Charge Transport in Lithium Thiophosphate. Chemistry of Materials, 2024, 36, 1482-1496.	6.7	O

#	Article	IF	CITATIONS
2794	Development of mesoporous abrasives and its unprecedented polishing performance elucidated by a novel atomic model. Materials Today Sustainability, 2024, 25, 100700.	4.1	0
2795	Enhanced Thermal Boundary Conductance across GaN/SiC Interfaces with AlN Transition Layers. ACS Applied Materials & Samp; Interfaces, 2024, 16, 8109-8118.	8.0	O
2796	Quasilocalized modes in crystalline and partially crystalline high-entropy alloys. Physical Review Research, 2024, 6, .	3.6	1
2797	In Situ X-ray Scattering Reveals Coarsening Rates of Superlattices Self-Assembled from Electrostatically Stabilized Metal Nanocrystals Depend Nonmonotonically on Driving Force. ACS Nano, 0, , .	14.6	0
2798	Crystal Lattice Structure Prediction of Fe-Based Compounds by a Molecular Dynamics Method. Minerals, Metals and Materials Series, 2024, , 633-643.	0.4	0
2799	Interplay between thermal vacancy and short-range order in complex concentrated alloys. Journal of Alloys and Compounds, 2024, 982, 173788.	5.5	0
2800	Virtual XRD Method in Molecular Dynamics Simulation and a Case Study for Fe16N2 and Fe8N Thin Films. Minerals, Metals and Materials Series, 2024, , 1693-1704.	0.4	0
2801	Can Silica Nanoparticles Improve Lithium Transport in Polymer Electrolytes?. Journal of Physical Chemistry C, 2024, 128, 2737-2747.	3.1	O
2802	Atomic cluster dynamics causes intermittent aging of metallic glasses. Acta Materialia, 2024, 267, 119730.	7.9	0
2803	Mechanical properties of silicon nanowires with native oxide surface state. Materials Today Communications, 2024, 38, 108321.	1.9	0
2804	Hydrogen-Induced Transformation of Dislocation Core in Fe and Its Effect on Dislocation Mobility. Minerals, Metals and Materials Series, 2024, , 1000-1007.	0.4	0
2805	Evolution of dislocation loops in irradiated α-Uranium: An atomistically-informed cluster dynamics investigation. Acta Materialia, 2024, 270, 119728.	7.9	0
2806	Establishing Pinhole Deposition Mode of Zn via Scalable Monolayer Graphene Film. Advanced Materials, 2024, 36, .	21.0	0
2807	Spectroscopic and theoretical analyses of the reaction of SrO in molten chloride and fluoride salts. Journal of Nuclear Materials, 2024, 592, 154962.	2.7	0
2808	<i>Colloquium</i> : Sliding and pinning in structurally lubric 2D material interfaces. Reviews of Modern Physics, 2024, 96, .	45.6	0
2809	Transport of particles through RO membrane in steady state condition. ChemistrySelect, 2024, 9, .	1.5	0
2810	CLEAVING: a LAMMPS package to compute surface free energies. Journal of Open Source Software, 2024, 9, 5886.	4.6	0
2811	Coupling ReaxFF molecular dynamics with computational fluid dynamics on the enhanced heat sink of n-decane decomposition initiated by nitroethane in the regenerative cooling channels. Journal of Analytical and Applied Pyrolysis, 2024, 178, 106394.	5.5	O

#	Article	IF	CITATIONS
2812	Enhancing mechanical performance of Al <sub>0.3</sub> CoCrFeNi HEA films through graphene coating: insights from nanoindentation and dislocation mechanism analysis. Modelling and Simulation in Materials Science and Engineering, 2024, 32, 035012.	2.0	0
2813	Chain-Level Analysis of Reinforced Polyethylene through Stretch-Induced Crystallization. ACS Macro Letters, 0, , 247-251.	4.8	0
2814	Conformational variability of intrinsically isotropic polymers with varying stiffness immersed in nematogenic solvents. Polymer, 2024, 295, 126774.	3.8	1
2815	Earth's "Missing―Chlorine May Be in the Core. Journal of Geophysical Research: Solid Earth, 2024, 129,	3.4	0
2816	Buckling kinetics of graphene membranes under uniaxial compression. Physical Review E, 2024, 109, .	2.1	0
2817	Elaboration of a neural-network interatomic potential for silica glass and melt. Computational Materials Science, 2024, 236, 112848.	3.0	0
2818	Strain rate effects on the axial tensile behavior of crystalline polyethylene: Insights from molecular dynamics simulations. Polymer, 2024, 295, 126779.	3.8	0
2819	Stability and Phase Transformations in Au–Pd Nanoparticles Studied by Means of Combined Monte Carlo and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2024, 128, 3054-3063.	3.1	0
2820	Study on non-classical effects of Knudsen layer in planar Couette flow using molecular dynamics simulations. AIP Conference Proceedings, 2024, , .	0.4	0
2821	Ion Channels in Critical Membranes: Clustering, Cooperativity, and Memory Effects. , 2024, 2, .		0
2822	The role of deep learning in reducing computational cost when simulating chloride ion attack on hydrated calcium silicate with molecular dynamics. Construction and Building Materials, 2024, 417, 135257.	7.2	0
2823	Tribological Properties of Phosphate Ester Confined between Iron-Based Surfaces. Langmuir, 0, , .	3.5	0
2824	Oxygen Diffusion in Brownmillerite Sr <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub> is Two-Dimensional: Results from a Molecular Dynamics Study. Chemistry of Materials, 2024, 36, 2039-2048.	6.7	0
2825	Structural and thermal analyses in semiconducting and metallic zigzag single-walled carbon nanotubes using molecular dynamics simulations. PLoS ONE, 2024, 19, e0296916.	2.5	0
2826	Properties of packings and dispersions of superellipse sector particles. Physical Review E, 2024, 109, .	2.1	0
2827	Modeling of irradiation-induced microstructure evolution in Fe: Impact of Frenkel pair distribution. Computational Materials Science, 2024, 236, 112852.	3.0	0
2828	Effect of the Ion, Solvent, and Thermal Interaction Coefficients on Battery Voltage. Journal of the American Chemical Society, 2024, 146, 4592-4604.	13.7	0
2829	Unraveling the crystallization kinetics of the Ge2Sb2Te5 phase change compound with a machine-learned interatomic potential. Npj Computational Materials, 2024, 10, .	8.7	0

#	Article	IF	CITATIONS
2830	Molecular dynamics simulations of solid-state sintering in Fe35Ni alloy: understanding the process at the atomic scale. Journal of Materials Science, 2024, 59, 2954-2973.	3.7	0
2831	Polymeric surfactants at liquid–liquid interfaces: Dependence of structural and thermodynamic properties on copolymer architecture. Journal of Chemical Physics, 2024, 160, .	3.0	0
2832	A bond swap algorithm for simulating dynamically crosslinked polymers. Journal of Chemical Physics, 2024, 160, .	3.0	0
2833	Diffuse electron scattering reveals kinetic frustration as origin of order in CoCrNi medium entropy alloy. Acta Materialia, 2024, 268, 119753.	7.9	0
2834	Macromolecular crowding in chiral assembly of ellipsoidal nanoparticles. Journal of Chemical Physics, 2024, 160, .	3.0	0
2835	Gradual weakening down to complete disappearance of the velocity correlated cluster emission effect in keV collisions of C60 with light metallic targets: Microscopic insights via molecular dynamics simulations. Journal of Chemical Physics, 2024, 160, .	3.0	0
2836	Einstein–Stokes relation for small bubbles at the nanoscale. Journal of Chemical Physics, 2024, 160, .	3.0	0
2837	Investigation of the effect of off-stoichiometric composition on oxygen transport in layered perovskite materials for SOFC cathode. Materials Letters, 2024, 361, 136114.	2.6	0
2838	Simulation data for engineering graphene quantum dot epoxy nanocomposites using molecular dynamics. Data in Brief, 2024, 53, 110169.	1.0	0
2839	Formation of large loop-hydrogen complexes and related effects on mechanical properties of Zirconium investigated with molecular dynamics method. Materials Today Communications, 2024, 38, 108362.	1.9	0
2840	Amplifying Nanoparticle Reinforcement through Low Volume Topologically Controlled Chemical Coupling. ACS Macro Letters, 2024, 13, 280-287.	4.8	0
2841	An examination of the performance of molecular dynamics force fields: Silicon and silicon dioxide reactive ion etching. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2024, 42, .	2.1	0
2842	One Stone, Two Birds: Using High Electric Fields to Enhance the Mobility and the Concentration of Point Defects in Ion-Conducting Solids. Journal of the American Chemical Society, 2024, 146, 4783-4794.	13.7	0
2843	All-atom molecular dynamics simulations of nematic liquid crystal elastomers. International Journal of Solids and Structures, 2024, 291, 112717.	2.7	O
2844	Short-range ordering mechanics in FCC materials. International Journal of Plasticity, 2024, 174, 103919.	8.8	0
2845	Kinetic trapping of nanoparticles by solvent-induced interactions. Nanoscale, 2024, 16, 5374-5382.	5.6	0
2846	Investigation of the influence of aluminum surficial water on aluminum-plastic hybrids through a combined experimental and simulation approach. Applied Surface Science, 2024, 656, 159694.	6.1	0
2847	Extended magic phase in twisted graphene multilayers. Physical Review Research, 2024, 6, .	3.6	1

#	Article	IF	CITATIONS
2848	Influence of the mixing speed in the rheology of NMC622-based Li-ion battery electrode slurries. Journal of Power Sources Advances, 2024, 26, 100141.	5.1	1
2849	Exploring Thermoset Fracture with a Quantum Chemically Accurate Model of Bond Scission. Macromolecules, 2024, 57, 1414-1425.	4.8	O
2850	Molecular Dynamics Simulation of 40Cr/Q345 Hot Compression Process. Journal of Materials Engineering and Performance, 0, , .	2.5	0
2851	Nano-friction behavior and deformation study of hydroxyapatite in ultra-precision polishing process. Journal of Molecular Modeling, 2024, 30, .	1.8	0
2852	Anisotropic Deformation in a Polymer Slab Subjected to Fluid Adsorption. Langmuir, 2024, 40, 4382-4391.	3.5	0
2853	Nanoscale Hierarchical Structures Formed by Sequence-Defined Polycations and Homopolyanions for High Salt-Tolerance Adhesives. Macromolecules, 2024, 57, 1859-1867.	4.8	O
2854	Unveiling the multicomponent phase separation through molecular dynamics simulation and graph theory. Journal of Chemical Physics, 2024, 160, .	3.0	0
2855	Clustering Effects on the Structure of Ionomer Solutions: A Combined SANS and Simulations Study. Macromolecules, 2024, 57, 1688-1698.	4.8	1
2856	Atomistic simulations of nuclear fuel <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>UO</mml:mi><mml:mn>2<td>nn<b>₂.4</b>/mml:</td><td>m<b>e</b>ub&gt;</td></mml:mn></mml:msub></mml:math>	nn <b>₂.4</b> /mml:	m <b>e</b> ub>
2857	Design of saccharide based organic binder for low-grade iron ore pelletization using atomistic simulations and machine learning methods. Journal of Molecular Graphics and Modelling, 2024, 129, 108730.	2.4	0
2858	Multifidelity Gaussian Processes for Predicting Shear Viscosity over Wide Ranges of Liquid State Points Based on Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2024, 63, 3755-3765.	3.7	0
2859	PySAGES: flexible, advanced sampling methods accelerated with GPUs. Npj Computational Materials, 2024, 10, .	8.7	1
2860	Graphene-Induced Surface Stiffening of Copper Studied by Nanoindentation. Journal of Physical Chemistry C, 2024, 128, 3449-3459.	3.1	0
2861	Photo-excited charge transfer from adamantane to electronic bound states in water. Physical Chemistry Chemical Physics, 2024, 26, 8158-8176.	2.8	O
2862	Discrete network models of endothelial cells and their interactions with the substrate. Biomechanics and Modeling in Mechanobiology, 0, , .	2.8	0
2863	Molecular Dynamics Research on Fe Precipitation Behavior of Cu95Fe5 Alloys during Rapid Cooling. Metals, 2024, 14, 228.	2.3	O
2864	Large-scale atomistic model construction of subbituminous and bituminous coals for solvent extraction simulations with reactive molecular dynamics. Carbon, 2024, 222, 118939.	10.3	0
2865	A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture. Communications Chemistry, 2024, 7, .	4.5	O

#	Article	IF	CITATIONS
2866	Experimental and Theoretical Study on the Tribological Characteristics of Organophosphates on Metal Surfaces. Tribology Online, 2024, 19, 11-22.	0.9	0
2867	Inorganic siloxane-modified nanosheet-assembled MnOx hollow sphere catalyst for VOC removal from coal-fired flue gas: Enhanced water resistance and Activity. Chemical Engineering Journal, 2024, 484, 149638.	12.7	O
2868	Training dependency of neural network interatomic potential for molecular dynamics simulation of Ru-Si-O mixed system. Japanese Journal of Applied Physics, 2024, 63, 03SP88.	1.5	0
2869	Ca-dimers, solvent layering, and dominant electrochemically active species in Ca(BH4)2 in THF. Nature Communications, 2024, $15$ , .	12.8	0
2870	Atomic-Scale Dislocation Structure Evolution and Crystal Ordering Analysis of Melting and Crystallization Microprocesses in Laser Powder Bed Melting of Î <sup>3</sup> -TiAl Alloys. Metals, 2024, 14, 237.	2.3	0
2871	Driving mechanisms of quartz wettability alteration under in-situ H2 geo-storage conditions: Role of organic ligands and surface morphology. International Journal of Hydrogen Energy, 2024, 59, 1388-1398.	7.1	0
2872	Structural and Spectroscopic Properties of Butanediol-Modified Boehmite Materials. Journal of Physical Chemistry C, 2024, 128, 3533-3542.	3.1	0
2873	Mixing mechanisms of lead nanoparticles with mineral particles: implication of atmospheric transportation of lead. Environmental Science: Nano, 2024, 11, 1452-1461.	4.3	O
2874	Electrified fracture of nanotube films. Physical Review Materials, 2024, 8, .	2.4	0
2875	Pressure Anisotropy in Polymer Brushes and Its Effects on Wetting. Langmuir, 2024, 40, 4401-4409.	3.5	0
2876	Electrical Chain Rearrangement: What Happens When Polymers in Brushes Have a Charge Gradient?. Langmuir, 2024, 40, 4142-4151.	3.5	0
2877	Automated identification and tracking of deformation twin structures in molecular dynamics simulations. Computational Materials Science, 2024, 236, 112878.	3.0	0
2879	Thermal Conductivity of Bottle–Brush Polymers. Langmuir, 2024, 40, 4392-4400.	3.5	0
2880	Formation of hollow silver nanoparticles under irradiation with ultrashort laser pulses. Nanophotonics, 2024, 13, 1149-1157.	6.0	1
2881	Role of cluster structure on the deformation behavior of Zr58Cu36Al6 metallic glass. Materials Today Communications, 2024, 38, 108416.	1.9	0
2882	Molecular dynamics simulation of Cr–O–C discrete nuclei to reduce the binding force of nanocrystalline Cu/Ni complexes. Journal of Materials Science, 2024, 59, 3531-3543.	3.7	0
2883	Suppression mechanism of diamond tool wear by graphene nanofluid in micro-milling of TC4 alloy: A study combining experimental and molecular dynamics. Journal of Manufacturing Processes, 2024, 115, 310-322.	5.9	0
2884	The Effects of Attractive Interaction on Viscosity in Undercooled Kob–Andersen Liquids. Multiscale Science and Engineering, 2023, 5, 160-165.	1.7	0

#	ARTICLE	IF	Citations
2885	Architectural design of anode materials for superior alkali-ion (Li/Na/K) batteries storage. Scientific Reports, 2024, $14$ , .	3.3	0
2886	Effects of using nanofluids on thermal performance and mass transfer in a micro-flat plate heat pipe. Journal of Thermal Analysis and Calorimetry, 2024, 149, 3735-3757.	3.6	O
2887	ç¹°ã,Šè¿"ã⊷è•é‡ã,'å⊷ã•ã,‹éŠãƒŠãƒŽãƒ¯ã,Ħƒ∰®å¡'性å‰å½¢ã«é—¢ã™ã,‹å^†åå‹•åŠ›å¦æ³•è§£æžټ¼šçµæ™¶æ—¹	ä <b>₩2ã®</b> å½:	± <b>é</b> Ÿ¿. Zairyc
2889	Modeling the Effects of Varying the Ti Concentration on the Mechanical Properties of Cu–Ti Alloys. ACS Omega, 2024, 9, 10286-10298.	3.5	0
2890	Molecular Insights into the Influence of Ions on the Water Structure. I. Alkali Metal Ions in Solution. Journal of Physical Chemistry B, 2024, 128, 1953-1962.	2.6	0
2891	Implementation of New Boundary Condition in LAMMPS for Energetics of Screw Dislocation in BCC Iron. Zairyo/Journal of the Society of Materials Science, Japan, 2024, 73, 136-140.  Mechanical behavior of Nikmml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	0.2	O
2892	altimg="si47.svg" display="inline" id="d1e400"> <mml:msub><mml:mrow></mml:mrow><mml:mrow></mml:mrow><mml:miow></mml:miow></mml:msub> Ti <mml:math xxlmml:mi=""></mml:math> Ti <mml:math altimg="si7.svg" display="inline" id="d1e408" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow< td=""><td>1.9</td><td>0</td></mml:mrow<></mml:msub></mml:math>	1.9	0
2893	/> <mml:mrow><mml:mn>100</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi>x</mml:mrow> Bidispersity Improves the Toughness and Impact Resistance of Star-Polymer Thin Films. ACS Macro Letters, 2024, 13, 302-307.	ıb>4.8	math> O
2894	Sampling-free computation of finite temperature material properties in isochoric and isobaric ensembles using the mean-field anharmonic bond model. Physical Review B, 2024, 109, .	3.2	0
2895	Adsorption variations on the Ni $(111)$ surface: electron density diversity from oxygen-containing functional groups. Molecular Systems Design and Engineering, 2024, 9, 477-489.	3.4	0
2896	Complex phase diagram and supercritical matter. Physical Review E, 2024, 109, .	2.1	0
2897	Mixed Stochastic-Deterministic Approach for Many-Body Perturbation Theory Calculations. Physical Review Letters, 2024, 132, .	7.8	0
2898	Ligand-induced incompatible curvatures control ultrathin nanoplatelet polymorphism and chirality. Proceedings of the National Academy of Sciences of the United States of America, 2024, 121, .	7.1	0
2899	Competition between lanes and transient jammed clusters in driven binary mixtures. Physical Review E, $2024, 109, .$	2.1	0
2900	Cold-welded joint characteristics of gold nanowires via atomistic simulation. Materials Today Communications, 2024, 38, 108446.	1.9	0
2901	Challenges in molecular dynamics simulations of heat exchange statistics. Journal of Chemical Physics, 2024, 160, .	3.0	0
2902	Electric-field-aligned liquid crystal polymer for doubling anisotropic thermal conductivity. Communications Materials, 2024, 5, .	6.9	0
2903	Stability Criterion for Electrodeposition in Solid-State Batteries with Metallic Anodes. , 2024, 3, .		0

#	Article	IF	CITATIONS
2904	Cross-Linked Gold Nanoparticle Assemblies: What Can We Learn from Single Flat Interfaces?. Journal of Physical Chemistry C, 2024, 128, 3994-4008.	3.1	0
2905	Interfacial failure in epoxy/CNT nanocomposites from molecular origins: Kinetic concepts, local failure and molecular simulations. Polymer, 2024, 296, 126830.	3.8	0
2906	Tunable Ferroelectric Topological Defects on 2D Topological Surfaces: Complex Strain Engineering Skyrmionâ€Like Polar Structures in 2D Materials. Advanced Functional Materials, 0, , .	14.9	0
2907	Modeling Temperature-Dependent Electron Thermal Diffuse Scattering via Machine-Learned Interatomic Potentials and Path-Integral Molecular Dynamics. Physical Review Letters, 2024, 132, .	7.8	O
2908	Molecular dynamics simulation of the formation of W-centers in silicon by Ga ion irradiation. Physical Review B, 2024, 109, .	3.2	0
2909	Variation of first pop-in loads in nanoindentation to detect chemical short-range ordering in the equiatomic Cr-Co-Ni medium-entropy alloy. Acta Materialia, 2024, 269, 119775.	7.9	0
2910	Simulation and experimental evaluation of laser-induced graphene on the cellulose and lignin substrates. Scientific Reports, 2024, 14, .	3.3	0
2911	Effects of indentation depth and grain size on scratching behavior of nanograin FCC Fe polycrystalline substrate. Tribology International, 2024, 193, 109464.	5.9	0
2912	Investigation of fundamental interactions between rare earth elements and a series of carboxylate ligands to enhance separation performance: An experimental and computational approach. Separation and Purification Technology, 2024, 341, 126867.	7.9	0
2913	Deep Potential Molecular Dynamics Study of Propane Oxidative Dehydrogenation. Journal of Physical Chemistry A, 2024, 128, 1656-1664.	2.5	0
2914	Molecular dynamics study of electro-osmotic flow in a nanochannel with molybdenum disulfide walls. Microfluidics and Nanofluidics, 2024, 28, .	2.2	0
2915	New Insight into Toughness Enhancement in a Lath Martensitic Steel. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2024, 55, 1409-1417.	2.2	0
2916	Huge anharmonic effects in delta plutonium. Physical Review B, 2024, 109, .	3.2	0
2917	Modeling Germanene Monolayer: Interaction Potentials and Insights into the Phonon Thermal Conductivity. Advances in Sustainability Science and Technology, 2024, , 325-335.	0.6	O
2918	Robust training of machine learning interatomic potentials with dimensionality reduction and stratified sampling. Npj Computational Materials, 2024, 10, .	8.7	0
2919	Thermal transports of 2D phosphorous carbides by machine learning molecular dynamics simulations. International Journal of Heat and Mass Transfer, 2024, 224, 125359.	4.8	0
2920	Liquid–Liquid Crossover in Water Model: Local Structure vs Kinetics of Hydrogen Bonds. Journal of Physical Chemistry B, 2024, 128, 2337-2346.	2.6	0
2921	Characterization of iron(III) in aqueous and alkaline environments with $\langle i \rangle$ abÂinitio $\langle i \rangle$ and ReaxFF potentials. Journal of Chemical Physics, 2024, 160, .	3.0	O

#	ARTICLE	IF	CITATIONS
2922	Smoother Surfaces Enhance Diffusion of Nanorods in Entangled Polymer Melts. Macromolecules, 2024, 57, 2482-2489.	4.8	0
2923	Electric field tunable bandgap in twisted double trilayer graphene. Npj 2D Materials and Applications, 2024, 8, .	7.9	0
2924	On data benchmarking and verification of discrete granular simulations. Data in Brief, 2024, 53, 110252.	1.0	0
2925	Application of a multiscale approach for modeling the rheology of complex fluids in industrial mixing equipment. Physics of Fluids, 2024, 36, .	4.0	0
2926	Robust macroscale superlubricity on carbon-coated metallic surfaces. Applied Materials Today, 2024, 37, 102140.	4.3	0
2927	Understanding Self-Assembly and Molecular Packing in Methylcellulose Aqueous Solutions Using Multiscale Modeling and Simulations. Biomacromolecules, 2024, 25, 1682-1695.	5.4	O
2928	Temperature-dependent failure of atomically thin MoTe2. Journal of Molecular Modeling, 2024, 30, .	1.8	0
2929	Construction of macromolecular model of coal based on deep learning algorithm. Energy, 2024, 294, 130856.	8.8	O
2930	Effects of Chemical Short-Range Order and Temperature on Basic Structure Parameters and Stacking Fault Energies in Multi-Principal Element Alloys. Modelling, 2024, 5, 352-366.	1.4	0
2931	New modified embedded-atom method interatomic potential to understand deformation behavior in VNbTaTiZr refractory high entropy alloy. Computational Materials Science, 2024, 237, 112886.	3.0	O
2932	The behavior of 12⟠111⟠© screw dislocations in W–Mo alloys analyzed through atomistic simulations. Journal of Applied Physics, 2024, 135, .	2.5	0
2933	Effect of interlayer slipping on the geometric, thermal and adsorption properties of 2D covalent organic frameworks: a comprehensive review based on computational modelling studies. Physical Chemistry Chemical Physics, 2024, 26, 8577-8603.	2.8	O
2934	Thermal Diffuse Scattering from Nanocrystalline Systems. Crystal Growth and Design, 0, , .	3.0	0
2935	Plastic deformations and strain hardening in fully dense granular crystals. Journal of the Mechanics and Physics of Solids, 2024, 186, 105597.	4.8	O
2936	Thermal boundary conductance in heterogeneous integration between $\hat{l}^2$ -Ga2O3 and semiconductors. Ceramics International, 2024, 50, 18787-18796.	4.8	0
2937	Demixing in Binary Mixtures with Differential Diffusivity at High Density. Physical Review Letters, 2024, 132, .	7.8	0
2938	The Effect of Grain Boundary Facet Junctions on Segregation and Embrittlement. Acta Materialia, 2024, 269, 119805.	7.9	0
2939	Structure and self-diffusivity of mixed-cation electrolytes between neutral and charged graphene sheets. Journal of Chemical Physics, 2024, 160, .	3.0	0

#	Article	IF	CITATIONS
2940	Surface Oxidation of GaN(0001) Simulated by Chargeâ€Transferâ€Type Molecular Dynamics. Physica Status Solidi (B): Basic Research, 0, , .	1.5	0
2941	Molecular driving forces for water adsorption in MOF-808: A comparative analysis with UiO-66. Journal of Chemical Physics, 2024, 160, .	3.0	0
2942	A charge-dependent long-ranged force drives tailored assembly of matter in solution. Nature Nanotechnology, 2024, 19, 485-493.	31.5	0
2943	Copper Nanowires for Electrochemical CO <sub>2</sub> Reduction Reaction. ACS Applied Nano Materials, 0, , .	5.0	0
2944	Understanding relationships between aging induced variation of asphaltene aggregation morphology and asphalt properties through molecular dynamics simulation. Construction and Building Materials, 2024, 420, 135610.	7.2	0
2945	Effects of terraces and steps on the 4H-SiC BPD-TED conversion rate: A reaction pathway analysis. Journal of Applied Physics, 2024, 135, .	2.5	0
2946	Phase transition lowering in shock compressed single-crystal aluminum: Atomistic insights. Physical Review B, 2024, 109, .	3.2	0
2947	Molecular Dynamics on Hf-Nb-Ta-Ti-Zr High Entropy Alloy. , 0, , .		0
2948	Mechanical behavior of graphene quantum dot epoxy nanocomposites: A molecular dynamics study. Materials Letters, 2024, 362, 136206.	2.6	0
2949	Sequence-dependent material properties of biomolecular condensates and their relation to dilute phase conformations. Nature Communications, 2024, $15$ , .	12.8	0
2950	Exploration of the mechanical properties of carbon-incorporated amorphous silica using a universal neural network potential. Journal of Applied Physics, 2024, 135, .	2.5	0
2951	Molecular Insights of Excessive Water Cut during Cyclic Gas Injection in Liquid-Rich Shale Reservoirs: Contributions of Hydrocarbon Condensation and Water Trapping. SPE Journal, 2024, , 1-15.	3.1	0
2952	From Molecular Constraints to Macroscopic Dynamics in Associative Networks Formed by Ionizable Polymers: A Neutron Spin Echo and Molecular Dynamics Simulations Study. ACS Polymers Au, 2024, 4, 149-156.	4.1	0
2953	Machine-learned atomic cluster expansion potentials for fast and quantum-accurate thermal simulations of wurtzite AlN. Journal of Applied Physics, 2024, 135, .	2.5	0
2954	Fluid-mineral Equilibrium Under Nonhydrostatic Stress: Insight From Molecular Dynamics. Numerische Mathematik, 0, 324, .	1.4	0
2955	Programming Interfacial Porosity and Symmetry with Escherized Colloids. Journal of Chemical Theory and Computation, 2024, 20, 2209-2218.	5.3	0
2956	Dislocation descriptors of low and high angle grain boundaries with convolutional neural networks. Extreme Mechanics Letters, 2024, 68, 102138.	4.1	0
2957	Coalescence of sessile aqueous droplets laden with surfactant. Physics of Fluids, 2024, 36, .	4.0	0

#	Article	IF	CITATIONS
2958	Integrating uncertainty into deep learning models for enhanced prediction of nanocomposite materials $\hat{a} \in \mathbb{T}^{M}$ mechanical properties. , 2024, 2, .		0
2959	Unveiling the importance of surface ionization on desalination and ion-sieving performance of graphene oxide membranes. Separation and Purification Technology, 2024, 341, 126930.	7.9	0
2960	Machine learning accelerated discovery of corrosion-resistant high-entropy alloys. Computational Materials Science, 2024, 237, 112925.	3.0	0
2961	Modelling atomic and nanoscale structure in the silicon–oxygen system through active machine learning. Nature Communications, 2024, 15, .	12.8	0
2962	Molecular dynamics simulation of microstructural evolution and mechanical behavior of titanium alloy subjected to laser shock peening. Optics and Laser Technology, 2024, 175, 110748.	4.6	0
2963	Role of Cationic Organization on Water Dynamics in Saponite Clays. Journal of Physical Chemistry C, 2024, 128, 4233-4244.	3.1	0
2964	Self-Similar Velocity Profiles in Granular Flow in a Silo with Two Asymmetrically Located Exits. Lecture Notes in Mechanical Engineering, 2024, , 419-424.	0.4	0
2965	The first-principles study on electrochemical performance, mechanical properties, and lithium-ion migration of LiFePO4 modified by doping with Co and Nb. Journal of Solid State Electrochemistry, 0, , .	2.5	0
2966	Enabling an Inorganic-Rich Interface via Cationic Surfactant for High-Performance Lithium Metal Batteries. Nano-Micro Letters, 2024, 16, .	27.0	0
2967	The Effect of Polymerization Degree of Hydrate Inhibitor on Hydrate Formation: Molecular Dynamics Simulations and Experiments. Springer Series in Geomechanics and Geoengineering, 2024, , 265-275.	0.1	0
2968	Exploring the Strain-Enhanced Li-lon Migration in Li <sub>1.33</sub> Al <sub>0.33</sub> Ti <sub>1.67</sub> (PO <sub>4</sub> ) <sub>3</sub> Solid Electrolyte., 2024, 6, 1224-1230.		0
2969	Hugoniot measurements of the 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) formulation T2 up to 70 GPa. Journal of Applied Physics, 2024, 135, .	2.5	0
2970	Electronic and Charge Properties of Titanium 2 and 4 nm Nanoclusters. Physics of Atomic Nuclei, 2023, 86, 2352-2356.	0.4	0
2971	Structure and thermal conductivity of high-pressure-treated silica glass. A molecular dynamics study. Journal of Applied Physics, 2024, 135, .	2.5	0
2972	Thermoelastic properties of bridgmanite using deep-potential molecular dynamics. Physical Review B, 2024, 109, .	3.2	0
2973	Adaptive patch grid strategy for parallel protein folding using atomic burials with NAMD. Journal of Parallel and Distributed Computing, 2024, 189, 104868.	4.1	0
2974	Lithium magnesium silicate nanoparticles with unique cation acceleration channels as Li-ion rectifiers for stabilizing Li metal batteries. Energy Storage Materials, 2024, 67, 103323.	18.0	0
2975	How Do Deep Eutectic Solvents Form Porous Liquids? The Example of Methyltriphenylphosphonium Bromide: Glycerol and ZIF-8. Journal of Physical Chemistry B, 2024, 128, 2481-2489.	2.6	0

#	Article	IF	CITATIONS
2976	Comment on â€~Pseudo hard-sphere viscosities from equilibrium molecular dynamics'. Journal of Physics Condensed Matter, 2024, 36, 228001.	1.8	0
2977	Selective Vapor Condensation for the Synthesis and Assembly of Spherical Colloids with a Precise Rough Patch. Jacs Au, 2024, 4, 1107-1117.	7.9	0
2978	Multiple phase transitions in shock compressed high-entropy alloy Cr9Mn9Fe64Co9Ni9: Experiments and molecular dynamics simulations. Applied Physics Letters, 2024, 124, .	3.3	0
2979	Tracer dynamics in polymer networks: Generalized Langevin description. Journal of Chemical Physics, 2024, 160, .	3.0	0
2980	Phonon transport across GaAs/Ge heterojunctions by nonequilibrium molecular dynamics. Applied Physics Letters, 2024, 124, .	3.3	0
2981	Thermal Conductivity of MgSiO <sub>3</sub> â€H <sub>2</sub> O System Determined by Machine Learning Potentials. Geophysical Research Letters, 2024, 51, .	4.0	0
2982	A hybrid smoothed-particle hydrodynamics model of oxide skins on molten aluminum. Applied Mathematical Modelling, 2024, 130, 310-326.	4.2	0
2983	Predicting Spin-Dependent Phonon Band Structures of HKUST-1 Using Density Functional Theory and Machine-Learned Interatomic Potentials. International Journal of Molecular Sciences, 2024, 25, 3023.	4.1	0
2984	Effects of Salts on Thickness of Diffused Double Layer around Clay Particles Using Molecular Dynamics. , 2024, , .		0
2985	Searching for low thermal conductivity materials for thermal barrier coatings: A theoretical approach. Physical Review Materials, 2024, 8, .	2.4	0
2986	Force matching and iterative Boltzmann inversion coarse grained force fields for ZIF-8. Journal of Chemical Physics, 2024, 160, .	3.0	0
2987	A mini review of the recent progress in coarse-grained simulation of polymer systems. , 2024, , 100266.		0
2988	Viscoelastic relaxation and topological fluctuations in glass-forming liquids. Journal of Chemical Physics, 2024, 160, .	3.0	0
2989	Hydrogen sorption kinetics and mobility on Li-functionalized polycrystalline carbon nanotube bundles: A molecular dynamics study. Journal of Energy Storage, 2024, 86, 111129.	8.1	0
2990	Model Based on the River Meander Curve for Simulating the Adhesion of Cross-Linked Polymers to Rough Surfaces. Macromolecules, 2024, 57, 3862-3872.	4.8	0
2991	Exploring the frontiers of condensed-phase chemistry with a general reactive machine learning potential. Nature Chemistry, 0, , .	13.6	0
2992	Molecular Simulations of Hydrogen Sorption in Semicrystalline High-Density Polyethylene: The Impact of the Surface Fraction of Tie-Chains. Journal of Physical Chemistry B, 2024, 128, 2799-2810.	2.6	0
2993	Wetting Behavior of Kerogen Surfaces: Insights from Molecular Dynamics. Langmuir, 2024, 40, 5715-5724.	3.5	0

#	Article	IF	CITATIONS
2994	Elucidating the role of water in collagen self-assembly by isotopically modulating collagen hydration. Proceedings of the National Academy of Sciences of the United States of America, 2024, 121, .	7.1	0
2995	New Nonreactive Force Field for Accurate Molecular Dynamics Simulations of TATB at Extreme Conditions. Journal of Chemical & Engineering Data, 2024, 69, 1526-1545.	1.9	O
2996	Theory-based design principles for unprecedentedly high two-level CO2 utilization of CO2-derived metal-organic frameworks. Chemical Engineering Journal, 2024, 486, 150248.	12.7	0
2997	Simulation of Electrochemical Oxidation in Aqueous Environments under Applied Voltage Using Classical Molecular Dynamics. Journal of Physical Chemistry A, 2024, 128, 2236-2244.	2.5	0
2998	Expansion Kinetics of Flexible Polymers upon Release from a Disk-Shaped Confinement. ACS Omega, 2024, 9, 13797-13802.	3.5	0
2999	Area-selective atomic layer deposition on 2D monolayer lateral superlattices. Nature Communications, 2024, $15$ , .	12.8	0
3000	A data-driven method for optimization of classical interatomic potentials. MRS Advances, 0, , .	0.9	0
3001	Pressureâ€driven homogenization of lithium disilicate glasses. Journal of the American Ceramic Society, 0, , .	3.8	0
3002	Investigating the effect of pH on the swelling process, mechanical and thermal attributes of polyacrylamide hydrogel structure: A molecular dynamics study. Case Studies in Thermal Engineering, 2024, 55, 104148.	5.7	0
3003	Roughness Evolution Induced by Third-Body Wear. Tribology Letters, 2024, 72, .	2.6	0
3004	An All-Atom Force Field for Dry and Water-Lubricated Carbon Tribological Interfaces. Journal of Physical Chemistry C, 2024, 128, 4699-4721.	3.1	0
3005	He bubble-induced phase transformation of W grain boundaries revealed by accelerated molecular dynamics. Acta Materialia, 2024, 269, 119821.	7.9	0
3006	Mechanisms of plastic deformation and mechanical strengthening in nano-scale Ti-Ti2Cu eutectoids: A study combined molecular dynamics simulation and experiment. Journal of Materials Science and Technology, 2024, 193, 146-159.	10.7	0
3007	Deviation from the prediction of the Maier-Saupe theory of mixtures of charged discotic Gay-Berne and Lennard-Jones particles. Liquid Crystals, 0, , 1-10.	2.2	0
3008	Compression Eliminates Charge Traps by Stabilizing Perovskite Grain Boundary Structures: An Ab Initio Analysis with Machine Learning Force Field. Chemistry of Materials, 2024, 36, 2898-2906.	6.7	0
3009	Structural Modeling of T9SS Outer Membrane Proteins and Their Complexes. Methods in Molecular Biology, 2024, , 331-344.	0.9	0
3010	Exploring NH3 combustion in environments with CO2 and H2O via reactive molecular dynamics. Journal of the Energy Institute, 2024, 114, 101606.	5.3	0
3011	Diffusion-Limited Crystal Growth of Gallium Nitride Using Active Machine Learning. Crystal Growth and Design, 2024, 24, 2855-2863.	3.0	O

#	Article	IF	CITATIONS
3012	A multiscale study on the microstructure and hardening models of the irradiation defects on reactor pressure vessel steels: Modelling and experiment. Journal of Materials Research and Technology, 2024, 30, 520-531.	5.8	0
3013	Structural Coarse-Graining via Multiobjective Optimization with Differentiable Simulation. Journal of Chemical Theory and Computation, 2024, 20, 2605-2617.	5.3	0
3014	Modelling infrared spectra of the O-H stretches in liquid H <sub>2</sub> O based on a deep learning potential, the importance of nuclear quantum effects. Molecular Simulation, 2024, 50, 539-546.	2.0	0
3015	Molecular dynamics simulations of the effect of porosity on heat transfer in Li2TiO3. Fusion Engineering and Design, 2024, 202, 114344.	1.9	0
3016	A multiscale modeling framework for predicting strainâ€dependent electrical conductivity of carbon nanotubeâ€incorporated nanocomposites considering the electron tunneling effect. Polymer Composites, 0, , .	4.6	0
3017	Structural transformations driven by local disorder at interfaces. Physical Review Materials, 2024, 8,	2.4	O
3018	The feasibility of hydrogen storage in aquifers: A molecular dynamics simulation. Fuel, 2024, 367, 131469.	6.4	0
3019	Extraction of Mechanical Parameters via Molecular Dynamics Simulation: Application to Polyimides. Polymers, 2024, 16, 813.	4.5	0
3020	Towards atomistic modelling of solid Pb-O formation and dissolution in liquid lead coolant: Interatomic potential development. Journal of Nuclear Materials, 2024, 594, 155016.	2.7	0
3021	Highly stretchable graphene kirigami with tunable mechanical properties. Physical Review E, 2024, 109, .	2.1	0
3022	Potential energy landscape of a coarse grained model for water: ML-BOP. Journal of Chemical Physics, 2024, 160, .	3.0	0
3023	Formation of Polymer-like Nanochains with Short Lithium–Lithium Distances in a Water-in-Salt Electrolyte. Journal of the American Chemical Society, 2024, 146, 8142-8148.	13.7	0
3024	The synergetic effect of He and Kr irradiation on helium bubble evolution in SiC/SiC composite: Combining in-situ TEM observation with MD simulation. Journal of Materials Science and Technology, 2024, 197, 238-246.	10.7	0
3025	Insights into PFAS environmental fate through computational chemistry: A review. Science of the Total Environment, 2024, 926, 171738.	8.0	O
3026	Molecular dynamics to model carbon infiltration into a porous silicon matrix: An experimental and computational approach. Computational Materials Science, 2024, 238, 112949.	3.0	0
3028	Ab initio potential energy surfaces calculation via restricted Hartree–Fock for molecular dynamics simulation: a comprehensive review. Journal of the Korean Physical Society, 2024, 84, 550-565.	0.7	0
3029	The role of chemical functional groups in dewaterability of hydrochar: A molecular simulation study. Journal of Molecular Liquids, 2024, 400, 124482.	4.9	0
3030	Study on the ablative characteristics of steel target irradiated by nanosecond pulsed pseudo spark electron beams: Experiment and molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2024, 550, 165314.	1.4	O

#	Article	IF	Citations
3031	Probing the state of hydrogen in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi><math>\hat{i}</math></mml:mi><mml:mtext><math>\hat{a}</math></mml:mtext><mm .<="" 2024,="" 6,="" at="" conditions="" learning="" machine="" mantle="" physical="" potential.="" research,="" review="" td="" with=""><td>OOlAxim:</td><td>H<i>q</i>mml:mi&gt;</td></mm></mml:math>	OOlAxim:	H <i>q</i> mml:mi>
3032	Atomistic Simulation of the Effect of H-Phase Precipitate on the Transformation Temperatures and Stress-Induced Phase Transformation in Ni-Rich NiTiHf. Shape Memory and Superelasticity, 0, , .	2.2	0
3033	Structural basis for the preservation of a subset of topologically associating domains in interphase chromosomes upon cohesin depletion. ELife, $0,12,.$	6.0	0
3034	Micromechanical Dilution of PLA/PETG–Glass/Iron Nanocomposites: A More Efficient Molecular Dynamics Approach. ACS Omega, 2024, 9, 14887-14898.	3.5	O
3035	Robust wear performance of graphene-reinforced high entropy alloy composites. Carbon, 2024, 224, 119040.	10.3	0
3036	Studies of Ni-Cr complexation in FLiBe molten salt using machine learning interatomic potentials. Journal of Molecular Liquids, 2024, 400, 124521.	4.9	0
3037	Non-equilibrium nature of fracture determines the crack paths. Extreme Mechanics Letters, 2024, 68, 102151.	4.1	0
3038	Enhanced Sampling of Crystal Nucleation with Graph Representation Learnt Variables. Journal of Physical Chemistry B, 2024, 128, 3037-3045.	2.6	0
3039	A molecular dynamics study on the size effects of Fe <sub>3</sub> O <sub>4</sub> nanoparticles on the mechanical characteristics of polypyrrole/Fe <sub>3</sub> O <sub>4</sub> nanocomposite. Molecular Simulation, 2024, 50, 493-505.	2.0	0
3040	Investigation of Tribological Behavior and Lubrication Mechanisms of Zinc Oxide under Poly α-olefin Lubrication Enhanced by the Electric Field. Langmuir, 2024, 40, 6741-6749.	3.5	0
3041	Impact of Atomic Defects on Ceria Surfaces on Chemical Mechanical Polishing of Silica Glass Surfaces. Langmuir, 2024, 40, 6773-6785.	3.5	0
3042	Comparing machine learning potentials for water: Kernel-based regression and Behler–Parrinello neural networks. Journal of Chemical Physics, 2024, 160, .	3.0	0
3044	Molecular Simulations Revealing Effects of Non-concatenated Ring Topology on Phase Behavior of Symmetric Diblock Copolymers. Macromolecules, 0, , .	4.8	0
3045	Numerical Modelling and Imaging of Industrial-Scale Particulate Systems: A Review of Contemporary Challenges and Solutions. KONA Powder and Particle Journal, 2024, , .	1.7	0
3046	Modeling membrane formation. , 2024, , 345-394.		0
3047	Thermodynamic driving forces in contact electrification between polymeric materials. Nature Communications, 2024, 15, .	12.8	O
3048	Effects of high temperature and high humidity on the reliability of copper/epoxy bond. Applied Surface Science, 2024, 660, 159970.	6.1	0
3049	Molecular Dynamics simulations and discrete perturbation theory for systems interacting via the parabolic-well pair potential. Journal of Molecular Liquids, 2024, 400, 124522.	4.9	O

#	Article	IF	CITATIONS
3050	Water–Hydrocarbon Interactions in Anionic Pyrene Monohydrate. Journal of Physical Chemistry B, 2024, 128, 3200-3210.	2.6	0
3051	The lattice thermal conductivity of hafnia: The influence of high-order scatterings and phonon coherence. Journal of Applied Physics, 2024, 135, .	2.5	0
3052	Influence of grain size on α′ Cr precipitation in an isothermally aged Fe-21Cr-5Al alloy. Materialia, 2024, 34, 102047.	2.7	0
3054	Machine Learning Enabled Potential for (BA)2(MA)(nâ°1)Pbnl3n+1 2D Ruddlesden–Popper Perovskite Materials. Multiscale Science and Engineering, 0, , .	1.7	0
3055	Photo-activated dynamic isomerization induced large density changes in liquid crystal polymers: A molecular dynamics study. Journal of Chemical Physics, 2024, 160, .	3.0	0
3056	Multi-scale modeling of decohesion characteristics of second phase particles from the matrix in uniaxial tension in a high strength aluminum alloy. Engineering Fracture Mechanics, 2024, 301, 110013.	4.3	0
3057	Dynamic Copper Site Redispersion through Atom Trapping in Zeolite Defects. Journal of the American Chemical Society, 2024, 146, 8280-8297.	13.7	0
3058	Explosions of nanodroplets studied with molecular dynamics simulations. Physics of Fluids, 2024, 36, .	4.0	0
3059	Mechanistic Insights into Surfactant-Modulated Electrode–Electrolyte Interface for Steering H <sub>2</sub> O <sub>2</sub> Electrosynthesis. Journal of the American Chemical Society, 2024, 146, 7575-7583.	13.7	0
3060	Investigation on the Effect of the Self-generated Metal Vapour on the Cathode Spot Formation in Vacuum Arc by Molecular Dynamics Simulation. Lecture Notes in Electrical Engineering, 2024, , 248-255.	0.4	0
3061	Development of multi-scale computational frameworks to solve fusion materials science challenges. Journal of Nuclear Materials, 2024, 594, 155011.	2.7	0
3062	Deformation behavior of SmCo compounds via amorphization and recrystallization. Journal of Rare Earths, 2024, , .	4.8	0
3063	Shock Hugoniot Calculations of Newly Designed Thermoplastic Elastomers and Comparison with Classical Binder Estane. Journal of Physical Chemistry B, 2024, 128, 2831-2840.	2.6	0
3064	Enhanced phonon transport in sI-type methane hydrate under uniaxial compression strain: Unveiling the opening of an advantageous channel. International Journal of Heat and Mass Transfer, 2024, 225, 125399.	4.8	0
3065	Investigating the stability mechanisms of single bulk Nanobubbles: A molecular dynamics perspective. International Journal of Heat and Mass Transfer, 2024, 225, 125407.	4.8	0
3066	Effect of sand particle shape on micromechanical modeling in direct shear testing. Computers and Geotechnics, 2024, 169, 106222.	4.7	0
3067	Predicting hydrogen segregation energy distributions in strained regions of tungsten using artificial neural network. Nuclear Materials and Energy, 2024, 39, 101637.	1.3	0
3068	Direct observation of strong momentum-dependent electron-phonon coupling in a metal. Science Advances, 2024, 10, .	10.3	0

#	Article	IF	CITATIONS
3069	Triggered contraction of self-assembled micron-scale DNA nanotube rings. Nature Communications, $2024,15,$	12.8	0
3070	Maximum Entropy Theory of Multiscale Coarse-Graining via Matching Thermodynamic Forces: Application to a Molecular Crystal (TATB). Journal of Physical Chemistry B, 2024, 128, 2955-2971.	2.6	O
3071	Role of the Carbon Nanotube Junction in the Mechanical Performance of Carbon Nanotube/Polyethylene Nanocomposites: A Molecular Dynamics Study. Nanomaterials, 2024, 14, 520.	4.1	0
3072	Hydrogen adsorption and diffusion behavior in kaolinite slit for underground hydrogen storage: A hybrid GCMC-MD simulation study. Chemical Engineering Journal, 2024, 487, 150517.	12.7	O
3073	Equivariant graph neural network interatomic potential for Green-Kubo thermal conductivity in phase change materials. Physical Review Materials, 2024, 8, .	2.4	0
3074	Atomic-scale simulation of ultrasonic vibration-assisted polishing process for graphene/GaN-layered composites. Materials Science in Semiconductor Processing, 2024, 176, 108323.	4.0	O
3075	Enhancing the Output Performance of Triboelectric Nanogenerator Through Regulation of its Internal Nanoâ€Architecture. Small, 0, , .	10.0	0
3076	Adaptive Force Field Parameter Optimization for Expanding Reaction Simulations within Wide-Ranged Temperature. Journal of Physical Chemistry A, 2024, 128, 2487-2497.	2.5	O
3077	Combinatorial and high-throughput investigation of growth nanotwin formation. Acta Materialia, 2024, 270, 119839.	7.9	0
3078	Mechanism of enhanced thermal conductivity of hybrid nanofluids by adjusting mixing ratio of nanoparticles. Journal of Molecular Liquids, 2024, 400, 124518.	4.9	O
3080	Single-molecule analysis of solvent-responsive mechanically interlocked ring polymers and the effects of nanoconfinement from coarse-grained simulations. Journal of Chemical Physics, 2024, 160, .	3.0	0
3081	The Flux Operator. F1000Research, 0, 13, 203.	1.6	O
3082	On the thermal properties of pure and defective $\hat{\Gamma}$ -graphene nanotubes by molecular dynamics simulations. Journal of Mathematical Chemistry, 2024, 62, 1209-1221.	1.5	0
3083	Heat and mass transfer of molten carbonates at charged electrode interface and its anisotropic behavior: A molecular dynamics study. Journal of Molecular Liquids, 2024, 400, 124539.	4.9	O
3084	CRESTâ€"A program for the exploration of low-energy molecular chemical space. Journal of Chemical Physics, 2024, 160, .	3.0	0
3085	Molecular rheology of nanoconfined oligomer melts. Journal of Rheology, 2024, 68, 285-299.	2.6	O
3086	Valency of Ligand–Receptor Binding from Pair Potentials. Journal of Chemical Theory and Computation, 2024, 20, 2901-2907.	5 <b>.</b> 3	0
3088	Homogeneous water vapor condensation with a deep neural network potential model. Journal of Chemical Physics, 2024, $160$ , .	3.0	O

#	Article	IF	CITATIONS
3089	Improving the mechanical properties of Cantor-like alloys with Bayesian optimization. , 2024, 2, .		0
3090	Effect of Strain Rate, Temperature, Vacancy, and Microcracks on Mechanical Properties of 8-16-4 Graphyne. Nanomaterials, 2024, 14, 556.	4.1	0
3091	Molecular Dynamics Study on the Mechanism of Improved Tribological Properties of Nano-ZnO with Decanol Lubrication. Tribology Letters, 2024, 72, .	2.6	0
3092	Calculation of the Neutronic Characteristics of a HTGR for the Verification of the MCU-HTR Software Package. Physics of Atomic Nuclei, 2023, 86, 1827-1837.	0.4	0
3093	Dynamic Nanoindentation and Short-Range Order in Equiatomic NiCoCr Medium-Entropy Alloy Lead to Novel Density Wave Ordering. Physical Review Letters, 2024, 132, .	7.8	0
3094	Inverse design of metal–organic frameworks for direct air capture of CO <sub>2</sub> <i>via</i> deep reinforcement learning., 2024, 3, 728-741.		0
3095	Investigation of the behavior of water and oil droplets on nanostructured surfaces: a molecular dynamics simulation study. Journal of Mechanical Science and Technology, 2024, 38, 1249-1257.	1.5	0
3096	ASCOT: A web tool for the digital construction of energy minimized Ag, CuO, TiO2 spherical nanoparticles and calculation of their atomistic descriptors. Computational and Structural Biotechnology Journal, 2024, 25, 34-46.	4.1	0
3097	Impact of crystalline domains on longâ€term stability and mechanical performance of anisotropic silk fibroin sponges. Journal of Biomedical Materials Research - Part A, O, , .	4.0	0
3098	Proposing TODD-graphene as a novel porous 2D carbon allotrope designed for superior lithium-ion battery efficiency. Scientific Reports, 2024, 14, .	3.3	0
3099	Role of methane in ammonia combustion in air: From microscale to macroscale. Fuel Processing Technology, 2024, 256, 108075.	7.2	0
3100	Type Label Framework for Bonded Force Fields in LAMMPS. Journal of Physical Chemistry B, 2024, 128, 3282-3297.	2.6	0
3101	Synergistic effects of temperature and strain rate on tensile properties of simulated Ni-6Cu alloy with $\hat{1}$ £3 non-Arrhenius grain boundary. Molecular Simulation, 2024, 50, 547-559.	2.0	0
3102	Influence of H <sub>2</sub> O and O <sub>2</sub> on the Homogeneous Conversion of Toluene and the Underlying Reaction Mechanisms. Industrial & Engineering Chemistry Research, 2024, 63, 5678-5688.	3.7	0
3103	Mechanical response of monolayer graphene via a multi-probe approach. International Journal of Mechanical Sciences, 2024, 273, 109208.	6.7	0
3104	Enhancing the Quality and Reliability of Machine Learning Interatomic Potentials through Better Reporting Practices. Journal of Physical Chemistry C, 2024, 128, 6524-6537.	3.1	0
3105	New method of molecular modeling of liquid transport coefficients. Thermophysics and Aeromechanics, 2023, 30, 1021-1030.	0.5	0