Qing Peng

List of Publications by Year in descending order

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245 papers	6,596 citations	81900 39 h-index	95266 68 g-index
245 all docs	245 docs citations	245 times ranked	7699 citing authors

#	Article	IF	Citations
1	Mechanical properties of the hexagonal boron nitride monolayer: Ab initio study. Computational Materials Science, 2012, 56, 11-17.	3.0	349
2	New materials graphyne, graphdiyne, graphone, and graphane: review of properties, synthesis, and application in nanotechnology. Nanotechnology, Science and Applications, 2014, 7, 1.	4.6	241
3	Outstanding mechanical properties of monolayer MoS2 and its application in elastic energy storage. Physical Chemistry Chemical Physics, 2013, 15, 19427.	2.8	235
4	Mechanical properties of graphyne monolayers: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 13385.	2.8	222
5	Artificial intelligence: A powerful paradigm for scientific research. Innovation(China), 2021, 2, 100179.	9.1	200
6	Hydrogen Evolution Reaction on Hybrid Catalysts of Vertical MoS₂ Nanosheets and Hydrogenated Graphene. ACS Catalysis, 2018, 8, 1828-1836.	11.2	180
7	Mechanical stabilities of silicene. RSC Advances, 2013, 3, 13772.	3.6	161
8	Injectable and biodegradable thermosensitive hydrogels loaded with PHBHHx nanoparticles for the sustained and controlled release of insulin. Acta Biomaterialia, 2013, 9, 5063-5069.	8.3	126
9	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO₂ Reduction. Angewandte Chemie - International Edition, 2018, 57, 12675-12679.	13.8	108
10	Shockwave generates < 100 > dislocation loops in bcc iron. Nature Communications, 2018, 9, 4880.	12.8	106
11	A theoretical analysis of the effect of the hydrogenation of graphene to graphane on its mechanical properties. Physical Chemistry Chemical Physics, 2013, 15, 2003-2011.	2.8	105
12	When Density Functional Approximations Meet Iron Oxides. Journal of Chemical Theory and Computation, 2016, 12, 5132-5144.	5.3	102
13	Determinants of per- and polyfluoroalkyl substances (PFAS) in midlife women: Evidence of racial/ethnic and geographic differences in PFAS exposure. Environmental Research, 2019, 175, 186-199.	7.5	102
14	MÃ¶ssbauer Spectroscopy of Iron Carbides: From Prediction to Experimental Confirmation. Scientific Reports, 2016, 6, 26184.	3.3	82
15	A first-principles study of the mechanical properties of g-GeC. Mechanics of Materials, 2013, 64, 135-141.	3.2	81
16	In situ tuning of electronic structure of catalysts using controllable hydrogen spillover for enhanced selectivity. Nature Communications, 2020, 11, 4773.	12.8	81
17	Mechanical properties of g-GaN: a first principles study. Applied Physics A: Materials Science and Processing, 2013, 113, 483-490.	2.3	80
18	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers via biaxial straining. Nanoscale, 2019, 11, 2335-2342.	5.6	80

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19	Elastic properties of hybrid graphene/boron nitride monolayer. Acta Mechanica, 2012, 223, 2591-2596.	2.1	77
20	A Review of Current Development of Graphene Mechanics. Crystals, 2018, 8, 357.	2.2	68
21	Machine learning reveals the importance of the formation enthalpy and atom-size difference in forming phases of high entropy alloys. Materials and Design, 2020, 193, 108835.	7.0	68
22	Tunable band gaps of mono-layer hexagonal BNC heterostructures. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1662-1666.	2.7	67
23	Cadmium and Alzheimerâ€™s disease mortality in U.S. adults: Updated evidence with a urinary biomarker and extended follow-up time. Environmental Research, 2017, 157, 44-51.	7.5	67
24	Mechanical stabilities and properties of graphene-like aluminum nitride predicted from first-principles calculations. RSC Advances, 2013, 3, 7083.	3.6	64
25	A theoretical prediction of super high-performance thermoelectric materials based on MoS2/WS2 hybrid nanoribbons. Scientific Reports, 2016, 6, 21639.	3.3	64
26	A first principles investigation of the mechanical properties of g-ZnO: The graphene-like hexagonal zinc oxide monolayer. Computational Materials Science, 2013, 68, 320-324.	3.0	63
27	A highly efficient, stable, durable, and recyclable filter fabricated by femtosecond laser drilling of a titanium foil for oil-water separation. Scientific Reports, 2016, 6, 37591.	3.3	58
28	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. ACS Catalysis, 2018, 8, 3365-3375.	11.2	58
29	Resolving a Decade-Long Question of Oxygen Defects in Raman Spectra of Ceria-Based Catalysts at Atomic Level. Journal of Physical Chemistry C, 2019, 123, 18889-18894.	3.1	53
30	A Physical Interaction Between the Adaptor Proteins DOK3 and DAP12 Is Required to Inhibit Lipopolysaccharide Signaling in Macrophages. Science Signaling, 2013, 6, ra72.	3.6	49
31	Mechanical properties and stabilities of g-ZnS monolayers. RSC Advances, 2015, 5, 11240-11247.	3.6	49
32	The normal-auxeticity mechanical phase transition in graphene. 2D Materials, 2017, 4, 021020.	4.4	49
33	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. Materials Research Letters, 2018, 6, 584-591.	8.7	46
34	Recent Progress on Irradiation-Induced Defect Engineering of Two-Dimensional 2H-MoS2 Few Layers. Applied Sciences (Switzerland), 2019, 9, 678.	2.5	46
35	Distinct point defect behaviours in body-centered cubic medium-entropy alloy NbZrTi induced by severe lattice distortion. Acta Materialia, 2022, 229, 117806.	7.9	44
36	Stability of self-interstitial atoms in hcp-Zr. Journal of Nuclear Materials, 2012, 429, 233-236.	2.7	43

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37	First-principles study of the effects of mechanical strains on the radiation hardness of hexagonal boron nitride monolayers. Nanoscale, 2013, 5, 695-703.	5.6	43
38	Structures, Mechanical Properties, Equations of State, and Electronic Properties of Î²-HMX under Hydrostatic Pressures: A DFT-D2 study. Physical Chemistry Chemical Physics, 2014, 16, 19972-83.	2.8	42
39	Molecular dynamics simulations of scratching characteristics in vibration-assisted nano-scratch of single-crystal silicon. Applied Surface Science, 2021, 551, 149451.	6.1	42
40	Mechanical properties and instabilities of ordered graphene oxide C6O monolayers. RSC Advances, 2013, 3, 24337.	3.6	38
41	Elastic limit of silicane. Nanoscale, 2014, 6, 12071-12079.	5.6	38
42	Effect of Molybdenum Additives on Corrosion Behavior of (CoCrFeNi)100â^'xMox High-Entropy Alloys. Entropy, 2018, 20, 908.	2.2	38
43	Magic auxeticity angle of graphene. Carbon, 2019, 149, 350-354.	10.3	38
44	Mechanical properties and stabilities of Î±-boron monolayers. Physical Chemistry Chemical Physics, 2015, 17, 2160-2168.	2.8	37
45	Distinctive nanofriction of graphene coated copper foil. Computational Materials Science, 2016, 117, 406-411.	3.0	37
46	Origin of pyroelectricity in LiNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	3.2	36
47	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. ACS Catalysis, 2019, 9, 2768-2776.	11.2	36
48	DEFECT ENGINEERING OF 2D MONATOMIC-LAYER MATERIALS. Modern Physics Letters B, 2013, 27, 1330017.	1.9	35
49	Stacking-Mode-Induced Reactivity Enhancement for Twisted Bilayer Graphene. Chemistry of Materials, 2016, 28, 1034-1039.	6.7	35
50	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. Journal of Nuclear Materials, 2018, 509, 237-244.	2.7	34
51	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO₂ Reduction. Angewandte Chemie, 2018, 130, 12857-12861.	2.0	34
52	Theoretical Perspectives on the Modulation of Carbon on Transition-Metal Catalysts for Conversion of Carbon-Containing Resources. ACS Catalysis, 2021, 11, 2156-2181.	11.2	34
53	Quantum simulation of materials at micron scales and beyond. Physical Review B, 2008, 78, .	3.2	33
54	Urinary arsenic and insulin resistance in US adolescents. International Journal of Hygiene and Environmental Health, 2015, 218, 407-413.	4.3	33

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55	Theoretical and experimental investigations of nanosecond 177.3Ânm deep-ultraviolet light by second harmonic generation inÂKBBF. Applied Physics B: Lasers and Optics, 2009, 96, 415-422.	2.2	32
56	Chemically Tuning Mechanics of Graphene by BN. Advanced Engineering Materials, 2013, 15, 718-727.	3.5	32
57	A Density Functional Theory Study of the Mechanical Properties of Graphane With van der Waals Corrections. Mechanics of Advanced Materials and Structures, 2015, 22, 717-721.	2.6	32
58	Fabrication and application of 2,4,6-trinitrophenol sensors based on fluorescent functional materials. Journal of Hazardous Materials, 2022, 425, 127987.	12.4	32
59	Processing and machining mechanism of ultrasonic vibration-assisted grinding on sapphire. Materials Science in Semiconductor Processing, 2022, 142, 106470.	4.0	31
60	Arsenic exposure is associated with diminished insulin sensitivity in nonâ€diabetic Amish adults. Diabetes/Metabolism Research and Reviews, 2016, 32, 565-571.	4.0	30
61	Giant Thermal Expansion in 2D and 3D Cellular Materials. Advanced Materials, 2018, 30, e1705048.	21.0	30
62	Theoretical exploration of intrinsic facet-dependent CH4 and C2 formation on Fe5C2 particle. Applied Catalysis B: Environmental, 2020, 278, 119308.	20.2	30
63	Mesoporous RhRu Nanosponges with Enhanced Water Dissociation toward Efficient Alkaline Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 5052-5060.	8.0	30
64	Predicting Elastic Properties of Î²-HMX from First-Principles Calculations. Journal of Physical Chemistry B, 2015, 119, 5896-5903.	2.6	29
65	Molybdenum Carbide Nanocatalysts at Work in the in Situ Environment: A Density Functional Tight-Binding and Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2015, 137, 4249-4259.	13.7	28
66	Grain Boundary Plays a Key Role in Carbon Diffusion in Carbon Irons Revealed by a ReaxFF Study. Journal of Physical Chemistry C, 2018, 122, 23191-23199.	3.1	28
67	Quantum mechanical modeling of hydrogen assisted cracking in aluminum. Physical Review B, 2013, 88, .	3.2	27
68	Product Distribution Control for Glucosamine Condensation: Nuclear Magnetic Resonance (NMR) Investigation Substantiated by Density Functional Calculations. Industrial & Engineering Chemistry Research, 2017, 56, 2925-2934.	3.7	27
69	Theoretical prediction of a graphene-like structure of indium nitride: A promising excellent material for optoelectronics. Applied Materials Today, 2017, 7, 169-178.	4.3	27
70	Self-healing mechanism of irradiation defects in nickelâ€“graphene nanocomposite: An energetic and kinetic perspective. Journal of Alloys and Compounds, 2018, 765, 253-263.	5.5	27
71	Adsorption of Hexacyclic C₆H₆, C₆H₈, C₆H₁₀, and C₆H₁₂ on a Mo-Terminated Î±-Mo₂C (0001) Surface. Journal of Physical Chemistry C, 2013, 117, 7069-7080.	3.1	26
72	A first-principles study of the structural, mechanical and electronic properties of precipitates of Al₂Cu in Alâ€“Cu alloys. Physical Chemistry Chemical Physics, 2018, 20, 967-976.	2.8	26

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73	Mechanical degradation of graphene by epoxidation: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 19484-19490.	2.8	25
74	Insight into the Nanoparticle Growth in Supported Ni Catalysts during the Early Stage of CO Hydrogenation Reaction: The Important Role of Adsorbed CO Molecules. ACS Catalysis, 2018, 8, 6367-6374.	11.2	25
75	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. Journal of Nuclear Materials, 2019, 524, 60-66.	2.7	25
76	Mechanism of Graphene Formation via Detonation Synthesis: AÂDFTB Nanoreactor Approach. Journal of Chemical Theory and Computation, 2019, 15, 3654-3665.	5.3	25
77	Temperature dependence of Raman spectra of graphene on copper foil substrate. Journal of Materials Science: Materials in Electronics, 2016, 27, 3888-3893.	2.2	24
78	An experimental study on the interdiffusion behaviors and mechanical properties of Ni-Zr system. Journal of Alloys and Compounds, 2018, 752, 412-419.	5.5	24
79	Interaction of Edge Dislocations with Graphene Nanosheets in Graphene/Fe Composites. Crystals, 2018, 8, 160.	2.2	24
80	Phonon transport in single-layer boron nanoribbons. Nanotechnology, 2016, 27, 445703.	2.6	23
81	Pressure-induced insulator-to-metal transitions for enhancing thermoelectric power factor in bismuth telluride-based alloys. Physical Chemistry Chemical Physics, 2017, 19, 12784-12793.	2.8	23
82	Time-dependent potential-functional embedding theory. Journal of Chemical Physics, 2014, 140, 124113.	3.0	22
83	Thermal transport in MoS₂/Graphene hybrid nanosheets. Nanotechnology, 2015, 26, 375402.	2.6	22
84	Very high thermoelectric figure of merit found in hybrid transition-metal-dichalcogenides. Journal of Applied Physics, 2016, 120, .	2.5	22
85	Van der Waals Density Functional Theory vdW-DFq for Semihard Materials. Crystals, 2019, 9, 243.	2.2	22
86	A 200ÂW diode-side-pumped CW 2ÂÎ¼m Tm:YAG laser with water cooling at 8Â°C. Applied Physics B: Lasers and Optics, 2011, 103, 83-88.	2.2	21
87	Mechanical Properties of Vacancy Tuned Carbon Honeycomb. Nanomaterials, 2019, 9, 156.	4.1	21
88	Tensile mechanical properties of CoCrFeNiTiAl high entropy alloy via molecular dynamics simulations. Intermetallics, 2022, 142, 107444.	3.9	21
89	Coupling of double grains enforces the grinding process in vibration-assisted scratch: Insights from molecular dynamics. Journal of Materials Processing Technology, 2022, 304, 117551.	6.3	21
90	Insight into the structure and energy of Mo₂₇S_xO_yclusters. RSC Advances, 2017, 7, 9513-9520.	3.6	20

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91	A Molecular Dynamics Study of the Mechanical Properties of Twisted Bilayer Graphene. Micromachines, 2018, 9, 440.	2.9	20
92	Proton irradiation of graphene: insights from atomistic modeling. Nanoscale, 2019, 11, 20754-20765.	5.6	20
93	Reduction of dislocation, mean free path, and migration barriers using high entropy alloy: insights from the atomistic study of irradiation damage of CoNiCrFeMn. Nanotechnology, 2020, 31, 425701.	2.6	20
94	High-efficiency high-power QCW diode-side-pumped zigzag Nd:YAG ceramic slab laser. Applied Physics B: Lasers and Optics, 2013, 111, 111-116.	2.2	19
95	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischerâ€“Tropsch Synthesis. Catalysis Letters, 2019, 149, 645-664.	2.6	19
96	The structureâ€“activity relationship of Fe nanoparticles in CO adsorption and dissociation by reactive molecular dynamics simulations. Journal of Catalysis, 2019, 374, 150-160.	6.2	19
97	Effect of Angle, Temperature and Vacancy Defects on Mechanical Properties of PSI-Graphene. Crystals, 2019, 9, 238.	2.2	19
98	Visiting CH4 formation and C1â€¯+â€¯C1 couplings to tune CH4 selectivity on Fe surfaces. Journal of Catalysis, 2019, 372, 217-225.	6.2	19
99	Kadsura-Shaped Covalentâ€“Organic Framework Nanostructures for the Sensitive Detection and Removal of 2,4,6-Trinitrophenol. ACS Applied Nano Materials, 2022, 5, 6422-6429.	5.0	19
100	Pressure effect on stabilities of self-Interstitials in HCP-Zirconium. Scientific Reports, 2014, 4, 5735.	3.3	18
101	Properties of AlN film grown on Si (111). Journal of Crystal Growth, 2016, 435, 76-83.	1.5	18
102	Anisotropic and temperature dependent mechanical properties of carbon honeycomb. Nanotechnology, 2019, 30, 325704.	2.6	18
103	Graphene Surface Reinforcement of Iron. Nanomaterials, 2019, 9, 59.	4.1	18
104	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. Scripta Materialia, 2020, 187, 291-295.	5.2	18
105	Peculiar pressure effect on Poisson ratio of graphone as a strain damper. Nanoscale, 2015, 7, 9975-9979.	5.6	17
106	Atomistic Study of Mechanical Behaviors of Carbon Honeycombs. Nanomaterials, 2019, 9, 109.	4.1	17
107	Atomic Structure and Mechanical Properties of Twisted Bilayer Graphene. Journal of Composites Science, 2019, 3, 2.	3.0	17
108	Density functional study of benzene adsorption on the Î±-Mo2C(0001) surface. Structural Chemistry, 2012, 23, 1459-1466.	2.0	16

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109	Sensitive Five-Fold Local Symmetry to Kinetic Energy of Depositing Atoms in Cu-Zr Thin Film Growth. Materials, 2018, 11, 2548.	2.9	16
110	Hydrostatic pressure-tuning of thermoelectric properties of CsSnI3 perovskite by first-principles calculations. Computational Materials Science, 2022, 201, 110917.	3.0	16
111	Temperature-dependent phonon anharmonicity and thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">CuInTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2022, 105, .	3.2	16
112	Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals. Physical Review B, 2010, 82, .	3.2	15
113	Detailed characteristics of adsorption of bisphenol A by highly hydrophobic MCM-41 mesoporous molecular sieves. Research on Chemical Intermediates, 2016, 42, 7169-7183.	2.7	15
114	Developing ReaxFF to Visit CO Adsorption and Dissociation on Iron Surfaces. Journal of Physical Chemistry C, 2018, 122, 27582-27589.	3.1	15
115	Surface strengthening of stainless steels by nondestructive laser peening. Materials and Design, 2021, 205, 109754.	7.0	15
116	Athermal simulation of plastic deformation in amorphous solids at constant pressure. Journal of Polymer Science, Part B: Polymer Physics, 2004, 42, 2057-2065.	2.1	14
117	A first-principles study of the mechanical properties of AlN with Raman verification. Computational Materials Science, 2016, 112, 342-346.	3.0	14
118	Development of a reactive force field for the Feâ€“C interaction to investigate the carburization of iron. Physical Chemistry Chemical Physics, 2018, 20, 775-783.	2.8	14
119	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. Journal of Nuclear Materials, 2018, 512, 246-251.	2.7	14
120	Highly Efficient Polarized GeS/MoSe₂ van der Waals Heterostructure for Water Splitting from Ultraviolet to Nearâ€Infrared Light. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900582.	2.4	14
121	A combined experiment and first-principles study on lattice dynamics of thermoelectric CuInTe2. Journal of Alloys and Compounds, 2020, 822, 153610.	5.5	14
122	Carbon Deposition and Permeation on Nickel Surfaces in Operando Conditions: A Theoretical Study. Journal of Physical Chemistry C, 2021, 125, 7166-7177.	3.1	14
123	Atomistic insights of a chemical complexity effect on the irradiation resistance of high entropy alloys. Materials Advances, 2022, 3, 1680-1686.	5.4	14
124	High-power diode side-pumped Nd:YAG laser on the low gain three lines near 1.1ÂÎ¼m. Applied Physics B: Lasers and Optics, 2011, 104, 45-52.	2.2	13
125	Stress evolution in AlN and GaN grown on Si(111): experiments and theoretical modeling. Journal of Materials Science: Materials in Electronics, 2016, 27, 2004-2013.	2.2	13
126	Oxygen defects stabilize the crystal structure of MgAl2O4 spinel under irradiation. Journal of Nuclear Materials, 2019, 527, 151830.	2.7	13

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127	From predicting to correlating the bonding properties of iron sulfide phases. Computational Materials Science, 2019, 164, 99-107.	3.0	13
128	Enhanced surface bombardment resistance of the CoNiCrFeMn high entropy alloy under extreme irradiation flux. Nanotechnology, 2020, 31, 025703.	2.6	13
129	Temperature-dependent surface free energy and the Wulff shape of iron and iron carbide nanoparticles: A molecular dynamics study. Applied Surface Science, 2020, 509, 144859.	6.1	13
130	How far away are iron carbide clusters from the bulk?. Physical Chemistry Chemical Physics, 2016, 18, 32944-32951.	2.8	12
131	The Temperature-Sensitive Anisotropic Negative Poissonâ€™s Ratio of Carbon Honeycomb. Nanomaterials, 2019, 9, 487.	4.1	12
132	Graphene Adhesion Mechanics on Iron Substrates: Insight from Molecular Dynamic Simulations. Crystals, 2019, 9, 579.	2.2	12
133	The formation energy and interaction energy of point defects in ZrC. Journal of Nuclear Materials, 2021, 557, 153235.	2.7	12
134	Ambient-environment processed perovskite solar cells: A review. Materials Today Physics, 2021, 21, 100557.	6.0	12
135	A comparative study of fracture in Al: Quantum mechanical vs. empirical atomistic description. Journal of the Mechanics and Physics of Solids, 2011, 59, 775-786.	4.8	11
136	Comparison of graphene oxide and graphitic carbon nitride filled carbonâ€“phenolic composites: Thermomechanical properties and role of the strong electronegativity of nanofillers. Journal of Applied Polymer Science, 2018, 135, 46242.	2.6	11
137	The Mechanical Properties of Defective Graphyne. Crystals, 2018, 8, 465.	2.2	11
138	Lattice dynamics of thermoelectric palladium sulfide. Journal of Alloys and Compounds, 2019, 798, 484-492.	5.5	11
139	Divalent doping-induced thermoelectric power factor increase in p-type Bi2Te3 via electronic structure tuning. Journal of Applied Physics, 2019, 125, .	2.5	11
140	Adsorption and Diffusion of Hydrogen in Carbon Honeycomb. Nanomaterials, 2020, 10, 344.	4.1	11
141	Effect of interfacial bonding on dislocation strengthening in graphene nanosheet reinforced iron composite: A molecular dynamics study. Computational Materials Science, 2021, 191, 110309.	3.0	11
142	CNT-sandwiched copper composites as super thermal conductors for heat management. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 128, 114557.	2.7	11
143	A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery. Nanomaterials, 2022, 12, 1280.	4.1	11
144	Quantum mechanical study of solid solution effects on dislocation nucleation during nanoindentation. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 075003.	2.0	10

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145	Structure, mechanical and thermodynamic stability of vacancy clusters in Cu. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 055009.	2.0	10
146	Quantum mechanical simulations of nanoindentation of Al thin film. Computational Materials Science, 2010, 47, 769-774.	3.0	10
147	Scattering effect and laser performance for the Nd:YAG transparent ceramics. Applied Physics B: Lasers and Optics, 2011, 104, 625-631.	2.2	10
148	Axial ratio dependence of the stability of self-interstitials in HCP structures. Journal of Nuclear Materials, 2013, 437, 293-296.	2.7	10
149	An interatomic potential for simulation of defects and phase change of zirconium. Computational Materials Science, 2018, 147, 7-17.	3.0	10
150	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3C SiC. Journal of Nuclear Materials, 2018, 510, 596-602.	2.7	10
151	Tuning the Slide-Roll Motion Mode of Carbon Nanotubes via Hydroxyl Groups. Nanoscale Research Letters, 2018, 13, 138.	5.7	10
152	Grain size and hydroxyl-coverage dependent tribology of polycrystalline graphene. Nanotechnology, 2019, 30, 385701.	2.6	10
153	Carbon Nanotubes Enhance the Radiation Resistance of bcc Iron Revealed by Atomistic Study. Materials, 2019, 12, 217.	2.9	10
154	Nonlinear diffusion, bonding, and mechanics of the interface between austenitic steel and iron. Physical Chemistry Chemical Physics, 2019, 21, 1464-1470.	2.8	10
155	One-pot selective synthesis of azoxy compounds and imines via the photoredox reaction of nitroaromatic compounds and amines in water. Scientific Reports, 2019, 9, 1280.	3.3	10
156	Enhancement of toughness of SiC through compositing SiCâ€“Al interpenetrating phase composites. Nanotechnology, 2020, 31, 135706.	2.6	10
157	Green- and Red-Emitting Fluorescent Silicon Nanoparticles: Synthesis, Mechanism, and Acid Phosphatase Sensing. ACS Applied Bio Materials, 2022, 5, 295-304.	4.6	10
158	Error analysis and applications of a general QM/MM approach. Computational Materials Science, 2010, 50, 714-719.	3.0	9
159	Geometry, stability and thermal transport of hydrogenated graphene nanoquilts. Solid State Communications, 2015, 213-214, 31-36.	1.9	9
160	A combined computational and experimental study of the adsorption of sulfur containing molecules on molybdenum disulfide nanoparticles. Journal of Materials Research, 2018, 33, 3589-3603.	2.6	9
161	Fabrication of ceramics/high-entropy alloys gradient composites by combustion synthesis in ultra-high gravity field. Materials Letters, 2018, 233, 4-7.	2.6	9
162	Molecular Dynamics Simulation on Mechanical and Piezoelectric Properties of Boron Nitride Honeycomb Structures. Nanomaterials, 2019, 9, 1044.	4.1	9

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163	Age at Onset of Metabolic Syndrome Among Women With and Without Polycystic Ovary Syndromeâ€"Like Status. Journal of Clinical Endocrinology and Metabolism, 2019, 104, 1429-1439.	3.6	9
164	Massively Engineering the Wettability of Titanium by Tuning Nanostructures and Roughness via Laser Ablation. Journal of Physical Chemistry C, 2019, 123, 30382-30388.	3.1	9
165	Suggest a new approach to fabricate AlFe2B2. Computational Materials Science, 2020, 171, 109239.	3.0	9
166	Ultrahigh Ballistic Resistance of Twisted Bilayer Graphene. Crystals, 2021, 11, 206.	2.2	9
167	The preexisting edge dislocations as recombination center of point defects enhancing irradiation tolerance in CoCrCuFeNi high entropy alloy. Materialia, 2022, 21, 101307.	2.7	9
168	Pressureâ€Induced Amorphization and Crystallization of Heterophase Pd Nanostructures. Small, 2022, 18, e2106396.	10.0	9
169	A 3D Smoothed Particle Hydrodynamics Method with Reactive Flow Model for the Simulation of ANFO. Propellants, Explosives, Pyrotechnics, 2015, 40, 566-575.	1.6	8
170	Release of helium-related clusters through a nickelâ€"graphene interface: An atomistic study. Applied Surface Science, 2019, 487, 218-227.	6.1	8
171	High impact resistance in graphyne. RSC Advances, 2020, 10, 1697-1703.	3.6	8
172	Enhanced self-healing of irradiation defects near a Niâ€"graphene interface by damaged graphene: Insights from atomistic modeling. Journal of Physics and Chemistry of Solids, 2021, 151, 109909.	4.0	8
173	A 7.5ÂW quasi-continuous-wave sodium D2 laser generated fromÂsingle-pass sum-frequency generation in LBO crystal. Applied Physics B: Lasers and Optics, 2011, 102, 781-787.	2.2	7
174	Athermal repair of nanoscale defects in optical materials using a femtosecond laser. Nanoscale, 2017, 9, 17233-17240.	5.6	7
175	Strain-induced dimensional phase change of graphene-like boron nitride monolayers. Nanotechnology, 2018, 29, 405201.	2.6	7
176	A Grain Boundary Regulates the Friction Behaviors between Graphene and a Gold Substrate. Crystals, 2019, 9, 418.	2.2	7
177	Analytical bond-order potential for silver, palladium, ruthenium and iodine bulk diffusion in silicon carbide. Journal of Physics Condensed Matter, 2020, 32, 085702.	1.8	7
178	Electronic effects of transition metal dopants on Fe(100) and Fe5C2(100) surfaces for CO activation. Catalysis Science and Technology, 2020, 10, 2047-2056.	4.1	7
179	Highly efficient desalination performance of carbon honeycomb based reverse osmosis membranes unveiled by molecular dynamics simulations. Nanotechnology, 2021, 32, .	2.6	7
180	Atomic Insights into Fracture Characteristics of Twisted Tri-Layer Graphene. Crystals, 2021, 11, 1202.	2.2	7

#	Article	IF	Citations
181	A SPH Implementation with Ignition and Growth and Afterburning Models for Aluminized Explosives. International Journal of Computational Methods, 2017, 14, 1750046.	1.3	6
182	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. Computational Materials Science, 2019, 170, 109190.	3.0	6
183	Theoretical exploration of the interaction between hydrogen and pyrite-type FeS2 surfaces. Applied Surface Science, 2021, 537, 147900.	6.1	6
184	Atomistic Insights into Aluminum Doping Effect on Surface Roughness of Deposited Ultra-Thin Silver Films. Nanomaterials, 2021, 11, 158.	4.1	6
185	Impact of Polypyrrole Functionalization on the Anodic Performance of Boron Nitride Nanosheets: Insights From First-Principles Calculations. Frontiers in Chemistry, 2021, 9, 670833.	3.6	6
186	The effects of temperature and pressure on the physical properties and stabilities of point defects and defect complexes in B1-ZrC. Computational Materials Science, 2021, 198, 110694.	3.0	6
187	Surface structure and morphology evolution of iron borides under dynamic conditions: A theoretical study. Applied Surface Science, 2020, 525, 146462.	6.1	6
188	High-order nonlinear mechanical properties of g-SiC. Mechanics of Materials, 2020, 148, 103473.	3.2	6
189	A First Principles Investigation of the Mechanical Properties of g-TlN. Modeling and Numerical Simulation of Material Science, 2012, 02, 76-84.	0.3	6
190	A combined DFTB nanoreactor and reaction network generator approach for the mechanism of hydrocarbon combustion. Chemical Communications, 2021, 57, 11633-11636.	4.1	6
191	The Crack Angle of 60Â° Is the Most Vulnerable Crack Front in Graphene According to MD Simulations. Crystals, 2021, 11, 1355.	2.2	6
192	Effect of low-frequency optical phonons on the thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml:m molybdenum disulfide. Physical Review B, 2022, 105, .	3.2	6
193	Shift of Creep Mechanism in Nanocrystalline NiAl Alloy. Materials, 2019, 12, 2508.	2.9	5
194	Strain Enhanced Visibleâ€“Ultraviolet Absorption of Blue Phosphorene/MoX 2 (Xâ€‰=â€‰S,Se) Heterolayers. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800659.	2.4	5
195	Theoretical Insights into the Structure and Activity of Cobalt Modulated by Surface and Subsurface Carbon in Operando Conditions. Journal of Physical Chemistry C, 2020, 124, 18576-18586.	3.1	5
196	Defect, temperature, and strain effects on lattice heat conductivity of egg-tray graphene. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 045003.	2.0	5
197	Fragility under shocking: molecular dynamics insights into defect evolutions in tungsten lattice. Tungsten, 2021, 3, 234-242.	4.8	5
198	Evaluation of the inhibition performance of piperazine-based polyurea towards mild steel corrosion: The role of keto-enol tautomerization. Journal of Molecular Structure, 2022, 1248, 131485.	3.6	5

#	Article	IF	Citations
199	Assembly of Silicalite-1 Crystals Like Toy Lego Bricks into One-, Two-, and Three-Dimensional Architectures for Enhancing Its Adsorptive Separation and Catalytic Performances. ACS Applied Materials & Interfaces, 2021, 13, 58085-58095.	8.0	5
200	Quantifying the photocatalytic role and activity at the edge and surface of Pd co-catalysts using N₂ fixation as a case. Journal of Materials Chemistry A, 2021, 9, 26036-26044.	10.3	5
201	Physical properties and radiation tolerance of high-entropy pyrochlores Gd2(Ti0.25Zr0.25Sn0.25Hf0.25)2O7 and individual pyrochlores Gd2X2O7 (X= Ti, Zr, Sn, Hf) from first principles calculations. Scripta Materialia, 2022, 220, 114898.	5.2	5
202	Quasicontinuum Simulation of the Effect of Lotus-Type Nanocavity on the Onset Plasticity of Single Crystal Al during Nanoindentation. Nanomaterials, 2018, 8, 778.	4.1	4
203	Exploration of Properties from Both the Bulk and Surface of Iron Silicides: A Unified Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 11939-11949.	3.1	4
204	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. Journal of Materials Science, 2019, 54, 10284-10296.	3.7	4
205	First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide. Crystals, 2019, 9, 48.	2.2	4
206	Fivefold enhancement of yield and toughness of copper nanowires via coating carbon nanotubes. Nanotechnology, 2020, 31, 115703.	2.6	4
207	Relationship between the Behavior of Hydrogen and Hydrogen Bubble Nucleation in Vanadium. Materials, 2020, 13, 322.	2.9	4
208	Mapping surface morphology and phase evolution of iron sulfide nanoparticles. CrystEngComm, 2021, 23, 5645-5654.	2.6	4
209	Insights into Coke Formation and Removal under Operating Conditions with a Quantum Nanoreactor Approach. Journal of Physical Chemistry Letters, 2021, 12, 9413-9421.	4.6	4
210	Sintering enhances turn-over frequency of nanoparticles: A case study of FexCy catalyst using reactive MD simulations. Applied Surface Science, 2021, 570, 151018.	6.1	4
211	The effect of Sr doping on the structural, mechanical, electronic properties and radiation tolerance of MgAl2O4 spinel: A first-principles study. Journal of Alloys and Compounds, 2021, 889, 161614.	5.5	4
212	The Role of Sulphonic and Phosphoric Pendant Groups on the Diffusion of Monovalent Ions in Polyelectrolyte Membranes: A Molecular Dynamics Study. Membranes, 2021, 11, 940.	3.0	4
213	Hybridization-driven strong anharmonicity in Yb-filled skutterudites. Physical Review B, 2022, 105, .	3.2	4
214	Microscopic study of the equation of state of Î²-HMX using reactive molecular dynamics simulations. RSC Advances, 2015, 5, 55892-55900.	3.6	3
215	Reduced Plastic Dilatancy in Polymer Glasses. Macromolecular Theory and Simulations, 2021, 30, 2000063.	1.4	3
216	Achieve 100% transmission via grafting hydroxyl groups on CNT nanomotors. Current Applied Physics, 2021, 29, 59-65.	2.4	3

#	Article	IF	Citations
217	Oxygen Adsorption-Induced Morphological Evolution of HÃgg Iron Carbide at High Oxygen Chemical Potentials. Journal of Physical Chemistry C, 2021, 125, 3055-3065.	3.1	3
218	Effect of Microstructure on the Onset Strain and Rate per Strain of Deformation-Induced Martensite Transformation in Q&P Steel by Modeling. Materials, 2022, 15, 952.	2.9	3
219	What can we learn by differentiating between the physical processes behind interference and diffraction phenomena?. Proceedings of SPIE, 2009, , .	0.8	2
220	Density-functional-based tight-binding parameterization of Mo, C, H, O and Si for studying hydrogenation reactions on molybdenum carbide. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
221	Thermal transports of one-dimensional ultrathin carbon structures. Nanotechnology, 2019, 30, 475401.	2.6	2
222	Codoping Erâ€N to Suppress Selfâ€Compensation Donors for Stablepâ€Type Zinc Oxide. Advanced Theory and Simulations, 2019, 2, 1800133.	2.8	2
223	The Application of Godunov SPH in the Simulation of Energetic Materials. International Journal of Computational Methods, 2020, 17, 1950028.	1.3	2
224	The role of ligands in pressure-induced phase transition of gold nanoribbons. Phase Transitions, 2021, 94, 123-133.	1.3	2
225	Dynamic Impact of High-Density Aluminum Foam. Acta Mechanica Solida Sinica, 2022, 35, 198-214.	1.9	2
226	Aluminum Doping Effect on Surface Structure of Silver Ultrathin Films. Materials, 2022, 15, 648.	2.9	2
227	A Molecular Dynamics Study of the Stability and Mechanical Properties of a Nano-Engineered Fuzzy Carbon Fiber Composite. Journal of Composites Science, 2022, 6, 54.	3.0	2
228	Mechanical Properties and Buckling of Kagome Graphene under Tension: A Molecular Dynamics Study. Crystals, 2022, 12, 292.	2.2	2
229	Microstructure evolution in Si⁺ ion irradiated and annealed Ti₃SiC₂ MAX phase. Journal of the American Ceramic Society, 2022, 105, 5921-5928.	3.8	2
230	A first-principles study of the avalanche pressure of alpha zirconium. RSC Advances, 2016, 6, 72551-72558.	3.6	1
231	A micro-macro coupling approach of MD-SPH method for reactive energetic materials. AIP Conference Proceedings, 2017, , .	0.4	1
232	Reduction of defect generation and development of sinks at nanocluster boundary in oxide dispersion-strengthened steel. Journal of Applied Physics, 2019, 126, 084302.	2.5	1
233	Enhancement of Diffusion Assisted Bonding of the Bimetal Composite of Austenitic/Ferric Steels via Intrinsic Interlayers. Materials, 2021, 14, 2416.	2.9	1
234	Ab Initio Investigation of Helium Mobility in La2Zr2O7 Pyrochlore. Crystals, 2021, 11, 667.	2.2	1

#	Article	IF	Citations
235	Nanostructuring enforced sandwich-tubular CNT-Cu interconnects. Composite Structures, 2021, 278, 114705.	5.8	1
236	C2 weakens the turnover frequency during the melting of Fe_xC_y: insights from reactive MD simulations. New Journal of Chemistry, 2021, 46, 282-293.	2.8	1
237	Tuning Surfaceâ€Electron Spins on Fe₃O₄ (111) through Chemisorption of Carbon Monoxide. Angewandte Chemie, 2022, 134, .	2.0	1
238	Can the 'photon interferes only with itself' hypothesis be reconciled with superposition of light from multiple beams or sources?. , 2007, , .		0
239	First-Principles Quantum Simulations. , 0, , .		0
240	Mechanical Stabilities and Properties of Graphene and Its Modification by BN Predicted from First-Principles Calculations. , 2016, , 79-92.		0
241	Graphene Mechanics. Crystals, 2019, 9, 636.	2.2	0
242	Performance of SCAN Meta-GGA Functionals on Nonlinear Mechanics of Graphene-Like g-SiC. Crystals, 2021, 11, 120.	2.2	0
243	10.1063/5.0072285.1. , 2022, , .		0
244	Abnormal radiation resistance via direct-amorphization-induced defect recovery in HgTe. Applied Physics Letters, 2022, 120, 012101.	3.3	0
245	Ab initio investigation of properties and mobility of helium defects in La2Sn2O7 pyrochlore. Nuclear Materials and Energy, 2022, 30, 101135.	1.3	0