

A second-generation reactive empirical bond order (REBOND) method for hydrocarbons

Journal of Physics Condensed Matter

14, 783-802

DOI: [10.1088/0953-8984/14/4/312](https://doi.org/10.1088/0953-8984/14/4/312)

Citation Report

#	ARTICLE	IF	CITATIONS
8	Predictions of a Spiral Diffusion Path for Nonspherical Organic Molecules in Carbon Nanotubes. <i>Physical Review Letters</i> , 2002, 89, 278301.	2.9	53
9	Study of C ₃ H ₅ ⁺ ion deposition on polystyrene and polyethylene surfaces using molecular dynamics simulations. <i>Journal of Applied Physics</i> , 2002, 92, 3363-3367.	1.1	16
10	Mechanics of carbon nanotubes. <i>Applied Mechanics Reviews</i> , 2002, 55, 495-533.	4.5	983
11	Carbon cluster coagulation and fragmentation kinetics in shocked hydrocarbons. <i>Journal of Chemical Physics</i> , 2002, 117, 11352-11358.	1.2	13
12	Molecular dynamics simulation of thin film nucleation through molecular cluster beam deposition: Effect of incident angle. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2002, 195, 329-338.	0.6	7
13	Compression of Carbon Nanotubes Filled with C ₆₀ , CH ₄ , or Ne: Predictions from Molecular Dynamics Simulations. <i>Physical Review Letters</i> , 2002, 88, 205505.	2.9	204
14	Molecular-Scale Tribology of Amorphous Carbon Coatings: Effects of Film Thickness, Adhesion, and Long-Range Interactions. <i>Journal of the American Chemical Society</i> , 2002, 124, 7202-7209.	6.6	212
15	Three-Terminal Junctions of Carbon Nanotubes: Synthesis, Structures, Properties and Applications. <i>Journal of Nanoparticle Research</i> , 2003, 5, 473-484.	0.8	26
16	Molecular dynamics study of defect formation in GaN cascades. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003, 202, 93-99.	0.6	66
17	Matrix and substrate effects on the sputtering of a 2 kDa molecule: Insights from molecular dynamics. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003, 212, 414-419.	0.6	4
18	Chemisorption of atomic hydrogen in graphite and carbon nanotubes. <i>Surface Science</i> , 2003, 544, 24-34.	0.8	39
19	Analysis of carbon nanotube pull-out from a polymer matrix. <i>Surface Science</i> , 2003, 525, L103-L108.	0.8	152
20	Modification of carbon nanotube-polystyrene matrix composites through polyatomic-ion beam deposition predictions from molecular dynamics simulations. <i>Composites Science and Technology</i> , 2003, 63, 1663-1669.	3.8	42
21	The stress-strain behavior of polymer-nanotube composites from molecular dynamics simulation. <i>Composites Science and Technology</i> , 2003, 63, 1655-1661.	3.8	439
22	Sticking of carbon nanotube Y junction branches. <i>JETP Letters</i> , 2003, 78, 327-331.	0.4	7
23	Non-linear elastic response of fullerene balls under uniform and axial deformations. <i>Nanotechnology</i> , 2003, 14, 1197-1202.	1.3	11
24	Molecular Dynamics Simulations of Energetic Materials. <i>Theoretical and Computational Chemistry</i> , 2003, , 125-184.	0.2	3
25	Diffusivities of Ar and Ne in Carbon Nanotubes. <i>Molecular Simulation</i> , 2003, 29, 677-684.	0.9	146

#	ARTICLE	IF	CITATIONS
26	Molecular dynamics study of shock-induced chemistry in small condensed-phase hydrocarbons. Journal of Chemical Physics, 2003, 118, 9795-9801.	1.2	33
27	Derivation of an Interatomic Potential for Germanium- and Silicon-Containing Zeolites and Its Application to the Study of the Structures of Octadecasil, ASU-7, and ASU-9 Materials. Chemistry of Materials, 2003, 15, 1788-1796.	3.2	51
28	Enhancement of Sputtering Yields Due to C60 versus Ga Bombardment of Ag{111} As Explored by Molecular Dynamics Simulations. Analytical Chemistry, 2003, 75, 4402-4407.	3.2	194
29	The General Utility Lattice Program (GULP). Molecular Simulation, 2003, 29, 291-341.	0.9	1,921
30	Formation pathways for single-wall carbon nanotube multiterminal junctions. New Journal of Physics, 2003, 5, 119-119.	1.2	28
31	Mechanisms and Rates of Interstitial H ₂ Diffusion in Crystalline C ₆₀ . Physical Review Letters, 2003, 91, 105901.	2.9	32
32	The Effect of Chemical Functionalization on Mechanical Properties of Nanotube/Polymer Composites. , 2003, , .		14
33	Would Diamond Nanorods Be Stronger than Fullerene Nanotubes?. Nano Letters, 2003, 3, 805-809.	4.5	80
34	Computational study of the non-equilibrium flow of gases through carbon nanotubes. , 0, , .		0
35	Nanoscale Modeling of Shock-Induced Deformation of Diamond. Materials Research Society Symposia Proceedings, 2003, 800, 292.	0.1	1
36	Molecular dynamics investigation on liquid-liquid phase change in carbon with empirical bond-order potentials. Journal of Chemical Physics, 2003, 119, 6053-6056.	1.2	20
37	Bonding and Stability of Hybrid Diamond/Nanotube Structures. Molecular Simulation, 2003, 29, 259-268.	0.9	33
38	Molecular dynamics predictions for chemical modification of "nanopeapods" via ion beam deposition. , 0, , .		1
39	An Iterative Variable-timestep Algorithm for Molecular Dynamics Simulations. Molecular Simulation, 2003, 29, 177-186.	0.9	6
40	Collisional Reactions of Energetic Methane Molecules with Single-Walled Carbon Nanotubes. Chinese Physics Letters, 2004, 21, 1044-1047.	1.3	0
41	Nanoscale measurements and manipulation. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2004, 22, 1609.	1.6	50
42	Nanotube-Substrate Interactions: Distinguishing Carbon Nanotubes by the Helical Angle. Physical Review Letters, 2004, 92, 085503.	2.9	36
43	Intrinsic Energy Loss Mechanisms in a Cantilevered Carbon Nanotube Beam Oscillator. Physical Review Letters, 2004, 93, 185501.	2.9	149

#	ARTICLE	IF	CITATIONS
44	Magnetic properties of polymerized C ₆₀ : The influence of defects and hydrogen. <i>Physical Review B</i> , 2004, 70, .	1.1	71
45	Improved mechanical load transfer between shells of multiwalled carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	1.1	141
46	Atomistic Simulations of Uniaxial Tensile Behaviors of Single-walled Carbon Nanotubes. <i>Molecular Simulation</i> , 2004, 30, 543-547.	0.9	13
47	Formation of sp ³ Bonding in Nanoindented Carbon Nanotubes and Graphite. <i>Physical Review Letters</i> , 2004, 93, 245502.	2.9	76
48	A molecular dynamics study of round and flattened carbon nanotube structures. <i>Applied Physics Letters</i> , 2004, 85, 807-809.	1.5	33
49	Quantum molecular dynamics simulations of shocked nitrogen oxide. <i>Physical Review B</i> , 2004, 69, .	1.1	16
50	Parallel replica dynamics with a heterogeneous distribution of barriers: Application to hexadecane pyrolysis. <i>Journal of Chemical Physics</i> , 2004, 121, 9808-9819.	1.2	25
51	Overview of the Atomistic Modeling of the Chemical Erosion of Carbon. <i>Physica Scripta</i> , 2004, T111, 133.	1.2	8
52	Thermal Conductivity of Single-Wall Carbon Nanotubes. , 2004, , 65.		4
53	Tensile and bending properties of double-walled carbon nanotubes. <i>Journal Physics D: Applied Physics</i> , 2004, 37, 2358-2363.	1.3	33
54	Defect formation in a carbon onion upon irradiation with Ar ions. <i>JETP Letters</i> , 2004, 79, 375-380.	0.4	2
55	Irradiation effects in carbon nanotubes. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2004, 216, 355-366.	0.6	204
56	Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism. <i>Structural Chemistry</i> , 2004, 15, 479-486.	1.0	10
57	A reactive empirical bond order (REBO) potential for hydrocarbon-oxygen interactions. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 7261-7275.	0.7	91
58	Constant temperature molecular dynamics simulations of energetic particle-solid collisions: comparison of temperature control methods. <i>Journal of Computational Physics</i> , 2004, 200, 251-266.	1.9	41
59	Nanoscale view of shock-wave splitting in diamond. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2004, 35, 2647-2650.	1.1	4
60	Structural analysis of carbon clusters by using a global optimization algorithm with Brenner potential. <i>Computational and Theoretical Chemistry</i> , 2004, 678, 113-122.	1.5	26
61	An atomistic-based continuum theory for carbon nanotubes: analysis of fracture nucleation. <i>Journal of the Mechanics and Physics of Solids</i> , 2004, 52, 977-998.	2.3	126

#	ARTICLE	IF	CITATIONS
62	Analytic bond-order potentials for multicomponent systems. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2004, 365, 2-13.	2.6	53
63	Ab initio studies on the atomic-scale origin of friction between hydrocarbon layers. <i>Chemical Physics</i> , 2004, 299, 47-56.	0.9	11
64	An introduction to computational nanomechanics and materials. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2004, 193, 1529-1578.	3.4	346
65	Molecular dynamics simulations of the elastic moduli of polymer-carbon nanotube composites. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2004, 193, 1773-1788.	3.4	314
66	The atomic-scale finite element method. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2004, 193, 1849-1864.	3.4	243
67	On the study of elastic and plastic properties of multi-walled carbon nanotubes under axial tension using molecular dynamics simulation. <i>Acta Materialia</i> , 2004, 52, 2521-2527.	3.8	345
68	Sputtering of a polycyclic hydrocarbon molecule: TOF-SIMS experiments and molecular dynamic simulations. <i>Applied Surface Science</i> , 2004, 231-232, 48-53.	3.1	5
69	Role of lattice registry in the full collapse and twist formation of carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	1.1	59
70	KINETIC MONTE CARLO-MOLECULAR DYNAMICS APPROACH TO MODEL SOOT INCEPTION. <i>Combustion Science and Technology</i> , 2004, 176, 991-1005.	1.2	61
71	Molecular dynamics simulations of bending behavior of tubular graphite cones. <i>Applied Physics Letters</i> , 2004, 85, 1778-1780.	1.5	12
72	Dependence of plasma-induced modification of polymer surfaces on polyatomic ion chemistry. <i>Applied Physics Letters</i> , 2004, 84, 5118-5120.	1.5	11
73	Improved interatomic potentials for silicon-fluorine and silicon-chlorine. <i>Journal of Chemical Physics</i> , 2004, 120, 2405-2412.	1.2	53
74	Atomistic simulation of the torsion deformation of carbon nanotubes. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2004, 12, 1099-1107.	0.8	57
75	Dynamic Sliding Friction between Concentric Carbon Nanotubes. <i>Physical Review Letters</i> , 2004, 93, 065503.	2.9	125
76	Computational Studies of Non-Equilibrium Molecular Transport through Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9861-9870.	1.2	33
77	Kiloelectronvolt Argon-Induced Molecular Desorption from a Bulk Polystyrene Solid. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15652-15661.	1.2	27
78	Microscopic Insights into the Sputtering of Ag{111} Induced by C ₆₀ and Ga Bombardment. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7831-7838.	1.2	182
79	Nanostructure of Fluorocarbon Films Deposited on Polystyrene from Hyperthermal C ₃ F ₅ ⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9656-9664.	1.2	28

#	ARTICLE	IF	CITATIONS
80	Multiterminal junctions formed by heating ultrathin single-walled carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	1.1	33
81	Recombination and Exchange Reactions of Hydrogen and Dihydrogen Molecular Condensation in Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4711-4715.	1.2	5
82	Coarse-Grained Chemical Reaction Model. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1815-1821.	1.2	29
83	Electronic properties of diamond clusters: self-consistent tight binding simulation. <i>Diamond and Related Materials</i> , 2004, 13, 1826-1833.	1.8	25
84	Molecular Dynamics Simulations of the Chemical Modification of Polystyrene through CxFy+Beam Deposition. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18993-19001.	1.2	33
85	Theory of Carbon Nanocones: Mechanical Chiral Inversion of a Micron-Scale Three-Dimensional Object. <i>Physical Review Letters</i> , 2004, 93, 255504.	2.9	85
86	Molecular Dynamics Simulation Study of Carbon Nanotube Welding under Electron Beam Irradiation. <i>Nano Letters</i> , 2004, 4, 109-114.	4.5	112
87	Collapse of Single-Wall Carbon Nanotubes is Diameter Dependent. <i>Physical Review Letters</i> , 2004, 92, 095501.	2.9	328
88	Interatomic potentials for the simulation of the zinc-blende and wurtzite forms of ZnS and CdS: Bulk structure, properties, and phase stability. <i>Physical Review B</i> , 2004, 70, .	1.1	124
89	Hyperthermal chemistry in the gas phase and on surfaces: theoretical studies. <i>International Reviews in Physical Chemistry</i> , 2004, 23, 341-373.	0.9	58
90	Molecular Dynamics Studies of Orientation Dependence of Shock Structure in Solids. <i>AIP Conference Proceedings</i> , 2004, , .	0.3	1
91	Van Der Waal's Elastica. , 2005, , 277.		1
92	Molecular dynamics simulation of the impact behaviour of various hydrocarbon species on DLC. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005, 228, 315-318.	0.6	25
93	Modeling keV particle interactions with molecular and polymeric samples. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005, 236, 1-10.	0.6	13
94	Improved long-range reactive bond-order potential for carbon. I. Construction. <i>Physical Review B</i> , 2005, 72, .	1.1	230
95	Development of the ReaxFF Reactive Force Field for Describing Transition Metal Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 493-499.	1.1	390
96	Thermal stability of benzerods: Molecular-dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 24, 213-218.	1.3	3
97	The relative roles of acetylene and aromatic precursors during soot particle inception. <i>Proceedings of the Combustion Institute</i> , 2005, 30, 1343-1351.	2.4	32

#	ARTICLE	IF	CITATIONS
98	Shock-Induced Chemistry in Hydrocarbon Molecular Solids. , 2005, , 351-368.		3
99	The Computational Materials Design Facility (CMDf): A powerful framework for multi-paradigm multi-scale simulations. Materials Research Society Symposia Proceedings, 2005, 894, 1.	0.1	6
100	Radial compression of carbon nanotubes: deformation and damage, super-elasticity and super-hardness. Nanotechnology, 2005, 16, 1035-1039.	1.3	20
101	Buckling properties of carbon nanotube bundles. Applied Physics Letters, 2005, 87, 041901.	1.5	79
102	Analysis of fracture nucleation in carbon nanotubes through atomistic-based continuum theory. Physical Review B, 2005, 71, .	1.1	9
103	Structures and stability of defect-free multiwalled carbon toroidal rings. Journal of Applied Physics, 2005, 98, 113522.	1.1	9
104	Analytic bond-order potential for predicting structural trends across thesp-valent elements. Physical Review B, 2005, 72, .	1.1	49
105	Energy dissipation via quantum chemical hysteresis during high-pressure compression: A first-principles molecular dynamics study of phosphates. Physical Review B, 2005, 72, .	1.1	25
106	Contact forces at the sliding interface: Mixed versus pure model alkane monolayers. Journal of Chemical Physics, 2005, 122, 024701.	1.2	43
107	Prediction of molecular-dynamics simulation results using feedforward neural networks: Reaction of a C2 dimer with an activated diamond (100) surface. Journal of Chemical Physics, 2005, 123, 224711.	1.2	20
108	Oscillatory behavior of gigahertz oscillators based on multiwalled carbon nanotubes. Journal of Applied Physics, 2005, 98, 014301.	1.1	46
109	Multiscale modeling of carbon nanotubes under axial tension and compression. Physical Review B, 2005, 72, .	1.1	30
110	Structural and electronic properties of carbon in hybrid diamond-graphite structures. Physical Review B, 2005, 72, .	1.1	77
111	Cracking diamond anvil cells by compressed nanographite sheets near the contact edge. Applied Physics Letters, 2005, 87, 051907.	1.5	14
112	Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 94, 036801.	2.9	119
113	Effect of Nanotube Functionalization on the Elastic Properties of Polyethylene Nanotube Composites. AIAA Journal, 2005, 43, 1828-1835.	1.5	84
114	Understanding catalysed growth of single-wall carbon nanotubes. Nanotechnology, 2005, 16, S575-S581.	1.3	80
115	The radial breathing mode of carbon nanotubes. Molecular Simulation, 2005, 31, 135-141.	0.9	16

#	ARTICLE	IF	CITATIONS
116	An Equivalent Continuum-Atomistic Characterization Model for Nanographitic Materials. , 2005, , 471.		0
117	A Finite-Temperature Continuum Theory Based on Interatomic Potentials. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 408-416.	0.8	77
118	Analytical interatomic potential for modeling nonequilibrium processes in the Wâ€“Câ€“H system. Journal of Applied Physics, 2005, 98, 123520.	1.1	244
119	Virtual Computing Infrastructures for Nanoelectronics Simulation. Proceedings of the IEEE, 2005, 93, 1839-1847.	16.4	22
120	Equilibrium and Nonequilibrium Transport of Oxygen in Carbon Nanotubes. Nano Letters, 2005, 5, 793-798.	4.5	40
121	Thermodynamics of two-dimensional single-component elastic crystalline solids: single-wall carbon nanotubes. Philosophical Magazine, 2005, 85, 2249-2280.	0.7	12
122	Modeling a Suspended Nanotube Oscillator. Nano Letters, 2005, 5, 523-526.	4.5	78
123	Deflection of Nanotubes in Response to External Atomic Collisions. Nano Letters, 2005, 5, 263-268.	4.5	17
124	Microscopic Insights into the Sputtering of Thin Organic Films on Ag{111} Induced by C60 and Ga Bombardment. Journal of Physical Chemistry B, 2005, 109, 11973-11979.	1.2	88
125	Molecular Dynamics Simulations on the Effects of Diameter and Chirality on Hydrogen Adsorption in Single Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2005, 109, 3780-3786.	1.2	135
126	Interactions between Polymers and Carbon Nanotubes:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2005, 109, 10009-10014.	1.2	333
127	Thermal conduction of carbon nanotubes using molecular dynamics. Physical Review B, 2005, 71, .	1.1	131
128	Simulation of the elastic response and the buckling modes of single-walled carbon nanotubes. Computational Materials Science, 2005, 32, 141-146.	1.4	106
129	A modified embedded atom method interatomic potential for carbon. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 7-16.	0.7	74
130	An efficient approach for theoretical study on the low-energy isomers of large fullerenes C90â€“C140. Journal of Chemical Physics, 2005, 122, 184318.	1.2	32
131	Prediction of elastic properties of carbon nanotube reinforced composites. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2005, 461, 1685-1710.	1.0	136
132	STUDY OF THERMAL STABILITY OF FULLERENES BY MOLECULAR DYNAMICS. International Journal of Modern Physics B, 2005, 19, 2892-2898.	1.0	8
133	GULP: Capabilities and prospects. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	167

#	ARTICLE	IF	CITATIONS
134	Thermal stability of single and multi-walled carbon nanotubes. <i>Physical Review B</i> , 2005, 71, .	1.1	130
135	Molecular dynamics study of a low energy carbon ion moving in a single-wall carbon nanotube. <i>Nanotechnology</i> , 2005, 16, 2681-2684.	1.3	15
136	Atomistic simulations of formation and stability of carbon nanorings. <i>Physical Review B</i> , 2005, 72, .	1.1	18
137	Oscillatory behavior of C60-nanotube oscillators: A molecular-dynamics study. <i>Journal of Applied Physics</i> , 2005, 97, 094313.	1.1	96
138	Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations. <i>Physical Review B</i> , 2005, 71, .	1.1	238
139	Structural Transformations of Carbon Nanotubes under Hydrostatic Pressure. <i>Nano Letters</i> , 2005, 5, 2268-2273.	4.5	93
140	Atomic-scale finite element method in multiscale computation with applications to carbon nanotubes. <i>Physical Review B</i> , 2005, 72, .	1.1	118
141	Improved long-range reactive bond-order potential for carbon. II. Molecular simulation of liquid carbon. <i>Physical Review B</i> , 2005, 72, .	1.1	48
142	Enhancement of hydrogen physisorption on single-walled carbon nanotubes resulting from defects created by carbon bombardment. <i>Physical Review B</i> , 2005, 71, .	1.1	19
143	Mechanical properties of connected carbon nanorings via molecular dynamics simulation. <i>Physical Review B</i> , 2005, 72, .	1.1	65
144	Interfacial thermal resistance between carbon nanotubes: Molecular dynamics simulations and analytical thermal modeling. <i>Physical Review B</i> , 2006, 74, .	1.1	328
145	MD simulations of polymeric C60fullerene layers/chain under tension. <i>Molecular Simulation</i> , 2006, 32, 385-390.	0.9	2
146	Equilibrium configuration and continuum elastic properties of finite sized graphene. <i>Nanotechnology</i> , 2006, 17, 864-870.	1.3	326
147	Subatomic Imaging of Si (001) Surface by Molecular Dynamic Simulation. , 2006, , .		1
148	Structural studies of carbon nanotubes obtained by template deposition using high-energy X-ray scattering. <i>Diamond and Related Materials</i> , 2006, 15, 1036-1040.	1.8	6
149	Tensile and Compressive Behavior of Carbon Nanotubes: Effect of Functionalization and Topological Defects. <i>Mechanics of Advanced Materials and Structures</i> , 2006, 13, 115-127.	1.5	17
150	Transition states and minimum energy pathways for the collapse of carbon nanotubes. <i>Physical Review B</i> , 2006, 73, .	1.1	73
151	Molecular dynamics simulations of electron and ion beam irradiation of multiwalled carbon nanotubes: The effects on failure by inner tube sliding. <i>Physical Review B</i> , 2006, 73, .	1.1	52

#	ARTICLE	IF	CITATIONS
152	Hypothetical hard structures of carbon with cubic symmetry. <i>Physical Review B</i> , 2006, 74, .	1.1	66
153	The C60Formation Puzzle – Solved – QM/MD Simulations Reveal the Shrinking Hot Giant Road of the Dynamic Fullerene Self-Assembly Mechanism. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14531-14545.	1.2	232
154	Study of Stress-strain Behavior of Carbon-nanotube Reinforced Epon 862 Composites Using Molecular Dynamics. , 2006, , .		0
155	A Rigorous Finite Element Study on the Mechanical Properties of Single-Walled Carbon Nanotubes. , 2006, , .		0
156	Computational Investigation of the Chemical Modification of Polystyrene through Fluorocarbon and Hydrocarbon Ion Beam Deposition. <i>Chemistry of Materials</i> , 2006, 18, 914-921.	3.2	12
157	Stability and chirality effect on twist formation of collapsed double wall carbon nanotubes. <i>Transactions of Nonferrous Metals Society of China</i> , 2006, 16, s776-s779.	1.7	5
158	Graphitization of small diamond cluster – Molecular dynamics simulation. <i>Diamond and Related Materials</i> , 2006, 15, 1818-1821.	1.8	36
159	Raman characteristic peaks induced by the topological defects of carbon nanotube intramolecular junctions. <i>Physical Review B</i> , 2006, 73, .	1.1	34
160	Energetics, structure, and long-range interaction of vacancy-type defects in carbon nanotubes: Atomistic simulations. <i>Physical Review B</i> , 2006, 74, .	1.1	202
161	Mechanical properties of ultrathin carbon nanotube junctions. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2006, 14, S1-S8.	0.8	16
162	Irreversible Organic Crystalline Chemistry Monitored in Real Time. <i>Science</i> , 2006, 313, 1756-1760.	6.0	100
163	Energy relaxation and pulsed neutrons diffraction studies of carbon nanotubes. <i>Diamond and Related Materials</i> , 2006, 15, 1090-1093.	1.8	2
164	Carbon nanostructures for advanced composites. <i>Reports on Progress in Physics</i> , 2006, 69, 1847-1895.	8.1	194
165	A generalization of the charge equilibration method for nonmetallic materials. <i>Journal of Chemical Physics</i> , 2006, 125, 094108.	1.2	131
166	Catalytic Effects of Subsurface Carbon in the Chemisorption of Hydrogen on a Mg(0001) Surface: An Ab-initio Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1814-1819.	1.2	55
167	The environmental effect on the radial breathing mode of carbon nanotubes in water. <i>Journal of Chemical Physics</i> , 2006, 124, 234708.	1.2	43
168	The environmental effect on the radial breathing mode of carbon nanotubes. II. Shell model approximation for internally and externally adsorbed fluids. <i>Journal of Chemical Physics</i> , 2006, 125, 184705.	1.2	33
169	Prediction of Low-Energy Isomers of Large Fullerenes from C132 to C160. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9247-9253.	1.1	18

#	ARTICLE	IF	CITATIONS
170	Mesoscale Energy Deposition Footprint Model for Kiloelectronvolt Cluster Bombardment of Solids. <i>Analytical Chemistry</i> , 2006, 78, 7206-7210.	3.2	85
171	Sputtering of Water Ice Induced by C60 Bombardment: Onset of Plume Formation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1389-1392.	1.1	13
172	Amplitude Response of Single-Wall Carbon Nanotube Probes during Tapping Mode Atomic Force Microscopy: Modeling and Experiment. <i>Nano Letters</i> , 2006, 6, 1669-1673.	4.5	25
173	Postbuckling prediction of axially loaded double-walled carbon nanotubes with temperature dependent properties and initial defects. <i>Physical Review B</i> , 2006, 74, .	1.1	37
174	Nonequilibrium Green's function approach to mesoscopic thermal transport. <i>Physical Review B</i> , 2006, 74, .	1.1	190
175	Force field comparisons of the heat capacity of carbon nanotubes. <i>Molecular Simulation</i> , 2006, 32, 839-848.	0.9	11
176	Atomic Hydrogen Diffusion in Novel Magnesium Nanostructures: The Impact of Incorporated Subsurface Carbon Atoms. <i>Journal of Physics: Conference Series</i> , 2006, 29, 167-172.	0.3	9
177	A comparison of different methods of Young's modulus determination for single-wall carbon nanotubes (SWCNT) using molecular dynamics (MD) simulations. <i>Computational Materials Science</i> , 2006, 38, 271-281.	1.4	84
178	Simulation of amorphous carbon with a bond-order potential. <i>Physica Scripta</i> , 2006, T124, 58-64.	1.2	17
179	Multiscale-Based Mechanical Engineering Education. , 2006, , 165.		0
180	Analysis of the oscillatory behavior of double-walled carbon nanotube-based oscillators. <i>Carbon</i> , 2006, 44, 27-36.	5.4	41
181	Size effect of X-shaped carbon nanotube junctions. <i>Carbon</i> , 2006, 44, 1263-1266.	5.4	43
182	Molecular dynamics simulation of triaxial compression of C60 and C80 solids. <i>Carbon</i> , 2006, 44, 1484-1490.	5.4	7
183	Tensile and compressive properties of carbon nanotube bundles. <i>Acta Materialia</i> , 2006, 54, 225-231.	3.8	88
184	Development of an empirical force field CRACK for n-alkanes that allows for classical molecular dynamics simulations investigating the pyrolysis reactions. <i>Computers and Chemical Engineering</i> , 2006, 30, 1346-1353.	2.0	7
185	Role of atomic scale interfaces in the compressive behavior of carbon nanotubes in composites. <i>Composites Science and Technology</i> , 2006, 66, 2030-2038.	3.8	34
186	Molecular dynamics simulation of carbon nanotube structure. <i>Journal of Molecular Structure</i> , 2006, 792-793, 78-81.	1.8	10
187	Stone-Wales transformation: Precursor of fracture in carbon nanotubes. <i>International Journal of Mechanical Sciences</i> , 2006, 48, 1464-1470.	3.6	29

#	ARTICLE	IF	CITATIONS
188	Coarse-grained molecular dynamics studies of cluster-bombarded benzene crystals. Applied Surface Science, 2006, 252, 6436-6439.	3.1	52
189	Sputtering of amorphous ice induced by C60 and Au3 clusters. Applied Surface Science, 2006, 252, 6423-6425.	3.1	35
190	Load transfer issues in the tensile and compressive behavior of multiwall carbon nanotubes. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 429, 66-73.	2.6	53
191	Atomistic Models of OH Defects in Nominally Anhydrous Minerals. Reviews in Mineralogy and Geochemistry, 2006, 62, 67-83.	2.2	23
192	Elastic constants of diamond from molecular dynamics simulations. Journal of Physics Condensed Matter, 2006, 18, S1737-S1750.	0.7	44
193	Thickness of graphene and single-wall carbon nanotubes. Physical Review B, 2006, 74, .	1.1	564
194	Shapes and energies of giant icosahedral fullerenes. European Physical Journal B, 2006, 53, 395-400.	0.6	9
195	The bending-kinking analysis of a single-walled carbon nanotube—a combined molecular dynamics and continuum mechanics technique. Journal of Materials Science, 2006, 41, 3341-3347.	1.7	15
196	Deformation-promoted reactivity of single-walled carbon nanotubes. Nanotechnology, 2006, 17, 410-414.	1.3	31
197	Combustion-generated nanoparticles produced in a benzene flame: A multiscale approach. Journal of Chemical Physics, 2006, 125, 054302.	1.2	42
198	Studies of Size Effects on Carbon Nanotubes' Mechanical Properties by Using Different Potential Functions. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 9-16.	1.0	53
199	SPIN IN CARBON NANOTUBE-BASED OSCILLATORS. International Journal of Nanoscience, 2006, 05, 47-55.	0.4	7
200	A Cross-Scale Characterization of Interface Properties between Carbon Nanotubes and Polymer Matrix. Key Engineering Materials, 2006, 312, 217-222.	0.4	3
201	Axial-Strain-Induced Torsion in Single-Walled Carbon Nanotubes. Physical Review Letters, 2006, 96, 165501.	2.9	58
202	Coalescence, melting, and mechanical characteristics of carbon nanotube junctions. Physical Review B, 2006, 74, .	1.1	22
203	Twisting effects of carbon nanotube bundles subjected to axial compression and tension. Journal of Applied Physics, 2006, 99, 114312.	1.1	29
204	Surface reconstructions and stability of X-shaped carbon nanotube junction. Journal of Chemical Physics, 2006, 124, 024711.	1.2	10
205	Expressions for the stress and elasticity tensors for angle-dependent potentials. Journal of Chemical Physics, 2006, 125, 144506.	1.2	20

#	ARTICLE	IF	CITATIONS
206	Atomic Simulation of Structure and Deformation's Influence on the Mechanical Properties of Single-walled Carbon Nanotubes. Chinese Journal of Chemical Physics, 2006, 19, 294-300.	0.6	2
207	Postbuckling of carbon nanotubes by atomic-scale finite element. Journal of Applied Physics, 2006, 99, 124308.	1.1	40
208	Transient Deformation Regime in Bending of Single-Walled Carbon Nanotubes. Physical Review Letters, 2006, 97, 245501.	2.9	66
209	Temperature-dependent elastic properties of single-walled carbon nanotubes: Prediction from molecular dynamics simulation. Applied Physics Letters, 2006, 89, 081904.	1.5	118
210	Surface Sensitivity in Cluster-Ion-Induced Sputtering. Physical Review Letters, 2006, 96, 216104.	2.9	56
211	Energy absorption capacity of carbon nanotubes under ballistic impact. Applied Physics Letters, 2006, 89, 123127.	1.5	25
212	Mode-dependent energy transmission across nanotube junctions calculated with a lattice dynamics approach. Physical Review B, 2006, 74, .	1.1	28
213	Effect of chirality on buckling behavior of single-walled carbon nanotubes. Journal of Applied Physics, 2006, 100, 074304.	1.1	73
214	Molecular dynamics study of carbon nanotube oscillators revisited. Journal of Chemical Physics, 2006, 124, 134705.	1.2	35
215	Energies of sp ² carbon shapes with pentagonal disclinations and elasticity theory. Nanotechnology, 2006, 17, 3598-3606.	1.3	14
216	Extended tight-binding potential for modelling intertube interactions in carbon nanotubes. Nanotechnology, 2007, 18, 065706.	1.3	38
217	Atomic geometry and energetics of carbon nanotube necking. Philosophical Magazine Letters, 2007, 87, 567-574.	0.5	13
218	Molecular dynamics simulation of sputtering process of hydrogen and graphene sheets. Molecular Simulation, 2007, 33, 121-126.	0.9	15
219	Molecular Dynamic Simulation Study of AFM Single-Wall Carbon Nanotube Tip-Surface Interactions. Key Engineering Materials, 2007, 339, 206-210.	0.4	5
220	Chemical sputtering from amorphous carbon under bombardment by deuterium atoms and molecules. New Journal of Physics, 2007, 9, 209-209.	1.2	46
221	Self-healing in defective carbon nanotubes: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 386212.	0.7	23
222	Computer Modeling of Nanostructured Materials. , 2007, , 293-328.		1
223	On Elastic Properties of Single-walled Carbon Nanotubes as Composite Reinforcing Fillers. Journal of Composite Materials, 2007, 41, 1123-1135.	1.2	19

#	ARTICLE	IF	CITATIONS
224	RMDff: A smoothly transitioning, forcefield-based representation of kinetics for reactive molecular dynamics simulations. <i>Molecular Simulation</i> , 2007, 33, 361-368.	0.9	19
225	Chapter 9 Integrated Approach to Dielectric Film Growth Modeling: Growth Mechanisms and Kinetics. <i>Thin Films and Nanostructures</i> , 2007, 34, 467-522.	0.1	0
226	Critical Strain of Carbon Nanotubes: An Atomic-Scale Finite Element Study. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2007, 74, 347-351.	1.1	20
227	Thermal Conductivity of Individual Single-Wall Carbon Nanotubes. <i>Journal of Heat Transfer</i> , 2007, 129, 705-716.	1.2	286
228	Simulation and Validation of CNT Mechanical Properties - The Future Interconnection Material. , 2007, , .		2
229	Size effect in the tensile fracture of single-walled carbon nanotubes with defects. <i>Nanotechnology</i> , 2007, 18, 155708.	1.3	25
230	Characteristics of phonon transmission across epitaxial interfaces: a lattice dynamic study. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 236211.	0.7	17
231	Length Dependence of Thermal Conductivity of Single-Walled Carbon Nanotubes. <i>Chinese Physics Letters</i> , 2007, 24, 1321-1323.	1.3	25
232	Excitation of fullerene ions during grazing scattering from a metal surface. <i>Physical Review A</i> , 2007, 76, .	1.0	19
233	Buckling and postbuckling of single-walled carbon nanotubes under combined axial compression and torsion in thermal environments. <i>Physical Review B</i> , 2007, 75, .	1.1	33
234	Tensile mechanical behavior of hollow and filled carbon nanotubes under tension or combined tension-torsion. <i>Applied Physics Letters</i> , 2007, 90, 023102.	1.5	72
235	Elastic torsional responses of carbon nanotube systems. <i>Journal of Applied Physics</i> , 2007, 101, 084309.	1.1	76
236	Carbon nanocones under compression: Buckling and post-buckling behaviors. <i>Physical Review B</i> , 2007, 75, .	1.1	44
237	Atomistic and multiscale analyses of brittle fracture in crystal lattices. <i>Physical Review B</i> , 2007, 76, .	1.1	55
238	Effect of impact angle and substrate roughness on growth of diamondlike carbon films. <i>Journal of Applied Physics</i> , 2007, 101, 014901.	1.1	18
239	Nanomechanical Energy Transfer and Resonance Effects in Single-Walled Carbon Nanotubes. <i>Physical Review Letters</i> , 2007, 98, 125503.	2.9	30
240	Sliding orientation effects on the tribological properties of polytetrafluoroethylene. <i>Journal of Applied Physics</i> , 2007, 102, .	1.1	54
241	Reassembly of single-walled carbon nanotubes into hybrid multilayered nanostructures inside nanotube extruders. <i>Physical Review B</i> , 2007, 76, .	1.1	5

#	ARTICLE	IF	CITATIONS
242	Chemical modification of the poly(vinylidene fluoride-trifluoroethylene) copolymer surface through fluorocarbon ion beam deposition. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2007, 25, 1084-1092.	0.9	4
243	Theory of genus reduction in alkali-induced graphitization of nanoporous carbon. Physical Review B, 2007, 76, .	1.1	14
244	Self-folding of single- and multiwall carbon nanotubes. Applied Physics Letters, 2007, 90, 073107.	1.5	60
245	Effect of thickness on the self-positioning of nanostructures. Journal of Applied Physics, 2007, 102, 083501.	1.1	8
246	Calculation of point defect parameters in diamond. Physical Review B, 2007, 75, .	1.1	65
247	Thermal conductivity of an ultrathin carbon nanotube with an X-shaped junction. Physical Review B, 2007, 75, .	1.1	28
248	Ballistic resistance capacity of carbon nanotubes. Nanotechnology, 2007, 18, 475701.	1.3	78
249	Buckling analysis of abnormal multiwalled carbon nanotubes. Journal of Applied Physics, 2007, 102, 053511.	1.1	21
250	Bending Induced Rippling and Twisting of Multiwalled Carbon Nanotubes. Physical Review Letters, 2007, 98, 205502.	2.9	53
251	Non-Twisted and Twisted CNT Bundles under Axial Tensile and Compressive Loads. Solid State Phenomena, 2007, 121-123, 1415-1418.	0.3	1
252	Atomistic Study of the Strain- and Size-Dependence of Poisson's Ratio of Single-Walled Carbon Nanotubes. Solid State Phenomena, 2007, 121-123, 1021-1024.	0.3	1
253	Role of atomic transverse migration in growth of diamond-like carbon films. Chinese Physics B, 2007, 16, 2798-2802.	1.3	3
254	Continuum and all-atom description of the energetics of graphene nanocones. Nanotechnology, 2007, 18, 375705.	1.3	8
255	Phase separation in H ₂ O:N ₂ mixture: Molecular dynamics simulations using atomistic force fields. Journal of Chemical Physics, 2007, 126, 044510.	1.2	12
256	Hierarchical chemo-nanomechanics of proteins: entropic elasticity, protein unfolding and molecular fracture. Journal of Mechanics of Materials and Structures, 2007, 2, 1019-1057.	0.4	28
257	Theoretical Studies of Chemical Reactions—A Fascinating World of Chemistry from Gas-Phase Elementary Reactions through Nanostructure Formation and Homogeneous Catalysis to Reactions of Metalloenzymes. Bulletin of the Chemical Society of Japan, 2007, 80, 2247-2261.	2.0	20
258	Molecular Dynamics Simulations of Graphite at High Temperatures. Nuclear Technology, 2007, 160, 251-256.	0.7	11
259	Predictive Carbon Nanotube Models Using the Eigenvector Dimension Reduction (EDR) Method. , 2007, , .		0

#	ARTICLE	IF	CITATIONS
260	Multiscale modelling of carbon nanostructures. , 2007, , 220-260.		0
261	Chemical sputtering by impact of excited molecules. <i>Europhysics Letters</i> , 2007, 77, 33002.	0.7	25
262	Atomistic-continuum and ab initio estimation of the elastic moduli of single-walled carbon nanotubes. <i>Computational Materials Science</i> , 2007, 40, 147-158.	1.4	53
263	Nanoscale Fracture Mechanics. <i>Annual Review of Physical Chemistry</i> , 2007, 58, 185-209.	4.8	45
264	Two quantum mechanical/molecular mechanical coupling schemes appropriate for fracture mechanics studies. , 2007, , .		3
265	Calculation of local and average pressure tensors in molecular simulations. <i>Molecular Simulation</i> , 2007, 33, 747-758.	0.9	23
266	Numerical Simulation in Molecular Dynamics. , 2007, , .		4
267	Thermal rectification in carbon nanotube intramolecular junctions: Molecular dynamics calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	222
268	Electrostatic deflections of cantilevered semiconducting single-walled carbon nanotubes. <i>Physical Review B</i> , 2007, 75, .	1.1	28
269	Simulating fullerene ball bearings of ultra-low friction. <i>Nanotechnology</i> , 2007, 18, 115718.	1.3	16
270	Buckling behaviors of single-walled carbon nanotubes filled with metal atoms. <i>Applied Physics Letters</i> , 2007, 91, 051122.	1.5	42
271	Mechanical properties of carbon nanocones. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	62
272	Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets. <i>Physical Review B</i> , 2007, 75, .	1.1	293
273	Energetic Material/ Systems Prognostics. , 2007, , .		8
274	Torsional stiffening of carbon nanotube systems. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	38
275	Structural phase transition and failure of nanographite sheets under high pressure: a molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 346224.	0.7	6
276	Effect of molecular interactions on carbon nanotube friction. <i>Journal of Applied Physics</i> , 2007, 102, .	1.1	24
277	Effect of Cluster Size in Kiloelectronvolt Cluster Bombardment of Solid Benzene. <i>Analytical Chemistry</i> , 2007, 79, 494-499.	3.2	45

#	ARTICLE	IF	CITATIONS
278	Global Potential Energy Surfaces with Correct Permutation Symmetry by Multiconfiguration Molecular Mechanics. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 938-948.	2.3	14
279	Experimental and Atomistic Simulation Study of the Structural and Adsorption Properties of Faujasite Zeolite-templated Nanostructured Carbon Materials. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15863-15876.	1.5	54
280	Structural studies of disordered carbons by high-energy X-ray diffraction. <i>Philosophical Magazine</i> , 2007, 87, 4973-4986.	0.7	24
281	An efficient method for evaluating the nanohardness of layer-configured materials by atomistic simulation. <i>Nanotechnology</i> , 2007, 18, 295704.	1.3	4
282	Electrostatic deflections of cantilevered metallic carbon nanotubes via charge-dipole model. <i>Physical Review B</i> , 2007, 76, .	1.1	31
283	Reaction Dynamics Following keV Cluster Bombardment. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12822-12826.	1.5	31
284	Sputtering Polymers with Buckminsterfullerene Projectiles: A Coarse-Grain Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15312-15324.	1.5	61
285	Superior flexibility of super carbon nanotubes: Molecular dynamics simulations. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	36
286	Formation of Single-Walled Carbon Nanotube via the Interaction of Graphene Nanoribbons: Ab Initio Density Functional Calculations. <i>Nano Letters</i> , 2007, 7, 3349-3354.	4.5	24
287	Collapse and stability of single- and multi-wall carbon nanotubes. <i>Nanotechnology</i> , 2007, 18, 395703.	1.3	87
288	Two Distinct Buckling Modes in Carbon Nanotube Bending. <i>Nano Letters</i> , 2007, 7, 143-148.	4.5	62
289	Multiscale-failure criteria of carbon nanotube systems under biaxial tension-torsion. <i>Nanotechnology</i> , 2007, 18, 485715.	1.3	12
290	The Atomic-Scale Finite Element Method for Post-Buckling of Carbon Nanotubes. , 2007, , 48-59.		0
291	Fullerene Coalescence into Metallic Heterostructures in Boron Nitride Nanotubes: A Molecular Dynamics Study. <i>Nano Letters</i> , 2007, 7, 3709-3715.	4.5	19
292	Study of the polarizability of fullerenes with a monopole-dipole interaction model. <i>Diamond and Related Materials</i> , 2007, 16, 2145-2149.	1.8	19
293	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. <i>Journal of Computational Chemistry</i> , 2007, 28, 1724-1734.	1.5	13
294	Performance of the semiempirical AM1, PM3, MNDO, and tight-binding methods in comparison with DFT method for the large fullerenes C ₁₁₆ -C ₁₂₀ . <i>Computational and Theoretical Chemistry</i> , 2007, 817, 35-41.	1.5	14
295	Hydrocarbon film growth by energetic CH ₃ molecule impact on SiC (001) surface. <i>Applied Surface Science</i> , 2007, 253, 8517-8523.	3.1	9

#	ARTICLE	IF	CITATIONS
296	Atomistic simulations of interfacial sliding in amorphous carbon nanocomposites. <i>Composites Science and Technology</i> , 2007, 67, 1302-1310.	3.8	8
297	Characterization of single-walled carbon nanotubes containing defects from their local vibrational densities of states. <i>Carbon</i> , 2007, 45, 349-356.	5.4	24
298	Effect of strain rate on the buckling behavior of single- and double-walled carbon nanotubes. <i>Carbon</i> , 2007, 45, 514-523.	5.4	52
299	Insights on the nanoparticle formation process in counterflow diffusion flames. <i>Carbon</i> , 2007, 45, 2400-2410.	5.4	43
300	Postbuckling of double-walled carbon nanotubes with temperature dependent properties and initial defects under combined axial and radial mechanical loads. <i>International Journal of Solids and Structures</i> , 2007, 44, 1461-1487.	1.3	46
301	Modelling temperature-dependent fracture nucleation of SWCNTs using atomistic-based continuum theory. <i>International Journal of Solids and Structures</i> , 2007, 44, 3828-3839.	1.3	6
302	Reversible mechanical bistability of carbon nanotubes under radial compression. <i>Chemical Physics</i> , 2007, 334, 144-147.	0.9	8
303	Indentation across size scales and disciplines: Recent developments in experimentation and modeling. <i>Acta Materialia</i> , 2007, 55, 4015-4039.	3.8	403
304	Methane production by deuterium impact at carbon surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007, 255, 202-207.	0.6	21
305	Time scales of chemical sputtering of carbon. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007, 258, 274-277.	0.6	7
306	Combined computational and experimental study of Ar beam induced defect formation in graphite. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007, 262, 240-248.	0.6	30
307	Molecular dynamics study of the stress-strain behavior of carbon-nanotube reinforced Epon 862 composites. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2007, 447, 51-57.	2.6	200
308	Microstructural and stress properties of ultrathin diamondlike carbon films during growth: Molecular dynamics simulations. <i>Physical Review B</i> , 2007, 75, .	1.1	58
309	Parallel replica dynamics for driven systems: Derivation and application to strained nanotubes. <i>Physical Review B</i> , 2007, 75, .	1.1	34
310	QM/MM: what have we learned, where are we, and where do we go from here?. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 185-199.	0.5	1,053
311	Effect of simulation conditions on friction in polytetrafluoroethylene (PTFE). <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 239-246.	0.7	13
312	Mechanical interaction between single-walled carbon nanotubes during the formation of a bundle. <i>Journal of Materials Science</i> , 2007, 42, 4935-4941.	1.7	13
314	A molecular mechanics approach for analyzing tensile nonlinear deformation behavior of single-walled carbon nanotubes. <i>Acta Mechanica Sinica/Lixue Xuebao</i> , 2007, 23, 663-671.	1.5	7

#	ARTICLE	IF	CITATIONS
315	Molecular dynamics study of the initial stages of catalyzed single-wall carbon nanotubes growth: force field development. <i>Journal of Molecular Modeling</i> , 2007, 13, 595-600.	0.8	47
316	Atomistic modeling of hydrocarbon systems using analytic bond-order potentials. <i>Progress in Materials Science</i> , 2007, 52, 230-254.	16.0	27
317	Analytic bond-order potentials for modelling the growth of semiconductor thin films. <i>Progress in Materials Science</i> , 2007, 52, 196-229.	16.0	29
318	Angle of incidence effects in a molecular solid. <i>Applied Surface Science</i> , 2008, 255, 844-846.	3.1	23
319	Bending buckling of single-walled carbon nanotubes by atomic-scale finite element. <i>Composites Part B: Engineering</i> , 2008, 39, 202-208.	5.9	40
320	The dependence of electronic transport on compressive deformation of C60 molecule. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 4294-4297.	0.9	9
321	Mechanical property of carbon nanotubes with intramolecular junctions: Molecular dynamics simulations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 6661-6666.	0.9	97
322	Molecular dynamics simulation of the deposition process of hydrogenated diamond-like carbon (DLC) films. <i>Science Bulletin</i> , 2008, 53, 1094-1099.	4.3	4
323	Modeling fracture in carbon nanotubes using a meshless atomic-scale finite-element method. <i>Jom</i> , 2008, 60, 50-55.	0.9	2
324	Material and structural instabilities of single-wall carbon nanotubes. <i>Acta Mechanica Sinica/Lixue Xuebao</i> , 2008, 24, 285-288.	1.5	5
325	Mechanical Behavior of Single-Walled Carbon Nanotubes in Water under Tensile Loadings: A Molecular Dynamics Study. <i>Chinese Journal of Catalysis</i> , 2008, 29, 1113-1116.	6.9	7
326	Enhanced Mechanical Properties of Prestressed Multi-Walled Carbon Nanotubes. <i>Small</i> , 2008, 4, 733-737.	5.2	30
327	Can nanotubes display auxetic behaviour?. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 2373-2382.	0.7	32
328	Computational view of surface based organic mass spectrometry. <i>Mass Spectrometry Reviews</i> , 2008, 27, 289-315.	2.8	139
329	Application of the higher-order Cauchy-Born rule in mesh-free continuum and multiscale simulation of carbon nanotubes. <i>International Journal for Numerical Methods in Engineering</i> , 2008, 75, 1238-1258.	1.5	54
330	Molecular Dynamics Simulation of Hydrogen Isotope Injection into Graphene. <i>Contributions To Plasma Physics</i> , 2008, 48, 265-269.	0.5	12
331	Empirical bond-order potential for hydrocarbons: Adaptive treatment of van der Waals interactions. <i>Journal of Computational Chemistry</i> , 2008, 29, 601-611.	1.5	27
332	The Intramolecular Junctions of Carbon Nanotubes. <i>Advanced Materials</i> , 2008, 20, 2815-2841.	11.1	126

#	ARTICLE	IF	CITATIONS
333	Torsion induced by axial strain of double-walled carbon nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 3488-3492.	0.9	27
334	Theoretical and computational hierarchical nanomechanics of protein materials: Deformation and fracture. <i>Progress in Materials Science</i> , 2008, 53, 1101-1241.	16.0	168
335	The intrinsic stiffness of single-wall carbon nanotubes. <i>Mechanics Research Communications</i> , 2008, 35, 2-9.	1.0	8
336	Molecular dynamics study of structure and graphitization process of nanodiamonds. <i>Journal of Molecular Structure</i> , 2008, 887, 34-40.	1.8	28
337	Optical properties of soot nanoparticles. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2008, 109, 1791-1801.	1.1	20
338	An atomistic-based finite-deformation shell theory for single-wall carbon nanotubes. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 279-292.	2.3	124
339	Internal lattice relaxation of single-layer graphene under in-plane deformation. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 1609-1623.	2.3	164
340	Can a single-wall carbon nanotube be modeled as a thin shell?. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 2213-2224.	2.3	87
341	Mechanics of hydrogen storage in carbon nanotubes. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 3224-3241.	2.3	55
342	Nonlocal shell model for elastic wave propagation in single- and double-walled carbon nanotubes. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 3475-3485.	2.3	369
343	Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2008, 197, 3190-3202.	3.4	22
344	Ar beam modification of nanotube based composites using molecular dynamics simulations. <i>Composites Science and Technology</i> , 2008, 68, 2049-2055.	3.8	22
345	Molecular dynamics evidences of the full graphitization of a nanodiamond annealed at 1500K. <i>Chemical Physics Letters</i> , 2008, 454, 299-304.	1.2	34
346	Formation and coalescence of linear chains in growth of nanostructured sp ³ -sp ² amorphous carbon films. <i>Chemical Physics Letters</i> , 2008, 462, 104-108.	1.2	6
347	Energetics and stability of C ₆₀ molecules encapsulated in carbon nanotubes. <i>Carbon</i> , 2008, 46, 649-655.	5.4	9
348	Length dependence of critical measures in single-walled carbon nanotubes. <i>International Journal of Solids and Structures</i> , 2008, 45, 4902-4920.	1.3	37
349	Energy transfer phenomena of keV fullerenes during grazing scattering from an Al(001) surface. <i>Vacuum</i> , 2008, 82, 895-899.	1.6	5
350	Structural relaxation of amorphous silicon carbide thin films in thermal annealing. <i>Thin Solid Films</i> , 2008, 516, 3855-3861.	0.8	14

#	ARTICLE	IF	CITATIONS
351	Hydrogen isotope sputtering of graphite by molecular dynamics simulation. <i>Thin Solid Films</i> , 2008, 516, 6553-6559.	0.8	20
352	Quantum thermal transport in nanostructures. <i>European Physical Journal B</i> , 2008, 62, 381-404.	0.6	503
353	Theoretical study of the stable states of small carbon clusters C_n Physical Review B, 2008, 78, .	1.1	34
354	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a review <i>Molecular Simulation</i> , 2008, 34, 119-146.	0.9	102
355	Dominoes in Carbon Nanotubes. <i>Physical Review Letters</i> , 2008, 101, 175501.	2.9	82
356	Dipole polarizability of onion-like carbons and electromagnetic properties of their composites. <i>Nanotechnology</i> , 2008, 19, 115706.	1.3	39
357	Control of the motion of nanoelectromechanical systems based on carbon nanotubes by electric fields. <i>Journal of Experimental and Theoretical Physics</i> , 2008, 107, 653-661.	0.2	10
358	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. <i>Nature Nanotechnology</i> , 2008, 3, 626-631.	15.6	972
359	Theoretical studies of the stretching behavior of carbon nanowires and their superplasticity. <i>Scripta Materialia</i> , 2008, 59, 479-482.	2.6	17
360	Möbius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. <i>Journal of Chemical Physics</i> , 2008, 128, 164719.	1.2	54
361	Nanoscale fracture of tetrahedral amorphous carbon by molecular dynamics: Flaw size insensitivity. <i>Physical Review B</i> , 2008, 77, .	1.1	15
362	Molecular simulation of protein-surface interactions: Benefits, problems, solutions, and future directions (Review). <i>Biointerphases</i> , 2008, 3, FC2-FC12.	0.6	153
363	State-of-the-art models for the phase diagram of carbon and diamond nucleation. <i>Molecular Physics</i> , 2008, 106, 2011-2038.	0.8	58
364	Strain-dependent twist stretch elasticity in chiral filaments. <i>Journal of the Royal Society Interface</i> , 2008, 5, 303-310.	1.5	24
365	Elastic constants of silicon materials calculated as a function of temperature using a parametrization of the second-generation reactive empirical bond-order potential. <i>Physical Review B</i> , 2008, 77, .	1.1	53
366	Functionalized Nanoscale Materials, Devices and Systems. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , .	0.2	31
367	Atomic contributions to friction and load for tip self-assembled monolayers interactions. <i>Physical Review B</i> , 2008, 78, .	1.1	28
368	Analytical carbon-oxygen reactive potential. <i>Journal of Chemical Physics</i> , 2008, 128, 234706.	1.2	6

#	ARTICLE	IF	CITATIONS
369	Structural studies of nanodiamond by high-energy X-ray diffraction. <i>Diamond and Related Materials</i> , 2008, 17, 1186-1193.	1.8	29
370	Effect of defects on oscillation characteristics and instability of carbon nanotube-based oscillators. <i>Applied Physics Letters</i> , 2008, 93, .	1.5	28
371	Molecular simulation of the carbon nanotube growth mode during catalytic synthesis. <i>Applied Physics Letters</i> , 2008, 92, 233121.	1.5	59
372	Molecular dynamics (MD) simulations of the dependence of C-C bond lengths and bond angles on the tensile strain in single-wall carbon nanotubes (SWCNT). <i>Computational Materials Science</i> , 2008, 41, 450-456.	1.4	32
373	Structures and stabilities of multi-terminal carbon nanotube junctions. <i>Computational Materials Science</i> , 2008, 43, 531-539.	1.4	12
374	Theoretical study of the vibrational edge modes in graphene nanoribbons. <i>Physical Review B</i> , 2008, 78, .	1.1	86
375	The running-in of amorphous hydrocarbon tribocoatings: a comparison between experiment and molecular dynamics simulations. <i>International Journal of Materials Research</i> , 2008, 99, 1136-1143.	0.1	28
376	Predicting the elastic properties of double-walled carbon nanotubes by molecular dynamics simulation. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 055404.	1.3	66
377	Thermal rectifiers from deformed carbon nanohorns. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 175211.	0.7	58
378	Single-walled carbon nanotubes filled with bimetallic alloys: Structures and buckling behaviors. <i>Journal of Applied Physics</i> , 2008, 103, 083519.	1.1	14
379	Fullerene-like structure of activated carbons. <i>Diamond and Related Materials</i> , 2008, 17, 1633-1638.	1.8	27
380	Interlayer energy-optimum stacking registry for two curved graphene sheets of nanometre dimensions. <i>Molecular Simulation</i> , 2008, 34, 813-819.	0.9	2
381	Mechanism for Superelongation of Carbon Nanotubes at High Temperatures. <i>Physical Review Letters</i> , 2008, 100, 175501.	2.9	44
382	Nanomechanical Resonance Spectroscopy: A Novel Route to Ultrasensitive Label-Free Detection. <i>Nano Letters</i> , 2008, 8, 2648-2652.	4.5	8
383	Molecular Dynamics Simulations of Carbon-Supported Ni Clusters Using the Reax Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12663-12668.	1.5	28
384	Microscopic Insight into the Sputtering of Thin Polystyrene Films on Ag{111} Induced by Large and Slow Ar Clusters. <i>Journal of Physical Chemistry C</i> , 2008, 112, 521-531.	1.5	53
385	Effects of boron nitride impurities on the elastic properties of carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 445703.	1.3	24
386	Evidence for Metal-Semiconductor Transitions in Twisted and Collapsed Double-Walled Carbon Nanotubes by Scanning Tunneling Microscopy. <i>Nano Letters</i> , 2008, 8, 3350-3356.	4.5	46

#	ARTICLE	IF	CITATIONS
387	High Thermal Conductivity of Single Polyethylene Chains Using Molecular Dynamics Simulations. <i>Physical Review Letters</i> , 2008, 101, 235502.	2.9	337
388	Actuation of a suspended nano-graphene sheet by impact with an argon cluster. <i>Nanotechnology</i> , 2008, 19, 505501.	1.3	38
389	An interatomic potential model for molecular dynamics simulation of silicon etching by Br ⁺ -containing plasmas. <i>Journal of Applied Physics</i> , 2008, 104, .	1.1	22
390	A critical assessment of the elastic properties and effective wall thickness of single-walled carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 075705.	1.3	111
391	Mechanical properties of functionalized carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 395702.	1.3	74
392	Deposition mechanism of nano-structured single-layered C ₃₆ film on a diamond (100) crystal plane. <i>Chinese Physics B</i> , 2008, 17, 4260-4267.	0.7	3
393	Numerical distortion and effects of thermostat in molecular dynamics simulations of single-walled carbon nanotubes. <i>Chinese Physics B</i> , 2008, 17, 4253-4259.	0.7	13
394	The application of molecular dynamics to the study of plasma-surface interactions: CF _x with silicon. <i>International Reviews in Physical Chemistry</i> , 2008, 27, 229-271.	0.9	32
395	Energy dissipation of high-speed nanobearings from double-walled carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 465703.	1.3	21
396	Mechanics of Carbon Nanotubes and Their Composites. , 2008, , 174-208.		0
397	Friction between solids. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2008, 366, 1469-1495.	1.6	36
398	A Finite-Deformation Shell Theory for Carbon Nanotubes Based on the Interatomic Potential—Part I: Basic Theory. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2008, 75, .	1.1	8
399	A Finite-Deformation Shell Theory for Carbon Nanotubes Based on the Interatomic Potential—Part II: Instability Analysis. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2008, 75, .	1.1	8
400	Molecular Dynamics Studies on the Growth and Structural Properties of Hydrogenated DLC Films. <i>Key Engineering Materials</i> , 0, 373-374, 108-112.	0.4	0
401	Modeling of Nanoimprinting of Metals by Nanotube Arrays. <i>Materials Research Society Symposia Proceedings</i> , 2008, 1137, 101301.	0.1	0
402	Nonlinear Deformation Processes and Damage Modes of Super Carbon Nanotubes with Armchair-Armchair Topology. <i>Chinese Physics Letters</i> , 2008, 25, 2577-2580.	1.3	5
403	Hyperthermal Ar atom scattering from a C(0001) surface. <i>Journal of Chemical Physics</i> , 2008, 128, 224708.	1.2	34
404	Integrating experimental and simulation length and time scales in mechanistic studies of friction. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 354012.	0.7	9

#	ARTICLE	IF	CITATIONS
405	Torsional responses of double-walled carbon nanotubes via molecular dynamics simulations. Journal of Physics Condensed Matter, 2008, 20, 455214.	0.7	28
406	Comparative Study of Plasma Source-Dependent Charging Polarity in Metal-Oxide-Semiconductor Field Effect Transistors with High-kand SiO ₂ Gate Dielectrics. Japanese Journal of Applied Physics, 2008, 47, 2369-2374.	0.8	17
407	Coupling of <i>ab initio</i> density functional theory and molecular dynamics for the multiscale modeling of carbon nanotubes. Nanotechnology, 2008, 19, 055702.	1.3	8
408	Elucidating atomic-scale friction using molecular dynamics and specialized analysis techniques. Journal of Physics Condensed Matter, 2008, 20, 354009.	0.7	38
409	Oscillation of gas molecules in carbon nanotubes. Nanotechnology, 2008, 19, 215707.	1.3	6
410	Bilinear responses and rippling morphologies of multiwalled carbon nanotubes under torsion. Applied Physics Letters, 2008, 93, .	1.5	15
411	Shear stresses in shock-compressed diamond from density functional theory. Physical Review B, 2008, 78, .	1.1	6
412	Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range. Physical Review B, 2008, 78, .	1.1	149
413	Many-body effects in bcc metals: An embedded atom model extension of the modified Johnson pair potential for iron. Physical Review B, 2008, 77, .	1.1	8
414	Tuning the torsional properties of carbon nanotube systems with axial prestress. Applied Physics Letters, 2008, 92, 253114.	1.5	21
415	A mimetic porous carbon model by quench molecular dynamics simulation. Journal of Chemical Physics, 2008, 128, 234707.	1.2	68
416	Examining the effects of wall numbers on buckling behavior and mechanical properties of multiwalled carbon nanotubes via molecular dynamics simulations. Journal of Applied Physics, 2008, 103, .	1.1	23
417	Pathways of bond topology transitions at the interface of silicon nanocrystals and amorphous silica matrix. Physical Review B, 2008, 77, .	1.1	19
418	Transversely isotropic elastic properties of single-walled carbon nanotubes by a rectangular beam model for the C-C bonds. Journal of Applied Physics, 2008, 103, .	1.1	43
419	Energy and angle spectra of sputtered particles for low-energy deuterium impact of deuterated amorphous carbon. Journal of Applied Physics, 2008, 104, .	1.1	15
420	Spontaneous generation and propagation of transverse coaxial traveling waves in multiwalled carbon nanotubes. Applied Physics Letters, 2008, 93, 013106.	1.5	5
421	Elasticity of ideal single-walled carbon nanotubes via symmetry-adapted tight-binding objective modeling. Applied Physics Letters, 2008, 93, .	1.5	44
422	Measurement of radial deformation of single-wall carbon nanotubes induced by intertube van der Waals forces. Physical Review B, 2008, 77, .	1.1	23

#	ARTICLE	IF	CITATIONS
424	Science-based model for particle formation from novel fuels. Journal of Physics: Conference Series, 2008, 125, 012033.	0.3	1
425	Simulation science for fusion plasmas. Journal of Physics: Conference Series, 2008, 133, 012025.	0.3	1
426	Formation of linear carbon chains during the initial stage of nanostructured carbon film growth. Journal of Applied Physics, 2008, 104, 064904.	1.1	11
427	Effect of the sliding orientation on the tribological properties of polyethylene in molecular dynamics simulations. Journal of Applied Physics, 2008, 103, 083502.	1.1	33
428	Edge states induce boundary temperature jump in molecular dynamics simulation of heat conduction. Physical Review B, 2009, 80, .	1.1	45
429	A torsional parametric oscillator based on carbon nanotubes. Applied Physics Letters, 2009, 95, .	1.5	9
430	Multilayer friction and attachment effects on energy dissipation in graphene nanoresonators. Applied Physics Letters, 2009, 94, 101918.	1.5	46
431	Intrinsic anisotropy of thermal conductance in graphene nanoribbons. Applied Physics Letters, 2009, 95, .	1.5	176
432	Effective coarse-grained simulations of super-thick multi-walled carbon nanotubes under torsion. Journal of Applied Physics, 2009, 105, 033516.	1.1	19
433	Nanomechanically induced molecular conductance switch. Applied Physics Letters, 2009, 95, 232118.	1.5	14
434	Interfacial thermal transport between nanotubes. Journal of Applied Physics, 2009, 106, .	1.1	20
435	A kinetic model to study film deposition during dusty plasma chemical vapor deposition process. Journal of Applied Physics, 2009, 105, 063303.	1.1	4
436	An image-guided atomistic reconstruction of pyrolytic carbons. Applied Physics Letters, 2009, 95, .	1.5	34
437	The collective motion of carbon atoms in a (10,10) single wall carbon nanotube under axial tensile strain. Journal of Applied Physics, 2009, 106, 063504.	1.1	4
438	Localized modes in capped single-walled carbon nanotubes. Applied Physics Letters, 2009, 94, 111903.	1.5	17
439	The influence of tube length, radius and chirality on the buckling behavior of single-walled carbon nanotubes filled with copper atoms. Journal of Physics Condensed Matter, 2009, 21, 305301.	0.7	4
440	Atomic-scale simulations on the sliding of incommensurate surfaces: The breakdown of superlubricity. Physical Review B, 2009, 80, .	1.1	43
441	Analysis of diamond nanocrystal formation from multiwalled carbon nanotubes. Physical Review B, 2009, 80, .	1.1	18

#	ARTICLE	IF	CITATIONS
442	Multiwall Nanotubes Can Be Stronger than Single Wall Nanotubes and Implications for Nanocomposite Design. <i>Physical Review Letters</i> , 2009, 103, 045502.	2.9	80
443	Single-mode phonon transmission in symmetry-broken carbon nanotubes: Role of phonon symmetries. <i>Journal of Applied Physics</i> , 2009, 105, 063509.	1.1	17
444	Origin of the isotope effect on solid friction. <i>Physical Review B</i> , 2009, 80, .	1.1	24
445	Buckling of defective carbon nanotubes. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	49
446	Assessment of continuum mechanics models in predicting buckling strains of single-walled carbon nanotubes. <i>Nanotechnology</i> , 2009, 20, 395707.	1.3	113
447	Theoretical Study on the Propagation of Acoustic Phonon Modes in Single-Wall Carbon Nanotubes by Different Potential Models. <i>Chinese Physics Letters</i> , 2009, 26, 087101.	1.3	0
448	CONNECTION OF SINGLE-WALLED CARBON NANOTUBES BY BANDAGING WITH A BIGGER RADIUS SINGLE-WALLED CARBON NANOTUBE. <i>Modern Physics Letters B</i> , 2009, 23, 1005-1012.	1.0	1
449	Geometry-Dependent Nonlinear Decrease of the Effective Young's Modulus of Single-Walled Carbon Nanotubes Submitted to Large Tensile Loadings. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 1-10.	1.0	12
450	Molecular dynamics study of energetics of graphene flakes. <i>Journal of Applied Physics</i> , 2009, 106, 114305.	1.1	16
451	How to Compute the Atomic Stress Objectively?. <i>Journal of Computational and Theoretical Nanoscience</i> , 2009, 6, 1081-1089.	0.4	39
452	Computational and experimental studies of phase separation in pentacene:C[sub 60] mixtures. <i>Journal of Vacuum Science & Technology B</i> , 2009, 27, 169.	1.3	20
453	Thermal transport in polyethylene and at polyethylene-diamond interfaces investigated using molecular dynamics simulation. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 084219.	0.7	40
454	Effect of substrate on thermal conductivity of single-walled carbon nanotubes. <i>Europhysics Letters</i> , 2009, 88, 26004.	0.7	18
455	The effect of normal load on polytetrafluoroethylene tribology. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 144201.	0.7	28
456	Dissipation and fluctuations in nanoelectromechanical systems based on carbon nanotubes. <i>Nanotechnology</i> , 2009, 20, 105202.	1.3	23
457	Buckling of carbon nanotubes at high temperatures. <i>Nanotechnology</i> , 2009, 20, 215702.	1.3	46
458	Study of axial strain-induced torsion of single-wall carbon nanotubes using the 2D continuum anharmonic anisotropic elastic model. <i>New Journal of Physics</i> , 2009, 11, 113049.	1.2	14
459	Temperature dependence of frictional force in carbon nanotube oscillators. <i>Nanotechnology</i> , 2009, 20, 035704.	1.3	20

#	ARTICLE	IF	CITATIONS
460	Computational study of nanometer-scale self-propulsion enabled by asymmetric chemical catalysis. <i>Journal of Chemical Physics</i> , 2009, 131, 014705.	1.2	14
461	Torsional behaviour of carbon nanotubes with abnormal interlayer distances. <i>Journal Physics D: Applied Physics</i> , 2009, 42, 055414.	1.3	15
462	On the use of cellular automata algorithm for the atomic-based simulation of carbon nanotubes. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2009, 465, 193-206.	1.0	5
463	Onion-like-carbon-based composite films: Theoretical modeling of electromagnetic response. <i>Solid State Sciences</i> , 2009, 11, 1752-1756.	1.5	10
464	Molecular mechanics in the context of the finite element method. <i>International Journal for Numerical Methods in Engineering</i> , 2009, 77, 969-997.	1.5	62
465	Concurrently coupled atomistic and XFEM models for dislocations and cracks. <i>International Journal for Numerical Methods in Engineering</i> , 2009, 78, 354-378.	1.5	84
466	A multiscale framework for computational nanomechanics: Application to the modeling of carbon nanotubes. <i>International Journal for Numerical Methods in Engineering</i> , 2009, 78, 863-882.	1.5	9
467	Molecular dynamics study of effects of sp ³ interwall bridging upon torsional behavior of double-walled carbon nanotube. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 682-685.	0.9	17
468	Atomistic simulations of mechanical properties of graphene nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 3359-3362.	0.9	144
469	Molecular dynamics simulation of hydrogen atom sputtering on the surface of graphite with defect and edge. <i>Journal of Nuclear Materials</i> , 2009, 390-391, 183-187.	1.3	31
470	Numerical analyses for the atomistic-based shell theory of carbon nanotubes. <i>International Journal of Plasticity</i> , 2009, 25, 1879-1887.	4.1	6
471	Molecular dynamics simulations of atomic-scale friction in diamond-silver sliding system. <i>Science Bulletin</i> , 2009, 54, 4555-4559.	4.3	6
472	Molecular dynamics studies on the thermal conductivity of single-walled carbon nanotubes. <i>Frontiers of Physics in China</i> , 2009, 4, 389-392.	1.0	19
473	Milestones in molecular dynamics simulations of single-walled carbon nanotube formation: A brief critical review. <i>Nano Research</i> , 2009, 2, 755.	5.8	52
474	Modeling plasma facing materials for fusion power. <i>Materials Today</i> , 2009, 12, 38-44.	8.3	28
475	A Continuum Model for Axial-Strain-Induced Torsion in Single-Wall Carbon Nanotubes. <i>Acta Mechanica Solida Sinica</i> , 2009, 22, 283-286.	1.0	2
476	Subjecting a Graphene Monolayer to Tension and Compression. <i>Small</i> , 2009, 5, 2397-2402.	5.2	400
477	Controlled Carbon Nanotube Junctions Self-Assembled from Graphene Nanoribbons. <i>Small</i> , 2009, 5, 2802-2806.	5.2	24

#	ARTICLE	IF	CITATIONS
478	Molecular Dynamics Simulations of Ar ⁺ Organic Polymer Interactions. Plasma Processes and Polymers, 2009, 6, 320-334.	1.6	17
479	Friction laws at the nanoscale. Nature, 2009, 457, 1116-1119.	13.7	783
480	Molecular Dynamics Simulations of Interfacial Sliding in Carbon Nanotube/Diamond Nanocomposites. Journal of the American Ceramic Society, 2009, 92, 2331-2336.	1.9	31
481	Plasma-surface interactions of hydrogenated carbon. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 704-710.	0.6	6
482	Modification of poly(methyl methacrylate) by keV Ar deposition. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 2525-2531.	0.6	9
483	Film growth by polyatomic C ₂ H ₅ ⁺ bombarding a diamond (100) surfaces: Molecular dynamics study. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3238-3241.	0.6	3
484	Stability of single-walled carbon nanopeapods under combined axial compressive load and external pressure. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 513-517.	1.3	14
485	Molecular dynamics study of effects of radius and defect on oscillatory behaviors of C ₆₀ nanotube oscillators. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 1058-1061.	0.9	28
486	An atomistic-continuum Cosserat rod model of carbon nanotubes. Journal of the Mechanics and Physics of Solids, 2009, 57, 932-958.	2.3	62
487	An extended finite element method for dislocations in complex geometries: Thin films and nanotubes. Computer Methods in Applied Mechanics and Engineering, 2009, 198, 1872-1886.	3.4	35
488	Interatomic potentials for atomic scale modeling of metal matrix ceramic particle reinforced nanocomposites. Composites Part B: Engineering, 2009, 40, 461-467.	5.9	15
489	Nonlinear bending of functionally graded carbon nanotube-reinforced composite plates in thermal environments. Composite Structures, 2009, 91, 9-19.	3.1	962
490	Half metallicity in a zigzag double-walled nanotube nanodot: An ab initio prediction. Chemical Physics Letters, 2009, 468, 257-259.	1.2	3
491	Atomic-scale finite element analysis of vibration mode transformation in carbon nanorings and single-walled carbon nanotubes. International Journal of Solids and Structures, 2009, 46, 4342-4360.	1.3	16
492	The effects of grafted amine groups on the elastic properties of single-walled carbon nanotubes. Carbon, 2009, 47, 713-721.	5.4	22
493	Stretching-dominated deformation mechanism in a super square carbon nanotube network. Carbon, 2009, 47, 812-819.	5.4	32
494	Energetics and structures of carbon nanorings. Carbon, 2009, 47, 1664-1669.	5.4	18
495	Origin of friction in films of horizontally oriented carbon nanotubes sliding against diamond. Carbon, 2009, 47, 1693-1700.	5.4	31

#	ARTICLE	IF	CITATIONS
496	Thermally activated model for tensile yielding of pristine single-walled carbon nanotubes with nonlinear elastic deformation. <i>Carbon</i> , 2009, 47, 2070-2076.	5.4	11
497	Molecular dynamics investigation on the atomic-scale friction behaviors between copper(001) and diamond(111) surfaces. <i>Applied Surface Science</i> , 2009, 255, 7663-7668.	3.1	8
498	Alignment Controlled Growth of Single-Walled Carbon Nanotubes on Quartz Substrates. <i>Nano Letters</i> , 2009, 9, 4311-4319.	4.5	125
499	Thermal conductivity of single-walled carbon nanotubes. <i>Physical Review B</i> , 2009, 80, .	1.1	79
500	Modeling of an ultrahigh-frequency resonator based on the relative vibrations of carbon nanotubes. <i>Physical Review B</i> , 2009, 80, .	1.1	24
501	Young's modulus of graphene: A molecular dynamics study. <i>Physical Review B</i> , 2009, 80, .	1.1	348
502	Lattice thermal conductivity of single-walled carbon nanotubes: Beyond the relaxation time approximation and phonon-phonon scattering selection rules. <i>Physical Review B</i> , 2009, 80, .	1.1	152
503	Temperature Dependence of Iron-Catalyzed Continued Single-Walled Carbon Nanotube Growth Rates: Density Functional Tight-Binding Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2009, 113, 159-169.	1.5	40
504	Gigahertz breathing oscillators based on carbon nanoscrolls. <i>Applied Physics Letters</i> , 2009, 95, .	1.5	59
505	A nonlocal shell model for mode transformation in single-walled carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 455301.	0.7	5
506	Thermal expansion in single-walled carbon nanotubes and graphene: Nonequilibrium Green's function approach. <i>Physical Review B</i> , 2009, 80, .	1.1	160
507	Molecular dynamics simulation of tensile elongation of carbon nanotubes: Temperature and size effects. <i>Physical Review B</i> , 2009, 79, .	1.1	55
508	Wrinkling of monolayer graphene: A study by molecular dynamics and continuum plate theory. <i>Physical Review B</i> , 2009, 80, .	1.1	76
509	A framework for stress computation in single-walled carbon nanotubes under uniaxial tension. <i>Computational Materials Science</i> , 2009, 46, 1135-1143.	1.4	26
510	Molecular dynamics with quantum heat baths: Application to nanoribbons and nanotubes. <i>Physical Review B</i> , 2009, 80, .	1.1	25
511	Nanoengineering Heat Transfer Performance at Carbon Nanotube Interfaces. <i>ACS Nano</i> , 2009, 3, 2767-2775.	7.3	207
512	Formation of multiwall fullerenes from nanodiamonds studied by atomistic simulations. <i>Physical Review B</i> , 2009, 80, .	1.1	45
513	Strain controlled thermomutability of single-walled carbon nanotubes. <i>Nanotechnology</i> , 2009, 20, 185701.	1.3	130

#	ARTICLE	IF	CITATIONS
514	Modeling Nanomaterials. , 2009, , 261-298.		0
515	Nonlocal elastic beam models for flexural wave propagation in double-walled carbon nanotubes. Journal of Applied Physics, 2009, 106, 044301.	1.1	43
516	Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: Application to polycyclic aromatic hydrocarbon clusters. Journal of Chemical Physics, 2009, 130, 244304.	1.2	88
517	Parametrization of a reactive many-body potential for MoS systems. Physical Review B, 2009, 79, .	1.1	241
518	Effective elastic mechanical properties of single layer graphene sheets. Nanotechnology, 2009, 20, 065709.	1.3	438
519	Edge elastic properties of defect-free single-layer graphene sheets. Applied Physics Letters, 2009, 94, .	1.5	106
520	Temperature-dependent bending rigidity of graphene. Applied Physics Letters, 2009, 94, .	1.5	62
521	Mesoscopic Simulation of Self-assembly of Carbon Nanotubes into a Network of Bundles. , 2009, , .		6
522	Explicit Treatment of Hydrogen Atoms in Thermal Simulations of Polyethylene. Nanoscale and Microscale Thermophysical Engineering, 2009, 13, 99-108.	1.4	13
523	Computational study of thermocompression bonding of carbon nanotubes to metallic substrates. Journal of Applied Physics, 2009, 106, .	1.1	21
524	NONLINEAR MECHANICS OF SINGLE-ATOMIC-LAYER GRAPHENE SHEETS. International Journal of Applied Mechanics, 2009, 01, 443-467.	1.3	222
525	Angular-dependent embedded atom method potential for atomistic simulations of metal-covalent systems. Physical Review B, 2009, 80, .	1.1	35
526	Computational investigation of the mechanical properties of nanomaterials. Diamond and Related Materials, 2009, 18, 438-442.	1.8	7
527	Atomic hydrogen interactions with amorphous carbon thin films. Journal of Applied Physics, 2009, 106, .	1.1	33
528	Chapter 1 A Shell Theory for Carbon Nanotubes Based on the Interatomic Potential and Atomic Structure. Advances in Applied Mechanics, 2009, 43, 1-68.	1.4	12
529	Hydrogen storage enhanced in Li-doped carbon replica of zeolites: A possible route to achieve fuel cell demand. Journal of Chemical Physics, 2009, 130, 174717.	1.2	31
530	Elastic bending modulus of monolayer graphene. Journal Physics D: Applied Physics, 2009, 42, 102002.	1.3	326
531	Mechanical and dynamical behavior of carbon nanotube with defects:A molecular dynamics simulation. , 2009, , .		1

#	ARTICLE	IF	CITATIONS
532	C ₆₀ -derived nanobaskets: stability, vibrational signatures, and molecular trapping. <i>Nanotechnology</i> , 2009, 20, 395701.	1.3	8
533	Merging bond-order potentials with charge equilibration. <i>Journal of Chemical Physics</i> , 2009, 131, 241105.	1.2	22
534	Development of empirical bond-order-type interatomic potential for amorphous carbon structures. <i>Journal of Applied Physics</i> , 2009, 105, 064310.	1.1	19
535	Growth of ultrathin diamond-like carbon films by C ₆₀ cluster assembly: Molecular dynamics simulations. <i>Diamond and Related Materials</i> , 2009, 18, 88-94.	1.8	11
536	Evolution of carbon surfaces under simulated bombardment by deuterium. <i>Journal of Physics: Conference Series</i> , 2009, 194, 012059.	0.3	6
537	Chemical sputtering of carbon by H, D, and T impact. <i>Journal of Physics: Conference Series</i> , 2009, 194, 132028.	0.3	0
538	Wave propagation in carbon nanotubes: nonlocal elasticity-induced stiffness and velocity enhancement effects. <i>Journal of Mechanics of Materials and Structures</i> , 2010, 5, 459-476.	0.4	52
539	On using many-particle interatomic potentials to compute elastic properties of graphene and diamond. <i>Mechanics of Solids</i> , 2010, 45, 815-834.	0.3	23
540	Optimized Tersoff and Brenner empirical potential parameters for lattice dynamics and phonon thermal transport in carbon nanotubes and graphene. <i>Physical Review B</i> , 2010, 81, .	1.1	917
541	Carbon clusters: From ring structures to nanographene. <i>Physical Review B</i> , 2010, 81, .	1.1	60
542	Structural Stability of Carbon Nanotube Films: The Role of Bending Buckling. <i>ACS Nano</i> , 2010, 4, 6187-6195.	7.3	80
543	Stick-Spiral Model for Studying Mechanical Properties of Carbon Nanotubes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 297-322.	0.6	0
544	Fast diffusion of a graphene flake on a graphene layer. <i>Physical Review B</i> , 2010, 82, .	1.1	85
545	Plasticity in carbon nanotubes: Cooperative conservative dislocation motion. <i>Physical Review B</i> , 2010, 81, .	1.1	18
546	Thermal conductivity and phonon transport in empty and water-filled carbon nanotubes. <i>Physical Review B</i> , 2010, 81, .	1.1	133
547	Ion and electron irradiation-induced effects in nanostructured materials. <i>Journal of Applied Physics</i> , 2010, 107, .	1.1	878
548	Molecular dynamics simulations of nanopore processing in a graphene sheet by using gas cluster ion beam. <i>Applied Physics A: Materials Science and Processing</i> , 2010, 98, 787-794.	1.1	27
549	Thermal conductivity and thermal rectification in carbon nanotubes with geometric variations of doped nitrogen: Non-equilibrium molecular dynamics simulations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 4885-4889.	0.9	31

#	ARTICLE	IF	CITATIONS
550	Isotope dependence of chemical erosion of carbon. Journal of Nuclear Materials, 2010, 401, 1-12.	1.3	9
551	Coordinated buckling of thick multi-walled carbon nanotubes under uniaxial compression. Nano Research, 2010, 3, 32-42.	5.8	22
552	Is a nanorod (or nanotube) with a lower Young's modulus stiffer? Is not Young's modulus a stiffness indicator?. Science China: Physics, Mechanics and Astronomy, 2010, 53, 712-724.	2.0	54
553	Radial Corrugations of Multi-Walled Carbon Nanotubes Driven by Inter-Wall Nonbonding Interactions. Nanoscale Research Letters, 2011, 6, 53.	3.1	17
554	Radiation stability of carbon nanostructures. Journal of Engineering Physics and Thermophysics, 2010, 83, 393-400.	0.2	4
555	Formation and conversion of carbon nanostructures under radiation. Journal of Engineering Physics and Thermophysics, 2010, 83, 849-862.	0.2	8
556	MD investigation of the collective carbon atom behavior of a (17, 0) zigzag single wall carbon nanotube under axial tensile strain. Journal of Nanoparticle Research, 2010, 12, 2979-2987.	0.8	1
557	Friction Properties of Carbon Nano-Onions from Experiment and Computer Simulations. Tribology Letters, 2010, 37, 75-81.	1.2	75
558	Atomistic Insights into the Running-in, Lubrication, and Failure of Hydrogenated Diamond-Like Carbon Coatings. Tribology Letters, 2010, 39, 49-61.	1.2	126
559	A continuum-atomistic bridging domain method for composite lattices. International Journal for Numerical Methods in Engineering, 2010, 81, 1635-1658.	1.5	26
560	Dependency of Tritium Retention in Graphite on Temperature Control of Molecular Dynamics. Contributions To Plasma Physics, 2010, 50, 464-469.	0.5	4
561	Determination of the Local Chemical Structure of Graphene Oxide and Reduced Graphene Oxide. Advanced Materials, 2010, 22, 4467-4472.	11.1	1,044
564	Recent advances in graphene based polymer composites. Progress in Polymer Science, 2010, 35, 1350-1375.	11.8	2,949
565	Thermal buckling and postbuckling behavior of functionally graded carbon nanotube-reinforced composite plates. Materials & Design, 2010, 31, 3403-3411.	5.1	468
566	Mechanical properties of nickel-coated single-walled carbon nanotubes and their embedded gold matrix composites. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 1068-1072.	0.9	35
567	Molecular dynamical simulations on a-C:H film growth from atomic flux of C and H: Effect of H fraction. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 2150-2155.	0.9	9
568	Multiscale computations for carbon nanotubes based on a hybrid QM/QC (quantum mechanical and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.3	11
569	A molecular based anisotropic shell model for single-walled carbon nanotubes. Journal of the Mechanics and Physics of Solids, 2010, 58, 1422-1433.	2.3	114

#	ARTICLE	IF	CITATIONS
570	Mechanical properties and deformation morphologies of covalently bridged multi-walled carbon nanotubes: Multiscale modeling. <i>Journal of the Mechanics and Physics of Solids</i> , 2010, 58, 1847-1862.	2.3	19
571	Computational investigation of the temperature influence on the cleavage of a graphite surface. <i>Surface Science</i> , 2010, 604, 730-740.	0.8	23
572	Optimizing load transfer in multiwall nanotubes through interwall coupling: Theory and simulation. <i>Acta Materialia</i> , 2010, 58, 6324-6333.	3.8	24
573	Failure analysis and the optimal toughness design of carbon nanotube-reinforced composites. <i>Composites Science and Technology</i> , 2010, 70, 1360-1367.	3.8	104
574	Torsional buckling and postbuckling of double-walled carbon nanotubes by nonlocal shear deformable shell model. <i>Composite Structures</i> , 2010, 92, 1073-1084.	3.1	130
575	Pressure induced transformations in condensed and molecular phases of C60. <i>Carbon</i> , 2010, 48, 744-755.	5.4	10
576	Molecular dynamics of cleavage and flake formation during the interaction of a graphite surface with a rigid nanoasperity. <i>Carbon</i> , 2010, 48, 1234-1243.	5.4	29
577	Unique buckling responses of multi-walled carbon nanotubes incorporated as torsion springs. <i>Carbon</i> , 2010, 48, 1697-1701.	5.4	16
578	Compressive mechanical properties of carbon nanotubes encapsulating helical copper nanowires. <i>Carbon</i> , 2010, 48, 1586-1591.	5.4	33
579	A molecular dynamics investigation of the torsional responses of defective single-walled carbon nanotubes. <i>Carbon</i> , 2010, 48, 4100-4108.	5.4	55
580	Nanoscale fracture in graphene. <i>Chemical Physics Letters</i> , 2010, 494, 218-222.	1.2	111
581	Pressure-driven water flow through carbon nanotubes: Insights from molecular dynamics simulation. <i>International Journal of Thermal Sciences</i> , 2010, 49, 281-289.	2.6	140
582	Isotope Effect on the Thermal Conductivity of Graphene. <i>Journal of Nanomaterials</i> , 2010, 2010, 1-5.	1.5	45
583	Nanowires with Unimaginable Characteristics. , 0, , .		1
584	Adsorption and Phase Behaviour in Nanochannels and Nanotubes. , 2010, , .		23
585	Accelerated molecular dynamics simulation of low-velocity frictional sliding. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010, 18, 034003.	0.8	23
586	Molecular Dynamic Simulation on Graphitization and Dehydrogenization of Hydrogenated Carbon Films in Vacuum. <i>Chinese Physics Letters</i> , 2010, 27, 078103.	1.3	0
587	A Multiscale Modeling Approach for Carbon Nanotubes. <i>Advanced Materials Research</i> , 2010, 97-101, 4201-4205.	0.3	0

#	ARTICLE	IF	CITATIONS
588	Material Properties in Codimension > 0: Graphene Edge Properties. Materials Research Society Symposia Proceedings, 2010, 1258, 1.	0.1	0
589	Mechanical Properties of Ni-Coated Single Graphene Sheet and Their Embedded Aluminum Matrix Composites. Communications in Theoretical Physics, 2010, 54, 143-147.	1.1	18
590	Molecular Dynamical Simulations on a-C:H Film Growth from C and H Atomic Flux: Effect of Incident Energy. Chinese Physics Letters, 2010, 27, 088102.	1.3	3
592	Roughness picture of friction in dry nanoscale contacts. Physical Review B, 2010, 81, .	1.1	79
593	Capillary force induced structural deformation in liquid infiltrated elastic circular tubes. Physical Review B, 2010, 81, .	1.1	15
594	Formation mechanism of peapod-derived double-walled carbon nanotubes. Physical Review B, 2010, 82, .	1.1	29
595	Conditions for the existence of phonon localized edge-modes. Physical Review B, 2010, 81, .	1.1	12
596	Determination of the bulk melting temperature of nickel using Monte Carlo simulations: Inaccuracy of extrapolation from cluster melting temperatures. Physical Review B, 2010, 81, .	1.1	16
597	Effects of ion bombardment on a two-dimensional target: Atomistic simulations of graphene irradiation. Physical Review B, 2010, 81, .	1.1	341
598	Bending manipulation induced sp ² →sp ³ bond transition in carbon nanotubes. Journal of Applied Physics, 2010, 108, .	1.1	19
599	Reactive force fields for surface chemical reactions: A case study with hydrogen dissociation on Pd surfaces. Journal of Chemical Physics, 2010, 132, 014704.	1.2	39
600	Load transfer between cross-linked walls of a carbon nanotube. Physical Review B, 2010, 81, .	1.1	39
601	Load-driven morphological evolution in covalently bridged multiwalled carbon nanotubes. Applied Physics Letters, 2010, 96, 203106.	1.5	8
602	Carbon nanotube initiated formation of carbon nanoscrolls. Applied Physics Letters, 2010, 97, .	1.5	69
603	Macroscopic Behavior of Carbon Nanotube (CNT)-Reinforced Composite Accounting for Interface Cohesive Force. Journal of Adhesion, 2010, 86, 273-289.	1.8	9
604	Dependencies of the thermal conductivity of individual single-walled carbon nanotubes. Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanoengineering and Nanosystems, 2010, 224, 41-54.	0.1	2
605	A Cohesive Law for Carbon Nanotube/Polymer Interface Accounting for Chemical Covalent Bonds. Mathematics and Mechanics of Solids, 2010, 15, 718-732.	1.5	14
606	Water adsorption isotherms on porous onionlike carbonaceous particles. Simulations with the grand canonical Monte Carlo method. Journal of Chemical Physics, 2010, 133, 144702.	1.2	36

#	ARTICLE	IF	CITATIONS
607	Self-repairing in single-walled carbon nanotubes by heat treatment. Journal of Applied Physics, 2010, 108, .	1.1	6
608	Buckling Analyses of Double-Wall Carbon Nanotubes: A Shell Theory Based on the Interatomic Potential. Journal of Applied Mechanics, Transactions ASME, 2010, 77, .	1.1	11
609	Modeling of amorphous carbon structures with arbitrary structural constraints. Journal of Physics Condensed Matter, 2010, 22, 395402.	0.7	7
610	1D-to-3D transition of phonon heat conduction in polyethylene using molecular dynamics simulations. Physical Review B, 2010, 82, .	1.1	101
611	Bond-order potential for point and extended defect simulations in tungsten. Journal of Applied Physics, 2010, 107, .	1.1	76
612	Topological effect on thermal conductivity in graphene. Journal of Applied Physics, 2010, 108, 064307.	1.1	18
613	Molecular Modeling of Matter: Impact and Prospects in Engineering. Industrial & Engineering Chemistry Research, 2010, 49, 3026-3046.	1.8	98
614	Amorphous Carbon and Related Materials. Carbon Materials, 2010, , 129-169.	0.2	6
615	Thermal transport in graphene junctions and quantum dots. Physical Review B, 2010, 81, .	1.1	95
616	Molecular dynamics simulation of energy exchanges during hydrogen collision with graphite sheets. Journal of Applied Physics, 2010, 107, 113533.	1.1	7
617	Nano-Scale and Atomistic-Scale Modeling of Advanced Materials. , 2010, , 719-758.		0
618	Molecular dynamics modelling of nanocarbon cluster properties under conditions close to HE detonation. EPJ Web of Conferences, 2010, 10, 00032.	0.1	0
619	Liquid Carbon: Freezing Line and Structure Near Freezing. Carbon Materials, 2010, , 1-36.	0.2	4
620	A universal exponential factor in the dimensional crossover from graphene to graphite. Journal of Applied Physics, 2010, 108, 124311.	1.1	1
621	Molecular Simulation of Adsorption in Zeolites and Carbon Nanotubes. , 2010, , 9-40.		3
622	Recent Studies on Buckling of Carbon Nanotubes. Applied Mechanics Reviews, 2010, 63, .	4.5	117
623	Curvature-induced excess surface energy of fullerenes: Density functional theory and Monte Carlo simulations. Physical Review B, 2010, 81, .	1.1	27
624	Temperature-Induced Reversible Dominoes in Carbon Nanotubes. Nano Letters, 2010, 10, 3490-3493.	4.5	55

#	ARTICLE	IF	CITATIONS
625	Predicting phonon dispersion relations and lifetimes from the spectral energy density. <i>Physical Review B</i> , 2010, 81, .	1.1	285
626	Enhancement of Friction between Carbon Nanotubes: An Efficient Strategy to Strengthen Fibers. <i>ACS Nano</i> , 2010, 4, 312-316.	7.3	75
627	Curved graphene nanoribbons: structure and dynamics of carbon nanobelts. <i>Nanotechnology</i> , 2010, 21, 075710.	1.3	59
628	Topology-induced thermal rectification in carbon nanodevice. <i>Europhysics Letters</i> , 2010, 89, 46005.	0.7	41
629	Tunable dual-frequency oscillators of carbon nanotubes. <i>Journal of Applied Physics</i> , 2010, 108, 054304.	1.1	3
630	Fusion power: a challenge for materials science. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2010, 368, 3315-3328.	1.6	59
631	Application of a field-based method to spatially varying thermal transport problems in molecular dynamics. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010, 18, 085007.	0.8	13
632	Lattice Dynamics from Force-Fields as a Technique for Mineral Physics. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 391-411.	2.2	8
633	Nanotube-based nanoelectromechanical systems: Control versus thermodynamic fluctuations. <i>Physical Review B</i> , 2010, 81, .	1.1	22
634	Elastic properties of imperfect single-walled carbon nanotubes under axial tension. <i>Computational Materials Science</i> , 2010, 49, 143-147.	1.4	35
635	Computational modeling of the transverse-isotropic elastic properties of single-walled carbon nanotubes. <i>Computational Materials Science</i> , 2010, 49, 544-551.	1.4	20
636	Temperature effects on mechanical properties of the (3,3) carbon nanotube X-junctions. <i>Computational Materials Science</i> , 2010, 49, 916-919.	1.4	4
637	Influence of nickel coating on the interfacial bonding characteristics of carbon nanotube-aluminum composites. <i>Computational Materials Science</i> , 2010, 49, 899-903.	1.4	45
638	Self-assembly of carbon nanotubes and boron nitride nanotubes into coaxial structures. <i>Computational Materials Science</i> , 2010, 50, 645-650.	1.4	10
639	Interplay of Catalyst Size and Metal-Carbon Interactions on the Growth of Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6952-6958.	1.5	40
640	Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons. <i>Physical Review Letters</i> , 2010, 104, 136403.	2.9	1,777
641	Free Folding of Suspended Graphene Sheets by Random Mechanical Stimulation. <i>Physical Review Letters</i> , 2010, 104, 166805.	2.9	143
642	Isotopic effects on the thermal conductivity of graphene nanoribbons: Localization mechanism. <i>Journal of Applied Physics</i> , 2010, 107, .	1.1	125

#	ARTICLE	IF	CITATIONS
643	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4939-4949.	1.5	288
644	Geometry Controls Conformation of Graphene Sheets: Membranes, Ribbons, and Scrolls. <i>ACS Nano</i> , 2010, 4, 3869-3876.	7.3	227
645	Modeling of Thermal Transport in Pillared-Graphene Architectures. <i>ACS Nano</i> , 2010, 4, 1153-1161.	7.3	280
646	Magnetic graphene: A new class of cages formed from graphene sheets and carbon nanotubes. <i>Physical Review B</i> , 2010, 82, .	1.1	9
647	On the utility of vacancies and tensile strain-induced quality factor enhancement for mass sensing using graphene monolayers. <i>Nanotechnology</i> , 2010, 21, 105710.	1.3	31
648	Determination of mechanical property of nanostructure using nano-macro equivalent mechanics method. , 2010, , .		0
649	Friction law for water flowing in carbon nanotubes. , 2010, , .		3
650	Nonlocal shear deformable shell model for thermal postbuckling of axially compressed double-walled carbon nanotubes. <i>Philosophical Magazine</i> , 2010, 90, 3189-3214.	0.7	18
651	Nanoresonator Based on Relative Vibrations of the Walls of Carbon Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2010, 18, 523-530.	1.0	9
652	A translational nanoactuator based on carbon nanoscrolls on substrates. <i>Applied Physics Letters</i> , 2010, 96, .	1.5	81
653	Excess energy and deformation along free edges of graphene nanoribbons. <i>Physical Review B</i> , 2010, 81, .	1.1	78
654	<i>Colloquium</i> : Failure of molecules, bones, and the Earth itself. <i>Reviews of Modern Physics</i> , 2010, 82, 1459-1487.	16.4	42
655	Mechanisms of Ion-Beam Modification of Terthiophene Oligomers from Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23936-23945.	1.5	6
656	Interlayer interaction and relative vibrations of bilayer graphene. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5687.	1.3	149
657	From graphene sheets to graphene nanoribbons: Dimensional crossover signals in structural thermal fluctuations. <i>Physical Review B</i> , 2011, 83, .	1.1	11
658	Strain engineering of thermal conductivity in graphene sheets and nanoribbons: a demonstration of magic flexibility. <i>Nanotechnology</i> , 2011, 22, 105705.	1.3	346
659	A nonequilibrium Greenâ€™s function study of thermoelectric properties in single-walled carbon nanotubes. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	102
660	Effect of Fluorocarbon Molecules Confined between Sliding Self-Mated PTFE Surfaces. <i>Langmuir</i> , 2011, 27, 9910-9919.	1.6	9

#	ARTICLE	IF	CITATIONS
661	A new REBO potential based atomistic structural model for graphene sheets. <i>Nanotechnology</i> , 2011, 22, 295711.	1.3	22
662	Modelling materials for fusion power. <i>International Materials Reviews</i> , 2011, 56, 324-340.	9.4	7
663	A Stretched Carbon Nanotube with a High-Density of Topological Defect. <i>Advanced Materials Research</i> , 0, 236-238, 2225-2228.	0.3	0
664	Molecular Dynamics Simulations Elucidate the Synergy of C ₆₀ and Low-Energy Ar Cobombardment for Molecular Depth Profiling. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2635-2638.	2.1	9
665	Self-Assembly of Gold Nanowires along Carbon Nanotubes for Ultrahigh-Aspect-Ratio Hybrids. <i>Chemistry of Materials</i> , 2011, 23, 2760-2765.	3.2	20
666	Elastic Moduli of Carbon Nanohorns. <i>Journal of Nanomaterials</i> , 2011, 2011, 1-6.	1.5	7
667	Influence of hydrogen functionalization on thermal conductivity of graphene: Nonequilibrium molecular dynamics simulations. <i>Applied Physics Letters</i> , 2011, 98, .	1.5	113
668	Thermal Decomposition of Condensed-Phase Nitromethane from Molecular Dynamics from ReaxFF Reactive Dynamics. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6534-6540.	1.2	105
669	Joule heating and thermoelectric properties in short single-walled carbon nanotubes: Electron-phonon interaction effect. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	42
670	Diffusion and drift of graphene flake on graphite surface. <i>Journal of Chemical Physics</i> , 2011, 134, 104505.	1.2	43
671	Vibrational Properties and Specific Heat of Ultrananocrystalline Diamond: Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 21691-21699.	1.5	20
672	On the effective plate thickness of monolayer graphene from flexural wave propagation. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	22
673	Strains and pseudomagnetic fields in circular graphene rings. <i>Physical Review B</i> , 2011, 84, .	1.1	34
674	Vibration of Single- and Double-Layered Graphene Sheets. <i>Journal of Nanotechnology in Engineering and Medicine</i> , 2011, 2, .	0.8	76
675	Continuum theory of dislocations and buckling in graphene. <i>Physical Review B</i> , 2011, 84, .	1.1	53
676	Thermal conductivity reduction through isotope substitution in nanomaterials: predictions from an analytical classical model and nonequilibrium molecular dynamics simulations. <i>Nanoscale</i> , 2011, 3, 3714.	2.8	54
677	Nonlinear Mechanical Properties of Graphene Nanoribbons. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1284, 165.	0.1	1
678	Bending behavior of double-walled carbon nanotubes with <i>sp³</i> interwall bonds. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	11

#	ARTICLE	IF	CITATIONS
679	Lattice thermal properties of graphane: Thermal contraction, roughness, and heat capacity. <i>Physical Review B</i> , 2011, 83, .	1.1	47
680	A Molecular Dynamics Investigaation of the Torsional Responses of Defective Single-Walled Carbon Nanotubes. <i>Procedia Engineering</i> , 2011, 14, 1307-1311.	1.2	1
681	The integrated effects of temperature and stress on the formation of carbon linear atomic chains from graphene nanoribbons. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	8
682	A molecular dynamics study of the mechanical properties of graphene nanoribbon-embedded gold composites. <i>Nanoscale</i> , 2011, 3, 4307.	2.8	11
683	Heat conduction in graphene flakes with inhomogeneous mass interface. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2011, 2011, P10031.	0.9	14
684	Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 035401.	0.7	39
685	Nanoscale continuum calculation of basal dislocation core structures in graphite. <i>Philosophical Magazine</i> , 2011, 91, 1441-1463.	0.7	7
686	Bottom-up coarse-graining of a simple graphene model: The blob picture. <i>Journal of Chemical Physics</i> , 2011, 134, 064106.	1.2	37
687	Molecular dynamics simulations of thermal transport in porous nanotube network structures. <i>Nanoscale</i> , 2011, 3, 3679.	2.8	31
688	Carbon Nanotube-Based Sensors for Detection of Gas Atoms. <i>Journal of Nanotechnology in Engineering and Medicine</i> , 2011, 2, .	0.8	22
689	Effective Elastic Moduli Evaluation of Single Walled Carbon Nanotubes Using Flexural Vibrations. <i>Mechanics of Advanced Materials and Structures</i> , 2011, 18, 262-271.	1.5	11
690	Properties on the edge: graphene edge energies, edge stresses, edge warping, and the Wulff shape of graphene flakes. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011, 19, 054002.	0.8	18
691	Effect of the Metal-Substrate Interaction Strength on the Growth of Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7668-7675.	1.5	20
692	Cutting and controlled modification of graphene with ion beams. <i>Nanotechnology</i> , 2011, 22, 175306.	1.3	130
693	Atomistic simulation and continuum modeling of graphene nanoribbons under uniaxial tension. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011, 19, 054006.	0.8	121
694	Thermal conductivity and thermal rectification in unzipped carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 215301.	0.7	23
695	Diameter and Temperature Dependence of Thermal Conductivity of Single-Walled Carbon Nanotubes. <i>Chinese Physics Letters</i> , 2011, 28, 066104.	1.3	8
696	Transformation of nano-diamonds to carbon nano-onions studied by X-ray diffraction and molecular dynamics. <i>Diamond and Related Materials</i> , 2011, 20, 1333-1339.	1.8	33

#	ARTICLE	IF	CITATIONS
697	Methane in carbon nanotube: molecular dynamics simulation. <i>Molecular Physics</i> , 2011, 109, 1691-1699.	0.8	22
698	Molecular dynamics study of effects of intertube spacing on sliding behaviors of multi-walled carbon nanotube. <i>Computational Materials Science</i> , 2011, 50, 971-974.	1.4	11
699	A robust nano-mechanics approach for tensile and modal analysis using atomistic-continuum mechanics method. <i>Computational Materials Science</i> , 2011, 50, 2245-2248.	1.4	1
700	Size effect on mechanical properties of carbon nanotube X-junctions. <i>Computational Materials Science</i> , 2011, 50, 3067-3070.	1.4	12
701	Charge and Mass Effects on Low Energy Ion Channeling in Carbon Nanotubes. <i>Chinese Physics Letters</i> , 2011, 28, 066101.	1.3	2
702	Dependence of mechanical characteristics and the fracture and buckling behavior of single-walled carbon nanotubes on their geometry. <i>New Carbon Materials</i> , 2011, 26, 408-416.	2.9	11
703	Strength of ultrananocrystalline diamond controlled by friction of buried interfaces. <i>Journal Physics D: Applied Physics</i> , 2011, 44, 405401.	1.3	12
704	Molecular Dynamics Simulation Study on the Mechanical Properties and Fracture Behavior of Single-Wall Carbon Nanotubes. , 0, , .		3
705	Application of the Continuum-Lattice Thermodynamics. , 2011, , .		0
706	Mechanisms of Single-Walled Carbon Nanotube Nucleation, Growth and Chirality-Control: Insights from QM/MD Simulations. , 2011, , .		0
709	Molecular Dynamics Simulations on Tension of Graphene and Graphite Containing Vacancies. <i>Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A</i> , 2011, 77, 1279-1291.	0.2	0
710	Aspect ratio dependent buckling mode transition in single-walled carbon nanotubes under compression. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	37
711	Observation of nonclassical scaling laws in the quality factors of cantilevered carbon nanotube resonators. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	33
712	Tribological Aspects of Carbon-Based Nanocoatings - Theory and Simulation. <i>Zeitschrift Fur Physikalische Chemie</i> , 2011, 225, 379-387.	1.4	4
713	Thermal Rectification in Graphene and Carbon Nanotube Systems Using Molecular Dynamics Simulations. , 2011, , .		1
714	Anisotropic mechanical amorphization drives wear in diamond. <i>Nature Materials</i> , 2011, 10, 34-38.	13.3	282
715	Isotopic effects in the energy spectrum of molecules sputtered from carbon. <i>Journal of Nuclear Materials</i> , 2011, 415, S121-S124.	1.3	0
716	Improved hydrocarbon potentials for sputtering studies. <i>Journal of Nuclear Materials</i> , 2011, 415, S183-S186.	1.3	1

#	ARTICLE	IF	CITATIONS
717	Progress in modeling erosion and redeposition on plasma facing materials. <i>Journal of Nuclear Materials</i> , 2011, 415, S10-S18.	1.3	3
718	Nanotube/matrix interfacial friction and sliding in composites with an amorphous carbon matrix. <i>Scripta Materialia</i> , 2011, 65, 1014-1017.	2.6	19
719	Hyperelastic axial buckling of single wall carbon nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 44, 525-529.	1.3	11
720	Multiscale modeling of graphene- and nanotube-based reinforced polymer nanocomposites. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 4034-4040.	0.9	104
721	Ultrafast nano-oscillators based on interlayer-bridged carbon nanoscrolls. <i>Nanoscale Research Letters</i> , 2011, 6, 470.	3.1	30
722	A rod model for three dimensional deformations of single-walled carbon nanotubes. <i>International Journal of Solids and Structures</i> , 2011, 48, 2849-2858.	1.3	27
723	Shear-induced lamellar ordering and interfacial sliding in amorphous carbon films: A superlow friction regime. <i>Chemical Physics Letters</i> , 2011, 514, 325-329.	1.2	35
724	Graphene-based torsional resonator from molecular-dynamics simulation. <i>Europhysics Letters</i> , 2011, 96, 66007.	0.7	4
725	Reparameterization of the REBO-CHO potential for graphene oxide molecular dynamics simulations. <i>Physical Review B</i> , 2011, 84, .	1.1	35
726	Mechanical Properties of Vacancy-containing Graphene and Graphite Estimated by Molecular Dynamics Simulations. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1362, 1.	0.1	4
727	Morphologies of monolayer graphene under indentation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011, 19, 054004.	0.8	6
728	Molecular dynamics simulation of the self-retracting motion of a graphene flake. <i>Physical Review B</i> , 2011, 84, .	1.1	35
729	Radial deformation and its related energy variations of single-walled carbon nanotubes. <i>Physical Review B</i> , 2011, 83, .	1.1	35
730	Monte Carlo simulation of temperature-dependent elastic properties of graphene. <i>Physical Review B</i> , 2011, 84, .	1.1	23
731	Description for mechanical properties of graphene using particles with rotational degrees of freedom. <i>Doklady Physics</i> , 2011, 56, 527-530.	0.2	20
732	Interfacial sliding in carbon nanotube/diamond matrix composites. <i>Acta Materialia</i> , 2011, 59, 6700-6709.	3.8	30
733	Reversible phase transformation in graphene nano-ribbons: Lattice shearing based mechanism. <i>Acta Materialia</i> , 2011, 59, 6783-6789.	3.8	22
734	Thermal stability and morphological variation of carbon nanorings of different radii during the temperature elevating process: a molecular dynamics simulation study. <i>Journal of Nanoparticle Research</i> , 2011, 13, 1995-2006.	0.8	5

#	ARTICLE	IF	CITATIONS
735	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. Tribology Letters, 2011, 42, 193-201.	1.2	25
736	The effect of the target structure and composition on the ejection and transport of polymer molecules and carbon nanotubes in matrix-assisted pulsed laser evaporation. Applied Physics A: Materials Science and Processing, 2011, 105, 529-546.	1.1	31
737	A pulsed neutron diffraction study of the topological defects presence in carbon nanohorns. Chemical Physics Letters, 2011, 502, 87-91.	1.2	21
738	Multiscale modeling of the effect of carbon nanotube orientation on the shear deformation properties of reinforced polymer-based composites. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 1588-1597.	0.9	22
739	Detection of gas atoms via vibration of graphenes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 2411-2415.	0.9	90
740	Chemical versus thermal folding of graphene edges. Nano Research, 2011, 4, 1242-1247.	5.8	8
741	Elastic properties of various boron-nitride structures. Metals and Materials International, 2011, 17, 21-27.	1.8	27
742	Enhancing surface heat transfer by carbon nanofins: towards an alternative to nanofluids?. Nanoscale Research Letters, 2011, 6, 249.	3.1	27
743	Buckling of a non-Euclidean annular plate. Proceedings in Applied Mathematics and Mechanics, 2011, 11, 277-278.	0.2	2
744	Negative stiffness of a buckled carbon nanotube in composite systems via molecular dynamics simulation. Physica Status Solidi (B): Basic Research, 2011, 248, 88-95.	0.7	10
745	Sputtering soft materials with molecular projectiles: a microscopic view. Surface and Interface Analysis, 2011, 43, 16-19.	0.8	12
746	Torsional strain energy evolution of carbon nanotubes and their stability with encapsulated helical copper nanowires. Carbon, 2011, 49, 1408-1415.	5.4	26
747	Structure and energetics of hydrogen chemisorbed on a single graphene layer to produce graphane. Carbon, 2011, 49, 3258-3266.	5.4	54
748	A theoretical analysis of frictional and defect characteristics of graphene probed by a capped single-walled carbon nanotube. Carbon, 2011, 49, 3687-3697.	5.4	71
749	Mechanical properties of graphyne. Carbon, 2011, 49, 4111-4121.	5.4	385
750	Mechanical properties of bilayer graphene sheets coupled by sp bonding. Carbon, 2011, 49, 4511-4517.	5.4	219
751	Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. Combustion and Flame, 2011, 158, 217-226.	2.8	196
752	Sanders shell model for buckling of single-walled carbon nanotubes with small aspect ratio. Composite Structures, 2011, 93, 1683-1691.	3.1	80

#	ARTICLE	IF	CITATIONS
753	Molecular simulations on the chirality preference of single-walled carbon nanotubes upon ductile behavior under tensile stress at high temperature. <i>Chemical Physics Letters</i> , 2011, 503, 272-276.	1.2	8
754	C-directional compression of nano-graphite: a comparison between effects of uniform and non-uniform pressure. <i>Physica B: Condensed Matter</i> , 2011, 406, 2763-2766.	1.3	3
755	Effects of temperature and torsion speed on torsional properties of single-walled carbon nanotubes. <i>Materials Science and Engineering C</i> , 2011, 31, 452-457.	3.8	29
756	Evolution of carbon based surfaces under bombardment: Examining the steady-state surface properties and the effect of potential. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2011, 269, 1271-1275.	0.6	2
757	Analysis of the entanglements in carbon nanotube fibers using a self-folded nanotube model. <i>Journal of the Mechanics and Physics of Solids</i> , 2011, 59, 511-524.	2.3	43
758	Wave propagation in double-walled carbon nanotubes on a novel analytically nonlocal Timoshenko-beam model. <i>Journal of Sound and Vibration</i> , 2011, 330, 1704-1717.	2.1	60
759	Mechanism of swift chemical sputtering: Comparison of Be/C/W dimer bond breaking. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2011, 269, 1257-1261.	0.6	12
760	Chemical sputtering of deuterated carbon surfaces at various surface temperatures. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2011, 269, 1280-1283.	0.6	3
761	Molecular dynamics study of effects of nickel coating on torsional behavior of single-walled carbon nanotube. <i>Physica B: Condensed Matter</i> , 2011, 406, 992-995.	1.3	13
762	Hyperelastic modelling of post-buckling response in single wall carbon nanotubes under axial compression. <i>Procedia Engineering</i> , 2011, 10, 2256-2261.	1.2	5
763	Critical buckling temperature of single-walled carbon nanotubes embedded in a one-parameter elastic medium based on nonlocal continuum mechanics. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 1185-1191.	1.3	67
764	Graphene characterization: A fully non-linear spring-based finite element prediction. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 1833-1839.	1.3	53
765	The effects of vacancy defects and nitrogen doping on the thermal conductivity of armchair (10, 10) single-wall carbon nanotubes. <i>Solid State Communications</i> , 2011, 151, 1004-1008.	0.9	17
766	Hydrogenation and surface density changes in hydrocarbon films during erosion using Ar/H ₂ plasmas. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	18
767	Extension of Binary-Collision-Approximation-Based Simulation Applicable to Any Structured Target Material. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 01AB03.	0.8	7
768	Molecular Dynamics Simulation of Hydrogen Injection onto Diamond Surfaces. <i>Japanese Journal of Applied Physics</i> , 0, 50, 01AB04.	0.8	3
769	Step driven competitive epitaxial and self-limited growth of graphene on copper surface. <i>AIP Advances</i> , 2011, 1, .	0.6	21
770	Computational study of electron-irradiation effects in carbon nanomaterials on substrates. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2011, 29, 06FG09.	0.6	7

#	ARTICLE	IF	CITATIONS
771	Theoretical study of thermal conductivity in single-walled boron nitride nanotubes. Physical Review B, 2011, 84, .	1.1	31
772	Reaction between graphene and hydrogen under oblique injection. Journal of Applied Physics, 2011, 110, 084320.	1.1	5
773	Tuning thermal transport in nanotubes with topological defects. Applied Physics Letters, 2011, 99, 091905.	1.5	24
774	Thermal transport in graphene and effects of vacancy defects. Physical Review B, 2011, 84, .	1.1	199
775	Molecular dynamics simulation for heat transport in thin diamond nanowires. Physical Review B, 2011, 83, .	1.1	17
776	Tight binding within the fourth moment approximation: Efficient implementation and application to liquid Ni droplet diffusion on graphene. Physical Review B, 2011, 84, .	1.1	10
777	Structural and mechanical properties of partially unzipped carbon nanotubes. Physical Review B, 2011, 83, .	1.1	28
778	Periodic ripples in suspended graphene. Physical Review B, 2011, 83, .	1.1	67
779	Thermal-Induced Edge Barriers and Forces in Interlayer Interaction of Concentric Carbon Nanotubes. Physical Review Letters, 2011, 107, 105502.	2.9	81
780	Dynamic ripples in single layer graphene. Applied Physics Letters, 2011, 98, .	1.5	42
781	Commensurate-incommensurate phase transition in bilayer graphene. Physical Review B, 2011, 84, .	1.1	86
782	Friction of water slipping in carbon nanotubes. Physical Review E, 2011, 83, 036316.	0.8	80
783	Anomalous thermal relaxation in carbon nanoclusters. Applied Physics Letters, 2011, 98, 193106.	1.5	4
785	Packing efficiency and accessible surface area of crumpled graphene. Physical Review B, 2011, 84, .	1.1	110
786	Dynamic response of graphene to thermal impulse. Physical Review B, 2011, 84, .	1.1	66
787	Thermal transport in double-wall carbon nanotubes using heat pulse. Journal of Applied Physics, 2011, 110, .	1.1	17
788	Surface-adsorption-induced bending behaviors of graphene nanoribbons. Applied Physics Letters, 2011, 98, 121909.	1.5	35
789	Thermal conductivity of deformed carbon nanotubes. Journal of Applied Physics, 2011, 109, 074317.	1.1	9

#	ARTICLE	IF	CITATIONS
790	Interfacial properties and morphologies of graphene-graphane composite sheets. Journal of Applied Physics, 2011, 109, 054314.	1.1	25
791	Thermal conductance modulator based on folded graphene nanoribbons. Applied Physics Letters, 2011, 99, 233101.	1.5	50
792	Compressive dynamic scission of carbon nanotubes under sonication: fracture by atomic ejection. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1270-1289.	1.0	24
793	A Study on Mechanism of Tribological Behavior of Carbon Nanotubes. Advanced Materials Research, 0, 306-307, 1444-1449.	0.3	1
794	Mechanical Properties of Single Crystal Diamond Estimated by Molecular Dynamics Simulation with the Second-Generation REBO Potential. Materials Research Society Symposia Proceedings, 2011, 1362, 1.	0.1	0
795	Extrinsic morphology of graphene. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 054005.	0.8	20
796	Wetting of Liquid Iron in Carbon Nanotubes and on Graphene Sheets: A Molecular Dynamics Study. Chinese Physics Letters, 2011, 28, 036102.	1.3	10
797	Elastic Moduli of Carbon Nanotubes Using Second Generation Improved Brenner Potential. Journal of Nano Research, 2011, 15, 1-10.	0.8	12
798	Reassessing molecular sieving by kinked carbon nanotubes. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 085009.	0.8	6
799	A simple molecular mechanics potential for $\hat{1}/4m$ scale graphene simulations from the adaptive force matching method. Journal of Chemical Physics, 2011, 134, 184704.	1.2	51
800	Vanishing stick-slip friction in few-layer graphenes: the thickness effect. Nanotechnology, 2011, 22, 285708.	1.3	99
801	Molecular Dynamics Simulation of Nanoindentation on Diamond Crystal [100] Surface. Advanced Materials Research, 2011, 399-401, 751-759.	0.3	0
802	The Unravelling of Open-Ended Single Walled Carbon Nanotubes Using Molecular Dynamics Simulations. Journal of Electronic Packaging, Transactions of the ASME, 2011, 133, .	1.2	10
803	Thermal Conductivity of Carbon Nanotubes With Defects. , 2011, , .		4
804	Nanocatalyst structure as a template to define chirality of nascent single-walled carbon nanotubes. Journal of Chemical Physics, 2011, 134, 014705.	1.2	36
805	Thermal transport by phonons in zigzag graphene nanoribbons with structural defects. Journal of Physics Condensed Matter, 2011, 23, 315302.	0.7	60
806	Slip boundaries in nanopores. Molecular Simulation, 2011, 37, 1023-1030.	0.9	6
807	EXAMINATION OF CYLINDRICAL SHELL THEORIES FOR BUCKLING OF CARBON NANOTUBES. International Journal of Structural Stability and Dynamics, 2011, 11, 1035-1058.	1.5	33

#	ARTICLE	IF	CITATIONS
808	Tensile and compressive behaviors of open-tip carbon nanocones under axial strains. Journal of Materials Research, 2011, 26, 1577-1584.	1.2	21
809	Mechanical properties of grafold: a demonstration of strengthened graphene. Nanotechnology, 2011, 22, 405701.	1.3	75
810	Molecular Dynamics Simulation of Chemical Vapor Deposition of Amorphous Carbon: Dependence on H/C Ratio of Source Gas. Japanese Journal of Applied Physics, 2011, 50, 01AB01.	0.8	4
811	A Molecular Mechanics Study of Morphologic Interaction between Graphene and Si Nanowires on a SiO ₂ Substrate. Journal of Nanomaterials, 2011, 2011, 1-7.	1.5	4
812	Investigative Tools: Theory, Modeling, and Simulation. , 2011, , 29-69.		4
813	Size Dependence of the Nonlinear Elastic Softening of Nanoscale Graphene Monolayers under Plane-Strain Bulge Tests: A Molecular Dynamics Study. Journal of Nanomaterials, 2011, 2011, 1-6.	1.5	11
814	First-principles study of void induced stresses at a diamond (100) grain boundary. Journal of Applied Physics, 2011, 109, 033518.	1.1	6
815	Slip flow in graphene nanochannels. Journal of Chemical Physics, 2011, 135, 144701.	1.2	104
816	Effect of Defects on Oscillatory Behaviors of Double-Walled Carbon Nanotube Oscillators. Advanced Materials Research, 0, 308-310, 584-588.	0.3	1
817	Calculation of self-diffusion coefficients in diamond. Applied Physics Letters, 2012, 100, .	1.5	38
818	Nanomechanics of Nonideal Single- and Double-Walled Carbon Nanotubes. Journal of Nanomaterials, 2012, 2012, 1-9.	1.5	21
819	Critical Dispersion Distance of Silicon Nanoparticles Intercalated between Graphene Layers. Journal of Nanomaterials, 2012, 2012, 1-4.	1.5	4
820	Transitional Failure of Carbon Nanotube Systems under a Combination of Tension and Torsion. Journal of Nanomaterials, 2012, 2012, 1-6.	1.5	1
821	Molecular Dynamics Study on Formation of Carbon Nanotube X-Shaped Junction by Heat Welding. Advanced Materials Research, 0, 538-541, 1460-1463.	0.3	0
822	Anisotropic Bond Orientation of Amorphous Carbon by Deposition. Japanese Journal of Applied Physics, 2012, 51, 01AC05.	0.8	2
823	Investigation of the effects of commensurability on friction between concentric carbon nanotubes. Nanotechnology, 2012, 23, 015702.	1.3	3
824	Effects of heat treatment and contact resistance on the thermal conductivity of individual multiwalled carbon nanotubes using a Wollaston wire thermal probe. Journal of Applied Physics, 2012, 111, .	1.1	21
825	Rippled nanocarbons from periodic arrangements of reordered bivacancies in graphene or nanotubes. Journal of Chemical Physics, 2012, 136, 124705.	1.2	7

#	ARTICLE	IF	CITATIONS
826	Torsional stability of carbon nanotubes filled with copper atoms. <i>Physica Scripta</i> , 2012, 85, 045602.	1.2	7
827	Morphology and in-plane thermal conductivity of hybrid graphene sheets. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	56
828	Atomistic Modeling of Gas Adsorption in Nanocarbons. <i>Journal of Nanomaterials</i> , 2012, 2012, 1-32.	1.5	11
829	Prediction of Coefficients of Thermal Expansion of 3-D CNT-Graphene Junctioned Carbon Nanostructures. , 2012, , .		0
830	Assessment of the resonance frequency of cantilever carbon nanocones using molecular dynamics simulation. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	15
831	Interfacial slip friction at a fluid-solid cylindrical boundary. <i>Journal of Chemical Physics</i> , 2012, 136, 244704.	1.2	35
832	Nonlinear breatherlike localized modes in C ₆₀ nanocrystals. <i>Physical Review B</i> , 2012, 85, .	1.1	29
833	Study on the mechanical behavior of tilt bicrystal graphene by molecular dynamics simulations: Bulk versus nanoribbons. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	10
834	Slip length of water on graphene: Limitations of non-equilibrium molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2012, 136, 024705.	1.2	166
835	Bioinspired design of functionalised graphene. <i>Molecular Simulation</i> , 2012, 38, 695-703.	0.9	17
836	Influence of Intertube Additional Atoms on Sliding Behaviors of Double-Walled Carbon Nanotube. <i>Communications in Theoretical Physics</i> , 2012, 58, 432-436.	1.1	1
837	Stress-induced annihilation of Stone-Wales defects in graphene nanoribbons. <i>Journal Physics D: Applied Physics</i> , 2012, 45, 305303.	1.3	31
838	THE ROLE OF POTENTIAL FUNCTIONS IN THE MECHANICAL BEHAVIOR OF THE SINGLE WALL CARBON NANOTUBES. <i>International Journal of Nanoscience</i> , 2012, 11, 1240009.	0.4	1
839	Nanoengineering carbon nanotubes: The effects of electron irradiation on nanotube structure. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1407, 56.	0.1	1
840	Mechanical Properties of Hydrogen Functionalized Graphyne - A Molecular Dynamics Investigation. <i>Advanced Materials Research</i> , 0, 472-475, 1813-1817.	0.3	5
841	Nonlocal material properties of single-walled carbon nanotubes. <i>International Journal of Smart and Nano Materials</i> , 2012, 3, 141-151.	2.0	8
842	Enhancing the mass sensitivity of graphene nanoresonators via nonlinear oscillations: the effective strain mechanism. <i>Nanotechnology</i> , 2012, 23, 475501.	1.3	41
843	Forming electronic waveguides from graphene grain boundaries. <i>Journal of Nanophotonics</i> , 2012, 6, 061718.	0.4	6

#	ARTICLE	IF	CITATIONS
844	An MD Study of the Temperature Effect on H Interacting with SiC (100). Plasma Science and Technology, 2012, 14, 1121-1124.	0.7	0
845	Effects of Stone-Wales Defects on the Thermal Conductivity of Carbon Nanotubes. Journal of Heat Transfer, 2012, 134, .	1.2	13
846	Effect of vacancy defects on the thermal conductivity of graphene nanoribbons: a molecular dynamics study. International Journal of Materials and Structural Integrity, 2012, 6, 26.	0.1	4
847	Carbon nanotube-based charge-controlled speed-regulating nanoclutch. Journal of Applied Physics, 2012, 111, 114304.	1.1	15
848	Why edge effects are important on the intrinsic loss mechanisms of graphene nanoresonators. Journal of Applied Physics, 2012, 111, 054314.	1.1	41
849	Engineering materials properties in codimension > 0. Journal of Materials Research, 2012, 27, 619-626.	1.2	1
850	Investigation of thermal resistance for the graphene-Si interface by molecular dynamics. International Journal of Materials and Structural Integrity, 2012, 6, 65.	0.1	10
851	Natural torsion in chiral single-wall carbon nanotubes. Journal of Physics Condensed Matter, 2012, 24, 485302.	0.7	7
852	Tuning the band gap of bilayer graphene by ion implantation: Insight from computational studies. Physical Review B, 2012, 86, .	1.1	26
853	Thermal Transport in Functionalized Graphene. ACS Nano, 2012, 6, 9050-9057.	7.3	119
854	Graphene-like structure of activated anthracites. Journal of Physics Condensed Matter, 2012, 24, 495303.	0.7	5
855	Potential energy surface for graphene on graphene: Ab initio derivation, analytical description, and microscopic interpretation. Physical Review B, 2012, 86, .	1.1	128
857	Predictive modeling of formation of carbon nanostructures. Nanotechnologies in Russia, 2012, 7, 575-587.	0.7	1
858	Porous Carbon Nanotube Membranes for Separation of H ₂ /CH ₄ and CO ₂ /CH ₄ Mixtures. Journal of Physical Chemistry C, 2012, 116, 25904-25910.	1.5	59
859	Symmetry of chiral nanotubes: Natural torsion and diffraction evidence. Physica Status Solidi (B): Basic Research, 2012, 249, 2446-2449.	0.7	1
860	Atomistic simulations of diamond-like carbon growth. Thin Solid Films, 2012, 521, 239-244.	0.8	10
861	A molecular dynamics simulation study for the mechanical properties of different types of carbon nanotubes. Applied Nanoscience (Switzerland), 2012, 2, 377-383.	1.6	2
862	Acoustic and breathing phonon modes in bilayer graphene with Moiré patterns. Applied Physics Letters, 2012, 101, 023113.	1.5	25

#	ARTICLE	IF	CITATIONS
863	Nanomechanics of CNTs for sensor application. , 2012, , .		2
864	Tensile loading characteristics of free-form and water submerged single layer graphene sheet. , 2012, , .		4
865	Saddles, twists, and curls: shape transitions in freestanding nanoribbons. <i>Nanoscale</i> , 2012, 4, 3620.	2.8	14
866	Knitted graphene-nanoribbon sheet: a mechanically robust structure. <i>Nanoscale</i> , 2012, 4, 785-791.	2.8	22
867	Enhancing interwall load transfer by vacancy defects in carbon nanotubes. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	12
868	Top-down vs. bottom-up coarse-graining of graphene and CNTs for nanodevice simulation. , 2012, , .		0
869	Thermal control in graphene nanoribbons: thermal valve, thermal switch and thermal amplifier. <i>Nanoscale</i> , 2012, 4, 5217.	2.8	21
870	Comparing the effects of dispersed Stoneâ€“Throwerâ€“Wales defects and double vacancies on the thermal conductivity of graphene nanoribbons. <i>Nanotechnology</i> , 2012, 23, 385702.	1.3	56
871	Thermal rectification in asymmetric U-shaped graphene flakes. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2012, 2012, P06011.	0.9	18
872	Geometry and temperature effects of the interfacial thermal conductance in copperâ€“ and nickelâ€“graphene nanocomposites. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 245301.	0.7	79
873	Formation Enthalpies Derived from Pairwise Interactions: A Step toward More Transferable Reactive Potentials for Organic Compounds. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1295-1303.	2.3	4
874	Molecular Dynamics Simulations of Atomic H Etching SiC Surface. <i>Physics Procedia</i> , 2012, 32, 539-544.	1.2	2
875	Thermal transport in graphene. <i>Solid State Communications</i> , 2012, 152, 1321-1330.	0.9	165
876	Molecular dynamics study on the thermal conductivity and mechanical properties of boron doped graphene. <i>Solid State Communications</i> , 2012, 152, 1503-1507.	0.9	89
877	Bond-order potentials with split-charge equilibration: Application to C-, H-, and O-containing systems. <i>Journal of Chemical Physics</i> , 2012, 136, 164701.	1.2	25
878	Ultrathin Carbon Nanotube With Single, Double, and Triple Bonds. <i>Physical Review Letters</i> , 2012, 109, 105501.	2.9	8
879	Atomistic study on the strength of symmetric tilt grain boundaries in graphene. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	40
880	Buckling instability of carbon nanoscrolls. <i>Journal of Applied Physics</i> , 2012, 112, 063515.	1.1	26

#	ARTICLE	IF	CITATIONS
881	Nanofracture in graphene under complex mechanical stresses. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	89
882	Influence of typical defects on thermal conductivity of graphene nanoribbons: An equilibrium molecular dynamics simulation. <i>Applied Surface Science</i> , 2012, 258, 9926-9931.	3.1	43
883	Mechanics of thermophoretic and thermally induced edge forces in carbon nanotube nanodevices. <i>Journal of the Mechanics and Physics of Solids</i> , 2012, 60, 1676-1687.	2.3	55
884	Effects of single vacancy defect position on the stability of carbon nanotubes. <i>Microelectronics Reliability</i> , 2012, 52, 1279-1284.	0.9	39
885	Size- and shape-dependent effective properties of single-walled super carbon nanotubes via a generalized molecular structure mechanics method. <i>Computational Materials Science</i> , 2012, 61, 27-33.	1.4	11
886	Mechanical properties of graphyne and its family – A molecular dynamics investigation. <i>Computational Materials Science</i> , 2012, 61, 83-88.	1.4	189
887	Detection of gas atoms with graphene sheets. <i>Computational Materials Science</i> , 2012, 60, 245-249.	1.4	22
888	Tensile mechanical behaviors of cubic silicon carbide thin films. <i>Computational Materials Science</i> , 2012, 62, 195-202.	1.4	20
889	Fullerene and graphene formation from carbon nanotube fragments. <i>Computational and Theoretical Chemistry</i> , 2012, 987, 115-121.	1.1	13
890	Molecular dynamics simulations based on reactive force-fields for surface chemical reactions. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 152-158.	1.1	9
891	Adsorption of colloid nanoparticles on carbon nanotubes studied by means of molecular dynamics simulations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2012, 409, 149-158.	2.3	9
892	Nanomechanics of imperfectly straight single walled carbon nanotubes under axial compression by using molecular dynamics simulation. <i>Computational Materials Science</i> , 2012, 53, 268-277.	1.4	30
893	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. <i>Computational Materials Science</i> , 2012, 54, 91-96.	1.4	39
894	Molecular Dynamics Calculations of the Thermal Conductivity of Molecular Liquids, Polymers, and Carbon Nanotubes. <i>Soft Materials</i> , 2012, 10, 42-80.	0.8	41
895	Acoustic energy dissipation and thermalization in carbon nanotubes: Atomistic modeling and mesoscopic description. <i>Physical Review B</i> , 2012, 86, .	1.1	17
896	Computational aspects of many-body potentials. <i>MRS Bulletin</i> , 2012, 37, 513-521.	1.7	278
897	Kinetic nanofriction: a mechanism transition from quasi-continuous to ballistic-like Brownian regime. <i>Nanoscale Research Letters</i> , 2012, 7, 148.	3.1	28
898	Detection of hydrogen using graphene. <i>Nanoscale Research Letters</i> , 2012, 7, 198.	3.1	27

#	ARTICLE	IF	CITATIONS
900	A molecular dynamics investigation of the mechanical properties of graphene nanochains. Journal of Materials Chemistry, 2012, 22, 9798.	6.7	23
902	Bond order potentials for fracture, wear, and plasticity. MRS Bulletin, 2012, 37, 493-503.	1.7	49
903	Static and dynamic analysis of two-dimensional graphite lattices. Mechanics of Solids, 2012, 47, 517-524.	0.3	11
904	Carbon Nanotube Container: Complexes of $C_{50}H_{10}$ with Small Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4546-4555.	2.3	16
905	Modified reactive empirical bond-order potential for heterogeneous bonding environments. Journal of Chemical Physics, 2012, 137, 054102.	1.2	8
906	Theoretical Investigation of the Intrinsic Mechanical Properties of Single- and Double-Layer Graphene. Journal of Physical Chemistry C, 2012, 116, 22608-22618.	1.5	40
907	Mechanical behavior of MoS ₂ nanotubes under compression, tension, and torsion from molecular dynamics simulations. Journal of Applied Physics, 2012, 112, .	1.1	38
908	First-principles study of Cs and Sr sorption on carbon structures. Journal of Applied Physics, 2012, 111, .	1.1	10
909	An angular-dependent embedded atom method (A-EAM) interatomic potential to model thermodynamic and mechanical behavior of Al/Si composite materials. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 035007.	0.8	21
910	Theoretical Studies of UNCD Properties. , 2012, , 85-102.		1
911	Molecular dynamics simulation of hydrogenated carbon film growth from CH radicals. Applied Surface Science, 2012, 263, 339-344.	3.1	8
912	Fracture analysis of carbon nanotubes in the context of an atomic-based cellular automata algorithm. Computational Materials Science, 2012, 65, 85-90.	1.4	3
913	Heat welding of non-orthogonal X-junction of single-walled carbon nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 46, 30-32.	1.3	20
914	Nanomechanics of free form and water submerged single layer graphene sheet under axial tension by using molecular dynamics simulation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 556, 420-428.	2.6	44
915	Strong Adhesion and Friction Coupling in Hierarchical Carbon Nanotube Arrays for Dry Adhesive Applications. ACS Applied Materials & Interfaces, 2012, 4, 1972-1980.	4.0	32
916	A molecular dynamics study of the thermal conductivity of graphene nanoribbons containing dispersed Stone-Wales defects. Carbon, 2012, 50, 4887-4893.	5.4	150
917	Reactive Molecular Dynamics: Numerical Methods and Algorithmic Techniques. SIAM Journal of Scientific Computing, 2012, 34, C1-C23.	1.3	56
918	Surface-Induced Interphases During Curing Processes Between Bi- and Pentafunctional Components: Reactive Coarse-Grained Molecular Dynamics Simulations. Journal of Adhesion, 2012, 88, 903-923.	1.8	7

#	ARTICLE	IF	CITATIONS
919	Mechanical properties of polycrystalline graphene based on a realistic atomistic model. Physical Review B, 2012, 85, .	1.1	181
920	Transformation of non-orthogonal X-junction of single-walled carbon nanotubes into parallel junction by heating. Chemical Physics Letters, 2012, 547, 42-46.	1.2	6
921	Mechanics of SWCNT Aggregates Studied by Incremental Constrained Minimization. Journal of Nanomechanics & Micromechanics, 2012, 2, 15-22.	1.4	6
922	Simulation of Thermal and Electrical Transport in Nanotube and Nanowire Composites. Advanced Structured Materials, 2012, , 297-335.	0.3	0
923	Thermomechanical properties of graphene: valence force field model approach. Journal of Physics Condensed Matter, 2012, 24, 175303.	0.7	24
924	Molecular dynamics simulation of atomic-scale frictional behavior of corrugated nano-structured surfaces. Nanoscale, 2012, 4, 3937.	2.8	20
925	Intrinsic Strength and Failure Behaviors of Graphene Grain Boundaries. ACS Nano, 2012, 6, 2704-2711.	7.3	197
926	Wide-angle X-ray scattering as a quality test for carbon nanotubes. Diamond and Related Materials, 2012, 29, 18-22.	1.8	9
927	Molecular packing of fullerenes inside single-walled carbon nanotubes. Carbon, 2012, 50, 5450-5457.	5.4	10
928	How does folding modulate thermal conductivity of graphene?. Applied Physics Letters, 2012, 100, 093107.	1.5	82
929	A band-pass filter approach within molecular dynamics for the prediction of intrinsic quality factors of nanoresonators. Journal of Applied Physics, 2012, 112, .	1.1	14
930	Markovian dissipative coarse grained molecular dynamics for a simple 2D graphene model. Journal of Chemical Physics, 2012, 137, 234103.	1.2	7
931	Effect of SiO ₂ substrate on the irradiation-assisted manipulation of supported graphene: a molecular dynamics study. Nanotechnology, 2012, 23, 285703.	1.3	47
932	Simple optimized Brenner potential for thermodynamic properties of diamond. Philosophical Magazine, 2012, 92, 500-515.	0.7	2
933	Strain-engineered graphene through a nanostructured substrate. I. Deformations. Physical Review B, 2012, 85, .	1.1	57
934	Strain-engineered graphene through a nanostructured substrate. II. Pseudomagnetic fields. Physical Review B, 2012, 85, .	1.1	30
935	Extended graphynes: simple scaling laws for stiffness, strength and fracture. Nanoscale, 2012, 4, 7797.	2.8	167
936	Nanoengineered nonuniform strain in graphene using nanopillars. Physical Review B, 2012, 86, .	1.1	55

#	ARTICLE	IF	CITATIONS
937	Tuning thermal conductivity of bilayer graphene by inter-layer sp ³ bonding: A molecular dynamics study. <i>Applied Physics Letters</i> , 2012, 101, 053115.	1.5	58
938	Thermal Conductivity of Graphene Nanoribbons: Effect of the Edges and Ribbon Width. <i>Journal of Heat Transfer</i> , 2012, 134, .	1.2	4
939	Self-Assembly of Graphene Nanoribbons with Unsaturated Edges. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1407, 125.	0.1	0
941	Mechanical Properties of Graphene Nanobuds: A Molecular Dynamics Study. <i>Current Nanoscience</i> , 2012, 8, 89-96.	0.7	31
942	Microstructure and surface roughness of graphite-like carbon films deposited on silicon substrate by molecular dynamic simulation. <i>Surface and Interface Analysis</i> , 2012, 44, 837-843.	0.8	15
943	Hyperthermal Atomic Oxygen and Argon Modification of Polymer Surfaces Investigated by Molecular Dynamics Simulations. <i>Plasma Processes and Polymers</i> , 2012, 9, 690-700.	1.6	8
944	Extensions of DFTB to investigate molecular complexes and clusters. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 245-258.	0.7	30
945	Effect of amorphous carbon coatings on the mechanical behavior of silicon carbide nanowire. <i>Journal of Applied Physics</i> , 2012, 111, 094306.	1.1	18
946	Classical interatomic potential for orthorhombic uranium. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 235403.	0.7	23
947	Organic Semiconductors and their Applications in Photovoltaic Devices. <i>Polymer Reviews</i> , 2012, 52, 1-37.	5.3	100
948	Twisting graphene nanoribbons into carbon nanotubes. <i>Physical Review B</i> , 2012, 85, .	1.1	75
949	Thermal transport in grain boundary of graphene by non-equilibrium Green's function approach. <i>Applied Physics Letters</i> , 2012, 101, 043112.	1.5	51
950	Multiscale Experimental Mechanics of Hierarchical Carbon-Based Materials. <i>Advanced Materials</i> , 2012, 24, 2805-2823.	11.1	52
951	Classical Reactive Molecular Dynamics Implementations: State of the Art. <i>ChemPhysChem</i> , 2012, 13, 1127-1151.	1.0	73
952	Dynamic Models for Plasma-Wall Interactions. <i>Contributions To Plasma Physics</i> , 2012, 52, 465-477.	0.5	9
953	Thermal transport in graphyne nanoribbons. <i>Physical Review B</i> , 2012, 85, .	1.1	103
954	Patterned graphene—a novel template for molecular packing. <i>Nanotechnology</i> , 2012, 23, 165303.	1.3	27
955	A chemical route to control molecular mobility on graphene. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10533.	1.3	12

#	ARTICLE	IF	CITATIONS
956	Atomistic theory and simulation of the morphology and structure of ionic nanoparticles. <i>Nanoscale</i> , 2012, 4, 1051-1067.	2.8	15
957	Predictive carbon nanotube models using the eigenvector dimension reduction (EDR) method. <i>Journal of Mechanical Science and Technology</i> , 2012, 26, 1089-1097.	0.7	5
958	Chemical bonding assisted damage production in single-walled carbon nanotubes induced by low-energy ions. <i>Applied Physics A: Materials Science and Processing</i> , 2012, 108, 313-320.	1.1	7
959	Strength of graphenes containing randomly dispersed vacancies. <i>Acta Mechanica</i> , 2012, 223, 669-678.	1.1	31
960	Elastic behavior of bilayer graphene under in-plane loadings. <i>Current Applied Physics</i> , 2012, 12, 1173-1177.	1.1	43
961	Molecular dynamics simulation study of the growth of a rough amorphous carbon film by the grazing incidence of energetic carbon atoms. <i>Carbon</i> , 2012, 50, 404-410.	5.4	32
962	Influence of chemisorption on the thermal conductivity of graphene nanoribbons. <i>Carbon</i> , 2012, 50, 421-428.	5.4	49
963	Prediction of 3D elastic moduli and Poisson's ratios of pillared graphene nanostructures. <i>Carbon</i> , 2012, 50, 603-611.	5.4	59
964	Predicted mechanical properties of a coiled carbon nanotube. <i>Carbon</i> , 2012, 50, 968-976.	5.4	40
965	Molecular dynamics simulation of the interlayer sliding behavior in few-layer graphene. <i>Carbon</i> , 2012, 50, 1025-1032.	5.4	59
966	An atomistic study of the abrasive wear and failure of graphene sheets when used as a solid lubricant and a comparison to diamond-like-carbon coatings. <i>Carbon</i> , 2012, 50, 4078-4084.	5.4	82
967	Free transverse vibration of single-walled carbon nanocones. <i>Carbon</i> , 2012, 50, 4418-4423.	5.4	31
968	Structural features of pyrocarbon atomistic models constructed from transmission electron microscopy images. <i>Carbon</i> , 2012, 50, 4388-4400.	5.4	67
969	Wave propagation in graphene sheets with nonlocal elastic theory via finite element formulation. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2012, 223-224, 1-9.	3.4	78
970	A deformation-fluctuation hybrid method for fast evaluation of elastic constants with many-body potentials. <i>Computer Physics Communications</i> , 2012, 183, 261-265.	3.0	20
971	Postbuckling of sandwich plates with nanotube-reinforced composite face sheets resting on elastic foundations. <i>European Journal of Mechanics, A/Solids</i> , 2012, 35, 10-21.	2.1	120
972	Atomistic models for disordered nanoporous carbons using reactive force fields. <i>Microporous and Mesoporous Materials</i> , 2012, 154, 24-37.	2.2	76
973	Nitrogen doping and curvature effects on thermal conductivity of graphene: A non-equilibrium molecular dynamics study. <i>Solid State Communications</i> , 2012, 152, 261-264.	0.9	97

#	ARTICLE	IF	CITATIONS
974	MD simulation of the frictional behavior of CNTs with respect to orientation. Tribology International, 2012, 50, 51-56.	3.0	13
975	Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques. Parallel Computing, 2012, 38, 245-259.	1.3	716
976	Modeling of graphene-based NEMS. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 949-954.	1.3	41
977	Self-assembly of free-standing graphene nano-ribbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 973-977.	0.9	16
978	Mechanical deformation and fracture mode of polycrystalline graphene: Atomistic simulations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1942-1947.	0.9	26
979	Interactive physically-based structural modeling of hydrocarbon systems. Journal of Computational Physics, 2012, 231, 2581-2598.	1.9	19
980	Molecular dynamics simulation study of the diamond D5 substructures. Open Chemistry, 2012, 10, 1028-1033.	1.0	4
981	Nanoparticle manipulation by thermal gradient. Nanoscale Research Letters, 2012, 7, 154.	3.1	19
982	Design of Low Wear Polymer Composites. Tribology Letters, 2012, 45, 79-87.	1.2	7
983	Determination of best-fit potential parameters for a reactive force field using a genetic algorithm. Journal of Molecular Modeling, 2012, 18, 1049-1061.	0.8	30
984	Vacancy spatial distribution causes different magnetism in graphene. International Journal of Quantum Chemistry, 2013, 113, 792-796.	1.0	5
985	Classical atomistic simulations of surfaces and heterogeneous interfaces with the charge-optimized many body (COMB) potentials. Materials Science and Engineering Reports, 2013, 74, 255-279.	14.8	222
986	Parameterization of a reactive force field using a Monte Carlo algorithm. Journal of Computational Chemistry, 2013, 34, 1143-1154.	1.5	74
987	ESPreSo 3.1: Molecular Dynamics Software for Coarse-Grained Models. Lecture Notes in Computational Science and Engineering, 2013, , 1-23.	0.1	118
988	Computer Simulations of the Sputtering of Metallic, Organic, and Metal-Organic Surfaces with Bi _n and C ₆₀ Projectiles. Journal of Physical Chemistry C, 2013, 117, 2740-2752.	1.5	25
989	Molecular modeling of cracks at interfaces in nanoceramic composites. Journal of the Mechanics and Physics of Solids, 2013, 61, 1971-1982.	2.3	12
990	Atomic scale study of the life cycle of a dislocation in graphene from birth to annihilation. Nature Communications, 2013, 4, 2098.	5.8	149
991	Interfacial thermal conductance of partially unzipped carbon nanotubes: Linear scaling and exponential decay. Physical Review B, 2013, 87, .	1.1	33

#	ARTICLE	IF	CITATIONS
992	Irradiation effects in high-density polyethylene. Nuclear Instruments & Methods in Physics Research B, 2013, 312, 54-59.	0.6	9
993	H \langle mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle mml:msub \rangle \langle mml:mrow \rangle \langle mml:mn \rangle 2 \langle mml:mn \rangle \langle mml:msub \rangle \langle mml:math \rangle on corrugated graphene: Diffusion Monte Carlo calculations. Physical Review B, 2013, 88, .	1.1	10
994	Elementary processes of H ₂ plasma-graphene interaction: A combined molecular dynamics and density functional theory study. Journal of Applied Physics, 2013, 113, 114302.	1.1	35
995	Strength and fracture behavior of graphene grain boundaries: effects of temperature, inflection, and symmetry from molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 11794.	1.3	39
996	Localized vibrational, edges and breathing modes of graphene nanoribbons with topological line defects. European Physical Journal B, 2013, 86, 1.	0.6	1
997	Shear deformation characteristics of single walled carbon nanotube with water interactions by using molecular dynamics simulation. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 54, 206-213.	1.3	27
998	The Effect of Atomic-Scale Roughness on the Adhesion of Nanoscale Asperities: A Combined Simulation and Experimental Investigation. Tribology Letters, 2013, 50, 81-93.	1.2	110
999	Molecular dynamics simulation of benzene in graphite and amorphous carbon slit pores. Journal of Computational Chemistry, 2013, 34, 2615-2624.	1.5	8
1000	Adhesion between two radially collapsed single-walled carbon nanotubes. Acta Mechanica, 2013, 224, 2759-2770.	1.1	14
1001	Thermal conduction phenomena in carbon nanotubes and related nanostructured materials. Reviews of Modern Physics, 2013, 85, 1295-1326.	16.4	365
1002	Phonon energy inversion in graphene during transient thermal transport. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 721-726.	0.9	30
1003	Water permeation through single-layer graphyne membrane. Journal of Chemical Physics, 2013, 139, 064705.	1.2	58
1004	On the role of structural defects during particle channeling through carbon nanotubes. Journal of Surface Investigation, 2013, 7, 218-222.	0.1	1
1005	A theoretical quantification of the possible improvement in the mechanical properties of carbon nanotube bundles by carbon ion irradiation. Carbon, 2013, 53, 346-356.	5.4	29
1006	A possible self-healing mechanism in damaged graphene by heat treatment. Computational Materials Science, 2013, 68, 391-395.	1.4	13
1007	Molecular dynamics simulation on the failure mechanism of Y-junction single-walled carbon nanotubes. Computational Materials Science, 2013, 79, 362-367.	1.4	4
1008	Theoretical study of soft-to-hard transition of copper-filled carbon nanotubes. Computational Materials Science, 2013, 69, 22-28.	1.4	3
1009	Atomistic simulations of nanoindentation on the basal plane of crystalline molybdenum disulfide (MoS ₂). Modelling and Simulation in Materials Science and Engineering, 2013, 21, 045003.	0.8	133

#	ARTICLE	IF	CITATIONS
1010	The effect of non-covalent functionalization on the thermal conductance of graphene/organic interfaces. <i>Nanotechnology</i> , 2013, 24, 165702.	1.3	92
1011	Nanomechanics of single walled carbon nanotube with water interactions under axial tension by using molecular dynamics simulation. <i>Computational Materials Science</i> , 2013, 79, 519-526.	1.4	36
1012	Electronic transport through ordered and disordered graphene grain boundaries. <i>Carbon</i> , 2013, 64, 101-110.	5.4	35
1013	Screened environment-dependent reactive empirical bond-order potential for atomistic simulations of carbon materials. <i>Physical Review B</i> , 2013, 88, .	1.1	34
1014	Structural manipulation of the graphene/metal interface with Ar ⁺ irradiation. <i>Physical Review B</i> , 2013, 88, .	1.1	26
1015	Free-energy analyses of a proton transfer reaction by simulated-tempering umbrella sampling and first-principles molecular dynamics simulations. <i>Physical Review E</i> , 2013, 87, 023301.	0.8	11
1016	Superlubric to stick-slip sliding of incommensurate graphene flakes on graphite. <i>Physical Review B</i> , 2013, 88, .	1.1	98
1017	Surface segregation trends in transition metal alloys. <i>Physical Review B</i> , 2013, 88, .	1.1	7
1018	Atomistic simulations, mesoscopic modeling, and theoretical analysis of thermal conductivity of bundles composed of carbon nanotubes. <i>Journal of Applied Physics</i> , 2013, 114, 104301.	1.1	33
1019	What makes a dangling bond a binding site for thermal CH ₃ radicals? A combined molecular dynamics and potential energy analysis study on amorphous hydrocarbon films. <i>Diamond and Related Materials</i> , 2013, 40, 41-50.	1.8	5
1020	Fitting empirical potentials: Challenges and methodologies. <i>Current Opinion in Solid State and Materials Science</i> , 2013, 17, 263-270.	5.6	44
1021	Thermal conductivity for single-walled carbon nanotubes from Einstein relation in molecular dynamics. <i>Journal of Physics and Chemistry of Solids</i> , 2013, 74, 1599-1603.	1.9	14
1022	Molecular dynamics simulations of single-layer molybdenum disulphide (MoS ₂): Stillinger-Weber parametrization, mechanical properties, and thermal conductivity. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	331
1023	Effects of loading mode and orientation on deformation mechanism of graphene nano-ribbons. <i>Applied Physics Letters</i> , 2013, 103, 191906.	1.5	5
1024	The effect of empirical potential functions on modeling of amorphous carbon using molecular dynamics method. <i>Applied Surface Science</i> , 2013, 286, 287-297.	3.1	59
1025	A computational analysis of graphene adhesion on amorphous silica. <i>Journal of Applied Physics</i> , 2013, 113, 164901.	1.1	19
1026	Thermal conductivity of hybrid graphene/silicon heterostructures. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	25
1027	Wear minimization through utilization of atomic-scale functional surface structure. <i>Applied Physics Letters</i> , 2013, 103, 151904.	1.5	5

#	ARTICLE	IF	CITATIONS
1028	On the Fracture of Supported Graphene Under Pressure. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2013, 80, .	1.1	17
1029	Influence of doped nitrogen and vacancy defects on the thermal conductivity of graphene nanoribbons. <i>Journal of Molecular Modeling</i> , 2013, 19, 4781-4788.	0.8	20
1030	Effects of surface heterogeneity of carbon nanotubes in adsorption of colloid nanoparticles studied by means of computer simulations. <i>Adsorption</i> , 2013, 19, 611-618.	1.4	1
1032	Plasma enhanced growth of single walled carbon nanotubes at low temperature: A reactive molecular dynamics simulation. <i>Carbon</i> , 2013, 65, 269-276.	5.4	24
1033	Co-existing heat currents in opposite directions in graphene nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 2970-2978.	0.9	26
1034	Thermal conductivity and tensile response of defective graphene: A molecular dynamics study. <i>Carbon</i> , 2013, 63, 460-470.	5.4	229
1035	Ion selection of charge-modified large nanopores in a graphene sheet. <i>Journal of Chemical Physics</i> , 2013, 139, 114702.	1.2	95
1036	Nonlinear failure analysis of carbon nanotubes by using molecular-mechanics based models. <i>Composites Part B: Engineering</i> , 2013, 50, 150-157.	5.9	20
1037	A room-temperature non-volatile CNT-based molecular memory cell. <i>Journal of Applied Physics</i> , 2013, 113, 144302.	1.1	1
1038	Formation and Classification of Amorphous Carbon by Molecular Dynamics Simulation. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 01AL04.	0.8	3
1039	Mechanics of self-folding of single-layer graphene. <i>Journal Physics D: Applied Physics</i> , 2013, 46, 055308.	1.3	68
1040	The collapse of an elastic tube induced by encapsulated liquid droplets. <i>Soft Matter</i> , 2013, 9, 9774.	1.2	1
1041	Classical molecular dynamics simulations of carbon nanofiber nucleation: the effect of carbon concentration in Ni carbide. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16314.	1.3	11
1042	Rough contact is not always bad for interfacial energy coupling. <i>Nanoscale</i> , 2013, 5, 11598.	2.8	71
1043	Morphology of a graphene nanoribbon encapsulated in a carbon nanotube. <i>AIP Advances</i> , 2013, 3, .	0.6	13
1044	Thermoelectric properties of gamma-graphyne nanoribbons and nanojunctions. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	49
1045	Shear deformations in calcium silicate hydrates. <i>Soft Matter</i> , 2013, 9, 7333.	1.2	109
1046	Molecular dynamics study on the generation and propagation of heat signals in single-wall carbon nanotubes. <i>RSC Advances</i> , 2013, 3, 12855.	1.7	2

#	ARTICLE	IF	CITATIONS
1047	Nanocasting of hierarchical nanostructured porous carbon in molecular dynamics simulation. <i>Journal of Materials Chemistry A</i> , 2013, 1, 3886.	5.2	14
1048	Mechanisms for hyperthermal polyatomic hydrocarbon modification of PMMA surfaces from molecular dynamics simulations. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2013, 31, 061403.	0.9	0
1049	A New Multi-Physics Molecular Dynamics Finite Element Method for designing graphene based nano-structures. , 2013, , .		0
1050	Development of the ReaxFF reactive force field for aluminum-molybdenum alloy. <i>Journal of Materials Research</i> , 2013, 28, 1155-1164.	1.2	10
1051	Ion-irradiation-induced Defects in Isotopically-Labeled Two Layered Graphene: Enhanced In-situ Annealing of the Damage. <i>Advanced Materials</i> , 2013, 25, 1004-1009.	11.1	79
1052	How graphene crumples are stabilized?. <i>RSC Advances</i> , 2013, 3, 2720.	1.7	29
1053	A modified Tersoff potential for pure and hydrogenated diamond-like carbon. <i>Computational Materials Science</i> , 2013, 67, 146-150.	1.4	55
1054	Finite element analysis of single-walled carbon nanotubes based on a rod model including in-plane cross-sectional deformation. <i>International Journal of Solids and Structures</i> , 2013, 50, 49-56.	1.3	8
1055	Molecular dynamics study of the interfacial mechanical properties of the graphene-collagen biological nanocomposite. <i>Computational Materials Science</i> , 2013, 69, 29-39.	1.4	42
1056	Atomistic simulation study of brittle failure in nanocrystalline graphene under uniaxial tension. <i>Applied Physics Letters</i> , 2013, 102, .	1.5	65
1057	DFT-based prediction of fission product sorption on carbon structures under O2 ingress conditions. <i>Journal of Nuclear Materials</i> , 2013, 437, 389-400.	1.3	4
1058	An atomistic simulation study of the mechanisms and kinetics of surface bond strengthening in thermally-treated cone-stacked carbon nanofibers. <i>Carbon</i> , 2013, 56, 351-357.	5.4	9
1059	Selective etching of armchair edges in graphite. <i>Carbon</i> , 2013, 56, 332-338.	5.4	14
1060	Influence of oriented topological defects on the mechanical properties of carbon nanotube heterojunctions. <i>Journal of Applied Physics</i> , 2013, 114, 144306.	1.1	2
1061	Screened empirical bond-order potentials for Si-C. <i>Physical Review B</i> , 2013, 87, .	1.1	113
1062	A molecular dynamics study on tensile strength and failure modes of carbon nanotube junctions. <i>Journal Physics D: Applied Physics</i> , 2013, 46, 495301.	1.3	13
1063	Improved inter-tube coupling in CNT bundles through carbon ion irradiation. <i>Carbon</i> , 2013, 51, 173-184.	5.4	39
1064	The atomic scale structure of nanographene platelets studied by X-ray diffraction, high-resolution transmission electron microscopy and molecular dynamics. <i>Diamond and Related Materials</i> , 2013, 35, 40-46.	1.8	17

#	ARTICLE	IF	CITATIONS
1065	Effect of temperature on kinetic nanofriction of a Brownian adparticle. <i>Chemical Physics Letters</i> , 2013, 570, 70-74.	1.2	6
1066	Dangling bond induced cross-linking model in nanoscratched graphene layers. <i>Surface and Coatings Technology</i> , 2013, 237, 230-233.	2.2	20
1067	Iterative Method for Edge Length Equalization. <i>Procedia Computer Science</i> , 2013, 18, 481-490.	1.2	2
1068	Electron-irradiation-induced reinforcement of reduced graphene oxide papers. <i>Acta Materialia</i> , 2013, 61, 6466-6473.	3.8	21
1069	Heating induced microstructural changes in graphene/Cu nanocomposites. <i>Journal Physics D: Applied Physics</i> , 2013, 46, 065309.	1.3	11
1070	Characterization of carbon atomistic pathways during single-walled carbon nanotube growth on supported metal nanoparticles. <i>Carbon</i> , 2013, 57, 298-309.	5.4	23
1071	How fast does water flow in carbon nanotubes?. <i>Journal of Chemical Physics</i> , 2013, 138, 094701.	1.2	240
1072	Spiral graphone and one-sided fluorographene nanoribbons. <i>Physical Review B</i> , 2013, 87, .	1.1	17
1073	Developing Descriptors To Predict Mechanical Properties of Nanotubes. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 773-782.	2.5	11
1074	The Genetic Algorithm in Real-Space Representation. , 2013, , 11-35.		0
1075	Graphene-Based Polymer Composites and Their Applications. <i>Polymer-Plastics Technology and Engineering</i> , 2013, 52, 319-331.	1.9	465
1076	Structure, stability and defects of single layer hexagonal BN in comparison to graphene. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 045009.	0.7	47
1077	Experimental and multiscale modeling of thermal conductivity and elastic properties of PLA/expanded graphite polymer nanocomposites. <i>Thermochimica Acta</i> , 2013, 552, 106-113.	1.2	74
1078	Melting of graphene clusters. <i>Physical Review B</i> , 2013, 87, .	1.1	30
1079	Elastic in-plane properties of 2D linearized models of graphene. <i>Mechanics of Materials</i> , 2013, 62, 60-68.	1.7	42
1080	Vibration characteristics of wrinkled single-layered graphene sheets. <i>International Journal of Solids and Structures</i> , 2013, 50, 1812-1823.	1.3	31
1081	<i>Colloquium</i>: Modeling friction: From nanoscale to mesoscale. <i>Reviews of Modern Physics</i> , 2013, 85, 529-552.	16.4	436
1082	Pseudo Hallâ€“Petch Strength Reduction in Polycrystalline Graphene. <i>Nano Letters</i> , 2013, 13, 1829-1833.	4.5	172

#	ARTICLE	IF	CITATIONS
1083	Strength of graphene in biaxial tension. <i>European Journal of Mechanics, A/Solids</i> , 2013, 39, 291-297.	2.1	6
1084	Buckling of a Supported Annular Plate with a Non-Euclidean Metric. <i>Advanced Structured Materials</i> , 2013, , 155-166.	0.3	1
1085	Nanohinge-Induced Plasticity of Helical Carbon Nanotubes. <i>Small</i> , 2013, 9, 3561-3566.	5.2	44
1086	Thermal properties of fluorinated graphene. <i>Physical Review B</i> , 2013, 87, .	1.1	91
1087	Layered graphene structure of a hexagonal carbon. <i>Physica B: Condensed Matter</i> , 2013, 418, 73-75.	1.3	8
1088	Nanoscale Phononic Crystals and Structures. <i>Springer Series in Solid-state Sciences</i> , 2013, , 281-327.	0.3	0
1089	Atomistic modelling of CVD synthesis of carbon nanotubes and graphene. <i>Nanoscale</i> , 2013, 5, 6662.	2.8	88
1090	Investigation into the mechanical properties of single-walled carbon nanotube heterojunctions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11579.	1.3	6
1091	Ehrlich-Schwoebel Barriers and Island Nucleation in Organic Thin-Film Growth. <i>Springer Series in Materials Science</i> , 2013, , 79-106.	0.4	6
1092	Highly defective graphene: A key prototype of two-dimensional Anderson insulators. <i>Nano Research</i> , 2013, 6, 326-334.	5.8	59
1093	Molecular dynamics study of a new mechanism for ripple formation on graphene nanoribbons at very low temperatures based on H ₂ physisorption. <i>Solid State Communications</i> , 2013, 159, 84-87.	0.9	8
1094	Thermal transport in bent graphene nanoribbons. <i>Nanoscale</i> , 2013, 5, 734-743.	2.8	41
1095	Reactive Potentials for Advanced Atomistic Simulations. <i>Annual Review of Materials Research</i> , 2013, 43, 109-129.	4.3	184
1096	Tuning thermal conduction via extended defects in graphene. <i>Physical Review B</i> , 2013, 87, .	1.1	48
1097	Electronic and Field Emission Properties of Wrinkled Graphene. <i>Journal of Physical Chemistry C</i> , 2013, 117, 692-696.	1.5	75
1098	Fracture and negative Poisson's ratio of novel spanned-fullerenes nanotube networks under tension. <i>Computational Materials Science</i> , 2013, 80, 15-26.	1.4	19
1099	Localized defect modes in graphene. <i>Physical Review B</i> , 2013, 88, .	1.1	12
1100	Buckling induced delamination of graphene composites through hybrid molecular modeling. <i>Applied Physics Letters</i> , 2013, 102, .	1.5	15

#	ARTICLE	IF	CITATIONS
1101	A molecular dynamics study about two way tuning of thermal conductivity in graphene: Strain and doping. , 2013, , .		2
1102	Molecular dynamics simulation on thermal conductivity of single-walled carbon nanotubes. , 2013, , .		1
1103	Carbon nanotubes as heat dissipaters in microelectronics. European Physical Journal B, 2013, 86, 1.	0.6	4
1104	Structural Modeling of Dahlia-Type Single-Walled Carbon Nanohorn Aggregates by Molecular Dynamics. Journal of Physical Chemistry A, 2013, 117, 9057-9061.	1.1	17
1105	Structural Modelling of Silicon Carbide-Derived Nanoporous Carbon by Hybrid Reverse Monte Carlo Simulation. Journal of Physical Chemistry C, 2013, 117, 14081-14094.	1.5	60
1106	Transitional failure of hybrid carbon nanotubes under multiaxial loads. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 53, 95-100.	1.3	1
1107	Reactive Bond-Order Potential for Si-, C-, and H-Containing Materials. Journal of Physical Chemistry C, 2013, 117, 1323-1334.	1.5	10
1108	Coalescence of parallel finite length single-walled carbon nanotubes by heat treatment. Journal of Physics and Chemistry of Solids, 2013, 74, 436-440.	1.9	9
1109	Size Dependent Mechanical Properties of Graphene Nanoribbons: Molecular Dynamics Simulation. Materials Science Forum, 0, 749, 456-460.	0.3	4
1110	Effect of Confined Fluid Interaction on the Thermal Transport in Carbon Nanotubes. International Journal of Micro-nano Scale Transport, 2013, 4, 77-84.	0.2	1
1111	Permeation of low-Z atoms through carbon sheets: Density functional theory study on energy barriers and deformation effects. AIP Advances, 2013, 3, 122104.	0.6	8
1112	Molecular Dynamics Simulation to Study the Effect of Empirical Potential Functions on Modeling of Diamond-Like Carbon. , 2013, , .		0
1113	Structural Change of Single-Crystalline Graphite under Plasma Irradiation. Japanese Journal of Applied Physics, 2013, 52, 01AL02.	0.8	5
1114	Phonon mediated loss in a graphene nanoribbon. Journal of Applied Physics, 2013, 114, .	1.1	8
1115	Sensitivity of thermal conductivity of carbon nanotubes to defect concentrations and heat-treatment. Journal of Applied Physics, 2013, 113, .	1.1	43
1116	Buckling characterizations of an individual multi-walled carbon nanotube: Insights from quantitative <i>in situ</i> transmission electron microscope nanoindentation and molecular dynamics. Applied Physics Letters, 2013, 103, .	1.5	15
1117	Interior and Edge Elastic Waves in Graphene. Journal of Applied Mechanics, Transactions ASME, 2013, 80, .	1.1	2
1118	Markovian equations of motion for non-Markovian coarse-graining and properties for graphene blobs. New Journal of Physics, 2013, 15, 125015.	1.2	4

#	ARTICLE	IF	CITATIONS
1119	Mechanics Interpretation on the Bending Stiffness and Wrinkled Pattern of Graphene. Journal of Applied Mechanics, Transactions ASME, 2013, 80, .	1.1	10
1120	Numerical Analysis of Circular Graphene Bubbles. Journal of Applied Mechanics, Transactions ASME, 2013, 80, .	1.1	60
1121	The Thermal Conductivity of Carbon Nanotubes with Defects and Intramolecular Junctions. Journal of Nanomaterials, 2013, 2013, 1-7.	1.5	10
1122	Bioinspired Graphene Nanogut. Journal of Applied Mechanics, Transactions ASME, 2013, 80, .	1.1	4
1123	Mechanical Properties Investigation of Single-Walled Carbon Nanotube Using Finite Element Method. Key Engineering Materials, 2013, 550, 179-187.	0.4	1
1124	Analytical Bond-order Potential for hcp-Y. Chinese Journal of Chemical Physics, 2013, 26, 526-532.	0.6	5
1125	Mechanical and Thermal Properties of Graphene Nanomeshes. Materials Research Society Symposia Proceedings, 2013, 1505, 1.	0.1	2
1126	Predicting the mechanical characteristics of hydrogen functionalized graphene sheets using artificial neural network approach. Journal of Nanostructure in Chemistry, 2013, 3, 1.	5.3	38
1127	Adsorption Properties of Tetracycline onto Graphene Oxide: Equilibrium, Kinetic and Thermodynamic Studies. PLoS ONE, 2013, 8, e79254.	1.1	151
1128	Mechanical properties investigation of graphene coated with Ni. , 2013, , .		1
1129	Interfacial Strength Between Single Wall Carbon Nanotubes and Copper Material: Molecular Dynamics Simulation. Journal of Nanotechnology in Engineering and Medicine, 2013, 4, .	0.8	12
1130	Mechanical coupling in homogeneously deformed single-wall carbon nanotubes. Journal of Physics Condensed Matter, 2013, 25, 145301.	0.7	1
1131	Vibrational properties of nanographene. The Nanoscale Systems: Mathematical Modeling and Applications, 0, 2, 10-29.	0.3	3
1132	Atomic simulation of the formation and mechanical behavior of carbon nanoscrolls. Journal of Applied Physics, 2013, 113, .	1.1	27
1133	Effects of doping, Stone-Wales and vacancy defects on thermal conductivity of single-wall carbon nanotubes. Chinese Physics B, 2013, 22, 016501.	0.7	32
1134	Effect of vacancy defects on thermal conductivity of single-walled carbon nanotubes. , 2013, , .		0
1135	Atomistic simulations of stainless steels: a many-body potential for the Fe-Cr-C system. Journal of Physics Condensed Matter, 2013, 25, 445401.	0.7	51
1136	Buckling of double-walled carbon nanotubes under compression and bending: Influence of vacancy defects and effect of high-temperature annealing. Journal of Applied Physics, 2013, 114, 174308.	1.1	2

#	ARTICLE	IF	CITATIONS
1137	High-speed nano-bearings constructed from double-walled carbon nanotubes: Effect of flexile deformation. Journal of Applied Physics, 2013, 114, 174501.	1.1	3
1138	Nanoindentation study of size effects in nickel-graphene nanocomposites. Philosophical Magazine Letters, 2013, 93, 196-203.	0.5	49
1139	Molecular Mass Transportation Via Carbon Nanoscrolls. Journal of Applied Mechanics, Transactions ASME, 2013, 80, .	1.1	15
1140	The atomic scale structure of CXV carbon: wide-angle x-ray scattering and modeling studies. Journal of Physics Condensed Matter, 2013, 25, 454203.	0.7	8
1141	Equilibrium Configurations of Lipid Bilayer Membranes and Carbon Nanostructures. Communications in Theoretical Physics, 2013, 59, 213-228.	1.1	10
1142	TENSILE PROPERTIES OF GRAPHENE-NANOTUBE HYBRID STRUCTURES: A MOLECULAR DYNAMICS STUDY. International Journal of Computational Materials Science and Engineering, 2013, 02, 1350020.	0.5	9
1143	LOADING, CHARGING AND THERMAL EFFECTS ON THE MECHANISM OF WATER-CARBON NANOTUBE TRANSMISSION. International Journal of Computational Materials Science and Engineering, 2013, 02, 1350017.	0.5	1
1144	Quantum correction and phonon density of states analysis for thermal conductivity of single walled carbon nanotube with Finite Length. , 2013, , .		0
1145	Computational investigation of the mechanical and tribological responses of amorphous carbon nanoparticles. Journal of Applied Physics, 2013, 113, .	1.1	4
1146	Molecular Dynamics Study on Buckling Behavior of Non-Defective and Defective Triple-Walled Carbon Nanotubes. Journal of Solid Mechanics and Materials Engineering, 2013, 7, 403-416.	0.5	3
1147	Nanotribological Behavior of Carbon Based Thin Films: Friction and Lubricity Mechanisms at the Nanoscale. Lubricants, 2013, 1, 22-47.	1.2	50
1148	BUCKLING PROPERTIES OF PRE-STRESSED MULTI-WALLED CARBON NANOTUBES. International Journal for Multiscale Computational Engineering, 2013, 11, 17-26.	0.8	3
1149	Tensile properties of a boron/nitrogen-doped carbon nanotube-graphene hybrid structure. Beilstein Journal of Nanotechnology, 2014, 5, 329-336.	1.5	27
1150	Resonance of graphene nanoribbons doped with nitrogen and boron: a molecular dynamics study. Beilstein Journal of Nanotechnology, 2014, 5, 717-725.	1.5	6
1151	Combined CI-MD approach in formulation of engineering moduli of single layer graphene sheet. Simulation Modelling Practice and Theory, 2014, 48, 93-111.	2.2	26
1152	Motion and energy dissipation of single-walled carbon nanotube on graphite by molecular dynamics simulation. Materials Research Express, 2014, 1, 025046.	0.8	3
1153	Thermal transport properties of defective graphene: A molecular dynamics investigation. Chinese Physics B, 2014, 23, 106501.	0.7	4
1154	Molecular Dynamics Analysis on Compressive Strength of PAN-Based Carbon Fibers. International Journal of Nanoscience, 2014, 13, 1440004.	0.4	2

#	ARTICLE	IF	CITATIONS
1155	Mechanical and thermal stability of graphene and graphene-based materials. <i>Physics-Usppekhi</i> , 2014, 57, 970-989.	0.8	100
1156	Surface activation of cyclo olefin polymer by oxygen plasma discharge: a molecular dynamics study. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014, 22, 055020.	0.8	4
1157	Structure of Lennard-Jones nanowires encapsulated by carbon nanotubes. <i>Chinese Physics B</i> , 2014, 23, 016104.	0.7	0
1158	Nonlocal thermal transport across embedded few-layer graphene sheets. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 502101.	0.7	6
1159	Influence of chirality on the thermal conductivity of single-walled carbon nanotubes. <i>Chinese Physics B</i> , 2014, 23, 083101.	0.7	12
1160	Thermal expansion of free-standing graphene: benchmarking semi-empirical potentials. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 185401.	0.7	44
1161	Multiscale modelling of plasma-wall interactions in fusion reactor conditions. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 224018.	1.3	55
1162	On the time scale associated with Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2014, 141, 204104.	1.2	47
1163	Calculation of Decomposition Products from Components of Gunpowder by using ReaxFF Reactive Force Field Molecular Dynamics and Thermodynamic Calculations of Equilibrium Composition. <i>Propellants, Explosives, Pyrotechnics</i> , 2014, 39, 830-837.	1.0	12
1164	VIBRATION ANALYSIS OF A GRAPHENE NANORIBBON UNDER HARMONIC LORENTZ FORCE USING A HYBRID MODAL-MOLECULAR DYNAMICS METHOD. <i>International Journal of Structural Stability and Dynamics</i> , 2014, 14, 1350057.	1.5	4
1165	Modeling the interfacial thermal resistance of diamond nanorod composites and related materials. <i>International Journal of Computational Materials Science and Engineering</i> , 2014, 03, 1450014.	0.5	1
1166	Taming the Untamable-The Art and Science of Diamond Polishing. , 2014, , 81-98.		2
1167	A Hybrid Molecular Dynamics/Atomic-Scale Finite Element Method for Quasi-Static Atomistic Simulations at Finite Temperature. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2014, 81, .	1.1	5
1168	Topological Defects in Two-Dimensional Crystals: The Stress Buildup and Accumulation. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2014, 81, .	1.1	19
1169	Gas Sensing and Thermal Transport Through Carbon-Nanotube-Based Nanodevices. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2014, , 99-136.	0.6	1
1170	Tuneable Resonance Properties of Graphene by Nitrogen-Dopant. <i>Applied Mechanics and Materials</i> , 2014, 553, 3-9.	0.2	4
1171	Study of the Nanomechanics of CNTs under Tension by Molecular Dynamics Simulation Using Different Potentials. , 2014, 2014, 1-18.		14
1172	Molecular Dynamics Simulation and Continuum Shell Model for Buckling Analysis of Carbon Nanotubes. <i>Springer Series in Materials Science</i> , 2014, , 239-273.	0.4	10

#	ARTICLE	IF	CITATIONS
1173	Bombardment of gas molecules on single graphene layer at high temperature. , 2014, , .		0
1174	High temperature phonon dispersion in graphene using classical molecular dynamics. , 2014, , .		2
1175	A MECHANICAL MODEL FOR SELF-ASSEMBLED GRAPHENE AROUND NANOTUBE. International Journal of Applied Mechanics, 2014, 06, 1450036.	1.3	9
1176	Adsorbate migration effects on continuous and discontinuous temperature-dependent transitions in the quality factors of graphene nanoresonators. Nanotechnology, 2014, 25, 025501.	1.3	14
1177	Interfacial Carbon Nanoplatelet Formation by Ion Irradiation of Graphene on Iridium(111). ACS Nano, 2014, 8, 12208-12218.	7.3	29
1178	Quantifying energetics of topological frustration in carbon nanostructures. Physical Review B, 2014, 89, .	1.1	9
1179	Registry effect on the thermal conductivity of few-layer graphene. Journal of Applied Physics, 2014, 116, .	1.1	6
1180	Binding energy and mechanical stability of single- and multi-walled carbon nanotube serpentines. Journal of Chemical Physics, 2014, 140, 204704.	1.2	17
1181	Thermal conductivity of configurable two-dimensional carbon nanotube architecture and strain modulation. Applied Physics Letters, 2014, 105, .	1.5	26
1182	Low-energy irradiation effects in cellulose. Journal of Applied Physics, 2014, 115, 023521.	1.1	8
1183	Effect of defects on thermal conductivity of graphene. , 2014, , .		1
1184	A kinematic study of energy barriers for crack formation in graphene tilt boundaries. Journal of Applied Physics, 2014, 115, .	1.1	19
1185	Moiré Patterns as a Probe of Interplanar Interactions for Graphene on h-BN. Physical Review Letters, 2014, 113, 135504.	2.9	130
1186	Partial molar enthalpies and reaction enthalpies from equilibrium molecular dynamics simulation. Journal of Chemical Physics, 2014, 141, 144501.	1.2	20
1187	Radiation effects on the D and G Raman intensities of carbon nanotubes. Physical Review B, 2014, 89, .	1.1	17
1189	A coupled mechanical charge/dipole molecular dynamics finite element method, with multiscale applications to the design of graphene nano-devices. International Journal for Numerical Methods in Engineering, 2014, 100, 243-276.	1.5	6
1190	Controlling the number of graphene sheets exfoliated from graphite by designed normal loading and frictional motion. Journal of Applied Physics, 2014, 116, 024313.	1.1	6
1191	The effects of temperature and vacancies on dynamics of crack in graphene sheet. AIP Advances, 2014, 4, .	0.6	14

#	ARTICLE	IF	CITATIONS
1192	Phonon dispersion and quantization tuning of strained carbon nanotubes for flexible electronics. Journal of Applied Physics, 2014, 115, 243702.	1.1	9
1193	Energy barrier for configurational transformation of graphene nanoribbon on nanotube. Theoretical and Applied Mechanics Letters, 2014, 4, 041010.	1.3	3
1194	Effects of temperature and strain rate on the mechanical properties of hexagonal boron nitride nanosheets. Journal Physics D: Applied Physics, 2014, 47, 025303.	1.3	101
1196	Thermal transport in folded zigzag and armchair graphene nanoribbons. Applied Physics Letters, 2014, 104, .	1.5	20
1197	Molecular dynamics simulation of thermal ripples in graphene with bond-order-informed harmonic constraints. Nanotechnology, 2014, 25, 485701.	1.3	7
1198	Topological symmetry-induced width dependence of thermal conductance of edge-reconstructed graphene nanoribbons. Journal Physics D: Applied Physics, 2014, 47, 265303.	1.3	6
1199	Heat conduction study across metal/graphene interface by molecular dynamics. , 2014, , .		0
1200	Theoretical Study of Iron Heterogeneous Growth on the Surface of C ₆₀ Molecule. Advanced Materials Research, 0, 1081, 115-118.	0.3	0
1201	Properties of Diamond Nanomaterials. , 2014, , 555-574.		0
1202	The effect of deposition energy of energetic atoms on the growth and structure of ultrathin amorphous carbon films studied by molecular dynamics simulations. Journal Physics D: Applied Physics, 2014, 47, 245303.	1.3	12
1203	Temperature-induced unfolding of scrolled graphene and folded graphene. Journal of Applied Physics, 2014, 115, .	1.1	22
1204	Classical molecular dynamics investigations of biphenyl-based carbon nanomembranes. Beilstein Journal of Nanotechnology, 2014, 5, 865-871.	1.5	10
1205	Abrikosov-like lattices in organic crystals on graphite surface. Materials Research Society Symposia Proceedings, 2014, 1663, 30.	0.1	0
1206	Morphology of Irradiated Adjacent Single-Walled Carbon Nanotubes. Applied Mechanics and Materials, 0, 553, 88-93.	0.2	0
1207	Grain size dependence of penetration depth of hydrogen injection into polycrystalline graphite by molecular simulation. Japanese Journal of Applied Physics, 2014, 53, 11RF04.	0.8	4
1208	Graphene field effect Nanopore glycine detector. , 2014, , .		0
1209	Molecular Dynamics Study of Programmable Nanoporous Graphene. Journal of Nanomechanics & Micromechanics, 2014, 4, .	1.4	14
1210	Modeling Potential Energy Surfaces: From First-Principle Approaches to Empirical Force Fields. Entropy, 2014, 16, 322-349.	1.1	7

#	ARTICLE	IF	CITATIONS
1211	Computer modeling of scattering carbon atoms with graphene. , 2014, , .		0
1212	Modeling of interface cracking in copper-graphite composites by MD and CFE method. Composites Part B: Engineering, 2014, 58, 586-592.	5.9	42
1213	Hydrogenation induced deformation mode and thermal conductivity variations in graphene sheets. Carbon, 2014, 72, 185-191.	5.4	9
1214	Instability of supersonic crack in graphene. Physica B: Condensed Matter, 2014, 434, 145-148.	1.3	21
1215	PuReMD-GPU: A reactive molecular dynamics simulation package for GPUs. Journal of Computational Physics, 2014, 272, 343-359.	1.9	47
1216	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. Tribology Letters, 2014, 53, 119-126.	1.2	89
1217	Estimation of mechanical properties of nanomaterials using artificial intelligence methods. Applied Physics A: Materials Science and Processing, 2014, 116, 1099-1107.	1.1	31
1218	Plasma Bromination of Graphene for Covalent Bonding of Organic Molecules. Plasma Chemistry and Plasma Processing, 2014, 34, 621-645.	1.1	22
1219	On localized modes of free vibrations of single-walled carbon nanotubes embedded in nonhomogeneous elastic medium. ZAMM Zeitschrift Fur Angewandte Mathematik Und Mechanik, 2014, 94, 130-141.	0.9	17
1220	Anchor Points Reactive Potential for Bond-Breaking Reactions. Journal of Chemical Theory and Computation, 2014, 10, 924-933.	2.3	16
1221	Probing the evolution and morphology of hard carbon spheres. Carbon, 2014, 68, 104-111.	5.4	44
1222	Load transfer of graphene/carbon nanotube/polyethylene hybrid nanocomposite by molecular dynamics simulation. Composites Part B: Engineering, 2014, 63, 27-33.	5.9	95
1223	Atomistic and continuum modelling of temperature-dependent fracture of graphene. International Journal of Fracture, 2014, 187, 199-212.	1.1	106
1224	Tensile behavior of heat welded CNT network structures. Computational Materials Science, 2014, 88, 14-21.	1.4	19
1225	Growth of junctions in 3D carbon nanotube-graphene nanostructures: A quantum mechanical molecular dynamic study. Carbon, 2014, 67, 627-634.	5.4	46
1226	Measurement of properties of graphene sheets subjected to drilling operation using computer simulation. Measurement: Journal of the International Measurement Confederation, 2014, 50, 50-62.	2.5	47
1227	A nonlinear theory of prestressed elastic stick-and-spring structures. International Journal of Engineering Science, 2014, 80, 4-20.	2.7	16
1228	An embedded simulation approach for modeling the thermal conductivity of 2D nanoscale material. Simulation Modelling Practice and Theory, 2014, 44, 1-13.	2.2	25

#	ARTICLE	IF	CITATIONS
1229	Fracture toughness of graphene. Nature Communications, 2014, 5, 3782.	5.8	567
1230	Representing potential energy surfaces by high-dimensional neural network potentials. Journal of Physics Condensed Matter, 2014, 26, 183001.	0.7	252
1231	Atomistic modeling of mechanical properties of polycrystalline graphene. Nanotechnology, 2014, 25, 215704.	1.3	99
1232	Two-Dimensional Thermal Transport in Graphene: A Review of Numerical Modeling Studies. Nanoscale and Microscale Thermophysical Engineering, 2014, 18, 155-182.	1.4	52
1233	Dislocations in bilayer graphene. Nature, 2014, 505, 533-537.	13.7	185
1234	Atomistic simulation and the mechanism of graphene amorphization under electron irradiation. Nanoscale, 2014, 6, 2082.	2.8	14
1235	Channeling of protons in single-walled carbon nanotubes based on kinetic and molecular-dynamics treatment. Carbon, 2014, 71, 196-205.	5.4	10
1236	Lonsdaleite Films with Nanometer Thickness. Journal of Physical Chemistry Letters, 2014, 5, 541-548.	2.1	56
1237	Multiscale modelling of irradiation in nanostructures. Journal of Computational Electronics, 2014, 13, 122-141.	1.3	45
1238	MoS2 nanoresonators: intrinsically better than graphene?. Nanoscale, 2014, 6, 3618.	2.8	70
1239	Effects of welding on thermal conductivity of randomly oriented carbon nanotube networks. International Journal of Heat and Mass Transfer, 2014, 70, 803-810.	2.5	23
1240	Molecular dynamics simulations of thermal conductivity of carbon nanotubes: Resolving the effects of computational parameters. International Journal of Heat and Mass Transfer, 2014, 70, 954-964.	2.5	96
1241	Molecular mobility on graphene nanoribbons. Physical Chemistry Chemical Physics, 2014, 16, 2129-2135.	1.3	7
1242	Studying the rotation induced super-lattices on graphite using a type-criterion potential based molecular dynamics method. Computational Materials Science, 2014, 83, 39-44. Cu cluster deposition on ZnO	1.4	0
1243	accent="true">$1$$0$ morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014, 14, 7145-7152.	0.8	16
1244	Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014, 14, 7145-7152.	4.5	210
1245	Reversible Oxidation of Graphene Through Ultraviolet/Ozone Treatment and Its Nonthermal Reduction through Ultraviolet Irradiation. Journal of Physical Chemistry C, 2014, 118, 27372-27381.	1.5	66
1246	Complete characterization by Raman spectroscopy of the structural properties of thin hydrogenated diamond-like carbon films exposed to rapid thermal annealing. Journal of Applied Physics, 2014, 116, .	1.1	71

#	ARTICLE	IF	CITATIONS
1247	Thickness dependence of properties and structure of ultrathin tetrahedral amorphous carbon films: A molecular dynamics simulation. <i>Surface and Coatings Technology</i> , 2014, 258, 938-942.	2.2	8
1248	Growth mechanism of hydrogenated amorphous carbon films: Molecular dynamics simulations. <i>Surface and Coatings Technology</i> , 2014, 258, 901-907.	2.2	6
1249	A first principle study of adsorption of two proximate nitrogen atoms on graphene. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1619-1629.	1.0	8
1250	Graphene: A partially ordered non-periodic solid. <i>Journal of Chemical Physics</i> , 2014, 141, 144701.	1.2	9
1251	Folding of multi-layer graphene sheets induced by van der Waals interaction. <i>Acta Mechanica Sinica/Lixue Xuebao</i> , 2014, 30, 410-417.	1.5	19
1252	A charge optimized many-body potential for titanium nitride (TiN). <i>Journal of Physics Condensed Matter</i> , 2014, 26, 265004.	0.7	10
1253	Multiscale modeling of thermal conductivity of polycrystalline graphene sheets. <i>Nanoscale</i> , 2014, 6, 3344-3352.	2.8	98
1254	Molecular simulation of "hydrolytic weakening" A case study on silica. <i>Acta Materialia</i> , 2014, 80, 264-277.	3.8	50
1255	Carbon nanotube"fullerene hybrid nanostructures by C₆₀ bombardment: formation and mechanical behavior. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21615-21619.	1.3	18
1256	The reaction enthalpy of hydrogen dissociation calculated with the Small System Method from simulation of molecular fluctuations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19681.	1.3	7
1257	Mechanics of graphyne crumpling. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18233-18240.	1.3	35
1258	Growth mechanisms and mechanical properties of 3D carbon nanotube"graphene junctions: molecular dynamic simulations. <i>RSC Advances</i> , 2014, 4, 33848-33854.	1.7	15
1259	Vacancy inter-layer migration in multi-layered graphene. <i>Nanoscale</i> , 2014, 6, 5729-5734.	2.8	20
1260	Effect of Wrinkles on the Surface Area of Graphene: Toward the Design of Nanoelectronics. <i>Nano Letters</i> , 2014, 14, 6520-6525.	4.5	81
1261	Tunable anisotropic thermal conduction in graphane nanoribbons. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	15
1262	Computer simulations of plasma"biomolecule and plasma"tissue interactions for a better insight in plasma medicine. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 293001.	1.3	39
1263	Equilibrium limit of thermal conduction and boundary scattering in nanostructures. <i>Journal of Chemical Physics</i> , 2014, 140, 244112.	1.2	11
1264	Nanotube Dispersion and Polymer Conformational Confinement in a Nanocomposite Fiber: A Joint Computational Experimental Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9476-9485.	1.2	30

#	ARTICLE	IF	CITATIONS
1265	Rapid motion of liquid mercury column in carbon nanotubes driven by temperature gradient. <i>Journal of Applied Physics</i> , 2014, 116, 074307.	1.1	8
1266	Effect of hydrogenation on graphene thermal transport. <i>Carbon</i> , 2014, 80, 167-173.	5.4	38
1267	Tetrahedral Amorphous Carbon Coatings for Friction Reduction of the Valve Train in Internal Combustion Engines. <i>Advanced Engineering Materials</i> , 2014, 16, 1226-1233.	1.6	12
1268	Extensive Energy Landscape Sampling of Nanotube End-Caps Reveals No Chiral-Angle Bias for Their Nucleation. <i>ACS Nano</i> , 2014, 8, 1899-1906.	7.3	34
1269	Interfacial Thermal Conductance of a Silicene/Graphene Bilayer Heterostructure and the Effect of Hydrogenation. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 18180-18188.	4.0	123
1270	Asymmetrically-gated graphene self-switching diodes as negative differential resistance devices. <i>Nanoscale</i> , 2014, 6, 7628-7634.	2.8	25
1271	A molecular dynamics based artificial intelligence approach for characterizing thermal transport in nanoscale material. <i>Thermochimica Acta</i> , 2014, 594, 39-49.	1.2	26
1272	Achieving ultra-hard surface of mechanically polished diamond crystal by thermo-chemical refinement. <i>Applied Surface Science</i> , 2014, 316, 617-624.	3.1	24
1273	Tuning thermal conductance in the twisted graphene and gamma graphyne nanoribbons. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	23
1274	“Unsticking”™ and exposing the surface area of graphene bilayers via randomly distributed nanoparticles. <i>Chemical Physics Letters</i> , 2014, 609, 65-69.	1.2	3
1275	Ultra-strong collagen-mimic carbon nanotube bundles. <i>Carbon</i> , 2014, 77, 1040-1053.	5.4	30
1276	Emergent magnetism in irradiated graphene nanostructures. <i>Carbon</i> , 2014, 78, 196-203.	5.4	9
1277	Atomistic simulations of pristine and defective hexagonal BN and SiC sheets under uniaxial tension. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2014, 615, 481-488.	2.6	52
1278	Coarse-graining of cohesive zone at interface of amorphous material. <i>Journal of Mechanical Science and Technology</i> , 2014, 28, 2787-2796.	0.7	2
1279	Self-Enhanced Catalytic Activities of Functionalized Graphene Sheets in the Combustion of Nitromethane: Molecular Dynamic Simulations by Molecular Reactive Force Field. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 12235-12244.	4.0	44
1280	Giant room-temperature spin caloritronics in spin-semiconducting graphene nanoribbons. <i>Physical Review B</i> , 2014, 90, .	1.1	85
1281	Dynamics of Topological Defects in Single-Walled Carbon Nanotubes during Catalytic Growth. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4808-4817.	1.5	15
1282	Torsional Characteristics of SingleWalled Carbon Nanotube with Water Interactions by Using Molecular Dynamics Simulation. <i>Nano-Micro Letters</i> , 2014, 6, 268-279.	14.4	32

#	ARTICLE	IF	CITATIONS
1283	Crystallization in Carbon Nanostructures. <i>Communications in Mathematical Physics</i> , 2014, 328, 545-571.	1.0	39
1284	A novel method for studying the buckling of nanotubes considering geometrical imperfections. <i>Applied Physics A: Materials Science and Processing</i> , 2014, 117, 945-953.	1.1	2
1285	Strong mechanical coupling between the carbon nanotube and the inner streaming water flow. <i>Microfluidics and Nanofluidics</i> , 2014, 17, 1053-1060.	1.0	5
1286	Continual model of deformation of graphene. <i>Vestnik St Petersburg University: Mathematics</i> , 2014, 47, 47-55.	0.1	0
1287	Thermomechanics of monolayer graphene: Rippling, thermal expansion and elasticity. <i>Journal of the Mechanics and Physics of Solids</i> , 2014, 66, 42-58.	2.3	138
1288	Compressive characteristics of single walled carbon nanotube with water interactions investigated by using molecular dynamics simulation. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 570-576.	0.9	33
1289	Design of 3D carbon nanotube-based nanostructures and prediction of their extra-strong mechanical properties under tension and compression. <i>Computational Materials Science</i> , 2014, 85, 324-331.	1.4	7
1290	Molecular dynamics simulation on double-elastic deformation of zigzag graphene nanoribbons at low temperature. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2014, 180, 1-6.	1.7	24
1291	Five Orders of Magnitude Reduction in Energy Coupling across Corrugated Graphene/Substrate Interfaces. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 2809-2818.	4.0	53
1292	Transport characteristics of water molecules in carbon nanotubes investigated by using molecular dynamics simulation. <i>Computational Materials Science</i> , 2014, 89, 36-44.	1.4	36
1293	Thermal expansion behavior of holes in graphene nanomeshes. <i>Physical Review B</i> , 2014, 89, .	1.1	20
1294	Surface passivation and boundary lubrication of self-mated tetrahedral amorphous carbon asperities under extreme tribological conditions. <i>Friction</i> , 2014, 2, 193-208.	3.4	29
1295	Guest editorial: Special issue on superlubricity. <i>Friction</i> , 2014, 2, 93-94.	3.4	4
1296	SYMPLER: SYMbolic ParticLE simuloR with grid-computing interface. <i>Computer Physics Communications</i> , 2014, 185, 1085-1099.	3.0	4
1297	A charge optimized many-body (comb) potential for titanium and titania. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 315007.	0.7	21
1298	A Large-Scale Molecular Dynamics Study of the Divacancy Defect in Graphene. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8200-8216.	1.5	40
1299	Mechanical properties of polycrystalline boron-nitride nanosheets. <i>RSC Advances</i> , 2014, 4, 19137-19143.	1.7	90
1300	Thermal Gradients on Graphene to Drive Nanoflake Motion. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 722-730.	2.3	63

#	ARTICLE	IF	CITATIONS
1301	Nanoscale structure and texture of highly anisotropic pyrocarbons revisited with transmission electron microscopy, image processing, neutron diffraction and atomistic modeling. Carbon, 2014, 80, 472-489.	5.4	53
1302	Chirality-Controlled Carbon Nanotubes Fabricated by Self-Assembly of Graphene Nanoribbons. Journal of Physical Chemistry C, 2014, 118, 19477-19483.	1.5	17
1303	Mechanical properties of MoS ₂ /graphene heterostructures. Applied Physics Letters, 2014, 105, .	1.5	135
1304	Superlubricity-activated thinning of graphite flakes compressed by passivated crystalline silicon substrates for graphene exfoliation. Carbon, 2014, 80, 68-74.	5.4	6
1305	Application of the molecular mechanics method to simulation of buckling of single-walled carbon nanotubes. Engineering Fracture Mechanics, 2014, 130, 83-95.	2.0	14
1306	A molecular dynamics study of the mechanical properties of a double-walled carbon nanocoil. Computational Materials Science, 2014, 82, 92-99.	1.4	24
1307	Thermal transport and thermoelectric properties of beta-graphyne nanostructures. Nanotechnology, 2014, 25, 245401.	1.3	51
1308	Molecular Dynamics Simulations of the Traction-Separation Response at the Interface between PVDF Binder and Graphite in the Electrode of Li-Ion Batteries. Journal of the Electrochemical Society, 2014, 161, A1218-A1223.	1.3	49
1309	Hydrogen species in diamond: Molecular dynamics simulation in bulk diamond for fusion applications. Journal of Nuclear Materials, 2014, 452, 218-222.	1.3	1
1310	Heat conduction in extended X-junctions of single-walled carbon nanotubes. Journal of Physics and Chemistry of Solids, 2014, 75, 123-129.	1.9	9
1311	Fracture and toughening mechanisms in SiC nanofiber reinforced SiC matrix nanocomposites with amorphous carbon coatings. Computational Materials Science, 2014, 83, 255-260.	1.4	6
1312	Role of cone angle on the mechanical behavior of cup-stacked carbon nanofibers studied by atomistic simulations. Carbon, 2014, 66, 523-529.	5.4	19
1313	Structure manipulation of graphene by hydrogenation. Carbon, 2014, 69, 86-91.	5.4	32
1314	Structural and elastic properties of a hypothetical high density <i>sp</i> ² -rich amorphous carbon phase. Journal of Chemical Physics, 2014, 140, .	1.2	5
1315	Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials. Journal of Physical Chemistry Letters, 2014, 5, 2144-2149.	2.1	59
1316	The tunable mechanical property of water-filled carbon nanotubes under an electric field. Journal Physics D: Applied Physics, 2014, 47, 125302.	1.3	4
1317	Tight-binding theory of graphene bending. Physical Review B, 2014, 89, .	1.1	39
1318	Mechanical-Thermal-Electrical and Morphological Properties of Graphene Reinforced Polymer Composites: A Review. Transactions of the Indian Institute of Metals, 2014, 67, 803-816.	0.7	56

#	ARTICLE	IF	CITATIONS
1319	Structure-mediated thermal transport of monolayer graphene allotropes nanoribbons. Carbon, 2014, 77, 416-423.	5.4	35
1320	Thermal transport in monolayer graphene oxide: Atomistic insights into phonon engineering through surface chemistry. Carbon, 2014, 77, 351-359.	5.4	62
1321	Thermal rectification of a single-wall carbon nanotube: A molecular dynamics study. Solid State Communications, 2014, 179, 54-58.	0.9	17
1322	Theoretical investigation of thermally induced coalescence mechanism of single-wall carbon nanohorns and their mechanical properties. Computational Materials Science, 2014, 88, 76-80.	1.4	6
1324	A Network Model for the Thermal Conductivity of Pillared-Graphene Architectures. , 2014, , .		0
1325	Cohesive Zone Model for the Interface of Multiwalled Carbon Nanotubes and Copper: Molecular Dynamics Simulation. Journal of Nanotechnology in Engineering and Medicine, 2014, 5, .	0.8	12
1326	WAVY-SHAPED DEFORMATION ANALYSIS OF MULTI-WALLED CARBON NANOTUBES USING MOLECULAR DYNAMICS METHOD. Journal of Japan Society of Civil Engineers Ser A2 (Applied Mechanics (AM)), 2014, 70, I_25-I_32.	0.1	0
1327	Water filling and electric field-induced enhancement in the mechanical property of carbon nanotubes. Scientific Reports, 2015, 5, 17537.	1.6	7
1328	Low thermal conductivity of graphyne nanotubes from molecular dynamics study. Physical Review B, 2015, 91, .	1.1	65
1329	<i>Ab initio</i> calculation of the real contact area on the atomic scale. Physical Review B, 2015, 91, .	1.1	9
1330	Threshold displacement energies in graphene and single-walled carbon nanotubes. Physical Review B, 2015, 92, .	1.1	20
1331	Xe irradiation of graphene on Ir(111): From trapping to blistering. Physical Review B, 2015, 92, .	1.1	32
1332	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. Physical Review B, 2015, 92, .	1.1	215
1333	Large-scale experimental and theoretical study of graphene grain boundary structures. Physical Review B, 2015, 92, .	1.1	75
1334	Effect of Structural Relaxation on the Electronic Structure of Graphene on Hexagonal Boron Nitride. Physical Review Letters, 2015, 115, 186801.	2.9	93
1335	Quantum effects in a free-standing graphene lattice: Path-integral against classical Monte Carlo simulations. Physical Review B, 2015, 92, .	1.1	24
1336	Exploiting hydrogenation for thermal rectification in graphene nanoribbons. Physical Review B, 2015, 92, .	1.1	26
1337	Modelling heat conduction in polycrystalline hexagonal boron-nitride films. Scientific Reports, 2015, 5, 13228.	1.6	104

#	ARTICLE	IF	CITATIONS
1338	Mechanism of strength reduction along the graphenization pathway. <i>Science Advances</i> , 2015, 1, e1501009.	4.7	16
1339	A test on reactive force fields for the study of silica dimerization reactions. <i>Journal of Chemical Physics</i> , 2015, 143, 184113.	1.2	19
1340	Voltage equilibration for reactive atomistic simulations of electrochemical processes. <i>Journal of Chemical Physics</i> , 2015, 143, 054109.	1.2	46
1341	Thermal Conductivity of Phonon Modes in Graphene Nanoribbon at Localized High Heating. , 2015, , .		0
1342	Coupling between flexural modes in free vibration of single-walled carbon nanotubes. <i>AIP Advances</i> , 2015, 5, 127110.	0.6	15
1343	Elastic behavior of carbon nanocoils: A molecular dynamics study. <i>AIP Advances</i> , 2015, 5, .	0.6	15
1344	Minimal graphene thickness for wear protection of diamond. <i>AIP Advances</i> , 2015, 5, 017117.	0.6	8
1345	Tunable thermal conductivity in carbon allotrope sheets: Role of acetylenic linkages. <i>Journal of Applied Physics</i> , 2015, 118, .	1.1	13
1346	Thermal conductivity of penta-graphene from molecular dynamics study. <i>Journal of Chemical Physics</i> , 2015, 143, 154703.	1.2	85
1347	Thermal conductivity variation of graphene with patterned double-side hydrogen doping. <i>Journal of Applied Physics</i> , 2015, 118, 075102.	1.1	12
1348	Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. <i>Journal of Chemical Physics</i> , 2015, 142, 244703.	1.2	51
1349	Morphology of a columnar stack of coronene molecules encapsulated in a single-walled carbon nanotube. <i>AIP Advances</i> , 2015, 5, 117113.	0.6	8
1350	Effect of Intrinsic Ripples on Elasticity of the Graphene Monolayer. <i>Nanoscale Research Letters</i> , 2015, 10, 422.	3.1	11
1351	Quenching of liquid carbon under intensive heat transfer to the cold diamond substrate: Molecular-dynamic simulation. <i>Journal of Physics: Conference Series</i> , 2015, 653, 012091.	0.3	10
1352	Material Temperature Dependence of the Retention and Sputtering Yield of Single-Crystal Graphite under Hydrogen Plasma Irradiation. <i>Plasma and Fusion Research</i> , 2015, 10, 3403075-3403075.	0.3	2
1353	Computer simulation of the interaction of ringlike carbon clusters with nanographene. <i>Journal of Physics: Conference Series</i> , 2015, 640, 012023.	0.3	2
1354	Predicting the lifetime of superlubricity. <i>Europhysics Letters</i> , 2015, 112, 60007.	0.7	3
1355	An analytical bond-order potential for carbon. <i>Journal of Computational Chemistry</i> , 2015, 36, 1719-1735.	1.5	36

#	ARTICLE	IF	CITATIONS
1356	Combining a reactive potential with a harmonic approximation for molecular dynamics simulation of failure: construction of a reduced potential. Journal of Physics: Conference Series, 2015, 574, 012041.	0.3	3
1357	Equilibrium Molecular Dynamics (MD) Simulation Study of Thermal Conductivity of Graphene Nanoribbon: A Comparative Study on MD Potentials. Electronics (Switzerland), 2015, 4, 1109-1124.	1.8	62
1358	Kinetic behavior of subsonic solitary wave in graphene nanoribbon. Journal of Statistical Mechanics: Theory and Experiment, 2015, 2015, P06007.	0.9	6
1359	Intrinsic thermal conductivity in monolayer graphene is ultimately upper limited: A direct estimation by atomistic simulations. Physical Review B, 2015, 91, .	1.1	59
1360	Atomistic Simulation on Buckling Behavior of Monolayer Graphene. Advanced Materials Research, 0, 1095, 35-38.	0.3	0
1361	Under pressure: Control of strain, phonons and bandgap opening in rippled graphene. Carbon, 2015, 91, 266-274.	5.4	55
1362	Electrochemical Hierarchical Composites. , 2015, , 239-286.		1
1363	Toward the Ultra-incompressible Carbon Materials. Computational Simulation and Experimental Observation. Journal of Physical Chemistry Letters, 2015, 6, 2147-2152.	2.1	16
1364	Atom Vacancies on a Carbon Nanotube: To What Extent Can We Simulate their Effects?. Journal of Chemical Theory and Computation, 2015, 11, 3393-3400.	2.3	6
1365	Effect of Covalent Functionalization on Thermal Transport across Graphene-Polymer Interfaces. Journal of Physical Chemistry C, 2015, 119, 12731-12738.	1.5	126
1366	Thermal AND Gate Using a Monolayer Graphene Nanoribbon. Small, 2015, 11, 2910-2917.	5.2	24
1367	Modification of graphene supported on SiO ₂ substrate with swift heavy ions from atomistic simulation point. Carbon, 2015, 93, 169-179.	5.4	42
1368	Raman spectroscopy and molecular simulation studies of graphitic nanomaterials. , 2015, , 179-199.		1
1370	Atomistic simulation of the growth of defect-free carbon nanotubes. Chemical Science, 2015, 6, 4704-4711.	3.7	44
1371	Finite element modelling of the instability in rapid fracture of graphene. Engineering Fracture Mechanics, 2015, 141, 111-119.	2.0	19
1372	Elastic moduli of boron nitride, aluminium nitride and gallium nitride nanotubes using second generation reactive empirical bond order potential. Multidiscipline Modeling in Materials and Structures, 2015, 11, 2-15.	0.6	11
1373	Molecular Dynamics Simulations of Sound Wave Propagation in a Gas and Thermo-Acoustic Effects on a Carbon Nanotube. Journal of Computational Acoustics, 2015, 23, 1540012.	1.0	5
1374	Change in electronic properties of carbon nanotubes caused by local distortion under axial compressive strain. , 2015, , .		0

#	ARTICLE	IF	CITATIONS
1375	Effect of Molecular Rotation on Charge Transport Phenomena. Journal of Multiscale Modeling, 2015, 06, 1550005.	1.0	0
1376	Lattice shearing in nano-grained graphene sheets: a molecular dynamics simulation. RSC Advances, 2015, 5, 105194-105199.	1.7	4
1377	Theory and modelling of diamond fracture from an atomic perspective. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2015, 373, 20140139.	1.6	9
1378	Recent developments and simulations utilizing bond-order potentials. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 074003.	0.8	14
1379	Interpolation effects in tabulated interatomic potentials. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 074008.	0.8	20
1380	Beyond ZnO nanowires for piezotronics and nanogenerators. , 2015, , .		0
1381	Fracture Size Effects in Nanoscale Materials: The Case of Graphene. Physical Review Applied, 2015, 4, .	1.5	11
1382	Mechanical integrity of a carbon nanotube/copper-based through-silicon via for 3D integrated circuits: a multi-scale modeling approach. Nanotechnology, 2015, 26, 485705.	1.3	11
1383	Edge Forces in Contacting Graphene Layers. Journal of Applied Mechanics, Transactions ASME, 2015, 82, .	1.1	20
1384	Dependence of Thermal Conductivity of Carbon Nanopeapods on Filling Ratios of Fullerene Molecules. Journal of Physical Chemistry A, 2015, 119, 11226-11232.	1.1	22
1385	A molecular dynamics investigation of buckling behaviour of hydrogenated graphene. Molecular Simulation, 2015, 41, 1212-1218.	0.9	14
1386	Investigation of mechanical strength of 2D nanoscale structures using a molecular dynamics based computational intelligence approach. International Journal of Modern Physics B, 2015, 29, 1450242.	1.0	3
1387	Rippling, buckling, and melting of single- and multilayer MoS_2 . Physical Review B, 2015, 91, .	1.1	41
1388	Enhancement of thermoelectric performance in I^2 -graphyne nanoribbons by suppressing phononic thermal conductance. Carbon, 2015, 85, 24-27.	5.4	76
1389	Computational study on the effects of annealing on the mechanical properties of polycrystalline graphene. Carbon, 2015, 86, 338-349.	5.4	23
1390	Wrinkling in Graphene Subjected to Gradient Tension. Nano, 2015, 10, 1550037.	0.5	4
1391	Superplastic deformation and energy dissipation mechanism in surface-bonded carbon nanofibers. Computational Materials Science, 2015, 99, 190-194.	1.4	7
1392	Parameterizing Complex Reactive Force Fields Using Multiple Objective Evolutionary Strategies (MOES). Part 1: ReaxFF Models for Cyclotrimethylene Trinitramine (RDX) and 1,1-Diamino-2,2-dinitroethene (FOX-7). Journal of Chemical Theory and Computation, 2015, 11, 381-391.	2.3	36

#	ARTICLE	IF	CITATIONS
1393	Effects of nanotube size and roof-layer coating on viscoelastic properties of hybrid diamond-like carbon and carbon nanotube composites. Carbon, 2015, 86, 163-173.	5.4	11
1394	C ₆₀ /Collapsed Carbon Nanotube Hybrids: A Variant of Peapods. Nano Letters, 2015, 15, 829-834.	4.5	26
1395	Graphene-Based Resonant Sensors for Detection of Ultra-Fine Nanoparticles: Molecular Dynamics and Nonlocal Elasticity Investigations. Nano, 2015, 10, 1550024.	0.5	26
1396	A review on the flexural mode of graphene: lattice dynamics, thermal conduction, thermal expansion, elasticity and nanomechanical resonance. Journal of Physics Condensed Matter, 2015, 27, 083001.	0.7	73
1397	Atomic simulations of effects of contact size and interfacial interaction strength on superlubricity in incommensurate sliding interface. Applied Physics A: Materials Science and Processing, 2015, 118, 301-306.	1.1	5
1398	Effects of atomic structure on the frictional properties of amorphous carbon coatings. Surface and Coatings Technology, 2015, 263, 8-14.	2.2	16
1399	On the Vibrational Behavior of Graphynes and Its Family: a Molecular Dynamics Investigation. Brazilian Journal of Physics, 2015, 45, 206-212.	0.7	19
1400	On the Wrapping of Polyglycolide, Poly(Ethylene Oxide), and Polyketone Polymer Chains Around Single-Walled Carbon Nanotubes Using Molecular Dynamics Simulations. Brazilian Journal of Physics, 2015, 45, 10-18.	0.7	18
1401	AIREBO-M: A reactive model for hydrocarbons at extreme pressures. Journal of Chemical Physics, 2015, 142, 024903.	1.2	159
1402	Vertical Tunneling Graphene Heterostructure-Based Transistor for Pressure Sensing. IEEE Electron Device Letters, 2015, 36, 280-282.	2.2	8
1403	Molecular Dynamics Calculations of CH ₃ Sticking Coefficient onto Diamond Surfaces. Plasma Processes and Polymers, 2015, 12, 764-770.	1.6	13
1404	Study on wrinkling in graphene under gradient shear by molecular dynamics simulation. Journal of Molecular Modeling, 2015, 21, 31.	0.8	11
1405	Reversible stretching of pre-strained water-filled carbon nanotubes under electric fields. Microfluidics and Nanofluidics, 2015, 18, 1201-1207.	1.0	5
1406	Wetting and motion behaviors of water droplet on graphene under thermal-electric coupling field. Journal of Applied Physics, 2015, 117, .	1.1	15
1407	Wrinkling Behaviour of Annular Graphynes under Circular Shearing Load Using Molecular Dynamics Simulations. Nanomaterials and Nanotechnology, 2015, 5, 9.	1.2	9
1408	Etching mechanisms of graphene nanoribbons in downstream H ₂ plasmas: insights from molecular dynamics simulations. Journal Physics D: Applied Physics, 2015, 48, 195202.	1.3	21
1409	Reset and switch protocols at Landauer limit in a graphene buckled ribbon. Europhysics Letters, 2015, 111, 10004.	0.7	5
1410	Tunable thermal rectification in silicon-functionalized graphene nanoribbons by molecular dynamics simulation. International Journal of Thermal Sciences, 2015, 98, 24-31.	2.6	28

#	ARTICLE	IF	CITATIONS
1411	Relaxation of moiré patterns for slightly misaligned identical lattices: graphene on graphite. 2D Materials, 2015, 2, 034010.	2.0	164
1412	Nano level optimization of graphene allotropes by means of a hybrid parallel evolutionary algorithm. Computational Materials Science, 2015, 106, 161-169.	1.4	17
1413	Cutting a chemical bond with demon's scissors: Mode- and bond-selective reactivity of methane on metal surfaces. Surface Science, 2015, 640, 25-35.	0.8	41
1414	Torsional behavior of single-walled carbon nanotubes. Carbon, 2015, 94, 826-835.	5.4	9
1415	A temperature related study on bifurcation strain and force of carbon nanotubes. Computational Materials Science, 2015, 109, 129-136.	1.4	3
1416	Molecular dynamics simulations of supported metal nanocatalyst formation by plasma sputtering. Catalysis Today, 2015, 256, 3-12.	2.2	30
1417	Simulation of mechanical properties of carbon nanotubes with superlattice structure. Current Applied Physics, 2015, 15, 1216-1221.	1.1	3
1418	Grain-size dependent mechanical behavior of nanocrystalline metals. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2015, 646, 101-134.	2.6	172
1419	Impeded Mass Transportation Due to Defects in Thermally Driven Nanotube Nanomotor. Journal of Physical Chemistry C, 2015, 119, 17362-17368.	1.5	33
1420	Diffusion of Heat and Mass in a Chemically Reacting Mixture away from Equilibrium. Journal of Physical Chemistry C, 2015, 119, 12838-12847.	1.5	6
1421	Nanoscale elasticity of highly anisotropic pyrocarbons. Carbon, 2015, 94, 285-294.	5.4	24
1422	Combined Effects of Structural Transformation and Hydrogen Passivation on the Frictional Behaviors of Hydrogenated Amorphous Carbon Films. Journal of Physical Chemistry C, 2015, 119, 16148-16155.	1.5	44
1423	Elastic Deformations in 2D van der waals Heterostructures and their Impact on Optoelectronic Properties: Predictions from a Multiscale Computational Approach. Scientific Reports, 2015, 5, 10872.	1.6	76
1424	Temperature dependent structural properties and bending rigidity of pristine and defective hexagonal boron nitride. Journal of Physics Condensed Matter, 2015, 27, 315302.	0.7	44
1425	Effects of nanobuds and heat welded nanobuds chains on mechanical behavior of carbon nanotubes. Computational Materials Science, 2015, 109, 49-55.	1.4	13
1426	Thermal transport across atomic-layer material interfaces. Nanotechnology Reviews, 2015, 4, .	2.6	28
1427	Parametrization of Stillinger-Weber potential based on valence force field model: application to single-layer MoS ₂ and black phosphorus. Nanotechnology, 2015, 26, 315706.	1.3	214
1428	Molecular dynamics study of a CNT-buckyball-enabled energy absorption system. Physical Chemistry Chemical Physics, 2015, 17, 17311-17321.	1.3	13

#	ARTICLE	IF	CITATIONS
1429	A review on nanomechanical resonators and their applications in sensors and molecular transportation. <i>Applied Physics Reviews</i> , 2015, 2, .	5.5	106
1430	Atomistic-continuum coupled model for nonlinear analysis of single layer graphene sheets. <i>International Journal of Non-Linear Mechanics</i> , 2015, 76, 112-119.	1.4	13
1431	Application of artificial intelligence technique for modelling elastic properties of 2D nanoscale material. <i>Molecular Simulation</i> , 2015, 41, 1143-1152.	0.9	7
1432	Phonon-phonon scattering rates in single walled carbon nanotubes. <i>Computational Materials Science</i> , 2015, 103, 151-156.	1.4	9
1433	Nanoscratching of multi-layer graphene by molecular dynamics simulations. <i>Tribology International</i> , 2015, 88, 85-88.	3.0	28
1434	Optimized molecular reconstruction procedure combining hybrid reverse Monte Carlo and molecular dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 114112.	1.2	24
1435	An analytical bond-order potential for the copper-hydrogen binary system. <i>Journal of Materials Science</i> , 2015, 50, 2859-2875.	1.7	18
1436	Imaging the C black formation by acetylene pyrolysis with molecular reactive force field simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11469-11480.	1.3	42
1437	Macroscale superlubricity enabled by graphene nanoscroll formation. <i>Science</i> , 2015, 348, 1118-1122.	6.0	665
1438	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. <i>Tribology Letters</i> , 2015, 58, 1.	1.2	38
1439	Energetics of atomic scale structure changes in graphene. <i>Chemical Society Reviews</i> , 2015, 44, 3143-3176.	18.7	141
1440	On the origin of abnormal phonon transport of graphyne. <i>International Journal of Heat and Mass Transfer</i> , 2015, 85, 880-889.	2.5	27
1441	Energy filtering transmission electron microscopy and atomistic simulations of tribo-induced hybridization change of nanocrystalline diamond coating. <i>Carbon</i> , 2015, 87, 317-329.	5.4	68
1442	Full symmetry implementation in condensed matter and molecular physics-Modified group projector technique. <i>Physics Reports</i> , 2015, 581, 1-43.	10.3	21
1443	On the crumpling of polycrystalline graphene by molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6297-6304.	1.3	37
1444	Intrinsic defect-induced tailoring of interfacial shear strength in CNT/polymer nanocomposites. <i>Composite Structures</i> , 2015, 127, 108-119.	3.1	48
1445	Insights into carbon nanotube and graphene formation mechanisms from molecular simulations: a review. <i>Reports on Progress in Physics</i> , 2015, 78, 036501.	8.1	93
1446	Anisotropic Shock Response of Stone-Wales Defects in Graphene. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7453-7460.	1.5	18

#	ARTICLE	IF	CITATIONS
1447	Thermal transport across graphene and single layer hexagonal boron nitride. <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	103
1448	Thermal transport in a graphene-MoS ₂ bilayer heterostructure: a molecular dynamics study. <i>RSC Advances</i> , 2015, 5, 29193-29200.	1.7	83
1449	Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field. <i>Chemical Reviews</i> , 2015, 115, 5797-5890.	23.0	182
1450	Fracture and defect evolution in carbon nanocoil – A molecular dynamics study. <i>Computational Materials Science</i> , 2015, 103, 126-133.	1.4	13
1451	Tuning the resonance properties of 2D carbon nanotube networks towards a mechanical resonator. <i>Nanotechnology</i> , 2015, 26, 315501.	1.3	6
1452	Using molecular dynamics simulations and finite element method to study the mechanical properties of nanotube reinforced polyethylene and polyketone. <i>Modern Physics Letters B</i> , 2015, 29, 1550155.	1.0	16
1453	Pressure dependence of the interfacial structure of potassium chloride films on iron. <i>Thin Solid Films</i> , 2015, 593, 150-157.	0.8	4
1454	Effect of extended line defects on thermal conduction of carbon nanotubes: analyzing phonon structures by band unfolding. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 305402.	0.7	6
1455	Size dependency and potential field influence on deriving mechanical properties of carbon nanotubes using molecular dynamics. <i>Theoretical and Applied Mechanics Letters</i> , 2015, 5, 167-172.	1.3	49
1456	Wet adhesion of graphene. <i>Extreme Mechanics Letters</i> , 2015, 3, 130-140.	2.0	16
1457	Elastic properties of nanopolycrystalline diamond: The nature of ultrahigh stiffness. <i>Applied Physics Letters</i> , 2015, 107, .	1.5	14
1458	The atomic scale structure of graphene powder studied by neutron and X-ray diffraction. <i>Journal of Applied Crystallography</i> , 2015, 48, 1429-1436.	1.9	18
1459	Anomalous heat conduction in asymmetric graphene Y junctions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 3136-3140.	0.9	0
1460	The effect of time step, thermostat, and strain rate on ReaxFF simulations of mechanical failure in diamond, graphene, and carbon nanotube. <i>Journal of Computational Chemistry</i> , 2015, 36, 1587-1596.	1.5	81
1461	Vibration of Cantilevered Double-Walled Carbon Nanotubes Predicted by Timoshenko Beam Model and Molecular Dynamics. <i>International Journal of Computational Methods</i> , 2015, 12, 1540017.	0.8	11
1462	Defect- and dopant-controlled carbon nanotubes fabricated by self-assembly of graphene nanoribbons. <i>Nano Research</i> , 2015, 8, 2988-2997.	5.8	7
1463	First principles-based multiparadigm, multiscale strategy for simulating complex materials processes with applications to amorphous SiC films. <i>Journal of Chemical Physics</i> , 2015, 142, 174703.	1.2	10
1464	Thermal transport in MoS ₂ /Graphene hybrid nanosheets. <i>Nanotechnology</i> , 2015, 26, 375402.	1.3	22

#	ARTICLE	IF	CITATIONS
1465	Thermal transport across carbon nanotube-graphene covalent and van der Waals junctions. <i>Journal of Applied Physics</i> , 2015, 118, .	1.1	52
1466	Fracture of graphene: a review. <i>International Journal of Fracture</i> , 2015, 196, 1-31.	1.1	144
1467	Elastic, plastic, and fracture mechanisms in graphene materials. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 373002.	0.7	26
1468	Significant reduction of graphene thermal conductivity by phononic crystal structure. <i>International Journal of Heat and Mass Transfer</i> , 2015, 91, 428-432.	2.5	79
1469	Nanoimprint-Assisted Shear Exfoliation (NASE) for Producing Multilayer MoS ₂ Structures as Field-Effect Transistor Channel Arrays. <i>ACS Nano</i> , 2015, 9, 8773-8785.	7.3	48
1470	Tuning the thermal conductivity of multi-layer graphene with interlayer bonding and tensile strain. <i>Applied Physics A: Materials Science and Processing</i> , 2015, 120, 1275-1281.	1.1	32
1471	Two-dimensional graphene heterojunctions: The tunable mechanical properties. <i>Carbon</i> , 2015, 95, 1061-1068.	5.4	13
1472	Molecular Dynamics Modeling of Buckling Behavior of Hydrogenated Graphyne. <i>Nano</i> , 2015, 10, 1550105.	0.5	6
1473	Low damage pre-doping on CVD graphene/Cu using a chlorine inductively coupled plasma. <i>Carbon</i> , 2015, 95, 664-671.	5.4	47
1474	A molecular dynamics study on thermal and mechanical properties of graphene-“paraffin nanocomposites. <i>RSC Advances</i> , 2015, 5, 82638-82644.	1.7	48
1475	A semi-analytical approach to molecular dynamics. <i>Journal of Computational Physics</i> , 2015, 303, 336-354.	1.9	10
1476	A close look at the motion of C60 on gold. <i>Current Applied Physics</i> , 2015, 15, 1402-1411.	1.1	33
1477	Elastic properties of a single-walled carbon nanotube under a thermal environment. <i>Composite Structures</i> , 2015, 121, 337-343.	3.1	37
1478	Calculation of the vibrational frequencies of carbon clusters and fullerenes with empirical potentials. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3898-3908.	1.3	12
1479	A minimalist's reactive potential for efficient molecular modelling of chemistry. <i>Molecular Simulation</i> , 2015, 41, 3-12.	0.9	1
1480	Water transport in the nano-pore of the calcium silicate phase: reactivity, structure and dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1411-1423.	1.3	75
1481	Carbon nanoscrolls fabricated from graphene nanoribbons using Ni nanowire templates: A molecular dynamics simulation. <i>Surface Science</i> , 2015, 634, 3-8.	0.8	11
1482	Adsorbate-Induced Curvature and Stiffening of Graphene. <i>Nano Letters</i> , 2015, 15, 159-164.	4.5	24

#	ARTICLE	IF	CITATIONS
1483	Rotation, elongation and failure of CNT nanoropes induced by electric field. <i>Computational Materials Science</i> , 2015, 98, 333-339.	1.4	2
1484	Structure, reactivity and mechanical properties of water ultra-confined in the ordered crystal: A case study of jennite. <i>Microporous and Mesoporous Materials</i> , 2015, 204, 106-114.	2.2	19
1485	Defect-Detriment to Graphene Strength Is Concealed by Local Probe: The Topological and Geometrical Effects. <i>ACS Nano</i> , 2015, 9, 401-408.	7.3	66
1486	Effects of covalent functionalization on the thermal transport in carbon nanotube/polymer composites: A multi-scale investigation. <i>Polymer</i> , 2015, 56, 563-571.	1.8	42
1487	Formation of nanopore in a suspended graphene sheet with argon cluster bombardment: A molecular dynamics simulation study. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2015, 343, 48-51.	0.6	13
1488	Molecular dynamics simulation of graphene on Cu (1 0 0) and (1 1 1) surfaces. <i>Carbon</i> , 2015, 82, 538-547.	5.4	35
1489	Hydrogen storage in heat welded random CNT network structures. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 403-411.	3.8	44
1490	The role of defects in the tensile properties of silicene. <i>Applied Physics A: Materials Science and Processing</i> , 2015, 118, 1437-1445.	1.1	39
1491	Bending Behavior of a Carbon Nanotube with Internal Fluid Flow. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015, 23, 431-436.	1.0	1
1492	Quasi-static buckling simulation of single-layer graphene sheets by the molecular mechanics method. <i>Mathematics and Mechanics of Solids</i> , 2015, 20, 836-870.	1.5	16
1493	A simulation study on the significant nanomechanical heterogeneous properties of collagen. <i>Biomechanics and Modeling in Mechanobiology</i> , 2015, 14, 445-457.	1.4	13
1494	Effects of topological point reconstructions on the fracture strength and deformation mechanisms of graphene. <i>Computational Materials Science</i> , 2015, 97, 172-180.	1.4	23
1495	Nonlinear-elastic membrane-shell model for single-walled carbon nanotubes under uni-axial deformation. <i>Computational Materials Science</i> , 2015, 97, 237-244.	1.4	3
1496	Enhanced torsional stability of carbon nanotubes with tensile pre-strain. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 66, 263-267.	1.3	1
1497	A shear localization mechanism for lubricity of amorphous carbon materials. <i>Scientific Reports</i> , 2014, 4, 3662.	1.6	92
1498	Mechanical analysis of graphene-based woven nano-fabric. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2015, 620, 367-374.	2.6	20
1499	Molecular scale simulations on thermoset polymers: A review. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015, 53, 103-122.	2.4	179
1500	Atomistic origin of radial corrugation in a few-walled carbon nanotubes: A molecular dynamics study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 65, 135-140.	1.3	4

#	ARTICLE	IF	CITATIONS
1501	Formation of carbon nanoscrolls from graphene nanoribbons: A molecular dynamics study. Computational Materials Science, 2015, 96, 300-305.	1.4	31
1502	Molecular dynamics simulations of the adsorption of polymer chains on graphyne and its family. Physica B: Condensed Matter, 2015, 456, 41-49.	1.3	19
1503	All-Graphene Planar Self-Switching MISFEDs, Metal-Insulator-Semiconductor Field-Effect Diodes. Scientific Reports, 2014, 4, 3983.	1.6	42
1504	Thermal Transport in Graphene Oxide " From Ballistic Extreme to Amorphous Limit. Scientific Reports, 2014, 4, 3909.	1.6	195
1506	Thermal Transport of Flexural and In-Plane Phonons Modulated by Bended Graphene Nanoribbons. Journal of Nanomaterials, 2016, 2016, 1-7.	1.5	3
1507	Buckling Behavior of Substrate Supported Graphene Sheets. Materials, 2016, 9, 32.	1.3	22
1508	Ionic Adsorption and Desorption of CNT Nanoropes. Nanomaterials, 2016, 6, 177.	1.9	7
1509	Atomistic Model Analysis of Deformation of Carbon Nanotubes under Axial Compression. Key Engineering Materials, 0, 725, 451-455.	0.4	0
1510	Multiscale Modeling of Novel Carbon Nanotube/Copper-Composite Material Used in Microelectronics. Journal of Multiscale Modeling, 2016, 07, 1650001.	1.0	2
1512	Oscillators based on double-walled armchair@zigzag carbon nanotubes containing inner tubes with different helical rises. Nanotechnology, 2016, 27, 095705.	1.3	8
1513	Gold nanoparticles promote amorphous carbon to be ammonia gas sensor. Europhysics Letters, 2016, 114, 40001.	0.7	2
1514	Atomistically derived cohesive zone model of intergranular fracture in polycrystalline graphene. Journal of Applied Physics, 2016, 119, 245107.	1.1	18
1515	Strain engineering for mechanical properties in graphene nanoribbons revisited: The warping edge effect. Journal of Applied Physics, 2016, 119, 234301.	1.1	2
1516	A molecular dynamics analysis of ion irradiation of ultrathin amorphous carbon films. Journal of Applied Physics, 2016, 120, 125311.	1.1	0
1517	Self-assembly of water molecules using graphene nanoresonators. RSC Advances, 2016, 6, 110466-110470.	1.7	5
1518	Predicting the thermal conductivity in a graphene nanoflake from its response to a thermal impulse. Physical Review B, 2016, 94, .	1.1	2
1519	Anomalous thermal conductivity of monolayer boron nitride. Applied Physics Letters, 2016, 108, .	1.5	30
1520	Cleaning graphene: A first quantum/classical molecular dynamics approach. Journal of Applied Physics, 2016, 119, 125309.	1.1	8

#	ARTICLE	IF	CITATIONS
1521	Phonon thermal properties of graphene from molecular dynamics using different potentials. Journal of Chemical Physics, 2016, 145, 134705.	1.2	67
1522	The unexpected stability of multiwall nanotubes under high pressure and shear deformation. Applied Physics Letters, 2016, 109, .	1.5	19
1523	Investigation of mechanical behavior of single- and multi-layer graphene by using molecular dynamics simulation. International Journal of Precision Engineering and Manufacturing, 2016, 17, 1693-1701.	1.1	18
1524	Young's modulus of defective graphene sheet from intrinsic thermal vibrations. Journal of Physics: Conference Series, 2016, 759, 012048.	0.3	3
1525	Entropic effects of thermal rippling on van der Waals interactions between monolayer graphene and a rigid substrate. Journal of Applied Physics, 2016, 119, .	1.1	18
1526	Strain- and torsion-induced resonance energy tuning of Raman scattering in single-wall carbon nanotubes. Physica Status Solidi (B): Basic Research, 2016, 253, 2391-2395.	0.7	1
1527	Self-healing phenomena of graphene: potential and applications. Open Physics, 2016, 14, 364-370.	0.8	17
1528	Adsorption of metal atoms at a buckled graphene grain boundary using model potentials. AIP Advances, 2016, 6, .	0.6	5
1529	Mode-I stress intensity factor in single layer graphene sheets. Computational Materials Science, 2016, 118, 251-258.	1.4	38
1530	Nonlocal continuum-based modeling of mechanical characteristics of nanoscopic structures. Physics Reports, 2016, 638, 1-97.	10.3	140
1531	Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations. Chemical Reviews, 2016, 116, 7078-7116.	23.0	635
1532	Effect of Oxygen Chemistry in Sputtering of Polymers. Journal of Physical Chemistry Letters, 2016, 7, 1559-1562.	2.1	9
1533	Multifactorial global search algorithm in the problem of optimizing a reactive force field. Theoretical and Mathematical Physics(Russian Federation), 2016, 187, 603-617.	0.3	1
1534	Bond breaking in stretched molecules: multi-reference methods versus density functional theory. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
1535	Effect of non-covalent functionalisation on thermal and mechanical properties of graphene-polymer nanocomposites. Carbon, 2016, 102, 311-318.	5.4	108
1536	Elucidating the Properties of Surrogate Fuel Mixtures Using Molecular Dynamics. Energy & Fuels, 2016, 30, 784-795.	2.5	16
1537	Tersoff potential with improved accuracy for simulating graphene in molecular dynamics environment. Materials Research Express, 2016, 3, 035011.	0.8	85
1538	Nanomechanics analysis of perfect and defected graphene sheets via a novel atomic-scale finite element method. Superlattices and Microstructures, 2016, 94, 1-12.	1.4	16

#	ARTICLE	IF	CITATIONS
1539	Collective superlubricity of graphene flakes. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 134007.	0.7	12
1540	A novel oscillator based on heterogeneous carbon@MoS ₂ nanotubes. <i>Nano Research</i> , 2016, 9, 1775-1784.	5.8	16
1541	Cross-Linking-Induced Frictional Behavior of Multilayer Graphene: Origin of Friction. <i>Tribology Letters</i> , 2016, 62, 1.	1.2	13
1542	Atomistic Mechanisms of Chemical Mechanical Polishing of a Cu Surface in Aqueous H ₂ O ₂ : Tight-Binding Quantum Chemical Molecular Dynamics Simulations. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 11830-11841.	4.0	42
1543	Early and transient stages of Cu oxidation: Atomistic insights from theoretical simulations and in situ experiments. <i>Surface Science</i> , 2016, 652, 98-113.	0.8	37
1544	Self healing nature of bilayer graphene. <i>Superlattices and Microstructures</i> , 2016, 96, 26-35.	1.4	9
1545	Energetics of a Li Atom adsorbed on B/N doped graphene with monovacancy. <i>Journal of Solid State Chemistry</i> , 2016, 240, 67-75.	1.4	22
1546	The thermoelectric performance of bulk three-dimensional graphene. <i>Materials Chemistry and Physics</i> , 2016, 183, 6-10.	2.0	15
1547	Buckled graphene for efficient energy harvest, storage and conversion. <i>Nanotechnology</i> , 2016, 27, 405402.	1.3	4
1548	Central-force decomposition of spline-based modified embedded atom method potential. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 075003.	0.8	0
1549	Efficient implementation of the many-body Reactive Bond Order (REBO) potential on GPU. <i>Journal of Computational Physics</i> , 2016, 321, 556-570.	1.9	4
1550	Simulation of structure and stability of carbon nanoribbons. <i>Russian Journal of General Chemistry</i> , 2016, 86, 1777-1786.	0.3	2
1551	Knockout driven reactions in complex molecules and their clusters. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016, 49, 162001.	0.6	52
1552	Elastocaloric Effect in Carbon Nanotubes and Graphene. <i>Nano Letters</i> , 2016, 16, 7008-7012.	4.5	24
1553	Nonequilibrium Molecular Dynamics Investigation of the Reduction in Friction and Wear by Carbon Nanoparticles Between Iron Surfaces. <i>Tribology Letters</i> , 2016, 63, 1.	1.2	46
1555	Long-range interatomic forces can minimize heat transfer: From slowdown of longitudinal optical phonons to thermal conductivity minimum. <i>Physical Review B</i> , 2016, 94, .	1.1	5
1556	An analytical benchmark and a Mathematica program for MD codes: Testing LAMMPS on the 2nd generation Brenner potential. <i>Computer Physics Communications</i> , 2016, 207, 426-431.	3.0	10
1557	Thermal vibration of a single-layered graphene with initial stress predicted by semiquantum molecular dynamics. <i>Materials Research Express</i> , 2016, 3, 095601.	0.8	6

#	ARTICLE	IF	CITATIONS
1558	Graphitization of amorphous carbons: A comparative study of interatomic potentials. Carbon, 2016, 109, 681-693.	5.4	173
1559	Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation. ACS Nano, 2016, 10, 8376-8384.	7.3	113
1560	Molecular dynamics study on α -phase vanadium monohydride with machine learning potential. Physical Review B, 2016, 94, .	1.1	21
1561	Negative Thermophoresis in Concentric Carbon Nanotube Nanodevices. Nano Letters, 2016, 16, 6396-6402.	4.5	31
1562	The atomic scale structure of glass-like carbon obtained from fullerene extract via spark plasma sintering. Carbon, 2016, 110, 172-179.	5.4	6
1563	Influence of helium atoms on the shear behavior of the fiber/matrix interphase of SiC/SiC composite. Journal of Nuclear Materials, 2016, 479, 504-514.	1.3	9
1564	Thermal transport in oxidized polycrystalline graphene. Carbon, 2016, 108, 318-326.	5.4	17
1565	Structure and energetics of interlayer dislocations in bilayer graphene. Physical Review B, 2016, 93, .	1.1	36
1566	A modified embedded-atom method interatomic potential for ionic systems: 2NNMEAM+Qeq. Physical Review B, 2016, 93, .	1.1	19
1567	Interplay between nanometer-scale strain variations and externally applied strain in graphene. Physical Review B, 2016, 93, .	1.1	8
1568	Critical thickness for interface misfit dislocation formation in two-dimensional materials. Physical Review B, 2016, 93, .	1.1	16
1569	Intrinsic Negative Poisson's Ratio for Single-Layer Graphene. Nano Letters, 2016, 16, 5286-5290.	4.5	107
1570	Molecular Dynamic Simulation of Collision-Induced Third-Body Formation in Hydrogen-Free Diamond-Like Carbon Asperities. Tribology Letters, 2016, 63, 26.	1.2	16
1571	Structural Changes in 2D Materials Due to Scattering of Light Ions. Nanoscience and Technology, 2016, , 63-88.	1.5	1
1572	Atomistic Study of Carbon Nanotubes: Effect of Cut-Off Distance. , 2016, , 293-300.		1
1573	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. ACS Central Science, 2016, 2, 409-415.	5.3	16
1574	Sequential Molecular Dynamics Simulations: A Strategy for Complex Chemical Reactions and a Case Study on the Graphitization of Cooked 1,3,5-Triamino-2,4,6-trinitrobenzene. Journal of Physical Chemistry C, 2016, 120, 25237-25245.	1.5	27
1575	Macroscopic self-reorientation of interacting two-dimensional crystals. Nature Communications, 2016, 7, 10800.	5.8	108

#	ARTICLE	IF	CITATIONS
1576	Energy-filtered Electron Transport Structures for Low-power Low-noise 2-D Electronics. Scientific Reports, 2016, 6, 36167.	1.6	6
1577	Elastic interaction of hydrogen atoms on graphene: A multiscale approach from first principles to continuum elasticity. Physical Review B, 2016, 94, .	1.1	4
1578	Strain effect on the device characteristics of vertical tunneling graphene heterostructure-based transistor. , 2016, , .		0
1579	What can molecular simulation do for global warming?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 173-197.	6.2	32
1582	The morphology and temperature dependent tensile properties of diamond nanothreads. Carbon, 2016, 107, 304-309.	5.4	46
1583	Modeling of Forced Desorption Processes in a Regenerable Graphene Sorbent for Elemental Mercury Capture. Journal of Physical Chemistry C, 2016, 120, 13263-13274.	1.5	6
1584	A molecular dynamics investigation into the size-dependent buckling behavior of a novel three-dimensional metallic carbon nanostructure (T6). Superlattices and Microstructures, 2016, 97, 125-131.	1.4	5
1585	A hyperboloid structure as a mechanical model of the carbon bond. International Journal of Solids and Structures, 2016, 96, 145-152.	1.3	10
1586	Uniaxial compression of suspended single and multilayer graphenes. 2D Materials, 2016, 3, 025033.	2.0	21
1587	Hot spot formation and chemical reaction initiation in shocked HMX crystals with nanovoids: a large-scale reactive molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 17627-17645.	1.3	52
1588	Friction and nonlinear dynamics. Journal of Physics Condensed Matter, 2016, 28, 293001.	0.7	19
1589	Directional anisotropy, finite size effect and elastic properties of hexagonal boron nitride. Journal of Physics Condensed Matter, 2016, 28, 295302.	0.7	38
1590	Effects of Vacancies, Nitrogen Atoms, and sp ³ Bonds on Mechanical Properties of Graphene Using Molecular Dynamics Simulations. , 2016, , 41-60.		0
1591	Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure. Computer Methods in Applied Mechanics and Engineering, 2016, 305, 422-440.	3.4	1
1592	Thermal conductivity of graphene kirigami: Ultralow and strain robustness. Carbon, 2016, 104, 203-213.	5.4	69
1593	Template-directed growth and mechanical properties of carbon nanotube-graphene junctions with nano-fillets: molecular dynamic simulation. RSC Advances, 2016, 6, 56077-56082.	1.7	2
1594	Controllable deformation of salt water-filled carbon nanotubes using an electric field with application to molecular sieving. Nanotechnology, 2016, 27, 315702.	1.3	12
1595	Molecular dynamics simulation of defected carbon nanotubes. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications, 2016, 230, 654-662.	0.7	7

#	ARTICLE	IF	CITATIONS
1596	Influence of out-of-plane defects on vibration analysis of graphene: Molecular Dynamics and Non-local Elasticity approaches. Superlattices and Microstructures, 2016, 91, 331-344.	1.4	17
1597	Toughness and strength of nanocrystalline graphene. Nature Communications, 2016, 7, 10546.	5.8	158
1598	Tuneable graphene nanopores for single biomolecule detection. Nanoscale, 2016, 8, 10066-10077.	2.8	19
1599	Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide. Computational Materials Science, 2016, 114, 236-243.	1.4	26
1600	Geometry and Self-stress of Single-Wall Carbon Nanotubes and Graphene via a Discrete Model Based on a 2nd-Generation REBO Potential. Journal of Elasticity, 2016, 125, 1-37.	0.9	26
1601	Reactive molecular simulation on the ordered crystal and disordered glass of the calcium silicate hydrate gel. Ceramics International, 2016, 42, 4333-4346.	2.3	34
1602	Activation and mechanochemical breaking of C-C bonds initiate wear of diamond (110) surfaces in contact with silica. Carbon, 2016, 98, 474-483.	5.4	61
1603	Atomistic-scale simulations of the chemomechanical behavior of graphene under nanoparticle impact. Carbon, 2016, 99, 58-64.	5.4	92
1604	New aspects on the metal reinforcement by carbon nanofillers: A molecular dynamics study. Materials and Design, 2016, 91, 306-313.	3.3	54
1605	Negative Poisson's Ratio in Single-Layer Graphene Ribbons. Nano Letters, 2016, 16, 2657-2662.	4.5	115
1606	Molecular dynamics study on doping defected graphene by boron. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 363-370.	1.0	7
1607	On the elastic properties of single-walled carbon nanotubes/poly(ethylene oxide) nanocomposites using molecular dynamics simulations. Journal of Molecular Modeling, 2016, 22, 41.	0.8	21
1608	A comparison of empirical potentials for sliding simulations of MoS ₂ . Computational Materials Science, 2016, 115, 158-169.	1.4	38
1609	Molecular dynamics simulations on deformation and fracture of bi-layer graphene with different stacking pattern under tension. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 609-613.	0.9	9
1610	Superlubricity of graphene nanoribbons on gold surfaces. Science, 2016, 351, 957-961.	6.0	302
1611	Thermoelectric properties of gamma-graphyne nanoribbon incorporating diamond-like quantum dots. Journal Physics D: Applied Physics, 2016, 49, 135303.	1.3	5
1612	Opportunities and Challenges of Atomistic Modeling to Simulate Amorphous Carbon Properties for Computer Hard-Disk Applications. IEEE Transactions on Magnetics, 2016, 52, 1-12.	1.2	1
1613	Molecular dynamics study on the mechanical response and failure behaviour of graphene: performance enhancement via 5-7 defects. RSC Advances, 2016, 6, 26361-26373.	1.7	25

#	ARTICLE	IF	CITATIONS
1614	Some Aspects of Thermal Transport across the Interface between Graphene and Epoxy in Nanocomposites. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 8272-8279.	4.0	106
1615	Formation of single carbon chain bridging two SWCNTs via tensile deformation of nanobud junction. <i>Materials and Design</i> , 2016, 97, 86-92.	3.3	5
1616	Phonon Scattering Dynamics of Thermophoretic Motion in Carbon Nanotube Oscillators. <i>Nano Letters</i> , 2016, 16, 2174-2180.	4.5	11
1617	Molecular dynamics simulations of irradiation defects in graphite: Single crystal mechanical and thermal properties. <i>Computational Materials Science</i> , 2016, 113, 60-65.	1.4	23
1618	Simulations of inorganic–bioorganic interfaces to discover new materials: insights, comparisons to experiment, challenges, and opportunities. <i>Chemical Society Reviews</i> , 2016, 45, 412-448.	18.7	176
1619	Efficient Use of an Adapting Database of <i>Ab Initio</i> Calculations To Generate Accurate Newtonian Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 664-675.	2.3	1
1620	Thermal conductivity of a new carbon nanotube analog: The diamond nanothread. <i>Carbon</i> , 2016, 98, 232-237.	5.4	71
1621	Hydrogen Plasmas Processing of Graphene Surfaces. <i>Plasma Chemistry and Plasma Processing</i> , 2016, 36, 213-229.	1.1	23
1622	Large scale atomistic simulation of single-layer graphene growth on Ni(111) surface: molecular dynamics simulation based on a new generation of carbon–metal potential. <i>Nanoscale</i> , 2016, 8, 921-929.	2.8	38
1623	Structural, energetic, and electronic properties of gyroidal graphene nanostructures. <i>Carbon</i> , 2016, 96, 998-1007.	5.4	9
1624	Characterizing nanotube–polymer interaction using molecular dynamics simulation. <i>Computational Materials Science</i> , 2016, 112, 356-363.	1.4	46
1625	Mechanical properties of hypothetical graphene foams: Giant Schwarzites. <i>Carbon</i> , 2016, 96, 1191-1199.	5.4	42
1626	Potential routes to stronger carbon nanotube fibres via carbon ion irradiation and deposition. <i>Carbon</i> , 2016, 96, 1138-1156.	5.4	10
1627	Effect of Point and Line Defects on Mechanical and Thermal Properties of Graphene: A Review. <i>Critical Reviews in Solid State and Materials Sciences</i> , 2016, 41, 47-71.	6.8	100
1628	Nanoscale origin and evolution of kinetically induced defects in carbon spheres. <i>Carbon</i> , 2016, 96, 647-660.	5.4	5
1629	Torsional failure of water-filled carbon nanotubes. <i>International Journal of Damage Mechanics</i> , 2016, 25, 87-97.	2.4	5
1630	Advances in atomic-scale tribological mechanisms of solid interfaces. <i>Tribology International</i> , 2016, 94, 1-13.	3.0	25
1631	Modelling of graphene functionalization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6351-6372.	1.3	190

#	ARTICLE	IF	CITATIONS
1632	Quantum and classical dynamics of reactive scattering of H ₂ from metal surfaces. Chemical Society Reviews, 2016, 45, 3658-3700.	18.7	137
1633	Investigation of the vibration and buckling of graphynes: A molecular dynamics-based finite element model. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 2017, 231, 1162-1178.	1.1	14
1634	H4-alkanes: A new class of hydrogen storage material?. International Journal of Hydrogen Energy, 2017, 42, 2223-2228.	3.8	6
1635	Vibration of single-walled carbon nanotubes with elastic boundary conditions. International Journal of Mechanical Sciences, 2017, 122, 156-166.	3.6	24
1636	Electron contributions to the heat conduction across Au/graphene/Au interfaces. Carbon, 2017, 115, 665-671.	5.4	24
1637	ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS ₂). Journal of Physical Chemistry Letters, 2017, 8, 631-640.	2.1	126
1638	The mechanics and design of a lightweight three-dimensional graphene assembly. Science Advances, 2017, 3, e1601536.	4.7	331
1639	An empirical force field for the simulation of the vibrational spectroscopy of carbon nanomaterials. Carbon, 2017, 113, 299-308.	5.4	12
1640	Frictional behavior of strained multilayer graphene: Tuning the atomic scale contact area. Diamond and Related Materials, 2017, 73, 273-277.	1.8	28
1641	Modelling of glass-like carbon structure and its experimental verification by neutron and X-ray diffraction. Journal of Applied Crystallography, 2017, 50, 36-48.	1.9	46
1642	Reactive molecular dynamics and experimental study of graphene-cement composites: Structure, dynamics and reinforcement mechanisms. Carbon, 2017, 115, 188-208.	5.4	301
1643	Impact of vacancies on the thermal conductivity of graphene nanoribbons: A molecular dynamics simulation study. AIP Advances, 2017, 7, .	0.6	40
1644	Classical Molecular Dynamics Simulations. , 2017, , 49-139.		1
1645	Interatomic Potential for Hydrocarbons on the Basis of the Modified Embedded-Atom Method with Bond Order (MEAM-BO). Journal of Physical Chemistry A, 2017, 121, 1502-1524.	1.1	18
1646	Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics. Journal of Physical Chemistry A, 2017, 121, 1051-1068.	1.1	204
1647	Fullerite-based nanocomposites with ultrahigh stiffness. Theoretical investigation. Carbon, 2017, 115, 546-549.	5.4	15
1648	A molecular dynamics simulation of the graphene growth on Cu(1 1 1) surface. Computational Materials Science, 2017, 130, 10-15.	1.4	20
1649	Weakening effect of nickel catalyst particles on the mechanical strength of the carbon nanotube/carbon fiber junction. Carbon, 2017, 115, 589-599.	5.4	21

#	ARTICLE	IF	CITATIONS
1650	Multiscale thermo-mechanical analysis of multi-layered coatings in solar thermal applications. Finite Elements in Analysis and Design, 2017, 127, 31-43.	1.7	14
1651	Thermal conductivity of graphene nanoribbons under shear deformation: A molecular dynamics simulation. Scientific Reports, 2017, 7, 41398.	1.6	53
1652	Fracture of monolayer boronitrene and its interface with graphene. International Journal of Fracture, 2017, 205, 151-168.	1.1	24
1653	Molecular dynamics investigation of the elastic and fracture properties of the R-graphyne under uniaxial tension. Physica B: Condensed Matter, 2017, 513, 29-39.	1.3	16
1654	A Catalytic Etching-Wetting-Dewetting Mechanism in the Formation of Hollow Graphitic Carbon Fiber. Chem, 2017, 2, 299-310.	5.8	44
1655	Initial Decay Mechanism of the Heated CL-20/HMX Cocrystal: A Case of the Cocrystal Mediating the Thermal Stability of the Two Pure Components. Journal of Physical Chemistry C, 2017, 121, 4899-4908.	1.5	68
1656	Interfacial thermal conductance in graphene/black phosphorus heterogeneous structures. Carbon, 2017, 117, 399-410.	5.4	85
1657	Phonon thermal properties of graphene on h-BN from molecular dynamics simulations. Applied Physics Letters, 2017, 110, .	1.5	45
1658	Atomistic mechanisms of Si chemical mechanical polishing in aqueous H2O2: ReaxFF reactive molecular dynamics simulations. Computational Materials Science, 2017, 131, 230-238.	1.4	68
1659	Thermophoretic transport of ionic liquid droplets in carbon nanotubes. Nanotechnology, 2017, 28, 155401.	1.3	12
1660	Enhancement of fracture toughness of graphene via crack bridging with stone-thrower-wales defects. Diamond and Related Materials, 2017, 74, 90-99.	1.8	33
1661	Transferable Reactive Force Fields: Extensions of ReaxFF- <i>lg</i> to Nitromethane. Journal of Physical Chemistry A, 2017, 121, 2001-2013.	1.1	19
1662	Methane Behavior in Carbon Nanotube as a Function of Pore Filling and Temperature Studied by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 4066-4073.	1.5	3
1663	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. Scientific Data, 2017, 4, 160125.	2.4	18
1664	Axial tensile strain effects on the contact thermal conductance between cross contacted single-walled carbon nanotubes. Journal of Applied Physics, 2017, 121, .	1.1	2
1665	Machine learning based interatomic potential for amorphous carbon. Physical Review B, 2017, 95, .	1.1	431
1666	Investigation of Overall Pyrolysis Stages for Liulin Bituminous Coal by Large-Scale ReaxFF Molecular Dynamics. Energy & Fuels, 2017, 31, 3675-3683.	2.5	62
1667	Aspect ratio effect on shear modulus and ultimate shear strength of graphene nanoribbons. Diamond and Related Materials, 2017, 74, 9-15.	1.8	11

#	ARTICLE	IF	CITATIONS
1668	Study on mechanical properties of graphyne nanostructures by molecular dynamics simulation. <i>Materials Research Express</i> , 2017, 4, 025603.	0.8	27
1669	Electrical and Thermal Transport in Coplanar Polycrystalline Graphene-hBN Heterostructures. <i>Nano Letters</i> , 2017, 17, 1660-1664.	4.5	62
1670	Confinement effects on the thermal stability of poly(ethylene oxide)/graphene nanocomposites: A reactive molecular dynamics simulation study. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2017, 55, 1026-1035.	2.4	16
1671	On the elastic and fracture properties of perfect and defective γ -graphynes: A molecular dynamics investigation. <i>Journal of Alloys and Compounds</i> , 2017, 713, 1-9.	2.8	11
1672	The atomic scale structure of saccharose-based carbons. <i>Philosophical Magazine</i> , 2017, 97, 1675-1697.	0.7	7
1673	Empirical potential influence and effect of temperature on the mechanical properties of pristine and defective hexagonal boron nitride. <i>Materials Research Express</i> , 2017, 4, 065005.	0.8	12
1674	Graphene helicoid as novel nanospring. <i>Carbon</i> , 2017, 120, 258-264.	5.4	42
1675	Effects of electron-phonon interactions on the spin-dependent Seebeck effect in graphene nanoribbons. <i>Carbon</i> , 2017, 119, 548-554.	5.4	20
1676	Thermal transmittance in graphene based networks for polymer matrix composites. <i>International Journal of Thermal Sciences</i> , 2017, 117, 98-105.	2.6	26
1677	Mechanical properties of single-walled carbon nanotubes: a comprehensive molecular dynamics study. <i>Materials Research Express</i> , 2017, 4, 055015.	0.8	16
1678	Stable carbon configurations. <i>Bolletino Dell Unione Matematica Italiana</i> , 2017, 10, 335-354.	0.6	4
1679	Enhancement of thermoelectric performance of gamma-graphyne through incorporating a hexagonal quantum dot. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2017, 25, 205-210.	1.0	2
1680	Anisotropic elastic modulus, high Poisson's ratio and negative thermal expansion of graphynes and graphdiynes. <i>Diamond and Related Materials</i> , 2017, 77, 57-64.	1.8	41
1681	Correcting for Tip Geometry Effects in Molecular Simulations of Single-Asperity Contact. <i>Tribology Letters</i> , 2017, 65, 1.	1.2	17
1682	A time-dependent atomistic reconstruction of severe irradiation damage and associated property changes in nuclear graphite. <i>Carbon</i> , 2017, 120, 111-120.	5.4	23
1683	Structure-dependent mechanical properties of extended beta-graphyne. <i>Carbon</i> , 2017, 120, 350-357.	5.4	21
1684	Investigation of Thermal Properties of Ni-Coated Graphene Nanoribbons Based on Molecular Dynamics Methods. <i>Journal of Electronic Materials</i> , 2017, 46, 4733-4739.	1.0	5
1685	Size effect on brittle and ductile fracture of two-dimensional interlinked carbon nanotube network. <i>Physica B: Condensed Matter</i> , 2017, 520, 82-88.	1.3	6

#	ARTICLE	IF	CITATIONS
1686	A mode-independent energy-based buckling analysis method and its application on substrate-supported graphene. <i>International Journal of Solids and Structures</i> , 2017, 124, 73-88.	1.3	5
1687	Effect of ripples on the finite temperature elastic properties of hexagonal boron nitride using strain-fluctuation method. <i>Superlattices and Microstructures</i> , 2017, 111, 360-372.	1.4	12
1688	Efficient molecular dynamics simulations with many-body potentials on graphics processing units. <i>Computer Physics Communications</i> , 2017, 218, 10-16.	3.0	126
1689	Length and temperature dependence of the mechanical properties of finite-size carbyne. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 93, 124-131.	1.3	14
1690	Transformation of Amorphous Carbon Clusters to Fullerenes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13396-13404.	1.5	22
1691	Grain boundaries guided vibration wave propagation in polycrystalline graphene. <i>RSC Advances</i> , 2017, 7, 24667-24673.	1.7	3
1692	Efficient embedded atom method interatomic potential for graphite and carbon nanostructures. <i>Molecular Simulation</i> , 2017, 43, 1480-1484.	0.9	5
1693	Mechanics of a Graphene Flake Driven by the Stiffness Jump on a Graphene Substrate. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2017, 84, .	1.1	8
1694	The normal-auxeticity mechanical phase transition in graphene. <i>2D Materials</i> , 2017, 4, 021020.	2.0	49
1695	Non-Hookean statistical mechanics of clamped graphene ribbons. <i>Physical Review B</i> , 2017, 95, .	1.1	55
1696	The atomic simulation environmentâ€”a Python library for working with atoms. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 273002.	0.7	1,933
1697	Abnormal nonlocal scale effect on static bending of single-layer MoS ₂ . <i>Nanotechnology</i> , 2017, 28, 215706.	1.3	1
1698	The Gaussian stiffness of graphene deduced from a continuum model based on Molecular Dynamics potentials. <i>Journal of the Mechanics and Physics of Solids</i> , 2017, 104, 96-114.	2.3	19
1699	The effects of intertube bridging through graphene nanoribbons on the mechanical properties of pillared graphene. <i>Composites Part B: Engineering</i> , 2017, 120, 1-9.	5.9	8
1700	Unraveling mechanics of armchair and zigzag graphene nanoribbons. <i>International Journal of Damage Mechanics</i> , 2017, 26, 447-462.	2.4	20
1701	An investigation on tensile properties of coiled carbon nanotubes using molecular dynamics simulation. <i>Diamond and Related Materials</i> , 2017, 74, 154-163.	1.8	11
1702	The best features of diamond nanothread for nanofibre applications. <i>Nature Communications</i> , 2017, 8, 14863.	5.8	62
1703	Plasticity resulted from phase transformation for monolayer molybdenum disulfide film during nanoindentation simulations. <i>Nanotechnology</i> , 2017, 28, 164005.	1.3	24

#	ARTICLE	IF	CITATIONS
1704	Chlorine-trapped CVD bilayer graphene for resistive pressure sensor with high detection limit and high sensitivity. <i>2D Materials</i> , 2017, 4, 025049.	2.0	34
1705	The enhancement of Hall mobility and conductivity of CVD graphene through radical doping and vacuum annealing. <i>RSC Advances</i> , 2017, 7, 16104-16108.	1.7	27
1706	Scaling properties of polycrystalline graphene: a review. <i>2D Materials</i> , 2017, 4, 012002.	2.0	62
1707	Blister-free ion beam patterning of supported graphene. <i>Nanotechnology</i> , 2017, 28, 055304.	1.3	5
1708	Elastic and electronic properties of oxygen plasma-treated graphene sheets from first principles. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750054.	1.0	0
1709	Characterizing Structural Complexity in Disordered Carbons: From the Slit Pore to Atomistic Models. <i>Langmuir</i> , 2017, 33, 831-847.	1.6	28
1710	Creating nanoporous graphene with swift heavy ions. <i>Carbon</i> , 2017, 114, 511-518.	5.4	52
1711	Impacts of potential models on calculating the thermal conductivity of graphene using non-equilibrium molecular dynamics simulations. <i>International Journal of Heat and Mass Transfer</i> , 2017, 107, 450-460.	2.5	67
1712	The atomic scale structure of dahlia-like single wall carbon nanohorns produced by direct vaporization of graphite. <i>Diamond and Related Materials</i> , 2017, 72, 26-31.	1.8	6
1713	Metal Ion Modeling Using Classical Mechanics. <i>Chemical Reviews</i> , 2017, 117, 1564-1686.	23.0	266
1714	An atomic-level understanding of the strengthening mechanism of aluminum matrix composites reinforced by aligned carbon nanotubes. <i>Computational Materials Science</i> , 2017, 128, 359-372.	1.4	54
1715	Tunable thermal conductivity along graphene/hexagonal boron-nitride polycrystalline heterostructures. <i>European Physical Journal Plus</i> , 2017, 132, 1.	1.2	11
1716	Suppressing Nanoscale Wear by Graphene/Graphene Interfacial Contact Architecture: A Molecular Dynamics Study. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 40959-40968.	4.0	43
1717	Liquid-assisted, etching-free, mechanical peeling of 2D materials. <i>Extreme Mechanics Letters</i> , 2017, 16, 33-40.	2.0	24
1718	Effect of room temperature lattice vibration on the electron transport in graphene nanoribbons. <i>Applied Physics Letters</i> , 2017, 111, 133107.	1.5	53
1719	Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. <i>RSC Advances</i> , 2017, 7, 45552-45581.	1.7	327
1720	Enhanced thermoelectric properties of the AGNR/CYNR heterojunctions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 3766-3772.	0.9	13
1721	Dynamic encapsulation of corannulene molecules into a single-walled carbon nanotube. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27704-27715.	1.3	7

#	ARTICLE	IF	CITATIONS
1722	Nonlinear vibrations of carbon chain resonators tuned by temperature. <i>Materials Research Express</i> , 2017, 4, 105026.	0.8	2
1723	Small-size effect on wrinkle and fracture of monolayer graphene subjected to in-plane shear. <i>Nanotechnology</i> , 2017, 28, 455702.	1.3	4
1724	Atomistic simulations of graphite etching at realistic time scales. <i>Chemical Science</i> , 2017, 8, 7160-7168.	3.7	6
1725	Spatial localization and thermal rectification in inhomogeneously deformed lattices. <i>Physical Review B</i> , 2017, 96, .	1.1	9
1726	A comparative study of the mechanical properties of multilayer MoS ₂ and graphene/MoS ₂ heterostructure: effects of temperature, number of layers and stacking order. <i>Current Applied Physics</i> , 2017, 17, 1483-1493.	1.1	19
1727	Remarkable reduction of thermal conductivity in graphyne nanotubes by local resonance. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 345301.	1.3	8
1728	Misorientation angle depended deformation of bilayer graphene sheets under in-plane loading. <i>Integrated Ferroelectrics</i> , 2017, 179, 120-129.	0.3	0
1729	Molecular Dynamics as the Tool for Investigation of Carbon Nanostructures Properties. , 2017, , 267-289.		9
1730	Tight-Binding Quantum Chemical Molecular Dynamics Study on the Friction and Wear Processes of Diamond-Like Carbon Coatings: Effect of Tensile Stress. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 34396-34404.	4.0	43
1731	Unraveling the influence of grain boundaries on the mechanical properties of polycrystalline carbon nanotubes. <i>Carbon</i> , 2017, 125, 180-188.	5.4	44
1732	Adsorption and Diffusion of Fluids in Defective Carbon Nanotubes: Insights from Molecular Simulations. <i>Langmuir</i> , 2017, 33, 11834-11844.	1.6	9
1733	Torsional behavior of chiral single-walled and double-walled carbon nanotubes. <i>Materials Research Express</i> , 2017, 4, 105004.	0.8	2
1734	Sliding friction of graphene/hexagonal boron nitride heterojunctions: a route to robust superlubricity. <i>Scientific Reports</i> , 2017, 7, 10851.	1.6	108
1735	Molecular dynamics study on the tensile properties of graphene/Cu nanocomposite. <i>International Journal of Computational Materials Science and Engineering</i> , 2017, 06, 1750021.	0.5	5
1736	Thermal transport in graphene/stanene hetero-bilayer nanostructures with vacancies: an equilibrium molecular dynamics study. <i>RSC Advances</i> , 2017, 7, 44780-44787.	1.7	26
1737	Negative differential thermal resistance in deformed carbon nanotubes. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2017, 2017, 053209.	0.9	4
1738	Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparametrization for Many-Body Dispersion Effects. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22826-22835.	1.5	61
1739	Graphene-Titanium Interfaces from Molecular Dynamics Simulations. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 33288-33297.	4.0	37

#	ARTICLE	IF	CITATIONS
1740	Growth speed of single edge pre-crack in graphene sheet under tension. <i>Engineering Fracture Mechanics</i> , 2017, 182, 337-355.	2.0	5
1741	Role of Interfaces in Elasticity and Failure of Clay-Organic Nanocomposites: Toughening upon Interface Weakening?. <i>Langmuir</i> , 2017, 33, 11457-11466.	1.6	17
1742	The chirality-dependent fracture properties of single-layer graphene sheets: Molecular dynamics simulations and finite element method. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	8
1743	Large anisotropic thermal conductivity and excellent thermoelectric properties observed in carbon foam. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	11
1744	Molecular dynamics study of the shear strength and fracture behavior of nanoporous graphene membranes. <i>Current Applied Physics</i> , 2017, 17, 1323-1328.	1.1	11
1745	Thermal fluctuations and effective bending stiffness of elastic thin sheets and graphene: A nonlinear analysis. <i>Journal of the Mechanics and Physics of Solids</i> , 2017, 107, 294-319.	2.3	49
1746	H+ ion-induced damage and etching of multilayer graphene in H2 plasmas. <i>Journal of Applied Physics</i> , 2017, 121, .	1.1	15
1747	Non-classic modeling of three-dimensional manipulation with different geometry of atomic force microscopy components: Multi-scale approach. <i>Mechanics Research Communications</i> , 2017, 84, 102-109.	1.0	2
1748	Site Dependent Atom Type ReaxFF for the Proton-Catalyzed Twin Polymerization. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15984-15992.	1.5	8
1749	Gas-like adhesion of two-dimensional materials onto solid surfaces. <i>Scientific Reports</i> , 2017, 7, 159.	1.6	15
1750	Modeling of tensile testing on perfect and defective graphenylene nanotubes using molecular dynamics simulations. <i>Materials Research Express</i> , 2017, 4, 085012.	0.8	4
1751	Graphene nanoribbons on gold: understanding superlubricity and edge effects. <i>2D Materials</i> , 2017, 4, 045003.	2.0	43
1752	Possibility of Improving Oscillation Performance of Double-Walled Nanotube Oscillators via Tuning Vacancy Defects. <i>Journal of Nano Research</i> , 2017, 48, 148-155.	0.8	5
1753	Identification of Graphene Properties in the Framework of Molecular Dynamics. <i>Springer Proceedings in Physics</i> , 2017, , 229-237.	0.1	0
1754	Size effect on interlayer shear between graphene sheets. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	7
1755	Determining the Gaussian Modulus and Edge Properties of 2D Materials: From Graphene to Lipid Bilayers. <i>Physical Review Letters</i> , 2017, 119, 068002.	2.9	29
1756	Morphology- and dehydrogenation-controlled mechanical properties in diamond nanothreads. <i>Carbon</i> , 2017, 124, 9-22.	5.4	22
1757	Stability and thermal behavior of molybdenum disulfide nanotubes: Nonequilibrium molecular dynamics simulation using REBO potential. <i>Journal of Applied Physics</i> , 2017, 122, 224303.	1.1	6

#	ARTICLE	IF	CITATIONS
1758	Atomistic simulations of the equation of state and hybridization of liquid carbon at a temperature of 6000 K in the pressure range of 1–25 GPa. <i>Journal of Chemical Physics</i> , 2017, 147, 214302.	1.2	16
1759	Exact expressions for the bending rigidity and elastic moduli of a graphene sheet derived with the geometric potential of carbon. <i>AIP Conference Proceedings</i> , 2017, , .	0.3	0
1760	Large stretchability and failure mechanism of graphene kirigami under tension. <i>Soft Matter</i> , 2017, 13, 8930-8939.	1.2	16
1761	Effective mechanical properties of multilayer nano-heterostructures. <i>Scientific Reports</i> , 2017, 7, 15818.	1.6	53
1762	Interface mechanical properties of graphene reinforced copper nanocomposites. <i>Materials Research Express</i> , 2017, 4, 115020.	0.8	17
1763	ChIMES: A Force Matched Potential with Explicit Three-Body Interactions for Molten Carbon. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6222-6229.	2.3	54
1764	A new material property of graphene: The bending Poisson coefficient. <i>Europhysics Letters</i> , 2017, 118, 26001.	0.7	7
1765	Laser structuring of carbon nanotubes in the albumin matrix for the creation of composite biostructures. <i>Journal of Biomedical Optics</i> , 2017, 22, 065003.	1.4	31
1766	Studying lowest energy structures of carbon clusters by bond-order empirical potentials. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	12
1767	Crystallization for a Brenner-like Potential. <i>Communications in Mathematical Physics</i> , 2017, 349, 1029-1061.	1.0	17
1768	Simulation of carbon nanotube welding through Ar bombardment. <i>Journal of Molecular Modeling</i> , 2017, 23, 148.	0.8	3
1769	High-temperature decomposition of the cellulose molecule: a stochastic molecular dynamics study. <i>Cellulose</i> , 2017, 24, 2713-2725.	2.4	63
1770	Water flow in carbon nanotubes: The effect of tube flexibility and thermostat. <i>Journal of Chemical Physics</i> , 2017, 146, 234701.	1.2	60
1771	Synergistic effects of grain boundaries and edges on fatigue deformations of sub-5Ånm graphene nanoribbons. <i>Journal of Materials Science</i> , 2017, 52, 10871-10878.	1.7	5
1772	New Coarse-Grained Model and Its Implementation in Simulations of Graphene Assemblies. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3706-3714.	2.3	21
1773	Mechanics of Materials Creation: Nanotubes, Graphene, Carbyne, Borophenes. <i>Procedia IUTAM</i> , 2017, 21, 17-24.	1.2	4
1774	Shock simulations of a single-site coarse-grain RDX model using the dissipative particle dynamics method with reactivity. <i>AIP Conference Proceedings</i> , 2017, , .	0.3	2
1775	Extremely high thermal conductivity anisotropy of double-walled carbon nanotubes. <i>AIP Advances</i> , 2017, 7, .	0.6	8

#	ARTICLE	IF	CITATIONS
1776	Application of Finite Element Method for the Design of Nanocomposites. , 2017, , 241-289.		1
1777	Sputtering of octatetraene by 15 keV C60 projectiles: Comparison of reactive interatomic potentials. Nuclear Instruments & Methods in Physics Research B, 2017, 393, 29-33.	0.6	4
1778	Pressurized CNTs under tension: A finite-deformation lattice model. Composites Part B: Engineering, 2017, 115, 223-235.	5.9	6
1779	Generation of amorphous carbon models using liquid quench method: A reactive molecular dynamics study. Carbon, 2017, 113, 87-99.	5.4	74
1780	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. Computer Physics Communications, 2017, 212, 8-24.	3.0	256
1781	Uniaxial-Strain Effects in the Paclitaxel Drug Molecule Adsorption on Nitrogen-Doped Graphene. International Journal of Nanoscience, 2017, 16, 1650027.	0.4	2
1782	How graphene flexes and stretches under concomitant bending couples and tractions. Meccanica, 2017, 52, 1601-1624.	1.2	15
1783	On the derivation of the elastic properties of lattice nanostructures: The case of graphene sheets. Composites Part B: Engineering, 2017, 115, 316-329.	5.9	52
1784	Computational Studies of Thermal Transport Properties of Carbon Nanotube Materials. , 2017, , 129-161.		6
1785	Phonon transmission of vacancy defected (10,0) carbon nanotube. , 2017, , .		3
1786	Parametric study on Topology of carbon Nanotubes Effects on Mechanical properties. Materials Today: Proceedings, 2017, 4, 9117-9125.	0.9	1
1787	Fullerene-water nanofluid confined in graphene nanochannel. AIP Advances, 2017, 7, 125208.	0.6	0
1788	Hierarchical deformation of super carbon nanotube under tensile load. , 2017, , .		0
1789	Thermal transport in defected armchair graphene nanoribbon: A molecular dynamics study. , 2017, , .		1
1790	Molecular dynamics simulation of elastic properties of multilayer MoS ₂ and graphene/MoS ₂ heterostructure. , 2017, , .		2
1791	METHOD FOR DETERMINING STRUCTURES OF NEW CARBON-BASED 2D MATERIALS WITH PREDEFINED MECHANICAL PROPERTIES. International Journal for Multiscale Computational Engineering, 2017, 15, 379-394.	0.8	8
1792	Molecular Mechanics of the Moisture Effect on Epoxy/Carbon Nanotube Nanocomposites. Nanomaterials, 2017, 7, 324.	1.9	27
1793	Arrangements of Carbon-Based Structures. , 2017, , 411-442.		2

#	ARTICLE	IF	CITATIONS
1794	A Molecular Dynamics Study on Wrinkles in Graphene with Simply Supported Boundary under In-Plane Shear. <i>Journal of Nanomaterials</i> , 2017, 2017, 1-10.	1.5	8
1795	Nonlocal Elasticity Theories. , 2017, , 301-334.		1
1796	Parameterization of Stillinger-Weber Potential for Two- Dimensional Atomic Crystals. , 0, , .		33
1797	Investigation of the Elastic Properties of Graphenylene Using Molecular Dynamics Simulations. <i>Materials Research</i> , 2017, 20, 1-9.	0.6	27
1798	Contribution of many-body effects into thermoelectricity and heat transport in graphene. , 2018, , 341-418.		0
1799	Calculating lattice thermal conductivity: a synopsis. <i>Physica Scripta</i> , 2018, 93, 043002.	1.2	40
1800	Deformation and spallation of shock-loaded graphene: Effects of orientation and grain boundary. <i>Carbon</i> , 2018, 132, 520-528.	5.4	21
1801	Capacitive Enhancement Mechanisms and Design Principles of High-Performance Graphene Oxide-Based All-Solid-State Supercapacitors. <i>Advanced Functional Materials</i> , 2018, 28, 1706721.	7.8	27
1802	Computational modeling of the effective Young's modulus values of fullerene molecules: a combined molecular dynamics simulation and continuum shell model. <i>Journal of Molecular Modeling</i> , 2018, 24, 71.	0.8	10
1803	Tensile loading characteristics of hydrogen stored carbon nanotubes in PEM fuel cell operating conditions using molecular dynamics simulation. <i>Molecular Simulation</i> , 2018, 44, 736-742.	0.9	8
1804	Thermophoretically driven water droplets on graphene and boron nitride surfaces. <i>Nanotechnology</i> , 2018, 29, 215401.	1.3	16
1805	Young's moduli of carbon materials investigated by various classical molecular dynamics schemes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 99, 215-219.	1.3	12
1806	Extending the accuracy of the SNAP interatomic potential form. <i>Journal of Chemical Physics</i> , 2018, 148, 241721.	1.2	129
1807	Mathematical Treatise to Model Dihedral Energy in the Multiscale Modeling of Two-Dimensional Nanomaterials. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2018, 85, .	1.1	3
1808	Temperature-dependent layer breathing modes in two-dimensional materials. <i>Physical Review B</i> , 2018, 97, .	1.1	8
1809	Decomposition of the Thermal Boundary Resistance across Carbon Nanotube-Graphene Junctions to Different Mechanisms. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 15226-15231.	4.0	10
1810	Thermal conduction of one-dimensional carbon nanomaterials and nanoarchitectures. <i>Chinese Physics B</i> , 2018, 27, 038103.	0.7	14
1811	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. <i>Physical Review Letters</i> , 2018, 120, 143001.	2.9	1,006

#	ARTICLE	IF	CITATIONS
1812	Atomistic modelling of crack-inclusion interaction in graphene. <i>Engineering Fracture Mechanics</i> , 2018, 195, 92-103.	2.0	13
1813	Shear Strength of Square Graphene Nanoribbons beyond Wrinkling. <i>Journal of Electronic Materials</i> , 2018, 47, 3891-3896.	1.0	7
1814	Investigating the thermal conductivity of concrete/graphene nanocomposite by a multi-scale modeling approach. <i>International Journal of Modern Physics B</i> , 2018, 32, 1850171.	1.0	6
1815	High-temperature annealing of graphite: A molecular dynamics study. <i>Journal of Nuclear Materials</i> , 2018, 503, 157-163.	1.3	8
1816	Effect of topological defects on mechanical properties of graphene sheets: a molecular dynamics study. <i>Materials Today: Proceedings</i> , 2018, 5, 6780-6788.	0.9	7
1817	Simulating the effects of carbon nanotube continuity and interfacial bonding on composite strength and stiffness. <i>Composites Science and Technology</i> , 2018, 166, 10-19.	3.8	25
1818	A unified framework for heat and mass transport at the atomic scale. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018, 26, 035014.	0.8	13
1819	Multiscale modeling of shock wave localization in porous energetic material. <i>Physical Review B</i> , 2018, 97, .	1.1	82
1820	Phase diagram of carbon and the factors limiting the quantity and size of natural diamonds. <i>Nanotechnology</i> , 2018, 29, 115603.	1.3	26
1821	Local strain field engineering on interfacial thermal resistance of graphene nanoribbon. <i>Applied Physics Letters</i> , 2018, 112, .	1.5	8
1822	Nanoscale Probing of Interaction in Atomically Thin Layered Materials. <i>ACS Central Science</i> , 2018, 4, 288-297.	5.3	6
1823	Contact mechanics of graphene-covered metal surfaces. <i>Applied Physics Letters</i> , 2018, 112, .	1.5	16
1824	Divergent effect of electric fields on the mechanical property of water-filled carbon nanotubes with an application as a nanoscale trigger. <i>Nanotechnology</i> , 2018, 29, 025707.	1.3	3
1825	Toward the multiscale nature of stress corrosion cracking. <i>Nuclear Engineering and Technology</i> , 2018, 50, 1-17.	1.1	16
1826	Fast crack propagation correlated with crack tip stress in 2D hexagonal atomic lattices. <i>International Journal of Fracture</i> , 2018, 210, 17-27.	1.1	2
1827	Single-crystal and polycrystalline diamond erosion studies in Pilot-PSI. <i>Journal of Nuclear Materials</i> , 2018, 500, 110-118.	1.3	3
1828	Phase Change of Carbon Atoms in Surface Layer Under Nanocutting During Diamond Lapping Process. <i>Journal of Tribology</i> , 2018, 140, .	1.0	2
1829	In situ atomic-scale observation of monolayer graphene growth from SiC. <i>Nano Research</i> , 2018, 11, 2809-2820.	5.8	21

#	ARTICLE	IF	CITATIONS
1830	Development of non- ϵ -bonded interaction parameters between graphene and water using particle swarm optimization. <i>Journal of Computational Chemistry</i> , 2018, 39, 721-734.	1.5	18
1831	Mesoscopic modeling of structural self-organization of carbon nanotubes into vertically aligned networks of nanotube bundles. <i>Carbon</i> , 2018, 130, 69-86.	5.4	13
1832	Stillinger-Weber potential for elastic and fracture properties in graphene and carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 055901.	0.7	33
1833	Atomistic perspective of how graphene protects metal substrate from surface damage in rough contacts. <i>Carbon</i> , 2018, 130, 672-679.	5.4	42
1834	Atomistic Simulations on the Tensile Deformation Behaviors of Three-Dimensional Graphene. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700680.	0.7	4
1835	Early Events of the Carburization of Fe Nanoparticles in Ethylene Pyrolysis: Reactive Force Field Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10835-10845.	1.5	12
1836	Chirality dependent interaction of ammonia with carbon nanotubes. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	0
1837	Molecular dynamics simulations of the thermal conductivity of cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains. <i>Diamond and Related Materials</i> , 2018, 86, 173-178.	1.8	26
1838	Structure of Amorphous Carbon. <i>Springer Series in Materials Science</i> , 2018, , 195-272.	0.4	4
1839	Investigation of Transport Parameters of Graphene-Based Nanostructures. <i>Russian Physics Journal</i> , 2018, 60, 1938-1945.	0.2	3
1840	Modal analysis of graphene-based structures for large deformations, contact and material nonlinearities. <i>Journal of Sound and Vibration</i> , 2018, 423, 161-179.	2.1	16
1841	Graphene Helicoid: Distinct Properties Promote Application of Graphene Related Materials in Thermal Management. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7605-7612.	1.5	25
1842	Interlocking Friction Governs the Mechanical Fracture of Bilayer MoS ₂ . <i>ACS Nano</i> , 2018, 12, 3600-3608.	7.3	40
1843	A REBO-Potential-Based Model for Graphene Bending by γ -Convergence. <i>Archive for Rational Mechanics and Analysis</i> , 2018, 229, 1153-1195.	1.1	2
1844	Nanotube-chirality-controlled tensile characteristics in coiled carbon metastructures. <i>Carbon</i> , 2018, 133, 335-349.	5.4	37
1845	Thermal conductivity of carbon nanotube superlattices: Comparative study with defective carbon nanotubes. <i>Chinese Physics B</i> , 2018, 27, 026501.	0.7	4
1846	The possibility of creation tissue-engineered structures with a structured internal nanocarbon scaffold in an organic matrix for repairing tissues of the cardiovascular system. , 2018, , .		0
1847	Nanomechanics and modelling of hydrogen stored carbon nanotubes under compression for PEM fuel cell applications. <i>Computational Materials Science</i> , 2018, 146, 176-183.	1.4	19

#	ARTICLE	IF	CITATIONS
1848	Tribochemical reactions and graphitization of diamond-like carbon against alumina give volcano-type temperature dependence of friction coefficients: A tight-binding quantum chemical molecular dynamics simulation. <i>Carbon</i> , 2018, 133, 350-357.	5.4	52
1849	Mesoscopic modeling of the uniaxial compression and recovery of vertically aligned carbon nanotube forests. <i>Composites Science and Technology</i> , 2018, 166, 66-85.	3.8	23
1850	Anisotropic thermal conductivity in carbon honeycomb. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 155702.	0.7	15
1851	Graphitization resistance determines super hardness of lonsdaleite, nanotwinned and nanopolycrystalline diamond. <i>Carbon</i> , 2018, 133, 69-76.	5.4	26
1852	Vibration of carbon nanotubes with defects: order reduction methods. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2018, 474, 20170555.	1.0	3
1853	Force constants of BN, SiC, AlN and GaN sheets through discrete homogenization. <i>Meccanica</i> , 2018, 53, 593-611.	1.2	22
1854	Design of robust energy consumption model for manufacturing process considering uncertainties. <i>Journal of Cleaner Production</i> , 2018, 172, 119-132.	4.6	13
1855	Structural and electronic transformation in low-angle twisted bilayer graphene. <i>2D Materials</i> , 2018, 5, 015019.	2.0	122
1856	Spurious heat conduction behavior of finite-size graphene nanoribbon under extreme uniaxial strain caused by the AIREBO potential. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 96, 46-53.	1.3	17
1857	Multi-layer graphene reinforced aluminum " Manufacturing of high strength composite by friction stir alloying. <i>Composites Part B: Engineering</i> , 2018, 136, 63-71.	5.9	134
1858	Atomistic simulation of Al-graphene thin film growth on polycrystalline Al substrate. <i>Applied Surface Science</i> , 2018, 433, 540-545.	3.1	11
1859	Interatomic potential suitable for the modeling of penta-graphene: Molecular statics/molecular dynamics studies. <i>Carbon</i> , 2018, 126, 165-175.	5.4	37
1860	Quantifying Parameter Sensitivity and Uncertainty for Interatomic Potential Design: Application to Saturated Hydrocarbons. <i>ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering</i> , 2018, 4, .	0.7	4
1861	Nanotribological behavior analysis of graphene/metal nanocomposites via MD simulations: New concepts and underlying mechanisms. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 115, 49-58.	1.9	16
1862	Self-Folding Mechanics of Surface Wettability Patterned Graphene Nanoribbons by Liquid Evaporation. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2018, 85, .	1.1	7
1863	Sub-nanometre channels embedded in two-dimensional materials. <i>Nature Materials</i> , 2018, 17, 129-133.	13.3	97
1864	Molecular junctions for thermal transport between graphene nanoribbons: Covalent bonding vs. interdigitated chains. <i>Computational Materials Science</i> , 2018, 142, 255-260.	1.4	11
1865	Nonlinear elastic properties of graphene sheet using MM3 potential under finite deformation. <i>Composites Part B: Engineering</i> , 2018, 136, 81-91.	5.9	17

#	ARTICLE	IF	CITATIONS
1866	Influence of chemical bonding on the variability of diamond-like carbon nanoscale adhesion. Carbon, 2018, 128, 267-276.	5.4	42
1867	Chain-like ground states in three dimensions. Transactions of Mathematics and Its Applications, 2018, 2, .	1.6	2
1868	Atomistic Simulations of Mechanical Properties of Circular and Collapsed Carbon Nanotubes With Covalent Cross-Links. , 2018, , .		0
1869	Interlayer Interactions in Low-Dimensional Layered Hetero-Structures: Modeling and Applications. , 2018, , 1-25.		0
1870	Elastic and failure properties of carbon nanocones using molecular dynamics simulation. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 777-789.	1.0	3
1871	A Self-Adaptive Umbrella Model for Vibration Analysis of Graphene. Materials, 2018, 11, 2497.	1.3	0
1872	Phase transformation in two-dimensional covalent organic frameworks under compressive loading. Physical Chemistry Chemical Physics, 2018, 20, 29462-29471.	1.3	15
1873	Mechanics of Carbon Nanotubes and Their Composites. , 2018, , 1-67.		0
1874	The effects of diamond amorphous layer on the diamond lapping surface. Procedia CIRP, 2018, 71, 140-143.	1.0	4
1875	Specific Features of Structure, Electrical Conductivity and Interlayer Adhesion of the Natural Polymer Matrix from the Layers of Branched Carbon Nanotube Networks Filled with Albumin, Collagen and Chitosan. Coatings, 2018, 8, 378.	1.2	4
1876	Computer simulation of electrical characteristics of singlewalled carbon nanotube (9,0) with Stone-Wales defect. Journal of Physics: Conference Series, 2018, 1015, 032124.	0.3	0
1877	Micro-Mechanism of Interfacial Separation and Slippage of Graphene/Aluminum Nanolaminated Composites. Nanomaterials, 2018, 8, 1046.	1.9	17
1878	Structure of amorphous carbon quenched from liquid in the pressure range 1â€“40 GPa: Molecular dynamic modeling. Journal of Physics: Conference Series, 2018, 946, 012086.	0.3	2
1879	Emergent D_{6h} symmetry in fully relaxed magic-angle twisted bilayer graphene. Physical Review B, 2018, 98, .		0
1880	Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures. Physical Review B, 2018, 98, .	1.1	41
1881	Interatomic Potentials for Nuclear Materials. , 2018, , 1-19.		0
1882	Mechanics and Electromechanics of Two-Dimensional Atomic Membranes. , 2018, , 1-37.		0
1883	Carbon Nanocones with Curvature Effects Close to the Vertex. Nanomaterials, 2018, 8, 624.	1.9	5

#	ARTICLE	IF	CITATIONS
1884	Buckling Analysis of Vacancy-Defected Graphene Sheets by the Stochastic Finite Element Method. <i>Materials</i> , 2018, 11, 1545.	1.3	11
1885	Effect of temperature and strain-rate on mechanical properties of defected graphene sheet: A molecular dynamics study. <i>IOP Conference Series: Materials Science and Engineering</i> , 2018, 402, 012020.	0.3	1
1886	Phonon Transport of Zigzag/Armchair Graphene Superlattice Nanoribbons. <i>International Journal of Thermophysics</i> , 2018, 39, 1.	1.0	2
1887	Effect of chemical structure on thermo-mechanical properties of epoxy polymers: Comparison of accelerated ReaxFF simulations and experiments. <i>Polymer</i> , 2018, 158, 354-363.	1.8	43
1888	Atomistic Simulations of the Efficiencies of Ge and Pt Ion Implantation into Graphene. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25700-25708.	1.5	6
1889	Molecular Dynamics Simulations of Non-equilibrium Systems. , 2018, , 1-33.		2
1890	Structure sensitivity of electronic transport across graphene grain boundaries. <i>Physical Review B</i> , 2018, 98, .	1.1	6
1891	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. <i>Chemistry of Materials</i> , 2018, 30, 7438-7445.	3.2	69
1892	Prediction of fluid slip in cylindrical nanopores using equilibrium molecular simulations. <i>Nanotechnology</i> , 2018, 29, 485404.	1.3	22
1893	Mechanical strength in hierarchically polycrystalline graphene with dislocation arrays-embedded grains. <i>Materials Research Express</i> , 2018, 5, 115019.	0.8	6
1894	Structural stability and buckling analysis of a series of carbon nanotorus using molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2018, 24, 263.	0.8	1
1895	Review of force fields and intermolecular potentials used in atomistic computational materials research. <i>Applied Physics Reviews</i> , 2018, 5, 031104.	5.5	101
1896	Tensile responses of carbon nanotubes-reinforced copper nanocomposites: Molecular dynamics simulation. <i>Computational Materials Science</i> , 2018, 151, 273-277.	1.4	30
1897	Cleaning of graphene surfaces by low-pressure air plasma. <i>Royal Society Open Science</i> , 2018, 5, 172395.	1.1	20
1898	Axial buckling behavior of single-walled carbon nanotubes: Atomistic structural instability analysis. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 103, 130-142.	1.3	5
1899	Mechanical abnormality in graphene-based lamellar superstructures. <i>Carbon</i> , 2018, 137, 196-206.	5.4	14
1900	Comparison of empirical potentials for calculating structural properties of amorphous carbon films by molecular dynamics simulation. <i>Computational Materials Science</i> , 2018, 151, 246-254.	1.4	38
1901	Mechanochemical formation of heterogeneous diamond structures during rapid uniaxial compression in graphite. <i>Physical Review B</i> , 2018, 97, .	1.1	20

#	ARTICLE	IF	CITATIONS
1902	Compressive response and buckling of graphene nanoribbons. <i>Scientific Reports</i> , 2018, 8, 9593.	1.6	25
1903	Atomistic Simulations of Carbon Nanotubes: Stiffness, Strength, and Toughness of Locally Buckled CNTs. , 2018, , 259-290.		0
1904	Multiscale Mechanics of Triply Periodic Minimal Surfaces of Three-Dimensional Graphene Foams. <i>Nano Letters</i> , 2018, 18, 4845-4853.	4.5	57
1905	Molecular dynamics simulations of acoustic absorption by a carbon nanotube. <i>Physics of Fluids</i> , 2018, 30, .	1.6	15
1906	Size- and temperature-dependent bending rigidity of graphene using modal analysis. <i>Carbon</i> , 2018, 139, 334-341.	5.4	42
1907	Continuum/Finite Element Modeling of Carbon Nanotube Reinforced Polymers. , 2018, , 385-409.		3
1908	High intrinsic dissipation of graphyne nanotubes. <i>Europhysics Letters</i> , 2018, 122, 46001.	0.7	6
1909	Size effects on the fracture of microscale and nanoscale materials. <i>Nature Reviews Materials</i> , 2018, 3, 211-224.	23.3	72
1910	Benchmark of ReaxFF force field for subcritical and supercritical water. <i>Journal of Chemical Physics</i> , 2018, 148, 234503.	1.2	34
1911	Robust microscale superlubricity in graphite/hexagonal boron nitride layered heterojunctions. <i>Nature Materials</i> , 2018, 17, 894-899.	13.3	292
1912	In-plane thermal transport in black phosphorene/graphene layered heterostructures: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21151-21162.	1.3	41
1913	Giant reduction and tunability of the thermal conductivity of carbon nanotubes through low-frequency resonant modes. <i>Physical Review B</i> , 2018, 98, .	1.1	14
1914	Thermoelastic damping of graphene nanobeams by considering the size effects of nanostructure and heat conduction. <i>Journal of Thermal Stresses</i> , 2018, 41, 1182-1200.	1.1	43
1915	Complex Behavior of Ordered and Icelike Water in Carbon Nanotubes near Its Bulk Boiling Point. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4746-4752.	2.1	8
1916	Interaction of Edge Dislocations with Graphene Nanosheets in Graphene/Fe Composites. <i>Crystals</i> , 2018, 8, 160.	1.0	24
1917	The Influence of Hydroxyl Groups on Friction of Graphene at Atomic Scale. <i>Crystals</i> , 2018, 8, 167.	1.0	11
1918	Investigation of N behavior during coal pyrolysis and oxidation using ReaxFF molecular dynamics. <i>Fuel</i> , 2018, 233, 867-876.	3.4	62
1919	The effect of defects on the fracture behavior of trilayer graphene. <i>Superlattices and Microstructures</i> , 2018, 123, 172-182.	1.4	7

#	ARTICLE	IF	CITATIONS
1920	Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. Journal of Physical Chemistry A, 2018, 122, 6633-6642.	1.1	96
1921	Small size effect on the wrinkling hierarchy in constrained monolayer graphene. International Journal of Engineering Science, 2018, 131, 19-25.	2.7	12
1922	Anomalous strength characteristics of Stone-Thrower-Wales defects in graphene sheets – a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 15203-15215.	1.3	13
1923	A molecular dynamics based cohesive zone model for predicting interfacial properties between graphene coating and aluminum. Computational Materials Science, 2018, 151, 117-123.	1.4	38
1924	Anisotropic thermal expansion coefficient of multilayer graphene reinforced copper matrix composites. Journal of Alloys and Compounds, 2018, 755, 114-122.	2.8	35
1925	Tuning the Slide-Roll Motion Mode of Carbon Nanotubes via Hydroxyl Groups. Nanoscale Research Letters, 2018, 13, 138.	3.1	10
1926	Sputtering of Graphite by Hydrogen Isotopes in the Fusion Environment: A Molecular Dynamics Simulation Study. Journal of Nuclear Engineering and Radiation Science, 2018, 4, .	0.2	0
1927	Vibrational analysis of single-walled carbon nanotubes filled with gold nanowires using MD simulations. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 104, 327-332.	1.3	10
1928	Piezoelectrically tunable resonance properties of boron nitride nanotube based resonators. Journal of Applied Physics, 2018, 124, 055103.	1.1	3
1929	Effect of interlayer space on the structure and Poisson's ratio of a graphene/MoS2 tubular van der Waals heterostructure. Journal of Applied Physics, 2018, 124, .	1.1	4
1930	Long triple carbon chains formation by heat treatment of graphene nanoribbon: Molecular dynamics study with revised Brenner potential. Carbon, 2018, 140, 543-556.	5.4	13
1931	Nanoserpents: Graphene Nanoribbon Motion on Two-Dimensional Hexagonal Materials. Nano Letters, 2018, 18, 6009-6016.	4.5	104
1932	Assessment of the mechanical properties of monolayer graphene using the energy and strain-fluctuation methods. RSC Advances, 2018, 8, 27283-27292.	1.7	42
1933	Effect of N-doping on hard carbon nano-balls as anode for Li-ion battery: improved hydrothermal synthesis and volume expansion study. Journal of Solid State Electrochemistry, 2018, 22, 3443-3455.	1.2	23
1934	Commensurate lattice constant dependent thermal conductivity of misoriented bilayer graphene. Carbon, 2018, 138, 451-457.	5.4	38
1935	Thermoelectric properties of graphene nanoribbons with surface roughness. Applied Physics Letters, 2018, 112, .	1.5	20
1936	Iodine nanoparticle-enhancing electrical and thermal transport for carbon nanotube fibers. Applied Thermal Engineering, 2018, 141, 913-920.	3.0	45
1937	Molecular statics simulation of CdTe grain boundary structures and energetics using a bond-order potential. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 045009.	0.8	3

#	ARTICLE	IF	CITATIONS
1938	Theoretical Modeling of CNT-Polymer Interactions. , 2018, , 347-383.		1
1939	An order reduction method for single-walled carbon nanotubes with multi-vacancy defects. Carbon, 2018, 138, 81-89.	5.4	7
1940	Impacts of environments on nanoscale wear behavior of graphene: Edge passivation vs. substrate pinning. Carbon, 2018, 139, 59-66.	5.4	62
1941	Pyrolysis of binary fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study. Fuel, 2019, 235, 194-207.	3.4	75
1942	Viscosity of carbon nanotube/water nanofluid. Journal of Thermal Analysis and Calorimetry, 2019, 135, 1787-1796.	2.0	40
1943	Using finite element codes as a numerical platform to run molecular dynamics simulations. Computational Mechanics, 2019, 63, 271-300.	2.2	1
1944	Reactive molecular dynamics simulation of the amorphous carbon growth: Effect of the carbon triple bonds. Computational Materials Science, 2019, 169, 109143.	1.4	5
1945	Graphynes: an alternative lightweight solution for shock protection. Beilstein Journal of Nanotechnology, 2019, 10, 1588-1595.	1.5	6
1946	The role of shock waves on the biodamage induced by ion beam radiation. Cancer Nanotechnology, 2019, 10, .	1.9	13
1947	Anomalous temperature dependent thermal conductivity of two-dimensional silicon carbide. Nanotechnology, 2019, 30, 445707.	1.3	49
1948	Mechanical properties of twin graphene subjected to uniaxial stress by molecular dynamic simulation. Materials Research Express, 2019, 6, 105611.	0.8	10
1949	Green function, quasi-classical Langevin and Kubo-Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	0.7	15
1950	Thermal transports of one-dimensional ultrathin carbon structures. Nanotechnology, 2019, 30, 475401.	1.3	2
1951	Tensile and Interfacial Loading Characteristics of Boron Nitride-Carbon Nanosheet Reinforced Polymer Nanocomposites. Polymers, 2019, 11, 1075.	2.0	16
1952	Finite element analysis and molecular dynamics simulations of nanoscale crack-hole interactions in chiral graphene nanoribbons. Engineering Fracture Mechanics, 2019, 218, 106571.	2.0	15
1953	Reactivity-Controlled Aggregation of Graphene Nanoflakes in Aluminum Matrix: Atomistic Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2019, 123, 18017-18027.	1.5	10
1954	Unidirectional Self-Driving Liquid Droplet Transport on a Monolayer Graphene-Covered Textured Substrate. ACS Applied Materials & Interfaces, 2019, 11, 28562-28570.	4.0	37
1955	Nickel nanoparticles inside carbon nanostructures: atomistic simulation. Mechanics of Advanced Materials and Modern Processes, 2019, 5, .	2.2	17

#	ARTICLE	IF	CITATIONS
1956	Geometry and chiral symmetry breaking of ripple junctions in 2D materials. <i>Journal of the Mechanics and Physics of Solids</i> , 2019, 131, 337-343.	2.3	6
1957	Transferability in interatomic potentials for carbon. <i>Carbon</i> , 2019, 155, 624-634.	5.4	55
1958	A Review on Brittle Fracture Nanomechanics by All-Atom Simulations. <i>Nanomaterials</i> , 2019, 9, 1050.	1.9	19
1959	A novel super-elastic carbon nanofiber with cup-stacked carbon nanocones and a screw dislocation. <i>Carbon</i> , 2019, 154, 98-107.	5.4	14
1960	Dramatic effect of a transverse electric field on frictional properties of graphene. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 385301.	1.3	3
1961	Fracture toughness of various percentage of doping of boron atoms on the mechanical properties of polycrystalline graphene: A molecular dynamics study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 114, 113614.	1.3	14
1962	The Princess and the Nanoscale Pea: Long-Range Penetration of Surface Distortions into Layered Materials Stacks. <i>ACS Nano</i> , 2019, 13, 7603-7609.	7.3	23
1963	Grain size and hydroxyl-coverage dependent tribology of polycrystalline graphene. <i>Nanotechnology</i> , 2019, 30, 385701.	1.3	10
1964	On the Mechanical Properties of the Graphdiyne Nanotubes: a Molecular Dynamics Investigation. <i>Brazilian Journal of Physics</i> , 2019, 49, 654-666.	0.7	4
1965	Generalized Scaling Law of Structural Superlubricity. <i>Nano Letters</i> , 2019, 19, 7735-7741.	4.5	42
1966	Crosslinking and interfacial behavior of carboxylic functionalized carbon nanotube Epon nanocomposites: a molecular dynamic simulation approach. <i>SN Applied Sciences</i> , 2019, 1, 1.	1.5	5
1967	Controlling the Diffusive Motion of Fullerene-Wheeled Nanocars Utilizing a Hybrid Substrate. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26018-26030.	1.5	22
1968	Tensile characteristics of carbene-functionalized CNTs subjected to physisorption of polymer chains: a molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2019, 25, 318.	0.8	11
1969	Atomistic modelling of the hypervelocity dynamics of shock-compressed graphite and impacted graphene armours. <i>Computational Materials Science</i> , 2019, 170, 109152.	1.4	7
1970	Insight into Geometry-Controlled Mechanical Properties of Spiral Carbon-Based Nanostructures. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3226-3238.	1.5	22
1971	Bending and interlayer shear moduli of ultrathin boron nitride nanosheet. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 465301.	1.3	26
1972	Unveiling Carbon Ring Structure Formation Mechanisms in Polyacrylonitrile-Derived Carbon Fibers. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 42288-42297.	4.0	36
1973	Atomistic simulation of the nanoindentation behavior of graphene/Al multilayered nanocomposites. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 531, 012055.	0.3	1

#	ARTICLE	IF	CITATIONS
1974	Effects of Divacancy and Extended Line Defects on the Thermal Transport Properties of Graphene Nanoribbons. <i>Nanomaterials</i> , 2019, 9, 1609.	1.9	9
1975	ReaxFF Parameter Optimization with Monte-Carlo and Evolutionary Algorithms: Guidelines and Insights. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6799-6812.	2.3	54
1976	Role of Nitrogen on the Mechanical Properties of the Novel Carbon Nitride Nanothreads. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28977-28984.	1.5	13
1977	Evaporation-driven crumpling and assembling of two-dimensional (2D) materials: A rotational spring "mechanical slider model. <i>Journal of the Mechanics and Physics of Solids</i> , 2019, 133, 103722.	2.3	23
1978	Observation of a threshold behavior in an ultracold endothermic atom-exchange process involving Feshbach molecules. <i>Physical Review A</i> , 2019, 100, .	1.0	8
1979	Buckling-induced band-gap modulation in zigzag carbon nanotubes. <i>Physical Review B</i> , 2019, 100, .	1.1	7
1980	Thermal and Mechanical Behavior of Wood Plastic Composites by Addition of Graphene Nanoplatelets. <i>Polymers</i> , 2019, 11, 1365.	2.0	17
1981	Theoretical analysis of spectral lineshapes from molecular dynamics. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	6
1982	Atomistic Simulation of Anisotropic Crystal Structures at Nanoscale. , 2019, , .		3
1983	Dissipative particle dynamics with reactions: Application to RDX decomposition. <i>Journal of Chemical Physics</i> , 2019, 151, 114112.	1.2	20
1984	Rapid Water Harvesting and Nonthermal Drying in Humid Air by N-Doped Graphene Micropads. <i>Langmuir</i> , 2019, 35, 12389-12399.	1.6	6
1985	Double-Vacancy Controlled Friction on Graphene: The Enhancement of Atomic Pinning. <i>Langmuir</i> , 2019, 35, 12898-12907.	1.6	14
1986	Interfacial properties of 3D metallic carbon nanostructures (T6 and T14)-reinforced polymer nanocomposites: A molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 341-356.	1.3	12
1987	Thickness of monolayer h-BN nanosheet and edge effect on free vibration behaviors. <i>International Journal of Mechanical Sciences</i> , 2019, 164, 105163.	3.6	17
1988	A Universal Length-Dependent Vibrational Mode in Graphene Nanoribbons. <i>ACS Nano</i> , 2019, 13, 13083-13091.	7.3	36
1989	Molecular Dynamics Simulation of Polymer-Matrix Composites Using BIOVIA Materials Studio, LAMMPS, and GROMACS. , 2019, , 141-225.		0
1990	Flexural Wave Propagation in Mass Chain-Filled Carbon Nanotubes. <i>Materials</i> , 2019, 12, 2986.	1.3	2
1991	High Performance of Carbon Nanotube Refrigerators. <i>Annalen Der Physik</i> , 2019, 531, 1800502.	0.9	12

#	ARTICLE	IF	CITATIONS
1992	Mechanical Properties of Vacancy Tuned Carbon Honeycomb. <i>Nanomaterials</i> , 2019, 9, 156.	1.9	21
1993	Atomic Structure and Mechanical Properties of Twisted Bilayer Graphene. <i>Journal of Composites Science</i> , 2019, 3, 2.	1.4	17
1994	Layer-dependent anisotropic frictional behavior in two-dimensional monolayer hybrid perovskite/ITO layered heterojunctions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2540-2546.	1.3	31
1995	Chirality-dependent motion transmission between aligned carbon nanotubes. <i>Carbon</i> , 2019, 151, 130-135.	5.4	13
1996	An efficient graphyne membrane for water desalination. <i>Polymer</i> , 2019, 175, 310-319.	1.8	33
1997	Insights into the atomistic behavior in diamond chemical mechanical polishing with OH environment using ReaxFF molecular dynamics simulation. <i>Computational Materials Science</i> , 2019, 166, 136-142.	1.4	22
1998	An adjustable permeation membrane up to the separation for multicomponent gas mixture. <i>Scientific Reports</i> , 2019, 9, 7380.	1.6	12
1999	Graphene layer of hybrid graphene/hexagonal boron nitride model upon heating. <i>Carbon Letters</i> , 2019, 29, 521-528.	3.3	13
2000	Chirality dependent mechanical properties of carbon nano-structures. <i>Materials Research Express</i> , 2019, 6, 095018.	0.8	6
2001	Dynamic profiles of tar products during NaomaoHu coal pyrolysis revealed by large-scale reactive molecular dynamic simulation. <i>Fuel</i> , 2019, 253, 910-920.	3.4	42
2002	Mapping the structural diversity of C ₆₀ carbon clusters and their infrared spectra. <i>Astronomy and Astrophysics</i> , 2019, 625, L11.	2.1	19
2003	Ultra-low friction of graphene/C60/graphene coatings for realistic rough surfaces. <i>Carbon</i> , 2019, 152, 727-737.	5.4	17
2004	Investigation on the Tensile Behavior of Graphene-Aluminum Nano-Laminated Composites by Molecular Dynamics Simulation. <i>Key Engineering Materials</i> , 0, 804, 1-6.	0.4	6
2005	Understanding the improved electrochemical performance of nitrogen-doped hard carbons as an anode for sodium ion battery. <i>Electrochimica Acta</i> , 2019, 317, 164-172.	2.6	70
2006	Optimizing the thermoelectric performance of $\hat{1}^3$ -graphyne nanoribbons via introducing disordered surface fluctuation. <i>Solid State Communications</i> , 2019, 298, 113646.	0.9	5
2007	Machine-Learning Based Stacked Ensemble Model for Accurate Analysis of Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5190-5198.	1.1	26
2008	Determination of pressure-viscosity relation of 2,2,4-trimethylhexane by all-atom molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , 2019, 495, 28-32.	1.4	18
2009	Atomistic Scale Analysis of the Carbonization Process for C/H/O/N-Based Polymers with the ReaxFF Reactive Force Field. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5357-5367.	1.2	123

#	ARTICLE	IF	CITATIONS
2010	Molecular Dynamics Simulation of Nanofilm Boiling on Graphene-Coated Surface. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900065.	1.3	16
2011	Multistability of armchair single-walled carbon nanotubes: a molecular dynamics investigation. <i>Materials Research Express</i> , 2019, 6, 0850f4.	0.8	0
2012	Multi-objective optimization of interatomic potentials with application to MgO. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019, 27, 074007.	0.8	7
2013	On the in-plane failure and post-failure behaviour of pristine and perforated single-layer graphene sheets. <i>Mathematics and Mechanics of Solids</i> , 2019, 24, 3418-3443.	1.5	12
2015	Flow of water through carbon nanotubes predicted by different atomistic water models. <i>Journal of Chemical Physics</i> , 2019, 150, 194501.	1.2	20
2016	Continuum models for twisted bilayer graphene: Effect of lattice deformation and hopping parameters. <i>Physical Review B</i> , 2019, 99, .	1.1	116
2017	Mechanochemistry of Stable Diamane and Atomically Thin Diamond Films Synthesis from Bi- and Multilayer Graphene: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15751-15760.	1.5	26
2018	Anisotropic Fracture Dynamics Due to Local Lattice Distortions. <i>ACS Nano</i> , 2019, 13, 5693-5702.	7.3	19
2019	A Kriging Surrogate Model for Uncertainty Analysis of Graphene Based on a Finite Element Method. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2355.	1.8	13
2020	A novel dual-signal output screwing oscillator based on carbon@MoS ₂ nanotubes. <i>Applied Physics Express</i> , 2019, 12, 065001.	1.1	5
2021	Coupling analysis of screwing motion of double-walled carbon nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 2309-2313.	0.9	2
2022	Estimation of Thermodynamic and Interfacial Parameters of Metallic Materials by Molecular Dynamics Simulations. <i>Materials Transactions</i> , 2019, 60, 180-188.	0.4	24
2023	Imaging covalent bond formation by H atom scattering from graphene. <i>Science</i> , 2019, 364, 379-382.	6.0	76
2024	azTotMD: Software for non-constant force field molecular dynamics. <i>SoftwareX</i> , 2019, 10, 100233.	1.2	9
2025	Misfit strain-induced energy dissipation for graphene/MoS ₂ heterostructure nanomechanical resonators. <i>Nanotechnology</i> , 2019, 30, 265701.	1.3	9
2026	Exploring the Effect of Dihedral Energy on the Nonlinear Mechanics of the Carbon Nanotubes Using a Multiscale Modeling. <i>Journal of Vibration and Acoustics, Transactions of the ASME</i> , 2019, 141, .	1.0	1
2027	Epoxy filled with bare and oxidized multi-layered graphene nanoplatelets: a comparative study of filler loading impact on thermal properties. <i>Journal of Materials Science</i> , 2019, 54, 9247-9266.	1.7	17
2028	Fracture Toughnesses and Crack Growth Angles of Single-Layer Graphyne Sheets. <i>Acta Mechanica Solida Sinica</i> , 2019, 32, 339-355.	1.0	6

#	ARTICLE	IF	CITATIONS
2029	Effect of Defects on the Mechanical and Thermal Properties of Graphene. <i>Nanomaterials</i> , 2019, 9, 347.	1.9	57
2030	Refined multiscale model based on the second generation interatomic potential for the mechanics of graphene sheets. <i>Mechanics of Materials</i> , 2019, 133, 26-36.	1.7	6
2031	Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials. <i>Physical Review B</i> , 2019, 99, .	1.1	77
2032	Free volume and internal structural evolution during creep in model amorphous polyethylene by Molecular Dynamics simulations. <i>Polymer</i> , 2019, 170, 85-100.	1.8	30
2033	Nanostructure of Gasification Charcoal (Biochar). <i>Environmental Science & Technology</i> , 2019, 53, 3538-3546.	4.6	20
2034	Multiscale molecular dynamics-FE modeling of polymeric nanocomposites reinforced with carbon nanotubes and graphene. <i>Composite Structures</i> , 2019, 217, 27-36.	3.1	23
2035	Carbon nanotube knots. <i>AIP Advances</i> , 2019, 9, 025030.	0.6	6
2036	Simulating the structural diversity of carbon clusters across the planar-to-fullerene transition. <i>Physical Review A</i> , 2019, 99, .	1.0	16
2037	Anisotropic and temperature dependent mechanical properties of carbon honeycomb. <i>Nanotechnology</i> , 2019, 30, 325704.	1.3	18
2038	A method for controlling absolute pressures at the entrance and exit of a nanochannel/nanotube. <i>Microfluidics and Nanofluidics</i> , 2019, 23, 1.	1.0	1
2039	Operational and environmental conditions regulate the frictional behavior of two-dimensional materials. <i>Applied Surface Science</i> , 2019, 483, 34-44.	3.1	29
2040	The Temperature-Sensitive Anisotropic Negative Poisson's Ratio of Carbon Honeycomb. <i>Nanomaterials</i> , 2019, 9, 487.	1.9	12
2041	Existence criteria and validity of plate models for graphene-like materials. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019, 62, 1.	2.0	3
2042	Alkyl group functionalization-induced phonon thermal conductivity attenuation in graphene nanoribbons. <i>Chinese Physics B</i> , 2019, 28, 016501.	0.7	6
2043	Combined molecular dynamics and phase-field modelling of crack propagation in defective graphene. <i>Computational Materials Science</i> , 2019, 163, 117-126.	1.4	16
2044	Twinning in two-dimensional materials and its application to electronic properties. <i>Electronic Structure</i> , 2019, 1, 025001.	1.0	7
2045	Novel nonlinear coarse-grained potentials of carbon nanotubes. <i>Journal of the Mechanics and Physics of Solids</i> , 2019, 128, 79-104.	2.3	37
2046	The origin of self-excited oscillation of double-walled carbon nanotubes. <i>Materials Research Express</i> , 2019, 6, 075033.	0.8	4

#	ARTICLE	IF	CITATIONS
2047	Intrinsic bending flexoelectric constants in two-dimensional materials. <i>Physical Review B</i> , 2019, 99, .	1.1	68
2048	Multiscale Design of Graphyne-Based Materials for High-Performance Separation Membranes. <i>Advanced Materials</i> , 2019, 31, e1805665.	11.1	30
2049	Application of ReaxFF-Reactive Molecular Dynamics and Continuum Methods in High-Temperature/Pressure Pyrolysis of Fuel Mixtures. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 161-185.	0.6	2
2050	Force Matching Approaches to Extend Density Functional Theory to Large Time and Length Scales. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 71-93.	0.6	5
2051	Functionalized Graphene-Based Nanocomposites for Energy Applications. , 2019, , 219-243.		30
2052	Accelerating AIREBO: Navigating the Journey from Legacy to High-Performance Code. <i>Journal of Computational Chemistry</i> , 2019, 40, 1471-1482.	1.5	6
2053	Multiphysics-Based Statistical Model for Investigating the Mechanics of Carbon Nanotubes Membranes for Proton-Exchange Membrane Fuel Cell Applications. <i>Journal of Electrochemical Energy Conversion and Storage</i> , 2019, 16, .	1.1	3
2054	Toward a Predictive Hierarchical Multiscale Modeling Approach for Energetic Materials. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 229-282.	0.6	16
2055	Negative Friction Coefficients in Superlubric Graphite-Hexagonal Boron Nitride Heterojunctions. <i>Physical Review Letters</i> , 2019, 122, 076102.	2.9	63
2056	Role of unsaturated hydrocarbon lubricant on the friction behavior of amorphous carbon films from reactive molecular dynamics study. <i>Computational Materials Science</i> , 2019, 161, 1-9.	1.4	18
2057	Temperature Dependent Thermal Conductivity of Graphene Nanoribbon (GNR) for Different Interatomic Potentials: An Equilibrium Molecular Dynamics Study. , 2019, , .		0
2058	Dodecagonal bilayer graphene quasicrystal and its approximants. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	53
2059	Interaction of Human Telomeric i-Motif DNA with Single-Walled Carbon Nanotubes: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10343-10353.	1.2	16
2060	Hybrid neural network potential for multilayer graphene. <i>Physical Review B</i> , 2019, 100, .	1.1	38
2061	A Non-Linear Spring Model for Predicting Modal Behavior of Oscillators Built from Double Walled Carbon Nanotubes. <i>Journal of Nano Research</i> , 0, 60, 21-32.	0.8	3
2062	Graphene Adhesion Mechanics on Iron Substrates: Insight from Molecular Dynamic Simulations. <i>Crystals</i> , 2019, 9, 579.	1.0	12
2063	Chain Model for Carbon Nanotube Bundle under Plane Strain Conditions. <i>Materials</i> , 2019, 12, 3951.	1.3	24
2064	A New Genetic Algorithm Approach Applied to Atomic and Molecular Cluster Studies. <i>Frontiers in Chemistry</i> , 2019, 7, 707.	1.8	19

#	ARTICLE	IF	CITATIONS
2065	Structural and elastic properties of amorphous carbon from simulated quenching at low rates. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 085009.	0.8	30
2066	Effect of boundary chain folding on thermal conductivity of lamellar amorphous polyethylene. RSC Advances, 2019, 9, 33549-33557.	1.7	13
2067	Tensile characteristics of single-walled carbon nanotubes endohedrally decorated with gold nanowires: A molecular dynamics study. Diamond and Related Materials, 2019, 92, 117-129.	1.8	14
2068	A new computationally efficient finite element formulation for nanoplates using second-order strain gradient Kirchhoff's plate theory. Composites Part B: Engineering, 2019, 168, 302-311.	5.9	51
2069	Nanoindentation of thin graphdiyne films: Experiments and molecular dynamics simulation. Carbon, 2019, 144, 72-80.	5.4	28
2070	An atomically-thin graphene reverse electrodialysis system for efficient energy harvesting from salinity gradient. Nano Energy, 2019, 57, 783-790.	8.2	58
2071	Machine Learning Classical Interatomic Potentials for Molecular Dynamics from First-Principles Training Data. Journal of Physical Chemistry C, 2019, 123, 6941-6957.	1.5	72
2072	On the atomistic energetics of carbon nanotube collapse from AIREBO potential. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 106, 319-325.	1.3	7
2073	Self-tearing and self-peeling of folded graphene nanoribbons. Carbon, 2019, 143, 230-239.	5.4	10
2074	Elastic constants of graphene: Comparison of empirical potentials and DFT calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 326-338.	1.3	47
2075	Insights on low-friction mechanism of amorphous carbon films from reactive molecular dynamics study. Tribology International, 2019, 131, 567-578.	3.0	41
2076	Complete steric exclusion of ions and proton transport through confined monolayer water. Science, 2019, 363, 145-148.	6.0	207
2077	Highly Switchable Adhesion of N-Doped Graphene Interfaces for Robust Micromanipulation. ACS Applied Materials & Interfaces, 2019, 11, 5544-5553.	4.0	7
2078	Multiscale structures in particle-fluid systems: Characterization, modeling, and simulation. Chemical Engineering Science, 2019, 198, 198-223.	1.9	85
2079	Graphene kirigami as reinforcement and interfacial bonding effect for toughness and strength of silicon-based nanocomposites. Computational Materials Science, 2019, 159, 306-315.	1.4	5
2080	Dislocation-blocking mechanism for the strengthening and toughening of laminated graphene/Al composites. Computational Materials Science, 2019, 160, 72-81.	1.4	33
2081	Difficulties and Virtues in Assessing the Potential Energy Surfaces of Carbon Clusters via DMBE Theory: Stationary Points of C_{10}^+ ($I^e = 2 \times 10$) at the Focal Point. Journal of Physical Chemistry A, 2019, 123, 3121-3130.	1.1	5
2082	Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C. Nature Communications, 2019, 10, 151.	5.8	118

#	ARTICLE	IF	CITATIONS
2083	Dimensional variation of reconfigurable serpentine graphene nanoribbon under tension. Journal of Applied Physics, 2019, 125, .	1.1	2
2084	A molecular dynamics study on the thermal conductivities of single- and multi-layer two-dimensional borophene. Nano Futures, 2019, 3, 015001.	1.0	22
2085	Stability analysis of endohedrally functionalized carbon nanotubes with pentagonal metallic nanowires: a molecular dynamics simulation approach. Materials Research Express, 2019, 6, 045056.	0.8	7
2086	Graphene Surface Reinforcement of Iron. Nanomaterials, 2019, 9, 59.	1.9	18
2087	Uncertainty analysis and estimation of robust AIREBO parameters for graphene. Carbon, 2019, 142, 300-310.	5.4	43
2088	Melting process of zigzag boron nitride nanoribbon. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 106, 95-100.	1.3	4
2089	Structural studies of carbons by neutron and x-ray scattering. Reports on Progress in Physics, 2019, 82, 016501.	8.1	15
2090	Determining porosity effect on the thermal conductivity of single-layer graphene using a molecular dynamics simulation. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 106, 90-94.	1.3	13
2091	Nanoindentation of circular multilayer graphene allotropes. Science China Technological Sciences, 2019, 62, 269-275.	2.0	5
2092	Laser Shock Tuning Dynamic Interlayer Coupling in Grapheneâ€“Boron Nitride MoirÃ© Superlattices. Nano Letters, 2019, 19, 283-291.	4.5	31
2093	Detachment Dynamics of Graphene Nanoribbons on Gold. ACS Nano, 2019, 13, 689-697.	7.3	14
2094	Strain engineering for thermal conductivity of diamond nanothread forests. Journal Physics D: Applied Physics, 2019, 52, 085301.	1.3	9
2095	Molecular simulations of carbon allotropes in processes with creation and destruction of chemical bonds. Carbon, 2019, 144, 177-184.	5.4	8
2096	Strain engineering of friction between graphene layers. Tribology International, 2019, 131, 686-693.	3.0	38
2097	Mechanical properties of two-dimensional materials and their applications. Journal Physics D: Applied Physics, 2019, 52, 083001.	1.3	97
2098	Application of the ChIMES Force Field to Nonreactive Molecular Systems: Water at Ambient Conditions. Journal of Chemical Theory and Computation, 2019, 15, 436-447.	2.3	23
2099	Theoretical Analysis on the Constitution of Calorific Values of Biomass Fuels. Journal of Energy Resources Technology, Transactions of the ASME, 2019, 141, .	1.4	6
2100	Molecular dynamics study of gold nano-clusters aggregation on a model defected graphene. Indian Journal of Physics, 2019, 93, 733-738.	0.9	0

#	ARTICLE	IF	CITATIONS
2101	Swift heavy-ion irradiation of graphene oxide: Localized reduction and formation of sp-hybridized carbon chains. <i>Carbon</i> , 2019, 141, 390-399.	5.4	17
2102	Recent progress on graphene-analogous 2D nanomaterials: Properties, modeling and applications. <i>Progress in Materials Science</i> , 2019, 100, 99-169.	16.0	235
2103	From high pressure radial collapse to graphene ribbon formation in triple-wall carbon nanotubes. <i>Carbon</i> , 2019, 141, 568-579.	5.4	31
2104	A computational study on the quantum transport properties of silicene-graphene nano-composites. <i>Microsystem Technologies</i> , 2019, 25, 1881-1899.	1.2	4
2105	Fracture behavior of the carbon nanotube/carbon fiber/polymer multiscale composites under bending test - A stochastic finite element method. <i>Mechanics of Advanced Materials and Structures</i> , 2019, 26, 1169-1177.	1.5	8
2106	Atomic-scale finite element modelling of mechanical behaviour of graphene nanoribbons. <i>International Journal of Mechanics and Materials in Design</i> , 2019, 15, 145-157.	1.7	10
2107	Comparison of fracture behavior of defective armchair and zigzag graphene nanoribbons. <i>International Journal of Damage Mechanics</i> , 2019, 28, 325-345.	2.4	26
2108	Recent advances in quantum-mechanical molecular dynamics simulations of proton transfer mechanism in various water-based environments. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1419.	6.2	10
2109	Adhesion and stress-enhanced elastocaloric effect in graphene. <i>Science China Technological Sciences</i> , 2020, 63, 297-302.	2.0	4
2110	Does vibration amplitude influence the evaluation of nonlocal small scale parameter of single layered graphene sheets?. <i>Mechanics of Advanced Materials and Structures</i> , 2020, 27, 493-504.	1.5	5
2111	Monitoring water and oxygen splitting at graphene edges and folds: Insights into the lubricity of graphitic materials. <i>Carbon</i> , 2020, 156, 93-103.	5.4	38
2112	Nonlinear vibrations of helical graphene resonators in the dynamic nano-indentation testing. <i>Nanotechnology</i> , 2020, 31, 025709.	1.3	5
2113	Investigation on thermal conductivity of graphene/Si heterostructure with different defect ratios and sizes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126077.	0.9	8
2114	Intelligent-ReaxFF: Evaluating the reactive force field parameters with machine learning. <i>Computational Materials Science</i> , 2020, 172, 109393.	1.4	34
2115	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 015901.	0.7	771
2116	Geometrical aspects of nanofillers influence the tribological performance of Al-based nanocomposites. <i>Wear</i> , 2020, 444-445, 203117.	1.5	15
2117	Ultrasoft slip-mediated bending in few-layer graphene. <i>Nature Materials</i> , 2020, 19, 305-309.	13.3	159
2118	In-plane breathing and shear modes in low-dimensional nanostructures. <i>Carbon</i> , 2020, 157, 364-370.	5.4	14

#	ARTICLE	IF	CITATIONS
2119	Improving the thermoelectric properties of carbon nanotubes through introducing graphene nanosprings. <i>Current Applied Physics</i> , 2020, 20, 150-154.	1.1	2
2120	A map between excitation magnitude and critical stable temperature for screwing oscillators built on double-walled nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113943.	1.3	4
2121	Comparing quantum, molecular and continuum models for graphene at large deformations. <i>Carbon</i> , 2020, 159, 478-494.	5.4	11
2122	Converting PBO fibers into carbon fibers by ultrafast carbonization. <i>Carbon</i> , 2020, 159, 432-442.	5.4	25
2123	A Bond Charge Model Ansatz for Intrinsic Bond Energies: Application to C-C Bonds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 176-184.	1.1	2
2124	Effect of planar torsional deformation on the thermal conductivity of 2D nanomaterials: A molecular dynamics study. <i>Materials Today Communications</i> , 2020, 22, 100706.	0.9	5
2125	Diameter-dependent polygonal cross section for holey phenine nanotubes. <i>Nanotechnology</i> , 2020, 31, 085702.	1.3	3
2126	Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 666-676.	2.3	39
2128	Energy barriers for collapsing large-diameter carbon nanotubes. <i>Carbon</i> , 2020, 159, 161-165.	5.4	9
2129	A temperature-calibrated continuum model for vibrational analysis of the fullerene family using molecular dynamics simulations. <i>Applied Mathematical Modelling</i> , 2020, 80, 115-125.	2.2	6
2130	Strain-Controlled Dynamic Rotation of Twisted 2D Atomic Layers for Tunable Nanomechanical Systems. <i>ACS Applied Nano Materials</i> , 2020, 3, 10878-10884.	2.4	3
2131	Unusual thermal properties of graphene origami crease: A molecular dynamics study. <i>Green Energy and Environment</i> , 2022, 7, 86-94.	4.7	18
2132	Voxelized Atomic Structure Potentials: Predicting Atomic Forces with the Accuracy of Quantum Mechanics Using Convolutional Neural Networks. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9093-9099.	2.1	10
2133	Molecular dynamics simulation of the coalescence behavior of small carbon clusters at high temperature. <i>Chemical Physics</i> , 2020, 539, 110931.	0.9	0
2134	Thermal Transport Behavior of Carbon Nanotube-Graphene Junction under Deformation. <i>International Journal of Nanoscience</i> , 2020, 19, 1950013.	0.4	3
2135	Stress concentration and instabilities in the atomistic process of brittle failure initiation. <i>International Journal of Fracture</i> , 2020, 224, 235-249.	1.1	3
2136	Theoretical study of collision dynamics of fullerenes on graphenylene and porous graphene membranes. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107664.	1.3	1
2137	Vibrational Analysis of Carbon Nanotube-Based Nanomechanical Resonators. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16714-16721.	1.5	4

#	ARTICLE	IF	CITATIONS
2138	Grain-size effect on plastic flow stress of nanolaminated polycrystalline aluminum/graphene composites. <i>Mechanics of Materials</i> , 2020, 148, 103530.	1.7	15
2139	Computational study of the water-driven graphene wrinkle life-cycle towards applications in flexible electronics. <i>Scientific Reports</i> , 2020, 10, 11315.	1.6	9
2140	Multilayer Structures of Graphene and Pt Nanoparticles: A Multiscale Computational Study. <i>Advanced Engineering Materials</i> , 2020, 22, 2000207.	1.6	4
2141	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. <i>Nature Communications</i> , 2020, 11, 5713.	5.8	111
2142	Predicted Confinement-Enhanced Stability and Extraordinary Mechanical Properties for Carbon Nanotube Wrapped Chains of Linear Carbon. <i>ACS Nano</i> , 2020, 14, 17071-17079.	7.3	29
2143	Effects of defects on heat conduction of graphene/hexagonal boron nitride heterointerface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126774.	0.9	9
2144	Evidence for Glass Behavior in Amorphous Carbon. <i>Journal of Carbon Research</i> , 2020, 6, 50.	1.4	5
2145	Bending vibrations of free and microdroplet-loaded graphene in the framework of the molecular dynamics method. <i>Journal of Physics: Conference Series</i> , 2020, 1556, 012053.	0.3	1
2146	Atomistic Modelling of Size-Dependent Mechanical Properties and Fracture of Pristine and Defective Cove-Edged Graphene Nanoribbons. <i>Nanomaterials</i> , 2020, 10, 1422.	1.9	11
2147	New automatic method for generating atomistic models of multi-branched and arbitrary-shaped seamless junctions of carbon nanostructures. <i>Computational Materials Science</i> , 2020, 184, 109943.	1.4	7
2148	Fracture analysis and tensile properties of perfect and defective carbon nanotubes functionalized with carbene using molecular dynamics simulations. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2020, 42, 1.	0.8	10
2149	Machine-learning models for Raman spectra analysis of twisted bilayer graphene. <i>Carbon</i> , 2020, 169, 455-464.	5.4	24
2150	Effect of interatomic potentials on modeling the nanostructure of amorphous carbon by liquid quenching method. <i>Computational Materials Science</i> , 2020, 184, 109939.	1.4	10
2151	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. <i>Physical Review B</i> , 2020, 102, .	1.1	44
2152	Twisted bilayer graphene as a linear nanoactuator. <i>Physical Review B</i> , 2020, 102, .	1.1	4
2153	Ripples in Graphene: A Variational Approach. <i>Communications in Mathematical Physics</i> , 2020, 379, 915-954.	1.0	1
2154	Probing the Effective Young's Modulus of "Magic Angle" Inspired Multifunctional Twisted Nano-Heterostructures. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000129.	1.3	17
2155	A Reactive Force Field with Coarse-Grained Electrons for Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9240-9247.	2.1	18

#	ARTICLE	IF	CITATIONS
2156	Integration of 3D nanographene into mesoporous germanium. <i>Nanoscale</i> , 2020, 12, 23984-23994.	2.8	6
2157	Species Separation and Hydrogen Streaming upon Shock Release from Polystyrene under Inertial Confinement Fusion Conditions. <i>Physical Review Letters</i> , 2020, 125, 105001.	2.9	11
2158	Heuristics for chemical species identification in dense systems. <i>Journal of Chemical Physics</i> , 2020, 153, 064102.	1.2	8
2159	Modeling the effect of ion-induced shock waves and DNA breakage with the reactive CHARMM force field. <i>Journal of Computational Chemistry</i> , 2020, 41, 2429-2439.	1.5	12
2160	An experimentally validated neural-network potential energy surface for H-atom on free-standing graphene in full dimensionality. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26113-26120.	1.3	14
2161	Many-body reactive force field development for carbon condensation in C/O systems under extreme conditions. <i>Journal of Chemical Physics</i> , 2020, 153, 054103.	1.2	17
2162	ReaxFF Reactive Force Field Study of Polymerization of a Polymer Matrix in a Carbon Nanotube-Composite System. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20488-20497.	1.5	31
2163	Uncertainty quantification in molecular simulations with dropout neural network potentials. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	42
2164	Exploring the Stability of Twisted van der Waals Heterostructures. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 45214-45221.	4.0	14
2165	Predicting tensile properties of monolayer white graphene involving edge effect. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2020, 42, 1.	0.8	2
2166	Finite-temperature mechanical properties of nanostructures with first-principles accuracy. <i>Physical Review B</i> , 2020, 102, .	1.1	8
2167	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. <i>Journal of Materials Chemistry A</i> , 2020, 8, 14054-14061.	5.2	8
2168	Surface slip on rotating graphene membrane enables the temporal selectivity that breaks the permeability-selectivity trade-off. <i>Science Advances</i> , 2020, 6, eaba9471.	4.7	54
2169	Mechanism of C60 rotation and translation on hexagonal boron-nitride monolayer. <i>Journal of Chemical Physics</i> , 2020, 153, 234702.	1.2	12
2170	Modeling for Structural Engineering and Synthesis of Two-Dimensional WSe ₂ Using a Newly Developed ReaxFF Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28285-28297.	1.5	20
2171	Topologically derived dislocation theory for twist and stretch moiré superlattices in bilayer graphene. <i>Physical Review B</i> , 2020, 102, .	1.1	12
2172	Calculation of the detonation state of HN3 with quantum accuracy. <i>Journal of Chemical Physics</i> , 2020, 153, 224102.	1.2	14
2173	Graphene origami structures with superflexibility and highly tunable auxeticity. <i>Physical Review B</i> , 2020, 102, .	1.1	26

#	ARTICLE	IF	CITATIONS
2174	Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4290-4304.	1.1	11
2175	Ten Facets, One Force Field: The GAL19 Force Field for Water–Noble Metal Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4565-4578.	2.3	26
2176	Flexural modes of graphene resonators derived from the reactive empirical bond-order potential. <i>Physical Review B</i> , 2020, 101, .	1.1	3
2177	Atomistic QM/MM simulations of the strength of covalent interfaces in carbon nanotube–polymer composites. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12007-12014.	1.3	5
2178	The effects of van der Waals interactions on the vibrational behavior of single-walled carbon nanotubes using the hammer impact test: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12613-12623.	1.3	6
2179	Negative friction coefficient in microscale graphite/mica layered heterojunctions. <i>Science Advances</i> , 2020, 6, eaaz6787.	4.7	17
2180	Stiffening offshore composite wind-blades bonding joints by carbon nanotubes reinforced resin – a new concept. <i>Journal of Structural Integrity and Maintenance</i> , 2020, 5, 87-103.	0.7	10
2181	Manipulation of mechanical properties of monolayer molybdenum disulfide: Kirigami and hetero-structure based approach. <i>Materials Chemistry and Physics</i> , 2020, 252, 123280.	2.0	5
2182	A comprehensive study on the mechanical properties and failure mechanisms of graphyne nanotubes (GNTs) in different phases. <i>Computational Materials Science</i> , 2020, 182, 109794.	1.4	23
2183	ReaxFF molecular dynamics simulations of electrolyte–water systems at supercritical temperature. <i>Journal of Chemical Physics</i> , 2020, 152, 204502.	1.2	11
2184	Effect of metallic nanowire encapsulation on the tensile behavior of single-walled carbon nanotubes: a molecular dynamics study. <i>European Physical Journal D</i> , 2020, 74, 1.	0.6	3
2185	Molecular dynamics simulation of size, temperature, heating and cooling rates on structural formation of Ag-Cu-Ni ternary nanoparticles (Ag ₃₄ -Cu ₃₃ -Ni ₃₃). <i>Computational Materials Science</i> , 2020, 183, 109842.	1.4	13
2186	Layer-based thermal migration of an ionic liquid nano-droplet on a graphene surface: a molecular dynamics study. <i>Molecular Simulation</i> , 2020, 46, 829-836.	0.9	3
2187	Computer Simulation of Spin Filtration Properties of Zigzag-Edged Octagraphene Nanoribbon Saturated with Hydrogen Atoms. <i>Russian Physics Journal</i> , 2020, 63, 303-310.	0.2	2
2188	Graphene Origami with Highly Tunable Coefficient of Thermal Expansion. <i>ACS Nano</i> , 2020, 14, 8969-8974.	7.3	36
2189	Atomistic simulation of tensile strength properties of graphene with complex vacancy and topological defects. <i>Acta Mechanica</i> , 2020, 231, 3387-3404.	1.1	8
2190	Structure, Reactivity, and Mechanical Properties of Sustainable Geopolymer Material: A Reactive Molecular Dynamics Study. <i>Frontiers in Materials</i> , 2020, 7, .	1.2	12
2191	Interlayer friction and superlubricity in bilayer graphene and MoS ₂ /MoSe ₂ van der Waals heterostructures. <i>Tribology International</i> , 2020, 151, 106483.	3.0	49

#	ARTICLE	IF	CITATIONS
2192	Molecular Investigation of Mechanical Properties and Fracture Behavior of Graphene Aerogel. Journal of Physical Chemistry B, 2020, 124, 6132-6139.	1.2	29
2193	Simulations of the Biodegradation of Citrate-Based Polymers for Artificial Scaffolds Using Accelerated Reactive Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 5311-5322.	1.2	14
2194	Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures. Materials Horizons, 2020, 7, 2359-2367.	6.4	124
2195	Benchmarking the Performance of the ReaxFF Reactive Force Field on Hydrogen Combustion Systems. Journal of Physical Chemistry A, 2020, 124, 5631-5645.	1.1	28
2196	Multiscale computational understanding and growth of 2D materials: a review. Npj Computational Materials, 2020, 6, .	3.5	89
2197	Neutral transport code for rovibrational population calculation of molecular hydrogen in large helical device plasmas. Contributions To Plasma Physics, 2020, 60, e201900153.	0.5	8
2198	Molecular dynamics simulation of graphene sinking during chemical vapor deposition growth on semi-molten Cu substrate. Npj Computational Materials, 2020, 6, .	3.5	29
2199	From Collisions to Bundles: An Adaptive Coarse-Grained Model for the Aggregation of High-Aspect-Ratio Carbon Nanotubes. Journal of Physical Chemistry C, 2020, 124, 8359-8370.	1.5	6
2200	Correlated states in twisted double bilayer graphene. Nature Physics, 2020, 16, 520-525.	6.5	374
2201	Efficient machine-learning based interatomic potentials for exploring thermal conductivity in two-dimensional materials. JPhys Materials, 2020, 3, 02LT02.	1.8	32
2202	Low interfacial thermal resistance between crossed ultra-thin carbon nanothreads. Carbon, 2020, 165, 216-224.	5.4	27
2203	A molecular dynamics study on the buckling behavior of single-walled carbon nanotubes filled with gold nanowires. Journal of Molecular Modeling, 2020, 26, 196.	0.8	6
2204	Enhancing mechanism of interfacial metal element on the thermal transport across Cu-graphene interfaces revealed by molecular dynamics simulations. Materials Today Communications, 2020, 25, 101431.	0.9	12
2205	Molecular dynamics simulation and experimental investigation of structural transformation and graphitization in diamond during friction. Computational Materials Science, 2020, 184, 109862.	1.4	19
2206	Characterization of a Microscale Superlubric Graphite Interface. Physical Review Letters, 2020, 125, 026101.	2.9	25
2207	Molecular dynamics simulation model of hydrogen recycling on carbon divertor for neutral transport analysis in large helical device. Contributions To Plasma Physics, 2020, 60, e201900152.	0.5	6
2208	Influence of Vacancies and Grain Boundaries on the Diffusive Motion of Surface Rolling Molecules. Journal of Physical Chemistry C, 2020, 124, 16629-16643.	1.5	13
2209	Thermal conductivity reduction in carbon nanotube by fullerene encapsulation: A molecular dynamics study. Carbon, 2020, 161, 800-808.	5.4	22

#	ARTICLE	IF	CITATIONS
2210	Adsorption and Diffusion of Hydrogen in Carbon Honeycomb. <i>Nanomaterials</i> , 2020, 10, 344.	1.9	11
2211	Moiré Flat Bands in Twisted Double Bilayer Graphene. <i>Nano Letters</i> , 2020, 20, 2410-2415.	4.5	107
2212	Rotational stability of twisted bilayer graphene. <i>Physical Review B</i> , 2020, 101, .	1.1	23
2213	Extended MARTINI water model for heat transfer studies. <i>Molecular Physics</i> , 2020, 118, e1692151.	0.8	5
2214	Soliton signature in the phonon spectrum of twisted bilayer graphene. <i>2D Materials</i> , 2020, 7, 025050.	2.0	34
2215	Molecular dynamics study on the thermal conductivity of bilayer graphene with nitrogen doping. <i>Solid State Communications</i> , 2020, 309, 113845.	0.9	9
2216	Mesoscopic computational model of covalent cross-links and mechanisms of load transfer in cross-linked carbon nanotube films with continuous networks of bundles. <i>Computational Materials Science</i> , 2020, 176, 109410.	1.4	4
2217	The Effect of Single Vacancy Defects on Graphene Nanoresonators. <i>Multiscale Science and Engineering</i> , 2020, 2, 1-6.	0.9	7
2218	Carbon rings as building blocks for single-walled carbon nanotubes. <i>Nano Futures</i> , 2020, 4, 025001.	1.0	0
2220	Bio-inspired self-folding strategy to break the trade-off between strength and ductility in carbon-nanoarchitected materials. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	14
2221	Single layer diamond - A new ultrathin 2D carbon nanostructure for mechanical resonator. <i>Carbon</i> , 2020, 161, 809-815.	5.4	42
2222	The COMPASS force field: Validation for carbon nanoribbons. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113937.	1.3	27
2223	Tuning the Mechanical and Adhesion Properties of Carbon Nanotubes Using Aligned Cellulose Wrap (Cellulose Nanotube): A Molecular Dynamics Study. <i>Nanomaterials</i> , 2020, 10, 154.	1.9	11
2224	Computer simulations and theoretical predictions. , 2020, , 11-50.		0
2225	Elastic straining of free-standing monolayer graphene. <i>Nature Communications</i> , 2020, 11, 284.	5.8	194
2226	Gram-scale bottom-up flash graphene synthesis. <i>Nature</i> , 2020, 577, 647-651.	13.7	438
2227	Anomalous Thermal Response of Graphene Kirigami Induced by Tailored Shape to Uniaxial Tensile Strain: A Molecular Dynamics Study. <i>Nanomaterials</i> , 2020, 10, 126.	1.9	7
2228	Buckling of cylindrical shells subjected to a finite number of lateral loads: application to single-walled carbon nanotubes. <i>Nanotechnology</i> , 2020, 31, 205711.	1.3	2

#	ARTICLE	IF	CITATIONS
2229	Dehydration-Determined Ion Selectivity of Graphene Subnanopores. ACS Applied Materials & Interfaces, 2020, 12, 24281-24288.	4.0	39
2230	Complex three-dimensional graphene structures driven by surface functionalization. Nanoscale, 2020, 12, 10172-10179.	2.8	18
2231	Icosahedral Geometry of Geodesic Domes, Fullerenes and Viruses: A Tutorial on the T-Number. Symmetry, 2020, 12, 556.	1.1	12
2232	The electrochemical interface in first-principles calculations. Surface Science Reports, 2020, 75, 100492.	3.8	89
2233	The effect of temperature on water desalination through two-dimensional nanopores. Journal of Chemical Physics, 2020, 152, 164701.	1.2	6
2234	Crease-induced targeted cutting and folding of graphene origami. Carbon, 2020, 165, 259-266.	5.4	11
2235	Mechanical behaviors of MoS nanowires under tension from molecular dynamics simulations. Computational Materials Science, 2020, 179, 109691.	1.4	5
2236	High density mechanical energy storage with carbon nanothread bundle. Nature Communications, 2020, 11, 1905.	5.8	45
2237	Surface-topology-controlled mechanical characteristics of triply periodic carbon Schwarzite foams. Soft Matter, 2020, 16, 4324-4338.	1.2	10
2238	Tribochemistry: A Review of Reactive Molecular Dynamics Simulations. Lubricants, 2020, 8, 44.	1.2	52
2239	Ab initio insights into graphene lubricity. , 2021, , 21-38.		0
2240	Reversible synthesis of GO: Role of differential bond structure transformation in fine-tuning photodetector response. Nanotechnology, 2021, 32, 045601.	1.3	4
2241	Mechanical modeling and simulation of aerogels: A review. Ceramics International, 2021, 47, 2981-2998.	2.3	31
2242	Strengthening mechanism of Al matrix composites reinforced by nickel-coated graphene: Insights from molecular dynamics simulation. Physica B: Condensed Matter, 2021, 601, 412620.	1.3	22
2243	Twisted bilayer graphene/h-BN under impact of a nano-projectile. Applied Surface Science, 2021, 538, 148030.	3.1	22
2244	Nanoindentation of Amorphous Carbon: a combined experimental and simulation approach. Acta Materialia, 2021, 203, 116485.	3.8	23
2245	Carbon nanotube (CNT) metal composites exhibit greatly reduced radiation damage. Acta Materialia, 2021, 203, 116483.	3.8	23
2246	Fitting of interatomic potentials by a differential evolution algorithm. Computational Materials Science, 2021, 187, 109929.	1.4	0

#	ARTICLE	IF	CITATIONS
2247	Graphene-based nanoscale version of da Vinci's reciprocal structures. <i>Computational Materials Science</i> , 2021, 187, 110105.	1.4	4
2248	Molecular Dynamics Simulations of the pH-Dependent Adsorption of Doxorubicin on Carbon Quantum Dots. <i>Molecular Pharmaceutics</i> , 2021, 18, 257-266.	2.3	5
2249	Energy transfers in a weakly coupled gas-surface system: The scattering of CO from MgO(001). <i>Surface Science</i> , 2021, 706, 121767.	0.8	2
2250	A molecular dynamics study on the tensile characteristics of various metallic glass nanocomposites reinforced by Weyl semimetals three-dimensional graphene network. <i>European Journal of Mechanics, A/Solids</i> , 2021, 85, 104104.	2.1	7
2251	A molecular dynamics study on the tribological behavior of molybdenum disulfide with grain boundary defects during scratching processes. <i>Friction</i> , 2021, 9, 1198-1212.	3.4	21
2252	Adsorption of Evans blue and Congo red on carbon nanotubes and its influence on the fracture parameters of defective and functionalized carbon nanotubes studied using computational methods. <i>Applied Surface Science</i> , 2021, 539, 148236.	3.1	16
2253	Effects of interlayer density and surfactant on coupled thermal stress and moisture absorption in modified montmorillonite/polypropylene nanocomposite. <i>Journal of Applied Polymer Science</i> , 2021, 138, 50186.	1.3	0
2254	Mechanical Properties of Soot Particles: The Impact of Crosslinked Polycyclic Aromatic Hydrocarbons. <i>Combustion Science and Technology</i> , 2021, 193, 643-663.	1.2	14
2255	Strain effect on the thermal transport property of gamma (Γ^3)-graphyne. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 0, , 1-17.	1.0	1
2256	Graphene-functionalized carbon/glass fiber reinforced polymer nanocomposites: fabrication and characterization for manufacturing applications. , 2021, , 57-78.		4
2257	Nano-scale and Atomistic-Scale Modeling of Advanced Materials. , 2021, , 555-577.		0
2258	Molecular modeling for predicting material and junction strengths of various carbon nanostructures. , 2021, , 67-102.		0
2259	Effects of Monovacancy on Thermal Properties of Bilayer Graphene Nanoribbons by Molecular Dynamics Simulations. <i>Journal of Thermal Science</i> , 2021, 30, 1917.	0.9	5
2260	Efficient Mechanical Stress Transfer in Multilayer Graphene with a Ladder-like Architecture. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 4473-4484.	4.0	9
2261	Reaction prediction via atomistic simulation: from quantum mechanics to machine learning. <i>IScience</i> , 2021, 24, 102013.	1.9	25
2262	Mechanisms of frictional energy dissipation at graphene grain boundaries. <i>Physical Review B</i> , 2021, 103, .	1.1	16
2263	Thermal conductivity of perfect and defective carbon nanotubes functionalized with carbene: a molecular dynamics study. <i>Molecular Simulation</i> , 0, , 1-9.	0.9	6
2264	How Does van der Waals Confinement Enhance Phonon Transport?*. <i>Chinese Physics Letters</i> , 2021, 38, 014401.	1.3	24

#	ARTICLE	IF	CITATIONS
2265	Bond order redefinition needed to reduce inherent noise in molecular dynamics simulations. <i>Scientific Reports</i> , 2021, 11, 3674.	1.6	1
2266	Study on the sorption mechanism of middle-temperature sorption thermal storage materials from the microscale simulation: A review. <i>International Journal of Energy Research</i> , 2021, 45, 9719-9752.	2.2	4
2267	Pattern Development and Control of Strained Solitons in Graphene Bilayers. <i>Nano Letters</i> , 2021, 21, 1772-1777.	4.5	16
2268	Effective Enhancement of a Carbon Nanothread on the Mechanical Properties of the Polyethylene Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5781-5792.	1.5	9
2269	Comparative studies of thermal conductivity for bilayer graphene with different potential functions in molecular dynamic simulations. <i>Results in Physics</i> , 2021, 22, 103894.	2.0	16
2270	Structural Defects, Mechanical Behaviors, and Properties of Two-Dimensional Materials. <i>Materials</i> , 2021, 14, 1192.	1.3	48
2271	Thermal boundary resistance at graphene-pentacene interface explored by a data-intensive approach. <i>Nanotechnology</i> , 2021, 32, 215404.	1.3	3
2272	Modeling buckling and topological defects in stacked two-dimensional layers of graphene and hexagonal boron nitride. <i>Physical Review Materials</i> , 2021, 5, .	0.9	9
2273	Theoretical investigations of the interaction between diatomic molecules and coinage metal atoms. <i>Molecular Physics</i> , 2021, 119, e1892224.	0.8	1
2274	Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics. <i>Physical Review B</i> , 2021, 103, .	1.1	4
2275	Free Transverse Vibration of Nickel Coated Carbon Nanotubes. <i>International Journal of Structural Stability and Dynamics</i> , 2021, 21, 2150085.	1.5	7
2276	Inelastic Scattering of H Atoms from Surfaces. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3059-3076.	1.1	14
2277	Shockwave response of graphene aerogels: An all-atom simulation study. <i>Computational Materials Science</i> , 2021, 189, 110252.	1.4	13
2278	Catalyst particle size dependent carbon nanotube cloning. <i>Carbon</i> , 2021, 175, 69-76.	5.4	12
2279	Soft Particles at Liquid Interfaces: From Molecular Particle Architecture to Collective Phase Behavior. <i>Langmuir</i> , 2021, 37, 5364-5375.	1.6	22
2280	Thermal conductivity of graphene/graphane/graphene heterostructure nanoribbons: Non-equilibrium molecular dynamics simulations. <i>Solid State Communications</i> , 2021, 328, 114249.	0.9	7
2281	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. <i>ACS Nano</i> , 2021, 15, 5959-5976.	7.3	30
2282	Self-Assembly of MoS ₂ Monolayer Sheets by Desulfurization. <i>Langmuir</i> , 2021, 37, 4971-4983.	1.6	6

#	ARTICLE	IF	CITATIONS
2283	Modification of the Interlayer Coupling and Chemical Reactivity of Multilayer Graphene through Wrinkle Engineering. <i>Chemistry of Materials</i> , 2021, 33, 2506-2515.	3.2	10
2284	Non-retraction rebound of the impacting nano-droplets. <i>Journal of Molecular Liquids</i> , 2021, 329, 115521.	2.3	10
2285	Tight-binding theory of graphene mechanical properties. <i>Microsystem Technologies</i> , 2021, 27, 3851-3858.	1.2	7
2286	INDEEDopt: a deep learning-based ReaxFF parameterization framework. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	21
2287	Parity-Dependent Moiré Superlattices in Graphene Heterostructures: A Route to Mechanomutable Metamaterials. <i>Physical Review Letters</i> , 2021, 126, 216101.	2.3	41
2288	Protonation of Cytosine-Rich Telomeric DNA Fragments by Carboxylated Carbon Nanotubes: Insights from Computational Studies. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5526-5536.	1.2	2
2289	Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3237-3251.	2.3	41
2290	Electronic localization in small-angle twisted bilayer graphene. <i>2D Materials</i> , 2021, 8, 035046.	2.0	25
2291	Role of OH Termination in Mitigating Friction of Diamond-like Carbon under High Load: A Joint Simulation and Experimental Study. <i>Langmuir</i> , 2021, 37, 6292-6300.	1.6	11
2292	Highly efficient desalination performance of carbon honeycomb based reverse osmosis membranes unveiled by molecular dynamics simulations. <i>Nanotechnology</i> , 2021, 32, .	1.3	7
2293	Multiscale Toughening of Composites with Carbon Nanotubes – Continuous Multiscale Reinforcement New Concept. <i>Journal of Composites Science</i> , 2021, 5, 135.	1.4	6
2294	Frontiers of graphene-based Hall-effect sensors. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 243002.	0.7	19
2295	Impact resistance of short carbon fibre-carbon nanotube-polymer matrix hybrid composites: A stochastic multiscale approach. <i>Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications</i> , 2021, 235, 1925-1936.	0.7	1
2296	A comprehensive assessment of empirical potentials for carbon materials. <i>APL Materials</i> , 2021, 9, .	2.2	26
2297	Infrared Spectroscopy of Chemically Diverse Carbon Clusters: A Data-Driven Approach. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5509-5518.	1.1	6
2298	Flat-to-Flat Polymerization of Single-Walled Carbon Nanotubes under High Pressure Mediated by Carbon Chain Encapsulation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12857-12869.	1.5	2
2299	Interplay of high-precision shock wave experiments with first-principles theory to explore molecular systems at extreme conditions: A perspective. <i>Journal of Applied Physics</i> , 2021, 129, .	1.1	3
2300	Nanopore creation in MoS ₂ and graphene monolayers by nanoparticles impact: a reactive molecular dynamics study. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	6

#	ARTICLE	IF	CITATIONS
2301	Multiscale Modeling on the Enhanced Heat Transfer Behavior of Thermal Interface Materials Based on Graphene. , 2021, , .		0
2302	Mechanical properties of graphene. Applied Physics Reviews, 2021, 8, .	5.5	37
2303	Tensile properties of functionalized carbon nanothreads. Nano Materials Science, 2022, 4, 220-226.	3.9	4
2304	A multilayer coarse-grained molecular dynamics model for mechanical analysis of mesoscale graphene structures. Carbon, 2021, 178, 528-539.	5.4	15
2305	Optical-Thermally Excited Graphene Resonant Mass Detection: A Molecular Dynamics Analysis. Nanomaterials, 2021, 11, 1924.	1.9	2
2306	Mechanical Properties of Single-Layer Diamond Reinforced Poly(vinyl alcohol) Nanocomposites through Atomistic Simulation. Macromolecular Materials and Engineering, 2021, 306, 2100292.	1.7	4
2307	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	23.0	287
2308	Comparing different multibody reactive potentials for the elastic properties and nonlinear mechanics of the carbon nanostructures. Mechanics of Materials, 2021, 158, 103858.	1.7	1
2309	Superlubricity in bilayer isomeric tellurene and graphene/tellurene van der Waals heterostructures. Tribology International, 2021, 159, 106974.	3.0	15
2310	Investigation of carbon nanosprings with the tunable mechanical properties controlled by the defect distribution. Carbon, 2021, 179, 240-255.	5.4	7
2311	Twisting or untwisting graphene twisted nanoribbons without rotation. Physical Review B, 2021, 104, .	1.1	3
2312	Multi-objective parametrization of interatomic potentials for large deformation pathways and fracture of two-dimensional materials. Npj Computational Materials, 2021, 7, .	3.5	9
2313	Atomistic simulation on frictional response of nanoscratched Al-graphene system. AIP Advances, 2021, 11, .	0.6	3
2314	Statistical abundance and stability of carbon nanostructures by combined condensation-annealing molecular dynamics simulations. Computational and Theoretical Chemistry, 2021, 1201, 113252.	1.1	3
2315	Reviewing computational studies of defect formation and behaviors in carbon fiber structural units. Computational Materials Science, 2021, 195, 110477.	1.4	6
2316	Supersonic Impact Response of Polymer Thin Films via Large-Scale Atomistic Simulations. Nano Letters, 2021, 21, 5991-5997.	4.5	10
2317	Robust Superlubricity and Moiré Lattice's Size Dependence on Friction between Graphdiyne Layers. ACS Applied Materials & Interfaces, 2021, 13, 40901-40908.	4.0	12
2318	A novel growth model for depositing ultrananocrystalline diamond films in CH ₄ /H ₂ chemistry. Surface and Coatings Technology, 2021, 419, 127280.	2.2	10

#	ARTICLE	IF	CITATIONS
2319	Strain Characterization in Two-Dimensional Crystals. <i>Materials</i> , 2021, 14, 4460.	1.3	7
2320	Negative interlayer shear effect on a double-layered van der Waals material resonator. <i>Physical Review B</i> , 2021, 104, .	1.1	5
2321	Evaluating the thermal conductivity coefficient of polypropylene/graphene nanocomposites: A hierarchical investigation. <i>Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications</i> , 2021, 235, 2762-2770.	0.7	3
2322	Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures. <i>Nature Materials</i> , 2022, 21, 47-53.	13.3	110
2323	Dynamic Behavior of Rotation Transmission Nano-System in Helium Environment: A Molecular Dynamics Study. <i>Molecules</i> , 2021, 26, 5199.	1.7	0
2324	Theoretical Study of Chemical Vapor Deposition Synthesis of Graphene and Beyond: Challenges and Perspectives. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7942-7963.	2.1	15
2325	Mechanical Behaviors of Si/CNT Core/Shell Nanocomposites under Tension: A Molecular Dynamics Analysis. <i>Nanomaterials</i> , 2021, 11, 1989.	1.9	5
2326	Influence of graphite crystalline orientation on the carbon dissolution reaction in liquid iron: A ReaxFF molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2021, 335, 115688.	2.3	1
2327	Nanoscale Continuous Directional Motion Driven by a Cyclic Thermal Field. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2021, 88, .	1.1	3
2328	Investigating mechanical properties and thermal conductivity of 2D carbon-based materials by computational experiments. <i>Computational Materials Science</i> , 2021, 196, 110493.	1.4	13
2329	Molecular dynamics simulations of the isotopic effect on nanoscale friction. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	1
2330	A molecular dynamics simulation on the atomic mass sensor made of monolayer diamond. <i>Nanotechnology</i> , 2021, 32, 475501.	1.3	6
2331	Elastocapillary cleaning of twisted bilayer graphene interfaces. <i>Nature Communications</i> , 2021, 12, 5069.	5.8	19
2332	Molecular dynamics study on the effect of polymer physisorption on the thermal conductivity of cross-linked functionalized carbon nanotubes. <i>Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science</i> , 2022, 236, 3663-3671.	1.1	1
2333	Implementation of the LAMMPS package using T-system with an Open Architecture. <i>Informatics and Automation</i> , 2021, 20, 971-999.	0.6	0
2334	A ReaxFF Force Field for 2D-WS ₂ and Its Interaction with Sapphire. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17950-17961.	1.5	10
2335	Influence of force field used in carbon nanostructure reconstruction on simulated phenol adsorption isotherms in aqueous medium. <i>Journal of Molecular Liquids</i> , 2021, 344, 117548.	2.3	3
2336	Physics-based, neural network force fields for reactive molecular dynamics: Investigation of carbene formation from [EMIM+][OAc ⁻]. <i>Journal of Chemical Physics</i> , 2021, 155, 104112.	1.2	6

#	ARTICLE	IF	CITATIONS
2337	LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. <i>Computer Physics Communications</i> , 2022, 271, 108171.	3.0	3,106
2338	The strategy of repairing defective graphene by graphene patch via interlayer cross-linking. <i>Computational Materials Science</i> , 2021, 197, 110645.	1.4	1
2339	Anisotropic frictional properties between Ti ₃ C ₂ T _x MXene/SiO ₂ layer-dependent heterojunctions. <i>Journal of Science: Advanced Materials and Devices</i> , 2021, 6, 488-493.	1.5	8
2340	Registry-Dependent Peeling of Layered Material Interfaces: The Case of Graphene Nanoribbons on Hexagonal Boron Nitride. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 43533-43539.	4.0	6
2341	Can force fields developed for carbon nanomaterials describe the isomerization energies of fullerenes?. <i>Chemical Physics Letters</i> , 2021, 779, 138853.	1.2	11
2342	Breakdown of Universal Scaling for Nanometer-Sized Bubbles in Graphene. <i>Nano Letters</i> , 2021, 21, 8103-8110.	4.5	23
2343	Superlubric polycrystalline graphene interfaces. <i>Nature Communications</i> , 2021, 12, 5694.	5.8	14
2344	Effect of misfit strain on the buckling of graphene/MoS ₂ van der Waals heterostructures. <i>Nanotechnology</i> , 2021, 32, 485701.	1.3	3
2345	Isotope effect of rovibrational distribution of hydrogen molecules desorbed from amorphous carbon. <i>Japanese Journal of Applied Physics</i> , 0, , .	0.8	1
2346	Tuning thermal conductance of graphene-polyethylene composites via graphene inclination and curvature. <i>International Journal of Heat and Mass Transfer</i> , 2021, 178, 121634.	2.5	9
2347	A nanoscale study of size scale, strain rate, temperature, and stress state effects on damage and fracture of polyethylene. <i>Mechanics of Materials</i> , 2021, 161, 104008.	1.7	7
2348	Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. <i>Carbon</i> , 2021, 183, 438-448.	5.4	3
2349	Enhanced surface and electrochemical properties of nitrogen-doped reduced graphene oxide by violet laser treatment for high charge storage and lower self-discharge supercapacitors. <i>Journal of Power Sources</i> , 2021, 513, 230517.	4.0	14
2350	Peeling of graphene/molybdenum disulfide heterostructure at different angles: A continuum model with accommodations for van der Waals interaction. <i>Composites Part A: Applied Science and Manufacturing</i> , 2021, 150, 106592.	3.8	7
2351	Exploring the necessary complexity of interatomic potentials. <i>Computational Materials Science</i> , 2021, 200, 110752.	1.4	8
2352	Stress-dominated growth of two-dimensional materials on nonplanar substrates. <i>Journal of the Mechanics and Physics of Solids</i> , 2021, 157, 104645.	2.3	4
2353	Phonon thermal transport in diamond and lonsdaleite: A comparative study of empirical potentials. <i>Diamond and Related Materials</i> , 2021, 120, 108618.	1.8	3
2354	An atomistic-continuum multiscale approach to determine the exact thickness and bending rigidity of monolayer graphene. <i>Journal of Sound and Vibration</i> , 2021, 514, 116464.	2.1	13

#	ARTICLE	IF	CITATIONS
2355	Multiscale Modeling and Applications of Bioinspired Materials with Gyroid Structures. Springer Series in Materials Science, 2021, , 629-644.	0.4	1
2356	Stoneâ€“Wales defects preserve hyperuniformity in amorphous two-dimensional networks. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	28
2357	Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, .	3.5	39
2358	Effect of graphene and carbon-nitride nanofillers on the thermal transport properties of polymer nanocomposites: A combined molecular dynamics and finite element study. Physical Review E, 2021, 103, 013310.	0.8	12
2360	Response of graphene reinforced concrete to the external compressive load: A multiscale approach. Structural Concrete, 2018, 19, 1702-1712.	1.5	3
2361	Molecular Dynamics Simulations of Hydrogen Adsorption in Finite and Infinite Bundles of Single Walled Carbon Nanotubes. Challenges and Advances in Computational Chemistry and Physics, 2007, , 469-485.	0.6	1
2362	Hierarchical Nanomechanics of Collagen Fibrils: Atomistic and Molecular Modeling. , 2008, , 175-247.		5
2363	Molecular Simulation of Protein-Surface Interactions. , 2009, , 69-95.		2
2364	A Comparison of Different Interatomic Potentials: Radius Effect of Single Wall Carbon Nanotubes. , 2007, , 121-134.		1
2365	Phase Transitions of Carbon Materials under High Pressure. , 2007, , 239-249.		1
2366	Atomic-Scale Simulations of the Mechanical Behavior of Carbon Nanotube Systems. Challenges and Advances in Computational Chemistry and Physics, 2010, , 255-295.	0.6	2
2367	Multiscale Modeling of Carbon Nanotubes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 367-388.	0.6	1
2368	Molecular Dynamics Simulations of Nanodiamond Graphitization. , 2010, , 35-54.		5
2369	Various Modeling Techniques for Nanostructures. Nanoscience and Technology, 2013, , 31-58.	1.5	2
2370	Improved Mechanical Performance of CNTs and CNT Fibres in Nanocomposites Through Inter-Wall and Inter-Tube Coupling. Springer Series in Materials Science, 2014, , 1-56.	0.4	3
2372	Challenges in Modeling Mixed Ionic-Covalent Glass Formers. Springer Series in Materials Science, 2015, , 87-112.	0.4	6
2373	Interatomic Potentials for Nuclear Materials. , 2020, , 2141-2159.		2
2374	Atomistic Study of Carbon Nanotubes: Effect of Cut-Off Distance. , 2016, , 293-300.		2

#	ARTICLE	IF	CITATIONS
2375	Computer Simulations of Nanometer-Scale Indentation and Friction. , 2017, , 301-370.		1
2376	Theoretical Aspects of Superlubricity. Nanoscience and Technology, 2007, , 177-199.	1.5	6
2377	Tensile properties of pillared graphene block. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2020, 257, 114557.	1.7	3
2378	Acoustic and double elastic shock waves in single-crystal graphene. Journal of Applied Physics, 2020, 127, 055101.	1.1	7
2379	Low energy chemical sputtering of ATJ graphite by atomic and molecular deuterium ions. Physica Scripta, 2007, T128, 50-54.	1.2	16
2380	Accuracy of Machine Learning Potential for Predictions of Multiple-Target Physical Properties*. Chinese Physics Letters, 2020, 37, 126301.	1.3	24
2381	Piezoelectric effects in boron nitride nanotubes predicted by the atomistic finite element method and molecular mechanics. Nanotechnology, 2017, 28, 355705.	1.3	13
2382	Simulated mechanical properties of finite-size graphene nanoribbons. Nanotechnology, 2021, 32, 045709.	1.3	7
2383	Concurrent Coupling of Atomistic and Continuum Models. , 2009, , 93-133.		3
2384	Collapsed carbon nanotubes as building blocks for high-performance thermal materials. Physical Review Materials, 2017, 1, .	0.9	11
2385	Molecular origins of anisotropic shock propagation in crystalline and amorphous polyethylene. Physical Review Materials, 2018, 2, .	0.9	18
2386	Theory of thin-film-mediated exfoliation of van der Waals bonded layered materials. Physical Review Materials, 2018, 2, .	0.9	18
2387	Interlayer Attraction Force in Concentric Carbon Nanotubes. Journal of Applied Mechanics, Transactions ASME, 2019, 86, .	1.1	4
2388	Pull-Out Testing of SWCNTs Simulated by Molecular Dynamics. International Journal of Theoretical and Applied Nanotechnology, 0, , .	0.0	6
2389	An Atomic-scale Finite Element Method for Single-Walled Carbon Nanotubes. , 2009, , .		1
2390	Modeling of Carbon Nanotube/Polymer Composites. , 2005, , .		1
2391	MD exercises with XMD and LAMMPS. , 2016, , 71-122.		1
2392	Nanocrystalline Diamond. , 2006, , .		8

#	ARTICLE	IF	CITATIONS
2393	Thermal Transport in Nanostructured Materials. The Electrical Engineering Handbook, 2012, , 545-572.	0.2	9
2395	Homogenized elastic properties of graphene for moderate deformations. Coupled Systems Mechanics, 2015, 4, 137-155.	0.4	2
2396	Research Progress on Resonant Characteristics of Graphene. Wuli Cailiao Xuebao/Journal of Inorganic Materials, 2016, 31, 673.	0.6	3
2397	Dependence of Melting Process on Size and Edge Type of Graphene Nanoribbon. Communications in Physics, 2017, 26, 381.	0.0	3
2398	How to Combine Binary Collision Approximation and Multi-Body Potential for Molecular Dynamics. Progress in Nuclear Science and Technology, 2011, 2, 44-50.	0.3	11
2399	Examination of Temperature Dependence of Chemical Sputtering on Graphite by Comparing the Langevin and Berendsen Thermostats. Plasma and Fusion Research, 2010, 5, S2020-S2020.	0.3	3
2400	Comparison of Hydrogen Adsorption on Diamond and Graphite Surfaces. Plasma and Fusion Research, 2010, 5, S2072-S2072.	0.3	1
2401	Molecular Dynamics Simulation of the Incident Angle Dependence of Reactions between Graphene and Hydrogen Atom. Plasma and Fusion Research, 2010, 5, S2076-S2076.	0.3	7
2402	Elucidation of Dynamic Mechanism for the Spontaneous Formation of C60 Structure and Thereafter-A New Realm of Computer Chemistry-. Journal of Computer Chemistry Japan, 2011, 10, A31-A38.	0.0	1
2404	A Systematic Molecular Dynamics Investigation on the Graphene Polymer Nanocomposites for Bulletproofing. Computers, Materials and Continua, 2020, 65, 2009-2032.	1.5	4
2406	Carbon Nanotubes and Short Cytosine-Rich Telomeric DNA Oligomers as Platforms for Controlled Release of Doxorubicinâ€”A Molecular Dynamics Study. International Journal of Molecular Sciences, 2020, 21, 3619.	1.8	16
2407	Influences of vacancy defects on tensile failure of open-tip carbon nanocones. AIMS Materials Science, 2017, 4, 178-193.	0.7	5
2410	Modeling and Simulation of Graphene Based Polymer Nanocomposites: Advances in the Last Decade. Graphene, 2016, 05, 96-142.	0.3	54
2411	Torsional Characteristics of Single Walled Carbon Nanotube with Water Interactions by Using Molecular Dynamics Simulation. Nano-Micro Letters, 2014, 6, 268.	14.4	1
2413	Molecular dynamics simulation on carbon nanotube bundles sandwiched between Si surfaces. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 016106.	0.2	5
2414	Relaxation properties of graphene nanoribbons at different ambient temperatures: a molecular dynamics study. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 200207.	0.2	9
2415	Influence of defects on friction and motion of carbon nanotube. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 056101.	0.2	6
2416	Quantum thermal transport and spin thermoelectrics in low-dimensional nano systems: application of nonequilibrium Green's function method. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 186302.	0.2	19

#	ARTICLE	IF	CITATIONS
2417	Molecular dynamics study on relaxation properties of monolayer MoS2 nanoribbons. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 160201.	0.2	5
2418	Investigation on the large tensile deformation and mechanical behaviors of graphene kirigami. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 066201.	0.2	4
2419	Molecular Dynamics Simulation of Chemical Vapor Deposition of Amorphous Carbon: Dependence on H/C Ratio of Source Gas. Japanese Journal of Applied Physics, 2011, 50, 01AB01.	0.8	1
2420	Extension of Binary-Collision-Approximation-Based Simulation Applicable to Any Structured Target Material. Japanese Journal of Applied Physics, 2011, 50, 01AB03.	0.8	5
2421	Molecular Dynamics Simulation of Hydrogen Injection onto Diamond Surfaces. Japanese Journal of Applied Physics, 2011, 50, 01AB04.	0.8	3
2422	Anisotropic Bond Orientation of Amorphous Carbon by Deposition. Japanese Journal of Applied Physics, 2012, 51, 01AC05.	0.8	6
2423	Spontaneous Polygonization of Multiwalled Carbon Nanotubes: Perturbation Analysis. Japanese Journal of Applied Physics, 2012, 51, 065101.	0.8	2
2424	Numerical Simulations to Study Growth of Single-Crystal Diamond by Using Microwave Plasma Chemical Vapor Deposition with Reactive (H, C, N) Species. Japanese Journal of Applied Physics, 2012, 51, 090105.	0.8	15
2425	Comparative Study of Carbon Force Fields for the Simulation of Carbon Onions. Australian Journal of Chemistry, 2021, 74, 709-714.	0.5	7
2426	Atomic Insights into Fracture Characteristics of Twisted Tri-Layer Graphene. Crystals, 2021, 11, 1202.	1.0	7
2427	Insight into acetylene plasma deposition using molecular dynamics simulations. Plasma Processes and Polymers, 2022, 19, e2100103.	1.6	8
2428	Introductory Roadmap to Current Reactive Force-Field Methodologies. , 2022, , 1-29.		0
2429	Fundamental frequency analysis of endohedrally functionalized carbon nanotubes with metallic nanowires: a molecular dynamics study. Journal of Molecular Modeling, 2021, 27, 313.	0.8	3
2430	LMFF. , 2021, , .		6
2431	Covalent-Binding Carbon Nanotube: Simulation of Formation Mechanisms and Energy Characteristics. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2004, , 279-282.	0.1	0
2432	Nanocrystalline Diamond. Advanced Materials and Technologies, 2006, , 175-209.	0.4	0
2433	Temperature and Loading-Rate Dependence on the Mechanical Behavior of Carbon Nanotubes. Transactions of the Korean Society of Mechanical Engineers, A, 2006, 30, 809-815.	0.1	0
2435	Compressive and Torsional Buckling Behavior of Carbon Nanotube Bundles. Transactions of the Korean Society of Mechanical Engineers, A, 2007, 31, 862-869.	0.1	1

#	ARTICLE	IF	CITATIONS
2436	Coarse-Graining in Time. , 2008, , 433-488.		1
2437	Friction between Diamond-Like Carbon (DLC) Filmsâ€”a Molecular Dynamics Study. , 2009, , 554-555.		0
2439	Molecular Dynamics Study on Carbon Nanotubes Sandwiched between Si Surface. , 2009, , 558-559.		0
2440	Predictive Modeling. , 2009, , 247-289.		0
2442	Computational Scale Linking in Biological Protein Materials. , 2010, , 491-531.		0
2443	Potentials for van der Waals Interaction in Nano-Scale Computation. Challenges and Advances in Computational Chemistry and Physics, 2010, , 323-333.	0.6	0
2444	Multiscale Modeling of Biological Protein Materials â€” Deformation and Failure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 473-533.	0.6	0
2445	Unusual Scaling Observations in the Quality Factors of Cantilevered Carbon Nanotube Resonators. , 2010, , .		0
2447	Molecular dynamical simulation on the mechanical property of hydrogenated diamond-like carbon films. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 5687.	0.2	3
2448	Molecular dynamics simulation of energy exchange during hydrogen collision with graphite sheet containing a vacancy. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 057901.	0.2	1
2449	Mechanical Properties of Carbon Nanotubes with One-Dimensional Intramolecular Junction. Zairyo/Journal of the Society of Materials Science, Japan, 2012, 61, 149-154.	0.1	0
2450	Computational Approaches and Simulation. Springer Series in Materials Science, 2012, , 213-263.	0.4	0
2451	Molecular dynamics simulation of energy exchanges between single hydrogen and graphite(001). Wuli Xuebao/Acta Physica Sinica, 2012, 61, 047901.	0.2	1
2452	Study of Interaction Between Graphene Layers: Fast Diffusion of Graphene Flake and Commensurate-Incommensurate Phase Transition. Carbon Nanostructures, 2012, , 177-180.	0.1	0
2453	Molecular dynamics simulation of energetic hydrogen isotopes bombarding the crystalline graphite(001). Wuli Xuebao/Acta Physica Sinica, 2012, 61, 055201.	0.2	0
2454	Growth mechanism of hydrogenated carbon films: molecular dynamics simulations of the effects of low energy CH radical. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 030701.	0.2	1
2455	Carbon Nanostructures and Nanocomposites. The Electrical Engineering Handbook, 2012, , 513-544.	0.2	0
2456	Energy Dissipation Analysis of Defected Carbon Nanotube Oscillators. , 2012, , .		0

#	ARTICLE	IF	CITATIONS
2457	Looking Back the Most Beautiful Molecule C60 after Quarter Century of Discovery. Visnik Nacional Noi Akademii Nauk Ukrai Ni, 2012, , 27-35.	0.0	0
2458	Efekti programirane nastave odbojke na nivo motoričkih sposobnosti i usvojenosti elemenata odbojkačke igre. Sportske Nauke I Zdravlje, 2013, 4, .	0.1	1
2459	Study on the mechanical properties of carbon nanocones using molecular dynamics simulation. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 016102.	0.2	5
2461	Helical Wrapping of Graphene Sheets and Their Self-Assembly into Core-Shelled Composite Nanostructures with Metallic Particles. Carbon Materials, 2013, , 1-40.	0.2	0
2462	Molecular Dynamics Simulation of Effect of Interlayer Spacing on Oscillate Behavior of Graphite Oscillator. Applied Physics, 2013, 03, 171-174.	0.0	0
2466	Molecular Modeling of the Microstructure of Soft Materials. , 2013, , .		0
2467	Reinforcement Application. , 2013, , 205-226.		0
2468	Interfacial Thermal Conductance Between Carbon Nanotubes From Nonequilibrium Green's Function Method. , 2013, , .		1
2469	Simulation of Thermal and Electrical Transport in Nanotube and Nanowire Composites. Advanced Structured Materials, 2014, , 47-85.	0.3	0
2470	The Molecular Dynamics Simulation on the Diamond-Like Carbon Films. Material Sciences, 2014, 04, 145-151.	0.0	0
2471	A Molecular Dynamics derived Finite Element Method for Structural Simulations and Failure of Graphene Nanocomposites. , 0, , .		0
2473	POSTMODERAN PRISTUP MASOVNOM KOMUNICIRANJU: ULOGA INTERNETA U OBRAZOVANJU I SAVREMENIM TRAJNIM KRETANJIMA. EMC Review - časopis Za Ekonomiju - APEIRON, 2015, 8, .	0.1	0
2474	Molecular dynamics study on tensile behavior of SiC nanofiber/C/SiC nanocomposites. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 117101.	0.2	2
2477	Deposition and thermal conductivity of diamond-like carbon film on a silicon substrate. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 096501.	0.2	2
2478	Reactive Empirical Bond-Order Potentials. , 2016, , 3419-3431.		0
2479	Influence of helical rise on the self-excited oscillation behavior of zigzag @ zigzag double-wall carbon nanotubes. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 148802.	0.2	2
2480	Collision reactions of CH radical on diamond and their effects on the carbon film growth. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 030701.	0.2	0
2482	A Molecular Dynamics Simulation Study of the Influence of Different Deposited Particle on the Properties of Hydrogenated Amorphous Carbon Films. Advances in Condensed Matter Physics, 2016, 05, 9-15.	0.1	0

#	ARTICLE	IF	CITATIONS
2483	Molecular dynamics study of the tensile mechanical properties of polycrystalline graphene. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 116101.	0.2	5
2484	Simulation Study of Topological Point Defects in Graphitic Layer - Curvature Effect and Pair Correlation Function Analysis. Acta Physica Polonica A, 2016, 130, 811-816.	0.2	1
2485	Simulation of Atomic-Bonds™ Break in Linear Monatomic Carbon Chain within the Wide Temperature Range. Metallofizika I Noveishie Tekhnologii, 2016, 36, 633-647.	0.2	0
2486	Based on the molecular dynamics characteristic research of heat conduction of graphyne nanoribbons with vacancy defects. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 136801.	0.2	2
2487	Molecular Dynamics Studies of Load Transfer in Nanocomposites Reinforced by Defective Carbon Nanotube. , 2018, , 71-121.		0
2488	Influences of hydroxyl groups on friction behavior and energy dissipation of carbon nanotube. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 076101.	0.2	0
2489	Influence of Information Technologies on the Company's Competitive Advantage on the Market in Conditions of the Global Crisis. JITA - Journal of Information Technology and Applications (Banja Luka) - APEIRON, 2018, 14, .	0.1	1
2490	Thermal Vibration of Carbon Nanostructures. , 2018, , 1-61.		0
2491	Characteristics of interaction between single-layer graphene on copper substrate and groove. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 033101.	0.2	0
2492	Deformed Carbon Nanotubes. SpringerBriefs in Applied Sciences and Technology, 2018, , 55-78.	0.2	0
2493	ANÁLISE DO EFEITO ELASTOCALÓRICO EM NANOTUBOS DE CARBONO POR SIMULAÇÕES DE DINÂMICA MOLECULAR. , 0, , .		0
2495	Simulation of static and dynamic mechanical characteristics of carbon nanotubes and carbon nano-peapods with defects. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 166101.	0.2	1
2496	Super square carbon nanotube networks: mechanical properties and electric conductivity. Letters on Materials, 2019, 9, 136-141.	0.2	2
2497	Stable carbon structures: fullerene+graphene where Cn is a liner cluster. Letters on Materials, 2019, 9, 344-348.	0.2	2
2498	Thermal Vibration of Carbon Nanostructures. , 2019, , 421-481.		1
2499	Mechanics of Carbon Nanotubes and Their Composites. , 2019, , 483-548.		0
2500	Vibrational Analysis of Fullerene Hydrides Using AIREBO Potential. Scientia Iranica, 2019, .	0.3	1

#	ARTICLE	IF	CITATIONS
2502	Graphene Growth and Characterization: Advances, Present Challenges and Prospects. Journal of Materials Science Research, 2020, 8, 37.	0.1	4
2504	Atomistic Modelling and Simulation of Transmission Electron Microscopy Images: Application to Intrinsic Defects of Graphene. Advances in Intelligent Systems and Computing, 2020, , 1-19.	0.5	0
2505	Deposition and growth mechanism of graphene on copper crystal surface based on molecular dynamics simulation. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 226102.	0.2	3
2506	Atomistic Mechanics of Torn Back Folded Edges of Triangular Voids in Monolayer WS ₂ . Small, 2021, 17, e2104238.	5.2	3
2507	Influence of temperature and point defects on the X-ray diffraction pattern of graphite. Carbon Trends, 2021, 5, 100124.	1.4	16
2508	Methodological Investigation for Hydrogen Addition to Small Cage Carbon Fullerenes. Crystals, 2021, 11, 1334.	1.0	5
2509	Interlayer Interactions in Low-Dimensional Layered Hetero-structures: Modeling and Applications. , 2020, , 635-659.		0
2510	Simulation of the processes of carbon atom and nanographene interaction with a molecule of fullerene C ₆₀ . Journal of Physics: Conference Series, 2020, 1686, 012060.	0.3	1
2511	Universal Intrinsic Dynamics and Freezing of Water in Small Nanotubes. Journal of Physical Chemistry C, 2021, 125, 946-956.	1.5	5
2512	Efficient approaches to solutions of partition function for condensed matters. Journal of Physics Condensed Matter, 2021, 33, 115901.	0.7	4
2513	Effect of grain boundary and defect on mechanical properties of bicrystalline graphene. Modern Physics Letters B, 2021, 35, 2150141.	1.0	0
2514	Mechanics and Electromechanics of Two-Dimensional Atomic Membranes. , 2020, , 1911-1947.		0
2515	Molecular Dynamics Simulations of Non-equilibrium Systems. , 2020, , 2161-2192.		0
2516	Algorithm for constructing full-atomic models of X- and T-shaped seamless junctions between single-walled carbon nanotubes. Letters on Materials, 2020, 10, 277-282.	0.2	1
2517	Ballistic phonon transport analysis of twisted graphene nanoribbons. Transactions of the JSME (in) Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50	0.1	0
2518	A novel triple-walled carbon nanotube screwing oscillator: a molecular dynamics simulation. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 228801.	0.2	0
2519	The Crack Angle of 60° Is the Most Vulnerable Crack Front in Graphene According to MD Simulations. Crystals, 2021, 11, 1355.	1.0	6
2520	Theoretical Study of the Adsorbed Small Molecule on Twisted Nanotubes by Atomic Scale Simulations. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , 449-456.	0.2	0

#	ARTICLE	IF	CITATIONS
2521	Development of a Molecular Dynamics Method with Heat Transfer into Bulk for Ion Injection into Materials. <i>Plasma and Fusion Research</i> , 2020, 15, 2403073-2403073.	0.3	2
2522	Graphdiyne family-tunable solution to shock resistance. <i>Materials Research Express</i> , 2020, 7, 115602.	0.8	4
2523	Size-dependent mechanical properties of twin graphene. <i>Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanomaterials, Nanoengineering and Nanosystems</i> , 2021, 235, 4-11.	0.5	1
2526	Emergence of carbon nanoscrolls from single walled carbon nanotubes: an oxidative route. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 27437-27448.	1.3	0
2527	KLIFF: A framework to develop physics-based and machine learning interatomic potentials. <i>Computer Physics Communications</i> , 2022, 272, 108218.	3.0	10
2528	Long-range in-plane elastic displacement fields of double vacancies in graphene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 137, 115075.	1.3	0
2529	Thermal conductance control of non-bonded interaction between loaded halogen molecules and carbon nanotubes: A molecular dynamics study. <i>International Journal of Heat and Mass Transfer</i> , 2022, 183, 122216.	2.5	5
2530	Accurate force field of two-dimensional ferroelectrics from deep learning. <i>Physical Review B</i> , 2021, 104, .	1.1	18
2531	Interfacial thermal conductance of graphene/MoS ₂ heterointerface. <i>Surfaces and Interfaces</i> , 2022, 28, 101640.	1.5	6
2532	The sp ² -sp ³ transition and shear slipping dominating the compressive deformation of diamond-like carbon. <i>Journal of Non-Crystalline Solids</i> , 2022, 577, 121318.	1.5	6
2533	High-Temperature Wear Mechanism of Diamond at the Nanoscale: A Reactive Molecular Dynamics Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2534	Precursor formation and crystal nucleation in stretched polyethylene/carbon nanotube nanocomposites. <i>Polymer</i> , 2022, 239, 124438.	1.8	8
2535	Ultralow friction of graphene-coated silica nanoparticle film. <i>Computational Materials Science</i> , 2022, 204, 111184.	1.4	3
2536	Rectilinear motion of carbon nanotube on gold surface. <i>International Journal of Mechanical Sciences</i> , 2022, 217, 107026.	3.6	13
2537	The Cohesive Energy and Vibration Characteristics of Parallel Single-Walled Carbon Nanotubes. <i>Molecules</i> , 2021, 26, 7470.	1.7	1
2538	Accelerating the prediction of large carbon clusters via structure search: Evaluation of machine-learning and classical potentials. <i>Carbon</i> , 2022, 191, 255-266.	5.4	11
2539	Collision of nanoparticles of covalently bound atoms: Impact of stress-dependent adhesion. <i>Physical Review E</i> , 2022, 105, 014607.	0.8	3
2540	Theoretical study of anisotropy and ultra-low thermal conductance of porous graphene nanoribbons. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, 71, 027803.	0.2	3

#	ARTICLE	IF	CITATIONS
2541	Simulation of a Patterned Core-Shell Double-Walled Carbon Nanotube with an Optimal Heat Capacity as Efficient Thermal Conductivity Modules. <i>ACS Applied Nano Materials</i> , 2022, 5, 1542-1552.	2.4	1
2542	Internal energy and temperature of a carbon nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 0, , 1-5.	1.0	0
2543	Chiral valley phonons and flat phonon bands in moiré materials. <i>Physical Review B</i> , 2022, 105, .	1.1	10
2544	Deformation mechanism of copper reinforced by three-dimensional graphene under torsion and tension. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2022, 30, 025004.	0.8	3
2545	Experimental and theoretical characterization of the interfacial adhesion of 2D heterogeneous materials: A review. <i>Journal of Micromechanics and Molecular Physics</i> , 2021, 06, 31-48.	0.7	4
2546	Superior performance of the machine-learning GAP force field for fullerene structures. <i>Structural Chemistry</i> , 2022, 33, 505-510.	1.0	5
2547	A Laboratory-driven Multiscale Investigation of X-Ray Induced Mass Loss and Photochemical Evolution in Cosmic Carbon and Silicate Dust. <i>Astrophysical Journal</i> , 2022, 925, 86.	1.6	2
2548	Applications of machine learning in computational nanotechnology. <i>Nanotechnology</i> , 2022, 33, 162501.	1.3	3
2549	Effects of elasticity and dislocation core structure on the interaction of dislocations with embedded CNTs in aluminium: An atomistic simulation study. <i>Materialia</i> , 2022, 21, 101347.	1.3	7
2550	Defect formation and bending properties in graphite under He atom implantation investigated by molecular dynamics method. <i>Carbon</i> , 2022, 191, 350-361.	5.4	2
2551	Chirality-Dependent Mechanical Properties of Bundles and Thin Films Composed of Covalently Cross-Linked Carbon Nanotubes. <i>Langmuir</i> , 2022, 38, 1977-1994.	1.6	10
2552	Dynamic aspects of graphene deformation and fracture from approximate density functional theory. <i>Carbon</i> , 2022, 190, 183-193.	5.4	8
2553	Correlation between the energetic and thermal properties of C40 fullerene isomers: An accurate machine-learning force field study. <i>Micro and Nano Engineering</i> , 2022, 14, 100105.	1.4	5
2554	Effective acetylene length dependence of the elastic properties of different kinds of graphynes. <i>Carbon Trends</i> , 2022, 7, 100152.	1.4	4
2555	Potential energy functions. , 2022, , 41-65.		0
2556	Methods for Measuring Thermal Conductivity of Two-Dimensional Materials: A Review. <i>Nanomaterials</i> , 2022, 12, 589.	1.9	7
2557	How Gas-Solid Interaction Matters in Graphene-Doped Silica Aerogels. <i>Langmuir</i> , 2022, 38, 2238-2247.	1.6	8
2558	Molecular dynamics study of silicon atomic layer etching by chlorine gas and argon ions. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2022, 40, .	0.6	10

#	ARTICLE	IF	CITATIONS
2559	Large-scale simulation of graphene and structural superlubricity with improved smoothed molecular dynamics method. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2022, 392, 114644.	3.4	4
2561	Electron Transport in Model Quasi-Two-Dimensional van der Waals Nanodevices. <i>Technical Physics Letters</i> , 2021, 47, 417-420.	0.2	2
2564	Thermal Properties of Carbon Nanothreads. <i>Materials Horizons</i> , 2022, , 157-193.	0.3	0
2565	Capillary Infiltration of Liquid Silicon in Carbon Nanotubes: A Molecular Dynamics Simulation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2566	Molecular Forcefield Methods for Describing Energetic Molecular Crystals: A Review. <i>Molecules</i> , 2022, 27, 1611.	1.7	9
2567	Flexible actuator by electric bending of saline solution-filled carbon nanotubes. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 215301.	1.3	1
2568	Dynamic pull-in instability of multilayer graphene NEMSs: non-classical continuum model and molecular dynamics simulations. <i>Acta Mechanica</i> , 2022, 233, 991-1018.	1.1	2
2569	Simultaneous stiffening and strengthening of nanodiamond by fivefold twins. <i>MRS Bulletin</i> , 2022, 47, 219-230.	1.7	5
2570	Mechanical Properties and Buckling of Kagome Graphene under Tension: A Molecular Dynamics Study. <i>Crystals</i> , 2022, 12, 292.	1.0	2
2571	Why Carbon Nanotubes Grow. <i>Journal of the American Chemical Society</i> , 2022, 144, 5606-5613.	6.6	27
2572	Breakdown of semiclassical description of thermoelectricity in near-magic angle twisted bilayer graphene. <i>Nature Communications</i> , 2022, 13, 1522.	5.8	12
2573	A Review on Mechanical Properties of Deformation Mechanism of Tubular Nanostructures: Molecular Dynamics Simulations. <i>Solid State Phenomena</i> , 0, 329, 79-86.	0.3	1
2574	Accurate tight-binding model for twisted bilayer graphene describes topological flat bands without geometric relaxation. <i>Physical Review B</i> , 2022, 105, .	1.1	9
2575	Molecular Simulations to Elucidate Transport Phenomena in Polymeric Membranes. <i>Environmental Science & Technology</i> , 2022, 56, 3313-3323.	4.6	25
2576	Atomistic understanding of the anisotropic tensile response and zero-stiffness of carbon honeycomb nanostructure. <i>Molecular Simulation</i> , 2022, 48, 965-975.	0.9	1
2577	Effect of hydrogenation of carbon atom on its deposition on graphene. <i>Letters on Materials</i> , 2022, 12, 27-31.	0.2	0
2578	Accessing negative Poisson's ratio of graphene by machine learning interatomic potentials. <i>Nanotechnology</i> , 2022, 33, 275710.	1.3	3
2579	Interfacial thermal transport between graphene and diamane. <i>Journal of Chemical Physics</i> , 2022, 156, 164703.	1.2	5

#	ARTICLE	IF	CITATIONS
2581	Atomistic Study on the Sintering Process and the Strengthening Mechanism of Al-Graphene System. <i>Materials</i> , 2022, 15, 2644.	1.3	5
2582	Molecular arrangement and fringe identification and analysis from molecular dynamics (MAFIA-MD): A tool for analyzing the molecular structures formed during reactive molecular dynamics simulation of hydrocarbons. <i>Computer Physics Communications</i> , 2022, 276, 108325.	3.0	2
2583	Graphene-Based Scaffolds: Fundamentals and Applications for Cardiovascular Tissue Engineering. <i>Frontiers in Bioengineering and Biotechnology</i> , 2021, 9, 797340.	2.0	21
2584	Mechanical behavior of single-layer graphdiyne via supersonic micro-projectile impact. <i>Nano Materials Science</i> , 2022, 4, 383-392.	3.9	4
2585	Modeling of electrotransport properties of Li-intercalated graphene film. <i>Journal of Physics: Conference Series</i> , 2021, 2140, 012025.	0.3	0
2586	Temperature-dependent thermal transport of single molecular junctions from semiclassical Langevin molecular dynamics. <i>Physical Review B</i> , 2021, 104, .	1.1	8
2587	The effect of graphene size and arrangement on crack propagation of Graphene/Aluminum composites. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, .	0.2	0
2588	The design of strongly bonded nanoarchitected carbon materials for high specific strength and modulus. <i>Carbon</i> , 2022, 195, 387-394.	5.4	5
2589	Radiative relaxation in isolated large carbon clusters: Vibrational emission versus recurrent fluorescence. <i>Journal of Chemical Physics</i> , 2022, 156, 144305.	1.2	11
2590	Interlayer Friction in Graphene/MoS ₂ , Graphene/NbSe ₂ , Tellurene/MoS ₂ and Tellurene/NbSe ₂ van der Waals Heterostructures. <i>Frontiers in Mechanical Engineering</i> , 2022, 8, .	0.8	2
2591	Molecular Dynamics Simulation on Wetting of Silver Nanosolder on a Diamond Surface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 7221-7229.	1.5	1
2592	An atomistic approach for the structural and electronic properties of twisted bilayer graphene-boron nitride heterostructures. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	22
2593	Investigation of structure and dynamics of water confined between hybrid layered materials of graphene, boron nitride, and molybdenum disulfide. <i>Journal of Materials Science</i> , 2022, 57, 10517-10534.	1.7	4
2594	High strain-rate effect on microstructure evolution and plasticity of aluminum 5052 alloy nano-multilayer: A molecular dynamics study. <i>Vacuum</i> , 2022, 201, 111104.	1.6	13
2601	Continuum and Atomic-Scale Modeling of Self-Positioning Microstructures and Nanostructures. <i>Computational Science, Engineering and Technology Series</i> , 0, , 271-294.	0.2	0
2603	Domino-like stacking order switching in twisted monolayer–multilayer graphene. <i>Nature Materials</i> , 2022, 21, 621-626.	13.3	28
2604	Microscopic Insight into Water Desalination through Nanoporous Graphene: The Influence of the Dipole Moment. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4029-4035.	2.1	6
2605	Dynamic penetration behaviors of single/multi-layer graphene using nanoparticle under hypervelocity impact. <i>Scientific Reports</i> , 2022, 12, 7440.	1.6	5

#	ARTICLE	IF	CITATIONS
2606	Competition between Sliding and Peeling of Graphene Nanoribbons under Horizontal Drag. <i>Materials</i> , 2022, 15, 3284.	1.3	0
2607	Exotic carbon microcrystals in meteoritic dust of the Chelyabinsk superbolide: experimental investigations and theoretical scenarios of their formation. <i>European Physical Journal Plus</i> , 2022, 137, .	1.2	3
2608	Catalytic Growth of Ultralong Graphene Nanoribbons on Insulating Substrates. <i>Advanced Materials</i> , 2022, 34, e2200956.	11.1	12
2610	Combining Experimental and Theoretical Techniques to Gain an Atomic Level Understanding of the Defect Binding Mechanism in Hard Carbon Anodes for Sodium Ion Batteries. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	38
2611	Tuning lattice thermal conductivity of bilayer and trilayer molybdenum disulfide thermoelectric materials through twist angles. <i>International Journal of Heat and Mass Transfer</i> , 2022, 194, 123005.	2.5	10
2612	Development of Chemical Kinetics Models from Atomistic Reactive Molecular Dynamics Simulations: Application to Iso-octane Combustion and Rubber Ablative Degradation. <i>Journal of Physical Chemistry A</i> , 2022, , .	1.1	2
2613	Anomalous layer-dependent lubrication on graphene-covered substrate: Competition between adhesion and plasticity. <i>Applied Surface Science</i> , 2022, 598, 153762.	3.1	6
2616	A discrete-continuum mosaic model for the buckling of inner tubes of double-walled carbon nanotubes under compression. <i>Mechanics of Materials</i> , 2022, 172, 104384.	1.7	0
2617	Effect of expanded graphite on the thermal conductivity of sodium sulfate decahydrate (Na ₂ SO ₄ ·10H ₂ O) phase change composites. <i>Journal of Energy Storage</i> , 2022, 52, 104949.	3.9	8
2621	Lattice relaxation and substrate effects on the electronic properties of graphene superlattice. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, .	0.2	0
2622	Adsorption of hydrogen isotopes on graphene. <i>Nuclear Engineering and Technology</i> , 2022, , .	1.1	0
2623	The Origin of Moiré Level Stick-Slip Behavior on Graphene/h-BN Heterostructures. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	20
2624	Development of potentials for molecular dynamics simulations of dry and hydrated calcium aluminosilicate glasses by force matching and refinement. <i>Journal of Non-Crystalline Solids</i> , 2022, 592, 121746.	1.5	4
2625	Spin-thermoelectric properties and giant tunneling magnetoresistance of boron-substituted graphene nanoribbon: a first principle study. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 345802.	0.7	2
2626	A continuum-discrete multiscale coupling method for pristine and defected single-walled carbon nanotubes. <i>Applied Mathematical Modelling</i> , 2022, 111, 176-200.	2.2	1
2627	Shock wave propagation in carbon honeycomb nanostructure and effect of cell vacancies. <i>Carbon Trends</i> , 2022, 8, 100186.	1.4	1
2628	Feature size coupling effect of nanolaminated graphene/copper composites. <i>International Journal of Mechanical Sciences</i> , 2022, 227, 107469.	3.6	6
2629	The influence of strain range, size and chiral on mechanical properties of graphene: Molecular dynamics insights. <i>Nanomaterials and Nanotechnology</i> , 2022, 12, 184798042211100.	1.2	1

#	ARTICLE	IF	CITATIONS
2630	Controlled Growth of Large-Area Monolayer Graphene on Ni (110) Facet: Insight from Molecular Dynamics Simulation. SSRN Electronic Journal, 0, , .	0.4	0
2631	Polarization-Dependent Selection Rules and Optical Spectrum Atlas of Twisted Bilayer Graphene Quantum Dots. Physical Review X, 2022, 12, .	2.8	8
2632	Mechanical Properties of Cubene Crystals. Materials, 2022, 15, 4871.	1.3	4
2633	Molecular dynamics study of phonon thermal transport in borophene with random vacancy defects. Modelling and Simulation in Materials Science and Engineering, 0, , .	0.8	0
2634	Discovery of Grapheneâ€Water Membrane Structure: Toward Highâ€Quality Graphene Process. Advanced Science, 2022, 9, .	5.6	6
2635	Mechanisms of elastic softening in highly anisotropic carbons under in-plane compression/indentation. Carbon, 2022, 197, 425-434.	5.4	5
2636	Non-symmetric stiffness of origami-graphene metamaterial plates. Composite Structures, 2022, 297, 115974.	3.1	13
2637	Hydrogenated Graphene with Tunable Poissonâ€™s Ratio Using Machine Learning: Implication for Wearable Devices and Strain Sensors. ACS Applied Nano Materials, 2022, 5, 10617-10627.	2.4	5
2638	Buckling of graphene under compressive strain: DFT calculations and second generation REBO potential. Extreme Mechanics Letters, 2022, 56, 101845.	2.0	2
2639	Highâ€Throughput Generation of 3D Graphene Metamaterials and Property Quantification Using Machine Learning. Small Methods, 2022, 6, .	4.6	12
2640	Diameter-Change-Induced Transition in Buckling Modes of Defective Zigzag Carbon Nanotubes. Nanomaterials, 2022, 12, 2617.	1.9	2
2641	Gas permeation through nanoporous single-walled carbon nanotubes: the confinement effect. Nanotechnology, 2022, 33, 455704.	1.3	0
2642	Molecular Dynamics Simulation of Coiled Carbon Nanotube Pull-Out from Matrix. International Journal of Molecular Sciences, 2022, 23, 9254.	1.8	2
2643	Machine Learning Methods for Multiscale Physics and Urban Engineering Problems. Entropy, 2022, 24, 1134.	1.1	0
2644	Comprehensive theoretical study of the correlation between the energetic and thermal stabilities for the entire set of 1812 C ₆₀ isomers. Journal of Applied Physics, 2022, 132, 064302.	1.1	1
2645	JAX-ReaxFF: A Gradient-Based Framework for Fast Optimization of Reactive Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 5181-5194.	2.3	8
2646	Electronic structure of lattice relaxed alternating twist tNG-multilayer graphene: from few layers to bulk AT-graphite. 2D Materials, 2022, 9, 044002.	2.0	5
2647	Strength and fracture behaviors of ultralong carbon nanotubes with defects. Carbon, 2022, 199, 300-317.	5.4	5

#	ARTICLE	IF	CITATIONS
2648	Controlled growth of large-area monolayer graphene on Ni (110) facet: Insight from molecular dynamics simulation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 144, 115465.	1.3	5
2649	Anomalous water transport in narrow-diameter carbon nanotubes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	4
2650	Atomistic Simulations of Temperature-Induced Switchable Morphology in Graphene Nanodrum. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2651	Tersoff and REBO Potentials. <i>Lecture Notes in Applied and Computational Mechanics</i> , 2022, , 187-203.	2.0	0
2652	Introduction to Interatomic Potentials/Forcefields. <i>Lecture Notes in Applied and Computational Mechanics</i> , 2022, , 21-49.	2.0	18
2653	Data-Driven Phase Selection, Property Prediction and Force-Field Development in Multi-Principal Element Alloys. <i>Lecture Notes in Applied and Computational Mechanics</i> , 2022, , 315-347.	2.0	4
2654	Evaluating the performance of ReaxFF potentials for sp ² carbon systems (graphene, carbon nanotubes,) Tj ETQq0 0 0 rgBT /Overlock 10	1.8	8
2655	Relaxation effects in twisted bilayer graphene: A multiscale approach. <i>Physical Review B</i> , 2022, 106, .	1.1	14
2656	From skeptic to believer: The power of models. <i>Tetrahedron</i> , 2022, 123, 132984.	1.0	1
2657	Atomistic simulations of $\langle 110 \rangle [111]$ grain boundary in diamond: Structure, stability, and properties. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	2
2658	Study on the Shear Behaviour and Fracture Characteristic of Graphene Kirigami Membranes via Molecular Dynamics Simulation. <i>Membranes</i> , 2022, 12, 886.	1.4	3
2659	Acceleration of hollow carbon nanospheres by gas leakage: An efficient nanomotor. <i>AIP Advances</i> , 2022, 12, 095204.	0.6	0
2660	Microscopic deformation and failure modes of high-functionality epoxy resins from bond breaking molecular dynamics simulations and experimental investigation. <i>Polymer Engineering and Science</i> , 2022, 62, 3952-3963.	1.5	3
2661	Linking atomic structural defects to mesoscale properties in crystalline solids using graph neural networks. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	15
2662	Thermal Stability and Melting Mechanism of Diamond Nanothreads: Insight from Molecular Dynamics Simulation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, , 130248.	2.3	0
2663	Finite-temperature stability of hydrocarbons: fullerenes versus flakes. <i>Journal of Chemical Physics</i> , 0, , .	1.2	3
2664	Thermal conductivity of the popgraphene monolayer tailored by strain and defect: A molecular dynamics study. <i>Diamond and Related Materials</i> , 2022, 130, 109409.	1.8	2
2665	Interatomic potentials: achievements and challenges. <i>Advances in Physics: X</i> , 2023, 8, .	1.5	11

#	ARTICLE	IF	CITATIONS
2666	High performance of carbon nanotube elastocaloric refrigerators over a large temperature span. <i>Physical Review B</i> , 2022, 106, .	1.1	5
2667	A Continuum Model for Circular Graphene Membranes Under Uniform Lateral Pressure. <i>Journal of Elasticity</i> , 2022, 151, 273-303.	0.9	3
2668	Low-energy moiré phonons in twisted bilayer van der Waals heterostructures. <i>Physical Review B</i> , 2022, 106, .	1.1	5
2669	Understanding the size and chirality dependence of bending stiffness of single-layer MoS_2 by a spring-driven method. <i>Physical Review B</i> , 2022, 106, .	1.1	5
2670	Thermal Conductance of Copper-Graphene Interface: A Molecular Simulation. <i>Materials</i> , 2022, 15, 7588.	1.3	3
2671	Molecular dynamics study on the thermal conductivity of a single polyethylene chain: Strain dependence and potential models' effect. <i>AIP Advances</i> , 2022, 12, 105223.	0.6	1
2672	From Cyclo[18]carbon to the Novel Nanostructures—Theoretical Predictions. <i>International Journal of Molecular Sciences</i> , 2022, 23, 12960.	1.8	2
2673	Bilayer Graphene Kirigami. <i>Carbon Trends</i> , 2022, , 100227.	1.4	0
2674	Modification of a force field for molecular dynamics simulations of silicon etching by chlorine atoms. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2022, 40, .	0.9	6
2675	Molecular dynamics study of the robust superlubricity in penta-graphene van der Waals layered structures. <i>Tribology International</i> , 2023, 177, 107988.	3.0	10
2676	Predicting char yield of high-temperature resins. <i>Carbon</i> , 2023, 202, 336-347.	5.4	5
2677	Controlling the Thermal Conductivity of Monolayer Graphene with Kirigami Structure. <i>Membranes</i> , 2022, 12, 1128.	1.4	0
2678	Simulated Pressure-temperature Carbon Structure Map obtained through uniaxial compression of Bulk C60. <i>Carbon</i> , 2023, 202, 554-560.	5.4	3
2679	Graphyne-type nano-metamaterials: A comprehensive molecular dynamics simulation. <i>Diamond and Related Materials</i> , 2023, 131, 109572.	1.8	2
2680	A ReaxFF molecular dynamics study of polycyclic aromatic hydrocarbon oxidation assisted by nitrogen oxides. <i>Combustion and Flame</i> , 2023, 248, 112571.	2.8	7
2681	Molecular dynamics of electric-field driven ionic systems using a universal neural-network potential. <i>Computational Materials Science</i> , 2023, 218, 111955.	1.4	2
2682	Capillary infiltration of liquid silicon in carbon nanotubes: A molecular dynamics simulation. <i>Journal of Materials Science and Technology</i> , 2023, 144, 219-223.	5.6	1
2683	Molecular dynamics studies on mechanical properties of graphene/nanotwinned aluminum matrix composites. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 147, 115597.	1.3	4

#	ARTICLE	IF	CITATIONS
2684	Voltage generation induced by thermo-driven ion solution flow in CNTs for low-grade thermal energy harvesting. <i>International Journal of Heat and Mass Transfer</i> , 2023, 202, 123751.	2.5	1
2685	One Dimensional Twisted Van der Waals Structures Constructed by Self-Assembling Graphene Nanoribbons on Carbon Nanotubes. <i>Materials</i> , 2022, 15, 8220.	1.3	4
2686	Machine learning interatomic potential for simulations of carbon at extreme conditions. <i>Physical Review B</i> , 2022, 106, .	1.1	16
2687	Chirality-Dependent and Intrinsic Auxeticity for Single-Walled Carbon Nanotubes. <i>Materials</i> , 2022, 15, 8720.	1.3	3
2688	Schwarz P^2 surface via isolated C_2 carbon heptagons: Design and properties. <i>Journal of Computational Chemistry</i> , 2023, 44, 954-961.	1.5	1
2689	Adsorption, Diffusion, and Transport of C_1 to C_3 Alkanes and Carbon Dioxide in Dual-Porosity Kerogens: Insights from Molecular Simulations. <i>Energy & Fuels</i> , 2023, 37, 492-508.	2.5	5
2690	Metal/Graphene Composites: A Review on the Simulation of Fabrication and Study of Mechanical Properties. <i>Materials</i> , 2023, 16, 202.	1.3	5
2691	ReaxFF-based nonadiabatic dynamics method for azobenzene derivatives. <i>Journal of Chemical Physics</i> , 2022, 157, 244101.	1.2	0
2692	Yukawa-Friedel-tail pair potentials for warm dense matter applications. <i>Physical Review E</i> , 2022, 106, .	0.8	4
2693	Accurate estimation of dynamical quantities for nonequilibrium nanoscale systems. <i>Physical Review E</i> , 2023, 107, .	0.8	1
2694	Effect of Interatomic Potential on Simulation of Fracture Behavior of Cu/Graphene Composite: A Molecular Dynamics Study. <i>Applied Sciences (Switzerland)</i> , 2023, 13, 916.	1.3	5
2695	Multiscale Theories and Applications: From Microstructure Design to Macroscopic Assessment for Carbon Nanotubes Networks. <i>Chinese Journal of Mechanical Engineering (English Edition)</i> , 2023, 36, .	1.9	4
2696	Stick-Slip Dynamics of Moiré Superstructures in Polycrystalline 2D Material Interfaces. <i>Physical Review Letters</i> , 2022, 129, .	2.9	3
2697	Molecular dynamics simulations of reactive neutral chemistry in an argon-methane plasma. <i>Plasma Processes and Polymers</i> , 2023, 20, .	1.6	3
2698	Mechanical Properties of Twisted Carbon Nanotube Bundles with Carbon Linkers from Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2473.	1.8	4
2699	Study on molecular dynamics simulation of graphene deposition and growth on WC-Co cemented carbides. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2023, .	0.2	0
2700	Raman spectroscopy and molecular dynamics simulation studies of graphitic nanomaterials. , 2023, , 363-399.		1
2701	Commensurate and incommensurate double moiré interference in twisted trilayer graphene. <i>Physical Review B</i> , 2023, 107, .	1.1	5

#	ARTICLE	IF	CITATIONS
2702	Modeling phonons in nanomaterials. , 2023, , 125-149.		0
2703	Multiwall Carbon Nanotubes for Solid Lubrication of Highly Loaded Contacts. ACS Applied Nano Materials, 2023, 6, 1755-1769.	2.4	3
2704	Atomistic Investigation on the Blocking Phenomenon of Crack Propagation in Cu Substrate Reinforced by CNT. Nanomaterials, 2023, 13, 575.	1.9	3
2705	A Review of the Mechanical Properties of Graphene Aerogel Materials: Experimental Measurements and Computer Simulations. Materials, 2023, 16, 1800.	1.3	3
2706	Fast proper orthogonal descriptors for many-body interatomic potentials. Physical Review B, 2023, 107, .	1.1	1
2707	Proper orthogonal descriptors for efficient and accurate interatomic potentials. Journal of Computational Physics, 2023, 480, 112030.	1.9	5
2708	Investigation of the heat transport in intersected graphene. International Journal of Heat and Mass Transfer, 2023, 209, 124162.	2.5	2
2709	Determine the Complete Configuration of Single-Walled Carbon Nanotubes by One Photograph of Transmission Electron Microscopy. Advanced Science, 0, , .	5.6	1
2710	Twisting Dynamics of Large Lattice-Mismatch van der Waals Heterostructures. ACS Applied Materials & Interfaces, 2023, 15, 19616-19623.	4.0	2
2712	Nanocutting mechanisms of Cu ₅₀ Zr ₅₀ amorphous alloy: A molecular dynamics simulation. Journal of Non-Crystalline Solids, 2023, 605, 122161.	1.5	3
2713	Superlubricity transition from ball bearing to nanocoating in the third-body lubrication. Tribology International, 2023, 181, 108320.	3.0	1
2714	Effects of interfacial molecular mobility on thermal boundary conductance at solid-liquid interface. Journal of Chemical Physics, 2023, 158, .	1.2	1
2715	Machine learning based modeling of disordered elemental semiconductors: understanding the atomic structure of a-Si and a-C. Semiconductor Science and Technology, 2023, 38, 043001.	1.0	1
2716	Nanoscale crack propagation in clay with water adsorption through reactive MD modeling. International Journal for Numerical and Analytical Methods in Geomechanics, 2023, 47, 1103-1133.	1.7	1
2717	Theoretical study on uniaxial compressive mechanical properties of three-dimensional graphene. International Journal of Mechanical Sciences, 2023, 249, 108250.	3.6	4
2718	Density dependence of elastic properties of graphynes. MRS Advances, 0, , .	0.5	0
2719	In silico approaches for aerogel. , 2023, , 399-477.		0
2720	Evolution of the Microstructure, Hybridization, and Internal Stress of Al-Doped Diamond-Like Carbon Coatings: A Molecular Dynamics Simulation. Langmuir, 2023, 39, 3895-3904.	1.6	3

#	ARTICLE	IF	CITATIONS
2721	Heterostrain and temperature-tuned twist between graphene/h-BN bilayers. <i>Scientific Reports</i> , 2023, 13, .	1.6	6
2722	Electronic properties of twisted bilayer graphene suspended and encapsulated with hexagonal boron nitride. <i>Physical Review B</i> , 2023, 107, .	1.1	3
2723	Fully atomistic molecular dynamics investigation of the simplest model of dry-draw fabrication of carbon nanotube fibers. <i>MRS Advances</i> , 0, , .	0.5	0
2724	Effect of Temperatures and Graphene on the Mechanical Properties of the Aluminum Matrix: A Molecular Dynamics Study. <i>Materials</i> , 2023, 16, 2722.	1.3	3
2725	Theoretical study of entropy-induced friction in graphene. <i>Thin-Walled Structures</i> , 2023, 186, 110724.	2.7	1
2726	Artificial Neural Network Potentials for Mechanics and Fracture Dynamics of Two-Dimensional Crystals. <i>Machine Learning: Science and Technology</i> , 0, , .	2.4	0
2727	Review on Molecular Dynamics Simulations of Effects of Carbon Nanotubes (CNTs) on Electrical and Thermal Conductivities of CNT-Modified Polymeric Composites. <i>Journal of Composites Science</i> , 2023, 7, 165.	1.4	15
2728	Recent advances in the mechanics of 2D materials. <i>International Journal of Extreme Manufacturing</i> , 2023, 5, 032002.	6.3	9
2729	Thermal Conductivity of a Two-Dimensional Diamondene Sheet: A Molecular Study. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	0
2768	Graphene Network with Ni and Al Nanoparticles as the Composite Precursor: Atomistic Simulation. , 2023, , .		0
2769	Multiscale mechanics and molecular dynamics simulations of the durability of fiber-reinforced polymer composites. <i>Communications Materials</i> , 2023, 4, .	2.9	3
2772	Modeling the Structural, Fractal and Mechanical Properties of Aerogels. <i>Springer Handbooks</i> , 2023, , 289-305.	0.3	1
2781	Machine Learning Interatomic Potentials: Keys to First-Principles Multiscale Modeling. <i>Computational Methods in Engineering & the Sciences</i> , 2023, , 427-451.	0.3	0
2783	Continuum Mechanics Applied for Studying Instabilities in Nanoparticles. <i>Advanced Structured Materials</i> , 2023, , 429-456.	0.3	0
2793	A Peridynamic Micro-Scale Model for Predicting Mechanical Properties of Graphene. <i>Mechanisms and Machine Science</i> , 2024, , 1-10.	0.3	0
2807	Practical classical molecular dynamics simulations for low-temperature plasma processing: a review. <i>Reviews of Modern Plasma Physics</i> , 2024, 8, .	2.2	0