Qing Peng

List of Publications by Year in Descending Order

226 papers	4,240 citations	32 h-index	55 g-index
245 ext. papers	5,369 ext. citations	4.7 avg, IF	6.06 L-index

#	Paper	IF	Citations
226	Atomistic insights of a chemical complexity effect on the irradiation resistance of high entropy alloys. *Materials Advances*, **2022**, 3, 1680-1686	3.3	1
225	Processing and machining mechanism of ultrasonic vibration-assisted grinding on sapphire. *Materials Science in Semiconductor Processing*, **2022**, 142, 106470	4.3	1
224	A Molecular Dynamics Study of the Stability and Mechanical Properties of a Nano-Engineered Fuzzy Carbon Fiber Composite. *Journal of Composites Science*, **2022**, 6, 54	3	
223	Ab initio investigation of properties and mobility of helium defects in La2Sn2O7 pyrochlore. *Nuclear Materials and Energy*, **2022**, 30, 101135	2.1	
222	Abnormal radiation resistance via direct-amorphization-induced defect recovery in HgTe. *Applied Physics Letters*, **2022**, 120, 012101	3.4	
221	The preexisting edge dislocations as recombination center of point defects enhancing irradiation tolerance in CoCrCuFeNi high entropy alloy. *Materialia*, **2022**, 21, 101307	3.2	0
220	Tensile mechanical properties of CoCrFeNiTiAl high entropy alloy via molecular dynamics simulations. *Intermetallics*, **2022**, 142, 107444	3.5	2
219	Hydrostatic pressure-tuning of thermoelectric properties of CsSnI3 perovskite by first-principles calculations. *Computational Materials Science*, **2022**, 201, 110917	3.2	1
218	The effect of Sr doping on the structural, mechanical, electronic properties and radiation tolerance of MgAl2O4 spinel: A first-principles study. *Journal of Alloys and Compounds*, **2022**, 889, 161614	5.7	
217	Evaluation of the inhibition performance of piperazine-based polyurea towards mild steel corrosion: The role of keto-enol tautomerization. *Journal of Molecular Structure*, **2022**, 1248, 131485	3.4	2
216	Mechanical Properties and Buckling of Kagome Graphene under Tension: A Molecular Dynamics Study. *Crystals*, **2022**, 12, 292	2.3	1
215	Hybridization-driven strong anharmonicity in Yb-filled skutterudites. *Physical Review B*, **2022**, 105,	3.3	1
214	Pressure-Induced Amorphization and Crystallization of Heterophase Pd Nanostructures.. *Small*, **2022**, e2106396	11	0
213	A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery.. *Nanomaterials*, **2022**, 12,	5.4	1
212	Distinct point defect behaviours in body-centered cubic medium-entropy alloy NbZrTi induced by severe lattice distortion. *Acta Materialia*, **2022**, 229, 117806	8.4	2
211	Coupling of double grains enforces the grinding process in vibration-assisted scratch: Insights from molecular dynamics. *Journal of Materials Processing Technology*, **2022**, 304, 117551	5.3	2
210	Effect of low-frequency optical phonons on the thermal conductivity of 2H molybdenum disulfide. *Physical Review B*, **2022**, 105,	3.3	1

209	C2 weakens the turnover frequency during the melting of FexCy: insights from reactive MD simulations. *New Journal of Chemistry*, **2021**, 46, 282-293	3.6	
208	The Crack Angle of 60° Is the Most Vulnerable Crack Front in Graphene According to MD Simulations. *Crystals*, **2021**, 11, 1355	2.3	3
207	Assembly of Silicalite-1 Crystals Like Toy Lego Bricks into One-, Two-, and Three-Dimensional Architectures for Enhancing Its Adsorptive Separation and Catalytic Performances. *ACS Applied Materials & Interfaces*, **2021**, 13, 58085-58095	9.5	3
206	Fabrication and application of 2,4,6-trinitrophenol sensors based on fluorescent functional materials.. *Journal of Hazardous Materials*, **2021**, 425, 127987	12.8	4
205	Quantifying the photocatalytic role and activity at the edge and surface of Pd co-catalysts using N2 fixation as a case. *Journal of Materials Chemistry A*, **2021**, 9, 26036-26044	13	1
204	A combined DFTB nanoreactor and reaction network generator approach for the mechanism of hydrocarbon combustion. *Chemical Communications*, **2021**, 57, 11633-11636	5.8	2
203	Atomic Insights into Fracture Characteristics of Twisted Tri-Layer Graphene. *Crystals*, **2021**, 11, 1202	2.3	4
202	Ambient-environment processed perovskite solar cells: A review. *Materials Today Physics*, **2021**, 21, 100557	8	1
201	Artificial intelligence: A powerful paradigm for scientific research. *Innovation(China)*, **2021**, 2, 100179	17.8	21
200	The role of ligands in pressure-induced phase transition of gold nanoribbons. *Phase Transitions*, **2021**, 94, 123-133	1.3	0
199	Defect, temperature, and strain effects on lattice heat conductivity of egg-tray graphene. *Modelling and Simulation in Materials Science and Engineering*, **2021**, 29, 045003	2	2
198	Impact of Polypyrrole Functionalization on the Anodic Performance of Boron Nitride Nanosheets: Insights From First-Principles Calculations. *Frontiers in Chemistry*, **2021**, 9, 670833	5	5
197	Enhanced self-healing of irradiation defects near a Ni graphene interface by damaged graphene: Insights from atomistic modeling. *Journal of Physics and Chemistry of Solids*, **2021**, 151, 109909	3.9	2
196	Effect of interfacial bonding on dislocation strengthening in graphene nanosheet reinforced iron composite: A molecular dynamics study. *Computational Materials Science*, **2021**, 191, 110309	3.2	3
195	CNT-sandwiched copper composites as super thermal conductors for heat management. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 128, 114557	3	6
194	Fragility under shocking: molecular dynamics insights into defect evolutions in tungsten lattice. *Tungsten*, **2021**, 3, 234-242	4.6	4
193	Molecular dynamics simulations of scratching characteristics in vibration-assisted nano-scratch of single-crystal silicon. *Applied Surface Science*, **2021**, 551, 149451	6.7	7
192	Ab Initio Investigation of Helium Mobility in La2Zr2O7 Pyrochlore. *Crystals*, **2021**, 11, 667	2.3	1

191	Surface strengthening of stainless steels by nondestructive laser peening. *Materials and Design*, **2021**, 205, 109754	8.1	5
190	Reduced Plastic Dilatancy in Polymer Glasses. *Macromolecular Theory and Simulations*, **2021**, 30, 2000063	1.5	1
189	Theoretical exploration of the interaction between hydrogen and pyrite-type FeS2 surfaces. *Applied Surface Science*, **2021**, 537, 147900	6.7	2
188	Mesoporous RhRu Nanosponges with Enhanced Water Dissociation toward Efficient Alkaline Hydrogen Evolution. *ACS Applied Materials & Interfaces*, **2021**, 13, 5052-5060	9.5	11
187	Performance of SCAN Meta-GGA Functionals on Nonlinear Mechanics of Graphene-Like g-SiC. *Crystals*, **2021**, 11, 120	2.3	
186	Mapping surface morphology and phase evolution of iron sulfide nanoparticles. *CrystEngComm*, **2021**, 23, 5645-5654	3.3	1
185	Ultrahigh Ballistic Resistance of Twisted Bilayer Graphene. *Crystals*, **2021**, 11, 206	2.3	5
184	Theoretical Perspectives on the Modulation of Carbon on Transition-Metal Catalysts for Conversion of Carbon-Containing Resources. *ACS Catalysis*, **2021**, 11, 2156-2181	13.1	9
183	Carbon Deposition and Permeation on Nickel Surfaces in Operando Conditions: A Theoretical Study. *Journal of Physical Chemistry C*, **2021**, 125, 7166-7177	3.8	3
182	Achieve 100% transmission via grafting hydroxyl groups on CNT nanomotors. *Current Applied Physics*, **2021**, 29, 59-65	2.6	0
181	Insights into Coke Formation and Removal under Operating Conditions with a Quantum Nanoreactor Approach. *Journal of Physical Chemistry Letters*, **2021**, 12, 9413-9421	6.4	1
180	The effects of temperature and pressure on the physical properties and stabilities of point defects and defect complexes in B1-ZrC. *Computational Materials Science*, **2021**, 198, 110694	3.2	0
179	Sintering enhances turn-over frequency of nanoparticles: A case study of FexCy catalyst using reactive MD simulations. *Applied Surface Science*, **2021**, 570, 151018	6.7	1
178	The formation energy and interaction energy of point defects in ZrC. *Journal of Nuclear Materials*, **2021**, 557, 153235	3.3	4
177	Nanostructuring enforced sandwich-tubular CNT-Cu interconnects. *Composite Structures*, **2021**, 278, 114705	5.3	
176	Oxygen Adsorption-Induced Morphological Evolution of Hägg Iron Carbide at High Oxygen Chemical Potentials. *Journal of Physical Chemistry C*, **2021**, 125, 3055-3065	3.8	1
175	Machine learning reveals the importance of the formation enthalpy and atom-size difference in forming phases of high entropy alloys. *Materials and Design*, **2020**, 193, 108835	8.1	29
174	Reduction of dislocation, mean free path, and migration barriers using high entropy alloy: insights from the atomistic study of irradiation damage of CoNiCrFeMn. *Nanotechnology*, **2020**, 31, 425701	3.4	3

173	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. *Scripta Materialia*, **2020**, 187, 291-295	5.6	7
172	Adsorption and Diffusion of Hydrogen in Carbon Honeycomb. *Nanomaterials*, **2020**, 10,	5.4	8
171	Electronic effects of transition metal dopants on Fe(100) and Fe5C2(100) surfaces for CO activation. *Catalysis Science and Technology*, **2020**, 10, 2047-2056	5.5	5
170	Relationship between the Behavior of Hydrogen and Hydrogen Bubble Nucleation in Vanadium. *Materials*, **2020**, 13,	3.5	2
169	High impact resistance in graphyne.. *RSC Advances*, **2020**, 10, 1697-1703	3.7	7
168	Surface structure and morphology evolution of iron borides under dynamic conditions: A theoretical study. *Applied Surface Science*, **2020**, 525, 146462	6.7	6
167	High-order nonlinear mechanical properties of g-SiC. *Mechanics of Materials*, **2020**, 148, 103473	3.3	3
166	Suggest a new approach to fabricate AlFe2B2. *Computational Materials Science*, **2020**, 171, 109239	3.2	1
165	Highly Efficient Polarized GeS/MoSe2 van der Waals Heterostructure for Water Splitting from Ultraviolet to Near-Infrared Light. *Physica Status Solidi - Rapid Research Letters*, **2020**, 14, 1900582	2.5	10
164	Analytical bond-order potential for silver, palladium, ruthenium and iodine bulk diffusion in silicon carbide. *Journal of Physics Condensed Matter*, **2020**, 32, 085702	1.8	3
163	A combined experiment and first-principles study on lattice dynamics of thermoelectric CuInTe2. *Journal of Alloys and Compounds*, **2020**, 822, 153610	5.7	9
162	Fivefold enhancement of yield and toughness of copper nanowires via coating carbon nanotubes. *Nanotechnology*, **2020**, 31, 115703	3.4	3
161	Temperature-dependent surface free energy and the Wulff shape of iron and iron carbide nanoparticles: A molecular dynamics study. *Applied Surface Science*, **2020**, 509, 144859	6.7	8
160	Enhancement of toughness of SiC through compositing SiC-Al interpenetrating phase composites. *Nanotechnology*, **2020**, 31, 135706	3.4	5
159	Theoretical exploration of intrinsic facet-dependent CH4 and C2 formation on Fe5C2 particle. *Applied Catalysis B: Environmental*, **2020**, 278, 119308	21.8	13
158	Theoretical Insights into the Structure and Activity of Cobalt Modulated by Surface and Subsurface Carbon in Operando Conditions. *Journal of Physical Chemistry C*, **2020**, 124, 18576-18586	3.8	2
157	The Application of Godunov SPH in the Simulation of Energetic Materials. *International Journal of Computational Methods*, **2020**, 17, 1950028	1.1	1
156	In situ tuning of electronic structure of catalysts using controllable hydrogen spillover for enhanced selectivity. *Nature Communications*, **2020**, 11, 4773	17.4	23

155	Enhanced surface bombardment resistance of the CoNiCrFeMn high entropy alloy under extreme irradiation flux. *Nanotechnology*, **2020**, 31, 025703	3.4	5
154	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. *Computational Materials Science*, **2019**, 170, 109190	3.2	5
153	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers via biaxial straining. *Nanoscale*, **2019**, 11, 2335-2342	7.7	42
152	Atomistic Study of Mechanical Behaviors of Carbon Honeycombs. *Nanomaterials*, **2019**, 9,	5.4	9
151	Mechanical Properties of Vacancy Tuned Carbon Honeycomb. *Nanomaterials*, **2019**, 9,	5.4	12
150	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischer–Tropsch Synthesis. *Catalysis Letters*, **2019**, 149, 645-664	2.8	13
149	Carbon Nanotubes Enhance the Radiation Resistance of bcc Iron Revealed by Atomistic Study. *Materials*, **2019**, 12,	3.5	6
148	Strain Enhanced Visible–Ultraviolet Absorption of Blue Phosphorene/MoX2 (X = S,Se) Heterolayers. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800659	2.5	5
147	Atomic Structure and Mechanical Properties of Twisted Bilayer Graphene. *Journal of Composites Science*, **2019**, 3, 2	3	13
146	Nonlinear diffusion, bonding, and mechanics of the interface between austenitic steel and iron. *Physical Chemistry Chemical Physics*, **2019**, 21, 1464-1470	3.6	5
145	Lattice dynamics of thermoelectric palladium sulfide. *Journal of Alloys and Compounds*, **2019**, 798, 484-492	5.7	7
144	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. *Journal of Nuclear Materials*, **2019**, 524, 60-66	3.3	12
143	Mechanism of Graphene Formation via Detonation Synthesis: A DFTB Nanoreactor Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 3654-3665	6.4	13
142	Determinants of per- and polyfluoroalkyl substances (PFAS) in midlife women: Evidence of racial/ethnic and geographic differences in PFAS exposure. *Environmental Research*, **2019**, 175, 186-199	7.9	59
141	Release of helium-related clusters through a nickel–graphene interface: An atomistic study. *Applied Surface Science*, **2019**, 487, 218-227	6.7	3
140	The structure–activity relationship of Fe nanoparticles in CO adsorption and dissociation by reactive molecular dynamics simulations. *Journal of Catalysis*, **2019**, 374, 150-160	7.3	11
139	Effect of Angle, Temperature and Vacancy Defects on Mechanical Properties of PSI-Graphene. *Crystals*, **2019**, 9, 238	2.3	8
138	Van der Waals Density Functional Theory vdW-DFq for Semihard Materials. *Crystals*, **2019**, 9, 243	2.3	15

137	Magic auxeticity angle of graphene. *Carbon*, **2019**, 149, 350-354	10.4	25
136	Resolving a Decade-Long Question of Oxygen Defects in Raman Spectra of Ceria-Based Catalysts at Atomic Level. *Journal of Physical Chemistry C*, **2019**, 123, 18889-18894	3.8	26
135	Exploration of Properties from Both the Bulk and Surface of Iron Silicides: A Unified Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 11939-11949	3.8	3
134	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. *Journal of Materials Science*, **2019**, 54, 10284-10296	4.3	1
133	Divalent doping-induced thermoelectric power factor increase in p-type Bi2Te3 via electronic structure tuning. *Journal of Applied Physics*, **2019**, 125, 165101	2.5	7
132	Visiting CH4 formation and C1 + C1 couplings to tune CH4 selectivity on Fe surfaces. *Journal of Catalysis*, **2019**, 372, 217-225	7.3	10
131	First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide. *Crystals*, **2019**, 9, 48	2.3	2
130	Age at Onset of Metabolic Syndrome Among Women With and Without Polycystic Ovary Syndrome-Like Status. *Journal of Clinical Endocrinology and Metabolism*, **2019**, 104, 1429-1439	5.6	8
129	From predicting to correlating the bonding properties of iron sulfide phases. *Computational Materials Science*, **2019**, 164, 99-107	3.2	9
128	Anisotropic and temperature dependent mechanical properties of carbon honeycomb. *Nanotechnology*, **2019**, 30, 325704	3.4	7
127	The Temperature-Sensitive Anisotropic Negative Poisson Ratio of Carbon Honeycomb. *Nanomaterials*, **2019**, 9,	5.4	11
126	Recent Progress on Irradiation-Induced Defect Engineering of Two-Dimensional 2H-MoS2 Few Layers. *Applied Sciences (Switzerland)*, **2019**, 9, 678	2.6	21
125	One-pot selective synthesis of azoxy compounds and imines via the photoredox reaction of nitroaromatic compounds and amines in water. *Scientific Reports*, **2019**, 9, 1280	4.9	9
124	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. *ACS Catalysis*, **2019**, 9, 2768-2776	13.1	23
123	Thermal transports of one-dimensional ultrathin carbon structures. *Nanotechnology*, **2019**, 30, 475401	3.4	2
122	Molecular Dynamics Simulation on Mechanical and Piezoelectric Properties of Boron Nitride Honeycomb Structures. *Nanomaterials*, **2019**, 9,	5.4	4
121	Grain size and hydroxyl-coverage dependent tribology of polycrystalline graphene. *Nanotechnology* , **2019**, 30, 385701	3.4	5
120	Reduction of defect generation and development of sinks at nanocluster boundary in oxide dispersion-strengthened steel. *Journal of Applied Physics*, **2019**, 126, 084302	2.5	0

119	Oxygen defects stabilize the crystal structure of MgAl2O4 spinel under irradiation. *Journal of Nuclear Materials*, **2019**, 527, 151830	3.3	5
118	A Grain Boundary Regulates the Friction Behaviors between Graphene and a Gold Substrate. *Crystals*, **2019**, 9, 418	2.3	1
117	Proton irradiation of graphene: insights from atomistic modeling. *Nanoscale*, **2019**, 11, 20754-20765	7.7	10
116	Graphene Adhesion Mechanics on Iron Substrates: Insight from Molecular Dynamic Simulations. *Crystals*, **2019**, 9, 579	2.3	8
115	Massively Engineering the Wettability of Titanium by Tuning Nanostructures and Roughness via Laser Ablation. *Journal of Physical Chemistry C*, **2019**, 123, 30382-30388	3.8	7
114	Codoping Er-N to Suppress Self-Compensation Donors for Stable p-Type Zinc Oxide. *Advanced Theory and Simulations*, **2019**, 2, 1800133	3.5	2
113	Graphene Surface Reinforcement of Iron. *Nanomaterials*, **2019**, 9,	5.4	11
112	Comparison of graphene oxide and graphitic carbon nitride filled carbon□phenolic composites: Thermomechanical properties and role of the strong electronegativity of nanofillers. *Journal of Applied Polymer Science*, **2018**, 135, 46242	2.9	9
111	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. *ACS Catalysis*, **2018**, 8, 3365-3375	13.1	42
110	Giant Thermal Expansion in 2D and 3D Cellular Materials. *Advanced Materials*, **2018**, 30, e1705048	24	18
109	An experimental study on the interdiffusion behaviors and mechanical properties of Ni-Zr system. *Journal of Alloys and Compounds*, **2018**, 752, 412-419	5.7	14
108	Hydrogen Evolution Reaction on Hybrid Catalysts of Vertical MoS2 Nanosheets and Hydrogenated Graphene. *ACS Catalysis*, **2018**, 8, 1828-1836	13.1	135
107	An interatomic potential for simulation of defects and phase change of zirconium. *Computational Materials Science*, **2018**, 147, 7-17	3.2	6
106	Interaction of Edge Dislocations with Graphene Nanosheets in Graphene/Fe Composites. *Crystals*, **2018**, 8, 160	2.3	17
105	Strain-induced dimensional phase change of graphene-like boron nitride monolayers. *Nanotechnology*, **2018**, 29, 405201	3.4	7
104	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. *Journal of Nuclear Materials*, **2018**, 509, 237-244	3.3	20
103	Tuning the Slide-Roll Motion Mode of Carbon Nanotubes via Hydroxyl Groups. *Nanoscale Research Letters*, **2018**, 13, 138	5	8
102	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO Reduction. *Angewandte Chemie - International Edition*, **2018**, 57, 12675-12679	16.4	78

101	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. *Materials Research Letters*, **2018**, 6, 584-591	7.4	27
100	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO2 Reduction. *Angewandte Chemie*, **2018**, 130, 12857-12861	3.6	29
99	Fabrication of ceramics/high-entropy alloys gradient composites by combustion synthesis in ultra-high gravity field. *Materials Letters*, **2018**, 233, 4-7	3.3	6
98	Insight into the Nanoparticle Growth in Supported Ni Catalysts during the Early Stage of CO Hydrogenation Reaction: The Important Role of Adsorbed CO Molecules. *ACS Catalysis*, **2018**, 8, 6367-6374	12.1	13
97	A first-principles study of the structural, mechanical and electronic properties of precipitates of AlCu in Al-Cu alloys. *Physical Chemistry Chemical Physics*, **2018**, 20, 967-976	3.6	15
96	Development of a reactive force field for the Fe-C interaction to investigate the carburization of iron. *Physical Chemistry Chemical Physics*, **2018**, 20, 775-783	3.6	10
95	Developing ReaxFF to Visit CO Adsorption and Dissociation on Iron Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 27582-27589	3.8	11
94	Shockwave generates dislocation loops in bcc iron. *Nature Communications*, **2018**, 9, 4880	17.4	74
93	A Molecular Dynamics Study of the Mechanical Properties of Twisted Bilayer Graphene. *Micromachines*, **2018**, 9,	3.3	14
92	Quasicontinuum Simulation of the Effect of Lotus-Type Nanocavity on the Onset Plasticity of Single Crystal Al during Nanoindentation. *Nanomaterials*, **2018**, 8,	5.4	2
91	Effect of Molybdenum Additives on Corrosion Behavior of (CoCrFeNi)Mo High-Entropy Alloys. *Entropy*, **2018**, 20,	2.8	15
90	The Mechanical Properties of Defective Graphyne. *Crystals*, **2018**, 8, 465	2.3	8
89	Sensitive Five-Fold Local Symmetry to Kinetic Energy of Depositing Atoms in Cu-Zr Thin Film Growth. *Materials*, **2018**, 11,	3.5	10
88	A combined computational and experimental study of the adsorption of sulfur containing molecules on molybdenum disulfide nanoparticles. *Journal of Materials Research*, **2018**, 33, 3589-3603	2.5	7
87	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. *Journal of Nuclear Materials*, **2018**, 512, 246-251	3.3	9
86	Grain Boundary Plays a Key Role in Carbon Diffusion in Carbon Irons Revealed by a ReaxFF Study. *Journal of Physical Chemistry C*, **2018**, 122, 23191-23199	3.8	19
85	A Review of Current Development of Graphene Mechanics. *Crystals*, **2018**, 8, 357	2.3	38
84	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3CSiC. *Journal of Nuclear Materials*, **2018**, 510, 596-602	3.3	7

83	Self-healing mechanism of irradiation defects in nickel–graphene nanocomposite: An energetic and kinetic perspective. *Journal of Alloys and Compounds*, **2018**, 765, 253-263	5.7	18
82	Product Distribution Control for Glucosamine Condensation: Nuclear Magnetic Resonance (NMR) Investigation Substantiated by Density Functional Calculations. *Industrial & Engineering Chemistry Research*, **2017**, 56, 2925-2934	3.9	20
81	Insight into the structure and energy of Mo27SxOy clusters. *RSC Advances*, **2017**, 7, 9513-9520	3.7	15
80	Cadmium and Alzheimer's disease mortality in U.S. adults: Updated evidence with a urinary biomarker and extended follow-up time. *Environmental Research*, **2017**, 157, 44-51	7.9	42
79	Pressure-induced insulator-to-metal transitions for enhancing thermoelectric power factor in bismuth telluride-based alloys. *Physical Chemistry Chemical Physics*, **2017**, 19, 12784-12793	3.6	15
78	The normal-auxeticity mechanical phase transition in graphene. *2D Materials*, **2017**, 4, 021020	5.9	35
77	Theoretical prediction of a graphene-like structure of indium nitride: A promising excellent material for optoelectronics. *Applied Materials Today*, **2017**, 7, 169-178	6.6	16
76	Athermal repair of nanoscale defects in optical materials using a femtosecond laser. *Nanoscale*, **2017**, 9, 17233-17240	7.7	3
75	A SPH Implementation with Ignition and Growth and Afterburning Models for Aluminized Explosives. *International Journal of Computational Methods*, **2017**, 14, 1750046	1.1	5
74	When Density Functional Approximations Meet Iron Oxides. *Journal of Chemical Theory and Computation*, **2016**, 12, 5132-5144	6.4	69
73	A first-principles study of the avalanche pressure of alpha zirconium. *RSC Advances*, **2016**, 6, 72551-72558	3.7	1
72	How far away are iron carbide clusters from the bulk?. *Physical Chemistry Chemical Physics*, **2016**, 18, 32944-32951	3.6	51
71	A theoretical prediction of super high-performance thermoelectric materials based on MoS2/WS2 hybrid nanoribbons. *Scientific Reports*, **2016**, 6, 21639	4.9	50
70	Mössbauer Spectroscopy of Iron Carbides: From Prediction to Experimental Confirmation. *Scientific Reports*, **2016**, 6, 26184	4.9	58
69	Detailed characteristics of adsorption of bisphenol A by highly hydrophobic MCM-41 mesoporous molecular sieves. *Research on Chemical Intermediates*, **2016**, 42, 7169-7183	2.8	11
68	Density-functional-based tight-binding parameterization of Mo, C, H, O and Si for studying hydrogenation reactions on molybdenum carbide. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
67	Mechanical Stabilities and Properties of Graphene and Its Modification by BN Predicted from First-Principles Calculations **2016**, 79-92		
66	Stacking-Mode-Induced Reactivity Enhancement for Twisted Bilayer Graphene. *Chemistry of Materials*, **2016**, 28, 1034-1039	9.6	23

65	Properties of AlN film grown on Si (111). *Journal of Crystal Growth*, **2016**, 435, 76-83	1.6	11
64	Arsenic exposure is associated with diminished insulin sensitivity in non-diabetic Amish adults. *Diabetes/Metabolism Research and Reviews*, **2016**, 32, 565-71	7.5	24
63	Stress evolution in AlN and GaN grown on Si(111): experiments and theoretical modeling. *Journal of Materials Science: Materials in Electronics*, **2016**, 27, 2004-2013	2.1	10
62	A highly efficient, stable, durable, and recyclable filter fabricated by femtosecond laser drilling of a titanium foil for oil-water separation. *Scientific Reports*, **2016**, 6, 37591	4.9	45
61	Very high thermoelectric figure of merit found in hybrid transition-metal-dichalcogenides. *Journal of Applied Physics*, **2016**, 120, 235109	2.5	18
60	A first-principles study of the mechanical properties of AlN with Raman verification. *Computational Materials Science*, **2016**, 112, 342-346	3.2	13
59	Distinctive nanofriction of graphene coated copper foil. *Computational Materials Science*, **2016**, 117, 406-411	3.2	25
58	Temperature dependence of Raman spectra of graphene on copper foil substrate. *Journal of Materials Science: Materials in Electronics*, **2016**, 27, 3888-3893	2.1	17
57	Phonon transport in single-layer boron nanoribbons. *Nanotechnology*, **2016**, 27, 445703	3.4	17
56	Mechanical degradation of graphene by epoxidation: insights from first-principles calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 19484-90	3.6	20
55	Microscopic study of the equation of state of β-HMX using reactive molecular dynamics simulations. *RSC Advances*, **2015**, 5, 55892-55900	3.7	3
54	Predicting elastic properties of β-HMX from first-principles calculations. *Journal of Physical Chemistry B*, **2015**, 119, 5896-903	3.4	21
53	Urinary arsenic and insulin resistance in US adolescents. *International Journal of Hygiene and Environmental Health*, **2015**, 218, 407-13	6.9	24
52	Geometry, stability and thermal transport of hydrogenated graphene nanoquilts. *Solid State Communications*, **2015**, 213-214, 31-36	1.6	5
51	Peculiar pressure effect on Poisson ratio of graphone as a strain damper. *Nanoscale*, **2015**, 7, 9975-9	7.7	11
50	Molybdenum carbide nanocatalysts at work in the in situ environment: a density functional tight-binding and quantum mechanical/molecular mechanical study. *Journal of the American Chemical Society*, **2015**, 137, 4249-59	16.4	20
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