

Qing Peng

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226
papers

4,240
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32
h-index

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245
ext. papers

5,369
ext. citations

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L-index

#	Paper	IF	Citations
226	Mechanical properties of the hexagonal boron nitride monolayer: Ab initio study. <i>Computational Materials Science</i> , 2012 , 56, 11-17	3.2	275
225	New materials graphyne, graphdiyne, graphone, and graphane: review of properties, synthesis, and application in nanotechnology. <i>Nanotechnology, Science and Applications</i> , 2014 , 7, 1-29	3.9	184
224	Mechanical properties of graphyne monolayers: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 13385-91	3.6	183
223	Outstanding mechanical properties of monolayer MoS ₂ and its application in elastic energy storage. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 19427-37	3.6	178
222	Hydrogen Evolution Reaction on Hybrid Catalysts of Vertical MoS ₂ Nanosheets and Hydrogenated Graphene. <i>ACS Catalysis</i> , 2018 , 8, 1828-1836	13.1	135
221	Mechanical stabilities of silicene. <i>RSC Advances</i> , 2013 , 3, 13772	3.7	130
220	Injectable and biodegradable thermosensitive hydrogels loaded with PHBHHx nanoparticles for the sustained and controlled release of insulin. <i>Acta Biomaterialia</i> , 2013 , 9, 5063-9	10.8	98
219	A theoretical analysis of the effect of the hydrogenation of graphene to graphane on its mechanical properties. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 2003-11	3.6	82
218	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO Reduction. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 12675-12679	16.4	78
217	Shockwave generates dislocation loops in bcc iron. <i>Nature Communications</i> , 2018 , 9, 4880	17.4	74
216	When Density Functional Approximations Meet Iron Oxides. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5132-5144	6.4	69
215	Elastic properties of hybrid graphene/boron nitride monolayer. <i>Acta Mechanica</i> , 2012 , 223, 2591-2596	2.1	67
214	Determinants of per- and polyfluoroalkyl substances (PFAS) in midlife women: Evidence of racial/ethnic and geographic differences in PFAS exposure. <i>Environmental Research</i> , 2019 , 175, 186-199	7.9	59
213	Mössbauer Spectroscopy of Iron Carbides: From Prediction to Experimental Confirmation. <i>Scientific Reports</i> , 2016 , 6, 26184	4.9	58
212	Tunable band gaps of mono-layer hexagonal BNC heterostructures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2012 , 44, 1662-1666	3	57
211	A first-principles study of the mechanical properties of g-GeC. <i>Mechanics of Materials</i> , 2013 , 64, 135-141	3.3	56
210	Mechanical properties of g-GaN: a first principles study. <i>Applied Physics A: Materials Science and Processing</i> , 2013 , 113, 483-490	2.6	55

209	Mechanical stabilities and properties of graphene-like aluminum nitride predicted from first-principles calculations. <i>RSC Advances</i> , 2013 , 3, 7083	3.7	53
208	A theoretical prediction of super high-performance thermoelectric materials based on MoS ₂ /WS ₂ hybrid nanoribbons. <i>Scientific Reports</i> , 2016 , 6, 21639	4.9	50
207	A first principles investigation of the mechanical properties of g-ZnO: The graphene-like hexagonal zinc oxide monolayer. <i>Computational Materials Science</i> , 2013 , 68, 320-324	3.2	50
206	A highly efficient, stable, durable, and recyclable filter fabricated by femtosecond laser drilling of a titanium foil for oil-water separation. <i>Scientific Reports</i> , 2016 , 6, 37591	4.9	45
205	Cadmium and Alzheimer's disease mortality in U.S. adults: Updated evidence with a urinary biomarker and extended follow-up time. <i>Environmental Research</i> , 2017 , 157, 44-51	7.9	42
204	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers via biaxial straining. <i>Nanoscale</i> , 2019 , 11, 2335-2342	7.7	42
203	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. <i>ACS Catalysis</i> , 2018 , 8, 3365-3375	13.1	42
202	First-principles study of the effects of mechanical strains on the radiation hardness of hexagonal boron nitride monolayers. <i>Nanoscale</i> , 2013 , 5, 695-703	7.7	40
201	A physical interaction between the adaptor proteins DOK3 and DAP12 is required to inhibit lipopolysaccharide signaling in macrophages. <i>Science Signaling</i> , 2013 , 6, ra72	8.8	38
200	A Review of Current Development of Graphene Mechanics. <i>Crystals</i> , 2018 , 8, 357	2.3	38
199	Elastic limit of silicane. <i>Nanoscale</i> , 2014 , 6, 12071-9	7.7	37
198	Structures, mechanical properties, equations of state, and electronic properties of HMX under hydrostatic pressures: a DFT-D2 study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 19972-83	3.6	37
197	The normal-auxeticity mechanical phase transition in graphene. <i>2D Materials</i> , 2017 , 4, 021020	5.9	35
196	Stability of self-interstitial atoms in hcp-Zr. <i>Journal of Nuclear Materials</i> , 2012 , 429, 233-236	3.3	33
195	DEFECT ENGINEERING OF 2D MONATOMIC-LAYER MATERIALS. <i>Modern Physics Letters B</i> , 2013 , 27, 13300167	0.67	32
194	Mechanical properties and stabilities of g-ZnS monolayers. <i>RSC Advances</i> , 2015 , 5, 11240-11247	3.7	32
193	Mechanical properties and instabilities of ordered graphene oxide C6O monolayers. <i>RSC Advances</i> , 2013 , 3, 24337	3.7	31
192	Mechanical properties and stabilities of Boron monolayers. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 2160-8	3.6	29

191	Machine learning reveals the importance of the formation enthalpy and atom-size difference in forming phases of high entropy alloys. <i>Materials and Design</i> , 2020 , 193, 108835	8.1	29
190	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO ₂ Reduction. <i>Angewandte Chemie</i> , 2018 , 130, 12857-12861	3.6	29
189	Quantum simulation of materials at micron scales and beyond. <i>Physical Review B</i> , 2008 , 78,	3.3	29
188	A Density Functional Theory Study of the Mechanical Properties of Graphane With van der Waals Corrections. <i>Mechanics of Advanced Materials and Structures</i> , 2015 , 22, 717-721	1.8	28
187	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. <i>Materials Research Letters</i> , 2018 , 6, 584-591	7.4	27
186	Chemically Tuning Mechanics of Graphene by BN. <i>Advanced Engineering Materials</i> , 2013 , 15, 718-727	3.5	27
185	Resolving a Decade-Long Question of Oxygen Defects in Raman Spectra of Ceria-Based Catalysts at Atomic Level. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 18889-18894	3.8	26
184	Origin of pyroelectricity in LiNbO ₃ . <i>Physical Review B</i> , 2011 , 83,	3.3	26
183	Magic auxeticity angle of graphene. <i>Carbon</i> , 2019 , 149, 350-354	10.4	25
182	Distinctive nanofriction of graphene coated copper foil. <i>Computational Materials Science</i> , 2016 , 117, 406-411	3.1	25
181	Urinary arsenic and insulin resistance in US adolescents. <i>International Journal of Hygiene and Environmental Health</i> , 2015 , 218, 407-13	6.9	24
180	Arsenic exposure is associated with diminished insulin sensitivity in non-diabetic Amish adults. <i>Diabetes/Metabolism Research and Reviews</i> , 2016 , 32, 565-71	7.5	24
179	Adsorption of Hexacyclic C ₆ H ₆ , C ₆ H ₈ , C ₆ H ₁₀ , and C ₆ H ₁₂ on a Mo-Terminated HMo ₂ C (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 7069-7080	3.8	24
178	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. <i>ACS Catalysis</i> , 2019 , 9, 2768-2776	13.1	23
177	Stacking-Mode-Induced Reactivity Enhancement for Twisted Bilayer Graphene. <i>Chemistry of Materials</i> , 2016 , 28, 1034-1039	9.6	23
176	In situ tuning of electronic structure of catalysts using controllable hydrogen spillover for enhanced selectivity. <i>Nature Communications</i> , 2020 , 11, 4773	17.4	23
175	Quantum mechanical modeling of hydrogen assisted cracking in aluminum. <i>Physical Review B</i> , 2013 , 88,	3.3	22
174	Theoretical and experimental investigations of nanosecond 177.3 nm deep-ultraviolet light by second harmonic generation in KBBF. <i>Applied Physics B: Lasers and Optics</i> , 2009 , 96, 415-422	1.9	22

173	Recent Progress on Irradiation-Induced Defect Engineering of Two-Dimensional 2H-MoS ₂ Few Layers. <i>Applied Sciences (Switzerland)</i> , 2019 , 9, 678	2.6	21
172	Predicting elastic properties of BHMx from first-principles calculations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 5896-903	3.4	21
171	Artificial intelligence: A powerful paradigm for scientific research. <i>Innovation(China)</i> , 2021 , 2, 100179	17.8	21
170	Product Distribution Control for Glucosamine Condensation: Nuclear Magnetic Resonance (NMR) Investigation Substantiated by Density Functional Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 2925-2934	3.9	20
169	Mechanical degradation of graphene by epoxidation: insights from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 19484-90	3.6	20
168	Molybdenum carbide nanocatalysts at work in the in situ environment: a density functional tight-binding and quantum mechanical/molecular mechanical study. <i>Journal of the American Chemical Society</i> , 2015 , 137, 4249-59	16.4	20
167	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. <i>Journal of Nuclear Materials</i> , 2018 , 509, 237-244	3.3	20
166	A 200 W diode-side-pumped CW 2 μ m Tm:YAG laser with water cooling at 8°C. <i>Applied Physics B: Lasers and Optics</i> , 2011 , 103, 83-88	1.9	20
165	Grain Boundary Plays a Key Role in Carbon Diffusion in Carbon Irons Revealed by a ReaxFF Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 23191-23199	3.8	19
164	Giant Thermal Expansion in 2D and 3D Cellular Materials. <i>Advanced Materials</i> , 2018 , 30, e1705048	24	18
163	Very high thermoelectric figure of merit found in hybrid transition-metal-dichalcogenides. <i>Journal of Applied Physics</i> , 2016 , 120, 235109	2.5	18
162	Self-healing mechanism of irradiation defects in nickel-graphene nanocomposite: An energetic and kinetic perspective. <i>Journal of Alloys and Compounds</i> , 2018 , 765, 253-263	5.7	18
161	Thermal transport in MoS ₂ /Graphene hybrid nanosheets. <i>Nanotechnology</i> , 2015 , 26, 375402	3.4	17
160	Interaction of Edge Dislocations with Graphene Nanosheets in Graphene/Fe Composites. <i>Crystals</i> , 2018 , 8, 160	2.3	17
159	Temperature dependence of Raman spectra of graphene on copper foil substrate. <i>Journal of Materials Science: Materials in Electronics</i> , 2016 , 27, 3888-3893	2.1	17
158	Phonon transport in single-layer boron nanoribbons. <i>Nanotechnology</i> , 2016 , 27, 445703	3.4	17
157	Theoretical prediction of a graphene-like structure of indium nitride: A promising excellent material for optoelectronics. <i>Applied Materials Today</i> , 2017 , 7, 169-178	6.6	16
156	High-efficiency high-power QCW diode-side-pumped zigzag Nd:YAG ceramic slab laser. <i>Applied Physics B: Lasers and Optics</i> , 2013 , 111, 111-116	1.9	16

- 155 Time-dependent potential-functional embedding theory. *Journal of Chemical Physics*, **2014**, 140, 124113, 3.9 16
- 154 Insight into the structure and energy of Mo₂₇S_xO_y clusters. *RSC Advances*, **2017**, 7, 9513-9520 3.7 15
- 153 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
- 152 Van der Waals Density Functional Theory vdW-DFq for Semihard Materials. *Crystals*, **2019**, 9, 243 2.3 15
- 151 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
- 150 Effect of Molybdenum Additives on Corrosion Behavior of (CoCrFeNi)Mo High-Entropy Alloys. *Entropy*, **2018**, 20, 2.8 15
- 149 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
- 148 Density functional study of benzene adsorption on the $\sqrt{3}\times\sqrt{3}$ Mo₂C(0001) surface. *Structural Chemistry*, **2012**, 23, 1459-1466 1.8 14
- 147 Athermal simulation of plastic deformation in amorphous solids at constant pressure. *Journal of Polymer Science, Part B: Polymer Physics*, **2004**, 42, 2057-2065 2.6 14
- 146 A Molecular Dynamics Study of the Mechanical Properties of Twisted Bilayer Graphene. *Micromachines*, **2018**, 9, 3.3 14
- 145 Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischer-Tropsch Synthesis. *Catalysis Letters*, **2019**, 149, 645-664 2.8 13
- 144 Atomic Structure and Mechanical Properties of Twisted Bilayer Graphene. *Journal of Composites Science*, **2019**, 3, 2 3 13
- 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 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
- 141 Theoretical exploration of intrinsic facet-dependent CH₄ and C₂ formation on Fe₅C₂ particle. *Applied Catalysis B: Environmental*, **2020**, 278, 119308 21.8 13
- 140 A first-principles study of the mechanical properties of AlN with Raman verification. *Computational Materials Science*, **2016**, 112, 342-346 3.2 13
- 139 Mechanical Properties of Vacancy Tuned Carbon Honeycomb. *Nanomaterials*, **2019**, 9, 5.4 12
- 138 Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. *Journal of Nuclear Materials*, **2019**, 524, 60-66 3.3 12

137	Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals. <i>Physical Review B</i> , 2010 , 82,	3.3	12
136	The structure-activity relationship of Fe nanoparticles in CO adsorption and dissociation by reactive molecular dynamics simulations. <i>Journal of Catalysis</i> , 2019 , 374, 150-160	7.3	11
135	The Temperature-Sensitive Anisotropic Negative Poisson's Ratio of Carbon Honeycomb. <i>Nanomaterials</i> , 2019 , 9,	5.4	11
134	Peculiar pressure effect on Poisson ratio of graphone as a strain damper. <i>Nanoscale</i> , 2015 , 7, 9975-9	7.7	11
133	Pressure effect on stabilities of self-interstitials in HCP-zirconium. <i>Scientific Reports</i> , 2014 , 4, 5735	4.9	11
132	Detailed characteristics of adsorption of bisphenol A by highly hydrophobic MCM-41 mesoporous molecular sieves. <i>Research on Chemical Intermediates</i> , 2016 , 42, 7169-7183	2.8	11
131	Properties of AlN film grown on Si (111). <i>Journal of Crystal Growth</i> , 2016 , 435, 76-83	1.6	11
130	Graphene Surface Reinforcement of Iron. <i>Nanomaterials</i> , 2019 , 9,	5.4	11
129	Mesoporous RhRu Nanosponges with Enhanced Water Dissociation toward Efficient Alkaline Hydrogen Evolution. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 5052-5060	9.5	11
128	Developing ReaxFF to Visit CO Adsorption and Dissociation on Iron Surfaces. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 27582-27589	3.8	11
127	Visiting CH ₄ formation and C1 + C1 couplings to tune CH ₄ selectivity on Fe surfaces. <i>Journal of Catalysis</i> , 2019 , 372, 217-225	7.3	10
126	Stress evolution in AlN and GaN grown on Si(111): experiments and theoretical modeling. <i>Journal of Materials Science: Materials in Electronics</i> , 2016 , 27, 2004-2013	2.1	10
125	Quantum mechanical study of solid solution effects on dislocation nucleation during nanoindentation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 075003	2	10
124	Highly Efficient Polarized GeS/MoSe ₂ van der Waals Heterostructure for Water Splitting from Ultraviolet to Near-Infrared Light. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020 , 14, 1900582	2.5	10
123	Proton irradiation of graphene: insights from atomistic modeling. <i>Nanoscale</i> , 2019 , 11, 20754-20765	7.7	10
122	Development of a reactive force field for the Fe-C interaction to investigate the carburization of iron. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 775-783	3.6	10
121	Sensitive Five-Fold Local Symmetry to Kinetic Energy of Depositing Atoms in Cu-Zr Thin Film Growth. <i>Materials</i> , 2018 , 11,	3.5	10
120	Atomistic Study of Mechanical Behaviors of Carbon Honeycombs. <i>Nanomaterials</i> , 2019 , 9,	5.4	9

119	From predicting to correlating the bonding properties of iron sulfide phases. <i>Computational Materials Science</i> , 2019 , 164, 99-107	3.2	9
118	One-pot selective synthesis of azoxy compounds and imines via the photoredox reaction of nitroaromatic compounds and amines in water. <i>Scientific Reports</i> , 2019 , 9, 1280	4.9	9
117	Comparison of graphene oxide and graphitic carbon nitride filled carbon/graphenic composites: Thermomechanical properties and role of the strong electronegativity of nanofillers. <i>Journal of Applied Polymer Science</i> , 2018 , 135, 46242	2.9	9
116	Axial ratio dependence of the stability of self-interstitials in HCP structures. <i>Journal of Nuclear Materials</i> , 2013 , 437, 293-296	3.3	9
115	High-power diode side-pumped Nd:YAG laser on the low gain three lines near 1.1 μ m. <i>Applied Physics B: Lasers and Optics</i> , 2011 , 104, 45-52	1.9	9
114	Scattering effect and laser performance for the Nd:YAG transparent ceramics. <i>Applied Physics B: Lasers and Optics</i> , 2011 , 104, 625-631	1.9	9
113	Quantum mechanical simulations of nanoindentation of Al thin film. <i>Computational Materials Science</i> , 2010 , 47, 769-774	3.2	9
112	A comparative study of fracture in Al: Quantum mechanical vs. empirical atomistic description. <i>Journal of the Mechanics and Physics of Solids</i> , 2011 , 59, 775-786	5	9
111	A combined experiment and first-principles study on lattice dynamics of thermoelectric CuInTe ₂ . <i>Journal of Alloys and Compounds</i> , 2020 , 822, 153610	5.7	9
110	Theoretical Perspectives on the Modulation of Carbon on Transition-Metal Catalysts for Conversion of Carbon-Containing Resources. <i>ACS Catalysis</i> , 2021 , 11, 2156-2181	13.1	9
109	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. <i>Journal of Nuclear Materials</i> , 2018 , 512, 246-251	3.3	9
108	Effect of Angle, Temperature and Vacancy Defects on Mechanical Properties of PSI-Graphene. <i>Crystals</i> , 2019 , 9, 238	2.3	8
107	Age at Onset of Metabolic Syndrome Among Women With and Without Polycystic Ovary Syndrome-Like Status. <i>Journal of Clinical Endocrinology and Metabolism</i> , 2019 , 104, 1429-1439	5.6	8
106	Adsorption and Diffusion of Hydrogen in Carbon Honeycomb. <i>Nanomaterials</i> , 2020 , 10,	5.4	8
105	Tuning the Slide-Roll Motion Mode of Carbon Nanotubes via Hydroxyl Groups. <i>Nanoscale Research Letters</i> , 2018 , 13, 138	5	8
104	Temperature-dependent surface free energy and the Wulff shape of iron and iron carbide nanoparticles: A molecular dynamics study. <i>Applied Surface Science</i> , 2020 , 509, 144859	6.7	8
103	Graphene Adhesion Mechanics on Iron Substrates: Insight from Molecular Dynamic Simulations. <i>Crystals</i> , 2019 , 9, 579	2.3	8
102	The Mechanical Properties of Defective Graphyne. <i>Crystals</i> , 2018 , 8, 465	2.3	8

101	Lattice dynamics of thermoelectric palladium sulfide. <i>Journal of Alloys and Compounds</i> , 2019 , 798, 484-492	3.7	7
100	Divalent doping-induced thermoelectric power factor increase in p-type Bi ₂ Te ₃ via electronic structure tuning. <i>Journal of Applied Physics</i> , 2019 , 125, 165101	2.5	7
99	Anisotropic and temperature dependent mechanical properties of carbon honeycomb. <i>Nanotechnology</i> , 2019 , 30, 325704	3.4	7
98	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. <i>Scripta Materialia</i> , 2020 , 187, 291-295	5.6	7
97	High impact resistance in graphyne.. <i>RSC Advances</i> , 2020 , 10, 1697-1703	3.7	7
96	Strain-induced dimensional phase change of graphene-like boron nitride monolayers. <i>Nanotechnology</i> , 2018 , 29, 405201	3.4	7
95	A 7.5 W quasi-continuous-wave sodium D2 laser generated from single-pass sum-frequency generation in LBO crystal. <i>Applied Physics B: Lasers and Optics</i> , 2011 , 102, 781-787	1.9	7
94	Structure, mechanical and thermodynamic stability of vacancy clusters in Cu. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 055009	2	7
93	Molecular dynamics simulations of scratching characteristics in vibration-assisted nano-scratch of single-crystal silicon. <i>Applied Surface Science</i> , 2021 , 551, 149451	6.7	7
92	Massively Engineering the Wettability of Titanium by Tuning Nanostructures and Roughness via Laser Ablation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 30382-30388	3.8	7
91	A combined computational and experimental study of the adsorption of sulfur containing molecules on molybdenum disulfide nanoparticles. <i>Journal of Materials Research</i> , 2018 , 33, 3589-3603	2.5	7
90	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3CSiC. <i>Journal of Nuclear Materials</i> , 2018 , 510, 596-602	3.3	7
89	Carbon Nanotubes Enhance the Radiation Resistance of bcc Iron Revealed by Atomistic Study. <i>Materials</i> , 2019 , 12,	3.5	6
88	An interatomic potential for simulation of defects and phase change of zirconium. <i>Computational Materials Science</i> , 2018 , 147, 7-17	3.2	6
87	How far away are iron carbide clusters from the bulk?. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 32944-32951	3.6	6
86	Fabrication of ceramics/high-entropy alloys gradient composites by combustion synthesis in ultra-high gravity field. <i>Materials Letters</i> , 2018 , 233, 4-7	3.3	6
85	A 3D Smoothed Particle Hydrodynamics Method with Reactive Flow Model for the Simulation of ANFO. <i>Propellants, Explosives, Pyrotechnics</i> , 2015 , 40, 566-575	1.7	6
84	Surface structure and morphology evolution of iron borides under dynamic conditions: A theoretical study. <i>Applied Surface Science</i> , 2020 , 525, 146462	6.7	6

83	CNT-sandwiched copper composites as super thermal conductors for heat management. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 128, 114557	3	6
82	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. <i>Computational Materials Science</i> , 2019 , 170, 109190	3.2	5
81	Strain Enhanced Visible-Ultraviolet Absorption of Blue Phosphorene/MoX ₂ (X = S,Se) Heterolayers. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019 , 13, 1800659	2.5	5
80	Nonlinear diffusion, bonding, and mechanics of the interface between austenitic steel and iron. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 1464-1470	3.6	5
79	Geometry, stability and thermal transport of hydrogenated graphene nanoquilts. <i>Solid State Communications</i> , 2015 , 213-214, 31-36	1.6	5
78	Electronic effects of transition metal dopants on Fe(100) and Fe ₅ C ₂ (100) surfaces for CO activation. <i>Catalysis Science and Technology</i> , 2020 , 10, 2047-2056	5.5	5
77	Grain size and hydroxyl-coverage dependent tribology of polycrystalline graphene. <i>Nanotechnology</i> , 2019 , 30, 385701	3.4	5
76	Oxygen defects stabilize the crystal structure of MgAl ₂ O ₄ spinel under irradiation. <i>Journal of Nuclear Materials</i> , 2019 , 527, 151830	3.3	5
75	A SPH Implementation with Ignition and Growth and Afterburning Models for Aluminized Explosives. <i>International Journal of Computational Methods</i> , 2017 , 14, 1750046	1.1	5
74	Error analysis and applications of a general QM/MM approach. <i>Computational Materials Science</i> , 2010 , 50, 714-719	3.2	5
73	Enhancement of toughness of SiC through compositing SiC-Al interpenetrating phase composites. <i>Nanotechnology</i> , 2020 , 31, 135706	3.4	5
72	Impact of Polypyrrole Functionalization on the Anodic Performance of Boron Nitride Nanosheets: Insights From First-Principles Calculations. <i>Frontiers in Chemistry</i> , 2021 , 9, 670833	5	5
71	Surface strengthening of stainless steels by nondestructive laser peening. <i>Materials and Design</i> , 2021 , 205, 109754	8.1	5
70	Enhanced surface bombardment resistance of the CoNiCrFeMn high entropy alloy under extreme irradiation flux. <i>Nanotechnology</i> , 2020 , 31, 025703	3.4	5
69	Ultrahigh Ballistic Resistance of Twisted Bilayer Graphene. <i>Crystals</i> , 2021 , 11, 206	2.3	5
68	Molecular Dynamics Simulation on Mechanical and Piezoelectric Properties of Boron Nitride Honeycomb Structures. <i>Nanomaterials</i> , 2019 , 9,	5.4	4
67	Fabrication and application of 2,4,6-trinitrophenol sensors based on fluorescent functional materials.. <i>Journal of Hazardous Materials</i> , 2021 , 425, 127987	12.8	4
66	A First Principles Investigation of the Mechanical Properties of g-TiN. <i>Modeling and Numerical Simulation of Material Science</i> , 2012 , 02, 76-84	0.7	4

65	Atomic Insights into Fracture Characteristics of Twisted Tri-Layer Graphene. <i>Crystals</i> , 2021 , 11, 1202	2.3	4
64	Fragility under shocking: molecular dynamics insights into defect evolutions in tungsten lattice. <i>Tungsten</i> , 2021 , 3, 234-242	4.6	4
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