Huiqiu Deng

List of Publications by Year in Descending Order

242 papers	3,307 citations	29 h-index	46 g-index
249 ext. papers	4,179 ext. citations	4.3 avg, IF	5.64 L-index

#	Paper	IF	Citations
242	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. *Metals*, **2022**, 12, 232	2.3	0
241	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. *Applied Physics Express*, **2022**, 15, 015503	2.4	2
240	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. *Metals*, **2022**, 12, 215	2.3	
239	Effect of nanopores on plasticity and their collapse mechanism in magnesium single crystal under shock loading. *Journal of Applied Physics*, **2022**, 131, 055903	2.5	1
238	Molecular dynamic simulations of displacement cascades in tungsten and tungsten□henium alloys: Effects of grain boundary and/or □phase. *Journal of Nuclear Materials*, **2022**, 561, 153543	3.3	1
237	Ta concentration effect on nucleation of defects in W-Ta alloy from first-principles model. *Materials Today Communications*, **2022**, 30, 103071	2.5	
236	The mechanism of plasticity and phase transition in iron single crystals under cylindrically divergent shock loading. *International Journal of Mechanical Sciences*, **2022**, 217, 107032	5.5	1
235	Atomic insight into iron corrosion exposed to supercritical water environment with an improved Fe-H2O reactive force field. *Applied Surface Science*, **2022**, 580, 152300	6.7	2
234	Molecular dynamics simulation study of helium bubble growth on W/Ta semi-coherent interface. *Journal of Nuclear Materials*, **2022**, 558, 153340	3.3	0
233	Study on the relationship between surface and dislocation of nanoporous copper under cyclic shear loading. *AIP Advances*, **2022**, 12, 035318	1.5	
232	Influence of titanium on the clustering of vacancy, rhenium and osmium in tungsten-titanium alloys: First-principles study. *Fusion Engineering and Design*, **2022**, 178, 113098	1.7	0
231	Molecular Dynamics Simulations of Xe Behaviors at the Grain Boundary in UO2. *Metals*, **2022**, 12, 763	2.3	1
230	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO2. *Metals*, **2022**, 12, 789	2.3	1
229	Orientation dependence of shock-induced change of habit plane for the 1/2<111> dislocation loop and plasticity in tungsten. *International Journal of Plasticity*, **2022**, 155, 103329	7.6	0
228	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. *International Journal of Mechanical Sciences*, **2022**, 107373	5.5	1
227	Shock-induced plasticity and phase transformation in single crystal magnesium: An interatomic potential and non-equilibrium molecular dynamics simulations.. *Journal of Physics Condensed Matter*, **2021**,	1.8	3
226	Roles of triple and quadruple junctions on plasticity by phase-field crystal approach. *Physica B: Condensed Matter*, **2021**, 626, 413449	2.8	

225	The interactions between nitrogen oxides and uranium surface. *Nuclear Materials and Energy*, **2021**, 26, 100945	2.1	
224	In-situ TEM investigation of 30 keV he+ irradiated tungsten: Effects of temperature, fluence, and sample thickness on dislocation loop evolution. *Acta Materialia*, **2021**, 206, 116618	8.4	18
223	Revealing the hardening mechanisms of ion-irradiated nanostructured multilayers/substrate systems: A theoretical model. *International Journal of Plasticity*, **2021**, 138, 102925	7.6	1
222	Wire-in-Wire TiO/C Nanofibers Free-Standing Anodes for Li-Ion and K-Ion Batteries with Long Cycling Stability and High Capacity. *Nano-Micro Letters*, **2021**, 13, 107	19.5	20
221	Energetics and diffusional properties of helium in W-Ta systems studied by a new ternary potential. *Journal of Nuclear Materials*, **2021**, 549, 152913	3.3	1
220	First-principles study on the dissolution and diffusion behavior of hydrogen in carbide precipitates. *International Journal of Hydrogen Energy*, **2021**, 46, 22030-22039	6.7	2
219	Atomistic insights into interactions between oxygen and Zr (101-1) surface. *Nuclear Materials and Energy*, **2021**, 27, 100974	2.1	
218	On the relationship between potential of zero charge and solvent dynamics in the reversible hydrogen electrode. *Journal of Catalysis*, **2021**, 398, 161-170	7.3	0
217	DFT study on the nucleation of He bubbles in Pd: Effect of H and self-interstitial atoms. *Journal of Nuclear Materials*, **2021**, 549, 152888	3.3	0
216	Double-layer honeycomb AlP as a promising catalyst for Li-O2 and Na-O2 batteries. *Applied Surface Science*, **2021**, 550, 149392	6.7	1
215	Molecular dynamics simulation of shock wave propagation and spall failure in single crystal copper under cylindrical impact. *Applied Physics Express*, **2021**, 14, 075504	2.4	2
214	A strategy to improve the electrochemical performance of Ni-rich positive electrodes: Na/F-co-doped LiNi0.6Mn0.2Co0.2O2 *. *Chinese Physics B*, **2021**, 30, 073101	1.2	0
213	Phase transformation and mechanical stability of niobium aluminide (Nb3Al) induced by high pressures. *Journal of Alloys and Compounds*, **2021**, 869, 159278	5.7	2
212	Unraveling the effects of anions in NixAy@CC (A=O, S, P) on Li-sulfur batteries. *Materials Today Nano*, **2021**, 13, 100106	9.7	3
211	Electroreduction of Carbon Dioxide Driven by the Intrinsic Defects in the Carbon Plane of a Single Fe-N Site. *Advanced Materials*, **2021**, 33, e2003238	24	92
210	Suppressing/enhancing effect of rhenium on helium clusters evolution in tungsten: Dependence on rhenium distribution. *Journal of Nuclear Materials*, **2021**, 543, 152545	3.3	0
209	Assessing Atomic-Phase Transitions and Ion Transport in Layered NaxNiO2 (x 0.67) Cathode Materials. *Journal of Physical Chemistry C*, **2021**, 125, 4930-4937	3.8	
208	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. *Journal of Applied Physics*, **2021**, 130, 015107	2.5	1

207	A First-Principles Study on Na and O Adsorption Behaviors on Mo (110) Surface. *Metals*, **2021**, 11, 1322	2.3	2
206	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. *Nano Letters*, **2021**, 21, 6875-6881	11.5	6
205	Modification of short-range repulsive interactions in ReaxFF reactive force field for Fe□Ni□Al alloy*. *Chinese Physics B*, **2021**, 30, 086110	1.2	1
204	Theoretical Evaluation of MBenes as Catalysts for the CO2 Reduction Reaction. *Journal of Physical Chemistry C*, **2021**, 125, 19183-19189	3.8	2
203	A Mechanistic Study of Clustering and Diffusion of Molybdenum and Rhenium Atoms in Liquid Sodium. *Metals*, **2021**, 11, 1430	2.3	1
202	Molecular dynamics simulation of the behavior of typical radiation defects under stress gradient field in tungsten. *Journal of Applied Physics*, **2021**, 130, 125103	2.5	0
201	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. *Ceramics International*, **2021**, 47, 29386-29391	5.1	1
200	In-situ TEM observation and MD simulation of the reaction and transformation of loops in tungsten during H2+ & He+ dual-beam irradiation. *Scripta Materialia*, **2021**, 204, 114154	5.6	3
199	Machine learning to predict aluminum segregation to magnesium grain boundaries. *Scripta Materialia*, **2021**, 204, 114150	5.6	2
198	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. *Journal of Nuclear Materials*, **2021**, 556, 153162	3.3	3
197	Finnis□Sinclair-type potential for atomistic simulation of defects behaviour in V-Ti-Ta ternary system. *Journal of Nuclear Materials*, **2021**, 557, 153231	3.3	1
196	Mechanisms for interstitial dislocation loops to diffuse in BCC iron. *Nature Communications*, **2021**, 12, 225	17.4	10
195	Chemistry of Defects in Crystalline Na2Se: Implications for the Na□Se Battery. *Journal of Physical Chemistry C*, **2020**, 124, 27930-27936	3.8	3
194	Effect of symmetrical tilt grain boundary on the compatibility between copper and liquid lithium: Atomistic simulations. *Journal of Alloys and Compounds*, **2020**, 835, 155212	5.7	0
193	New Insight into the Confinement Effect of Microporous Carbon in Li/Se Battery Chemistry: A Cathode with Enhanced Conductivity. *Small*, **2020**, 16, e2000266	11	24
192	Dielectric Polarization in Inverse Spinel-Structured Mg TiO Coating to Suppress Oxygen Evolution of Li-Rich Cathode Materials. *Advanced Materials*, **2020**, 32, e2000496	24	59
191	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. *Computational Materials Science*, **2020**, 183, 109845	3.2	4
190	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. *Fusion Engineering and Design*, **2020**, 159, 111850	1.7	3

189	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. *Acta Materialia*, **2020**, 196, 133-143	8.4	45
188	Carbide effects on tensile deformation behavior of [001] symmetric tilt grain boundaries in bcc Fe. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 035006	2	1
187	A better nanochannel tungsten film in releasing helium atoms. *Journal of Nuclear Materials*, **2020**, 532, 152044	3.3	5
186	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. *Computational Materials Science*, **2020**, 177, 109555	3.2	5
185	Double-Layer Honeycomb AlP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 2978-2986	3.8	5
184	Interatomic potentials of W□V and W□Mo binary systems for point defects studies. *Journal of Nuclear Materials*, **2020**, 531, 152020	3.3	5
183	Evaluation of tungsten interatomic potentials for radiation damage simulations. *Tungsten*, **2020**, 2, 3-14	4.6	3
182	Interaction between impurity elements (C, N and O) and hydrogen in hcp-Zr: a first-principles study. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 085007	2	
181	Effect of transmutation elements Re and Ta on the vacancy formation and dissociation behaviors in W bulk. *Computational Materials Science*, **2020**, 179, 109624	3.2	5
180	Boosting the charge transfer of LiTiSiO using nitrogen-doped carbon nanofibers: towards high-rate, long-life lithium-ion batteries. *Nanoscale*, **2020**, 12, 19702-19710	7.7	4
179	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Fe□10Ni□20Cr and Ni. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 075002	2	2
178	Segregation and aggregation of rhenium in tungsten grain boundary: Energetics, configurations and strengthening effects. *Journal of Nuclear Materials*, **2020**, 528, 151867	3.3	8
177	Effect of tungsten on the vacancy behaviors in Ta□W alloys from first-principles calculations. *Solid State Communications*, **2020**, 306, 113767	1.6	5
176	Constructing a 3D compact sulfur host based on carbon-nanotube threaded defective Prussian blue nanocrystals for high performance lithium□sulfur batteries. *Journal of Materials Chemistry A*, **2020**, 8, 1154-1163	13	16
175	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. *Computational Materials Science*, **2020**, 173, 109412	3.2	4
174	Interatomic potentials and defect properties of Fe□Cr□Al alloys. *Journal of Nuclear Materials*, **2020**, 541, 152421	3.3	6
173	Effect of titanium on the precipitation behaviors of transmutation elements in tungsten-titanium alloys from first-principles calculations. *Fusion Engineering and Design*, **2020**, 158, 111673	1.7	2
172	Electrospun Ta-doped TiO2/C nanofibers as a high-capacity and long-cycling anode material for Li-ion and K-ion batteries. *Journal of Materials Chemistry A*, **2020**, 8, 20666-20676	13	24

171	Molecular dynamics simulation of the diffusion of self-interstitial atoms and interstitial loops under temperature gradient field in tungsten. *Journal of Applied Physics*, **2020**, 128, 065103	2.5	4
170	Ductile-brittle transition of open-cell nanoporous Cu in tension: A reliance of specific surface area. *Scripta Materialia*, **2020**, 175, 43-48	5.6	4
169	Molecular dynamics simulations of shock loading of nearly fully dense granular Ni-Al composites. *Physical Chemistry Chemical Physics*, **2019**, 21, 20252-20261	3.6	3
168	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. *Journal of Nuclear Materials*, **2019**, 527, 151821	3.3	7
167	Molecular dynamics simulations of high-energy radiation damage in W and WRe alloys. *Journal of Nuclear Materials*, **2019**, 524, 9-20	3.3	12
166	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. *Journal of Nuclear Materials*, **2019**, 522, 200-211	3.3	16
165	Orientation and grain-boundary dependence of shock-induced plasticity and transformation in nanocrystalline Ti. *Physical Review B*, **2019**, 99,	3.3	11
164	Ab initio study of interstitial helium clusters in 3C-SiC. *Journal of Nuclear Materials*, **2019**, 521, 13-20	3.3	9
163	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. *Nuclear Fusion*, **2019**, 59, 076020	3.3	7
162	Effect of MCl3 (M=La, U or Sc) component on the local structures and transport properties of LiClKClMCl3 eutectic: A molecular dynamics study. *Electrochimica Acta*, **2019**, 306, 366-376	6.7	8
161	Development of a NiMo interatomic potential for irradiation simulation. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 045009	2	4
160	Development of the interatomic potentials for W-Ta system. *Computational Materials Science*, **2019**, 163, 91-99	3.2	10
159	Rectangular Tunnel-Structured Na0.4MnO2 as a Promising Cathode Material Withstanding a High Cutoff Voltage for Na-Ion Batteries. *ChemElectroChem*, **2019**, 6, 1711-1721	4.3	6
158	Intrinsic strain-induced segregation in multiply twinned Cu-Pt icosahedra. *Physical Chemistry Chemical Physics*, **2019**, 21, 4802-4809	3.6	6
157	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. *Energy Storage Materials*, **2019**, 17, 211-219	19.4	7
156	Clustering and dislocation loop punching induced by different noble gas bubbles in tungsten: a molecular dynamics study. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 084002	2	0
155	Theoretical insights into nitrogen fixation on Ti2C and Ti2CO2 in a lithium–nitrogen battery. *Journal of Materials Chemistry A*, **2019**, 7, 19950-19960	13	10
154	Interactions of plasticity and phase transformation under shock in iron bicrystals. *Journal of Applied Physics*, **2019**, 126, 045901	2.5	4

153	The adsorption and dissolution properties of iron surfaces in liquid lithium and lead under a fusion environment. *Journal of Nuclear Materials*, **2019**, 524, 200-208	3.3	2
152	Defect-rich one-dimensional MoS2 hierarchical architecture for efficient hydrogen evolution: Coupling of multiple advantages into one catalyst. *Applied Catalysis B: Environmental*, **2019**, 258, 117964	21.8	53
151	First-principles study of hydrogen-vacancy complexes in Be12Ti. *Journal of Nuclear Materials*, **2019**, 525, 7-13	3.3	5
150	Transition from ductilizing to hardening in tungsten: The dependence on rhenium distribution. *Acta Materialia*, **2019**, 181, 110-123	8.4	14
149	Effect of particle packing and density on shock response in ordered arrays of Ni + Al nanoparticles. *Physical Chemistry Chemical Physics*, **2019**, 21, 7272-7280	3.6	7
148	Dopant Segregation Boosting High-Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. *Advanced Materials*, **2019**, 31, e1904816	24	46
147	Shock-induced migration of asymmetry tilt grain boundary in iron bicrystal: A case study of Σ [110]. *Chinese Physics B*, **2019**, 28, 126201	1.2	1
146	Corrosion characteristics of copper in static liquid lithium under high vacuum. *Journal of Nuclear Materials*, **2019**, 513, 282-292	3.3	4
145	Atomistic studies of shock-induced plasticity and phase transition in iron-based single crystal with edge dislocation. *International Journal of Plasticity*, **2019**, 114, 215-226	7.6	24
144	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Na-Se Batteries. *ACS Applied Materials & Interfaces*, **2019**, 11, 4995-5002	9.5	19
143	Influence of hydrostatic strain on the behaviors of rhenium and osmium in tungsten. *Journal of Nuclear Materials*, **2019**, 516, 111-117	3.3	1
142	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. *Journal of Alloys and Compounds*, **2019**, 775, 1184-1198	5.7	17
141	Development of interatomic potentials for Fe-Cr-Al alloy with the particle swarm optimization method. *Journal of Alloys and Compounds*, **2019**, 780, 881-887	5.7	16
140	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. *Computational Materials Science*, **2019**, 156, 47-55	3.2	17
139	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. *Fusion Engineering and Design*, **2018**, 128, 75-81	1.7	13
138	Robust pseudo-capacitive Li-I2 battery enabled by catalytic, adsorptive N-doped graphene interlayer. *Energy Storage Materials*, **2018**, 14, 129-135	19.4	47
137	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. *Computational Materials Science*, **2018**, 148, 242-248	3.2	11
136	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. *Computational Materials Science*, **2018**, 149, 435-441	3.2	2

135	Towards understanding the mechanism of rhenium and osmium precipitation in tungsten and its implication for tungsten-based alloys. *Journal of Nuclear Materials*, **2018**, 505, 30-43	3.3	18
134	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 11713-11721	3.6	18
133	New interatomic potentials of W, Re and W-Re alloy for radiation defects. *Journal of Nuclear Materials*, **2018**, 502, 141-153	3.3	35
132	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. *Journal of Applied Physics*, **2018**, 123, 045105	2.5	19
131	A first-principles investigation of the ScO2 monolayer as the cathode material for alkali metal-ion batteries. *Journal of Materials Chemistry A*, **2018**, 6, 3171-3180	13	15
130	Oxygen adsorption and diffusion on □U(0 0 1) surface: Effect of titanium. *Computational Materials Science*, **2018**, 144, 85-91	3.2	6
129	An ab initio study for probing iodization reactions on metallic anode surfaces of Li□2 batteries. *Journal of Materials Chemistry A*, **2018**, 6, 7807-7814	13	6
128	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. *Computational Materials Science*, **2018**, 141, 293-301	3.2	16
127	First-Principles Calculations on the Wettability of Li Atoms on the (111) Surfaces of W and Mo Substrates. *Plasma Physics Reports*, **2018**, 44, 692-701	1.2	3
126	Compatibility of Molybdenum, Tungsten, and 304 Stainless Steel in Static Liquid Lithium Under High Vacuum. *Plasma Physics Reports*, **2018**, 44, 671-677	1.2	3
125	Nanochannel structures in W enhance radiation tolerance. *Acta Materialia*, **2018**, 153, 147-155	8.4	34
124	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 22351-22358	3.6	6
123	Effect of neon on the hydrogen behaviors in tungsten: A first-principles study. *Journal of Nuclear Materials*, **2018**, 510, 492-498	3.3	2
122	Modified analytic embedded atom method potential for chromium. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 065001	2	2
121	Local identification of chemical ordering: Extension, implementation, and application of the common neighbor analysis for binary systems. *Computational Materials Science*, **2018**, 143, 195-205	3.2	3
120	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. *Current Applied Physics*, **2018**, 18, 183-190	2.6	11
119	Shock wave propagation, plasticity, and void collapse in open-cell nanoporous Ta. *Physical Chemistry Chemical Physics*, **2018**, 20, 28039-28048	3.6	10
118	Retention and diffusion of transmutation H and He atoms in BeTi: first-principles calculations.. *RSC Advances*, **2018**, 8, 35735-35743	3.7	6

117	Shockwave generates dislocation loops in bcc iron. *Nature Communications*, **2018**, 9, 4880	17.4	74
116	Does the MgCl2 Battery Suffer Severe Shuttle Effect?. *Journal of Physical Chemistry C*, **2018**, 122, 28518-28527	3.7	3
115	Investigation of wettability of Li on 316L SS surface and interfacial interactions for fusion device. *Fusion Engineering and Design*, **2018**, 137, 420-426	1.7	2
114	Surface premelting/recrystallization governing the collapse of open-cell nanoporous Cu via thermal annealing. *Physical Chemistry Chemical Physics*, **2018**, 20, 16184-16192	3.6	5
113	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. *Journal of Alloys and Compounds*, **2018**, 763, 1-10	5.7	5
112	The effect of solutes on the precipitate/matrix interface properties in the Vanadium alloys: A first-principles study. *Computational Materials Science*, **2018**, 153, 113-118	3.2	3
111	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. *Fusion Engineering and Design*, **2017**, 117, 188-193	1.7	8
110	The effects of interstitial impurities on the mechanical properties of vanadium alloys: A first-principles study. *Journal of Alloys and Compounds*, **2017**, 701, 975-980	5.7	11
109	Behaviors of transmutation elements Re and Os and their effects on energetics and clustering of vacancy and self-interstitial atoms in W. *Nuclear Fusion*, **2017**, 57, 046006	3.3	22
108	A molecular dynamics study of the transport properties of LiF-BeF 2 -ThF 4 molten salt. *Journal of Molecular Liquids*, **2017**, 234, 220-226	6	7
107	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. *Journal of Materials Research*, **2017**, 32, 1474-1483	2.5	6
106	Atomistic simulations of solidification process in B2-LiPb solid(0 0 1)-liquid system. *Journal of Crystal Growth*, **2017**, 470, 113-121	1.6	3
105	Molecular dynamics simulations of the structure evolutions of Cu-Zr metallic glasses under irradiation. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 393, 77-81	1.2	7
104	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. *Physical Chemistry Chemical Physics*, **2017**, 19, 17607-17617	3.6	14
103	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. *Computational Materials Science*, **2017**, 137, 273-281	3.2	12
102	First-principles study of the adsorption properties of atoms and molecules on UN2 (001) surface. *Journal of Nuclear Materials*, **2017**, 493, 124-131	3.3	1
101	Simulation of radiation damages in molybdenum by combining molecular dynamics and OKMC. *Nuclear Science and Techniques/Hewuli*, **2017**, 28, 1	2.1	3
100	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. *Computational Materials Science*, **2016**, 111, 203-208	3.2	17

99	Ab initio solute–interstitial impurity interactions in vanadium alloys: the roles of vacancy. *RSC Advances*, **2016**, 6, 78621-78628	3.7	9
98	Clustering of Fe atoms in liquid Li and its effect on the viscosity of liquid Li. *Nuclear Fusion*, **2016**, 56, 046004	3.3	5
97	Orientation dependences of the Fe-Li solid-liquid interface properties: Atomistic simulations. *Journal of Alloys and Compounds*, **2016**, 687, 875-884	5.7	11
96	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. *Computational Materials Science*, **2016**, 122, 1-10	3.2	16
95	The energy and stability of helium-related cluster in nickel: A study of molecular dynamics simulation. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 368, 75-80	1.2	7
94	Development of a pair potential for Ni–He. *Journal of Nuclear Materials*, **2016**, 472, 105-109	3.3	9
93	Atomic simulation of helium trapping in displacement cascades. *RSC Advances*, **2016**, 6, 27113-27118	3.7	5
92	First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys. *Journal of Alloys and Compounds*, **2016**, 660, 55-61	5.7	25
91	The flow behavior of liquid Li in Cu micro-channels. *Wuli Xuebao/Acta Physica Sinica*, **2016**, 65, 104705	0.6	
90	Tensile mechanical properties of Ni-based superalloy of nanophases using molecular dynamics simulation. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 726-732	1.3	12
89	MD and OKMC simulations of the displacement cascades in nickel. *Nuclear Science and Techniques/Hewuli*, **2016**, 27, 1	2.1	1
88	Atomistic simulation of mechanical properties and crack propagation of irradiated nickel. *Computational Materials Science*, **2016**, 120, 21-28	3.2	6
87	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. *Computational Materials Science*, **2016**, 119, 114-119	3.2	12
86	Study of the corrosion behaviors of 304 austenite stainless steel specimens exposed to static liquid lithium at 600 K. *Journal of Nuclear Materials*, **2016**, 480, 25-31	3.3	11
85	Monte Carlo simulations of strain-driven elemental depletion or enrichment in Cu95Al5 and Cu90Al10 alloys. *Computational Materials Science*, **2015**, 106, 123-128	3.2	1
84	Diffusion mechanisms at the Pb solid–liquid interface: Atomic level point of view. *Chemical Physics Letters*, **2015**, 634, 108-112	2.5	2
83	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. *Journal of Nuclear Materials*, **2015**, 467, 398-405	3.3	13
82	A molecular dynamics study of helium diffusion and clustering in fcc nickel. *Computational Materials Science*, **2015**, 107, 54-57	3.2	15

81	Mesoscale elucidation of laser-assisted chemical deposition of Sn nanostructured electrodes. *Journal of Applied Physics*, **2015**, 117, 214301	2.5	2
80	Chemical Ordering and Surface Segregation in Cu–Pt Nanoalloys: The Synergetic Roles in the Formation of Multishell Structures. *Journal of Physical Chemistry C*, **2015**, 119, 21515-21527	3.8	25
79	Atomic simulation of fatigue crack propagation in Ni3Al. *Applied Physics A: Materials Science and Processing*, **2015**, 118, 1399-1406	2.6	12
78	Stability and diffusion properties of Ti atom on α-uranium surfaces: A first-principles study. *Computational Materials Science*, **2015**, 97, 201-208	3.2	2
77	Composition Dependence of Lithium Diffusion in Lithium Silicide: A Density Functional Theory Study. *ChemElectroChem*, **2015**, 2, 1292-1297	4.3	15
76	Oxygen Deficiency and Defect Chemistry in Delithiated Spinel LiNi0.5Mn1.5O4 Cathodes for Li-Ion Batteries. *ChemElectroChem*, **2015**, 2, 1182-1186	4.3	16
75	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. *International Journal of Plasticity*, **2015**, 71, 218-236	7.6	38
74	The alloying processes in solid–solid and liquid–solid Li–Pb interfaces with atomistic simulations. *Journal of Alloys and Compounds*, **2015**, 632, 467-472	5.7	5
73	Evaluating pristine and modified SnS2 as a lithium-ion battery anode: a first-principles study. *ACS Applied Materials & Interfaces*, **2015**, 7, 4000-9	9.5	59
72	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. *Scripta Materialia*, **2015**, 100, 106-109	5.6	15
71	Amorphization and thermal stability of aluminum-based nanoparticles prepared from the rapid cooling of nanodroplets: effect of iron addition. *Physical Chemistry Chemical Physics*, **2015**, 17, 6511-22	3.6	9
70	Study of erosion and deposition characteristics of Li during liquid Li limiter experiment in HT-7. *Wuli Xuebao/Acta Physica Sinica*, **2015**, 64, 212801	0.6	2
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