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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Size effect on alloying ability and phase stability of immiscible bimetallic nanoparticles. <i>European Physical Journal B</i> , 2006 , 54, 479-484	1.2	137
241	Surface Segregation and Structural Features of Bimetallic AuPt Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 11026-11032	3.8	106
240	AuAg Bimetallic Nanoparticles: Surface Segregation and Atomic-Scale Structure. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 11355-11363	3.8	92
239	Electroreduction of Carbon Dioxide Driven by the Intrinsic Defects in the Carbon Plane of a Single Fe-N Site. <i>Advanced Materials</i> , 2021 , 33, e2003238	24	92
238	Controlling magnetism of MoS ₂ sheets by embedding transition-metal atoms and applying strain. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 18464-70	3.6	81
237	An atomic study on the shock-induced plasticity and phase transition for iron-based single crystals. <i>International Journal of Plasticity</i> , 2014 , 59, 180-198	7.6	80
236	A new FeFe interatomic potential based on ab initio calculations in Fe. <i>Journal of Nuclear Materials</i> , 2011 , 418, 115-120	3.3	75
235	Shockwave generates dislocation loops in bcc iron. <i>Nature Communications</i> , 2018 , 9, 4880	17.4	74
234	Single-layered V ₂ O ₅ a promising cathode material for rechargeable Li and Mg ion batteries: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 8705-9	3.6	73
233	Point-defect properties in HCP rare earth metals with analytic modified embedded atom potentials. <i>European Physical Journal B</i> , 2003 , 34, 429-440	1.2	63
232	Temperature dependence of atomic relaxation and vibrations for the vicinal Ni(9 7 7) surface: a molecular dynamics study. <i>Surface Science</i> , 2004 , 572, 439-448	1.8	62
231	Dielectric Polarization in Inverse Spinel-Structured Mg TiO Coating to Suppress Oxygen Evolution of Li-Rich Cathode Materials. <i>Advanced Materials</i> , 2020 , 32, e2000496	24	59
230	Evaluating pristine and modified SnS ₂ as a lithium-ion battery anode: a first-principles study. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 4000-9	9.5	59
229	Defect-rich one-dimensional MoS ₂ hierarchical architecture for efficient hydrogen evolution: Coupling of multiple advantages into one catalyst. <i>Applied Catalysis B: Environmental</i> , 2019 , 258, 117964 ^{21.8}	21.8	53
228	Robust pseudo-capacitive Li-I ₂ battery enabled by catalytic, adsorptive N-doped graphene interlayer. <i>Energy Storage Materials</i> , 2018 , 14, 129-135	19.4	47
227	Dopant Segregation Boosting High-Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. <i>Advanced Materials</i> , 2019 , 31, e1904816	24	46
226	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. <i>Acta Materialia</i> , 2020 , 196, 133-143	8.4	45

225	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. <i>Physical Review B</i> , 2009 , 79,	3.3	43
224	Comparison of tetragonal and cubic tin as anode for Mg ion batteries. <i>ACS Applied Materials & Interfaces</i> , 2014 , 6, 6786-9	9.5	41
223	Monte Carlo simulation of the surface segregation of PtPd and PtIr alloys with an analytic embedded-atom method. <i>Surface Science</i> , 2002 , 517, 177-185	1.8	40
222	Molecular dynamics simulation of fatigue crack propagation in bcc iron under cyclic loading. <i>International Journal of Fatigue</i> , 2014 , 68, 253-259	5	38
221	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. <i>International Journal of Plasticity</i> , 2015 , 71, 218-236	7.6	38
220	Modelling and simulation of electron-rich effect on Li diffusion in group IVA elements (Si, Ge and Sn) for Li ion batteries. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 13976-13982	13	37
219	Atomistic studies of nucleation of He clusters and bubbles in bcc iron. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 68-71	1.2	36
218	Modified analytic EAM potentials for the binary immiscible alloy systems. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2003 , 355, 357-367	5.3	36
217	New interatomic potentials of W, Re and W-Re alloy for radiation defects. <i>Journal of Nuclear Materials</i> , 2018 , 502, 141-153	3.3	35
216	Hydrogen storage properties of destabilized MgH ₂ - α -AlH ₃ system. <i>International Journal of Hydrogen Energy</i> , 2010 , 35, 8122-8129	6.7	35
215	Nanochannel structures in W enhance radiation tolerance. <i>Acta Materialia</i> , 2018 , 153, 147-155	8.4	34
214	Diffusion of Co, Ru and Re in Ni-based superalloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2014 , 588, 163-169	5.7	32
213	Diffusion of small He clusters in bulk and grain boundaries in α -Fe. <i>Journal of Nuclear Materials</i> , 2013 , 442, S667-S673	3.3	29
212	Surface Segregation and Chemical Ordering Patterns of AgPd Nanoalloys: Energetic Factors, Nanoscale Effects, and Catalytic Implication. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 27850-27860	3.8	28
211	Carbon monoxide adsorption and dissociation on Mn-decorated Rh(111) and Rh(553) surfaces: A first-principles study. <i>Catalysis Today</i> , 2011 , 160, 228-233	5.3	26
210	Chemical Ordering and Surface Segregation in CuPt Nanoalloys: The Synergetic Roles in the Formation of Multishell Structures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 21515-21527	3.8	25
209	First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys. <i>Journal of Alloys and Compounds</i> , 2016 , 660, 55-61	5.7	25
208	New Insight into the Confinement Effect of Microporous Carbon in Li/Se Battery Chemistry: A Cathode with Enhanced Conductivity. <i>Small</i> , 2020 , 16, e2000266	11	24

207	Atomistic simulation of the segregation profiles in MoRe random alloys. <i>Surface Science</i> , 2003 , 543, 95-102	1.8	24
206	Electrospun Ta-doped TiO ₂ /C nanofibers as a high-capacity and long-cycling anode material for Li-ion and K-ion batteries. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 20666-20676	13	24
205	Atomistic studies of shock-induced plasticity and phase transition in iron-based single crystal with edge dislocation. <i>International Journal of Plasticity</i> , 2019 , 114, 215-226	7.6	24
204	Ferromagnetic and metallic properties of the semihydrogenated GaN sheet. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1442-1445	1.3	23
203	Behaviors of transmutation elements Re and Os and their effects on energetics and clustering of vacancy and self-interstitial atoms in W. <i>Nuclear Fusion</i> , 2017 , 57, 046006	3.3	22
202	Structure and electronic properties of transition metal dichalcogenide MX ₂ (M = Mo, W, Nb; X = S, Se) monolayers with grain boundaries. <i>Materials Chemistry and Physics</i> , 2014 , 147, 1068-1073	4.4	21
201	Computer simulations of interstitial loop growth kinetics in irradiated bcc Fe. <i>Journal of Nuclear Materials</i> , 2012 , 427, 259-267	3.3	21
200	Morphology, dimension, and composition dependence of thermodynamically preferred atomic arrangements in Ag-Pt nanoalloys. <i>Faraday Discussions</i> , 2013 , 162, 293-306	3.6	21
199	Wire-in-Wire TiO/C Nanofibers Free-Standing Anodes for Li-Ion and K-Ion Batteries with Long Cycling Stability and High Capacity. <i>Nano-Micro Letters</i> , 2021 , 13, 107	19.5	20
198	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. <i>Journal of Applied Physics</i> , 2018 , 123, 045105	2.5	19
197	First-principles study of magnetic properties in Ag-doped SnO ₂ . <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1961-1966	1.3	19
196	Analytic embedded-atom method approach to studying the surface segregation of AlMg alloys. <i>Applied Surface Science</i> , 2004 , 221, 408-414	6.7	19
195	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Na-Se Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 4995-5002	9.5	19
194	Towards understanding the mechanism of rhenium and osmium precipitation in tungsten and its implication for tungsten-based alloys. <i>Journal of Nuclear Materials</i> , 2018 , 505, 30-43	3.3	18
193	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 11713-11721	3.6	18
192	The stability and diffusion properties of foreign impurity atoms on the surface and in the bulk of vanadium: A first-principles study. <i>Computational Materials Science</i> , 2014 , 81, 191-198	3.2	18
191	In-situ TEM investigation of 300keV he ⁺ irradiated tungsten: Effects of temperature, fluence, and sample thickness on dislocation loop evolution. <i>Acta Materialia</i> , 2021 , 206, 116618	8.4	18
190	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. <i>Computational Materials Science</i> , 2016 , 111, 203-208	3.2	17

189	Diffusion of tungsten clusters on tungsten (110) surface. <i>European Physical Journal B</i> , 2009 , 68, 479-485	1.2	17
188	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. <i>Journal of Alloys and Compounds</i> , 2019 , 775, 1184-1198	5.7	17
187	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. <i>Computational Materials Science</i> , 2019 , 156, 47-55	3.2	17
186	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. <i>Journal of Nuclear Materials</i> , 2019 , 522, 200-213	3.3	16
185	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. <i>Computational Materials Science</i> , 2018 , 141, 293-301	3.2	16
184	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. <i>Computational Materials Science</i> , 2016 , 122, 1-10	3.2	16
183	Oxygen Deficiency and Defect Chemistry in Delithiated Spinel LiNi _{0.5} Mn _{1.5} O ₄ Cathodes for Li-Ion Batteries. <i>ChemElectroChem</i> , 2015 , 2, 1182-1186	4.3	16
182	Constructing a 3D compact sulfur host based on carbon-nanotube threaded defective Prussian blue nanocrystals for high performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 1154-1163	13	16
181	Development of interatomic potentials for Fe-Cr-Al alloy with the particle swarm optimization method. <i>Journal of Alloys and Compounds</i> , 2019 , 780, 881-887	5.7	16
180	A molecular dynamics study of helium diffusion and clustering in fcc nickel. <i>Computational Materials Science</i> , 2015 , 107, 54-57	3.2	15
179	A first-principles investigation of the ScO ₂ monolayer as the cathode material for alkali metal-ion batteries. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 3171-3180	13	15
178	Atomistic simulations of the Fe(001)/Ni solid-liquid interface. <i>Fusion Engineering and Design</i> , 2014 , 89, 2894-2901	1.7	15
177	Composition Dependence of Lithium Diffusion in Lithium Silicide: A Density Functional Theory Study. <i>ChemElectroChem</i> , 2015 , 2, 1292-1297	4.3	15
176	Atomistic simulations of solid solution strengthening in Ni-based superalloy. <i>Computational Materials Science</i> , 2013 , 68, 132-137	3.2	15
175	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. <i>Scripta Materialia</i> , 2015 , 100, 106-109	5.6	15
174	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 17607-17617	3.6	14
173	Transition from ductilizing to hardening in tungsten: The dependence on rhenium distribution. <i>Acta Materialia</i> , 2019 , 181, 110-123	8.4	14
172	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. <i>Journal of Nuclear Materials</i> , 2015 , 467, 398-405	3.3	13

171	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. <i>Fusion Engineering and Design</i> , 2018 , 128, 75-81	1.7	13
170	Strain-driven phase transition of molybdenum nanowire under uniaxial tensile strain. <i>Computational Materials Science</i> , 2010 , 50, 373-377	3.2	13
169	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. <i>Computational Materials Science</i> , 2017 , 137, 273-281	3.2	12
168	Molecular dynamics simulations of high-energy radiation damage in W and WRe alloys. <i>Journal of Nuclear Materials</i> , 2019 , 524, 9-20	3.3	12
167	Atomic simulation of fatigue crack propagation in Ni ₃ Al. <i>Applied Physics A: Materials Science and Processing</i> , 2015 , 118, 1399-1406	2.6	12
166	Atomic self-diffusion behaviors relevant to 2D homoepitaxy growth on stepped Pd(001) surface. <i>Surface Science</i> , 2014 , 624, 89-94	1.8	12
165	First-principles approach to the properties of point defects and small helium-vacancy clusters in palladium. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009 , 267, 3037-3040	1.2	12
164	Gibbs free energy approach to calculate the thermodynamic properties of copper nanocrystals. <i>Physica B: Condensed Matter</i> , 2011 , 406, 859-863	2.8	12
163	Atomic and molecular adsorption on RhMn alloy surface: a first principles study. <i>Journal of Chemical Physics</i> , 2008 , 129, 244711	3.9	12
162	Self-diffusion of Al and Pb atoms in AlPb immiscible alloy system. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2004 , 108, 253-257	3.1	12
161	Tensile mechanical properties of Ni-based superalloy of nanophases using molecular dynamics simulation. <i>Physica Status Solidi (B): Basic Research</i> , 2016 , 253, 726-732	1.3	12
160	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. <i>Computational Materials Science</i> , 2016 , 119, 114-119	3.2	12
159	The effects of interstitial impurities on the mechanical properties of vanadium alloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2017 , 701, 975-980	5.7	11
158	Orientation and grain-boundary dependence of shock-induced plasticity and transformation in nanocrystalline Ti. <i>Physical Review B</i> , 2019 , 99,	3.3	11
157	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. <i>Computational Materials Science</i> , 2018 , 148, 242-248	3.2	11
156	Orientation dependences of the Fe-Li solid-liquid interface properties: Atomistic simulations. <i>Journal of Alloys and Compounds</i> , 2016 , 687, 875-884	5.7	11
155	Thermodynamic properties of Li, Pb and Li ₁₇ Pb ₈₃ with molecular dynamics simulations. <i>Fusion Engineering and Design</i> , 2014 , 89, 2946-2952	1.7	11
154	First-principles calculation of self-diffusion coefficients in Ni ₃ Al. <i>Journal of Alloys and Compounds</i> , 2014 , 612, 361-364	5.7	11

153	Helium nanobubble release from Pd surface: An atomic simulation. <i>Journal of Materials Research</i> , 2011 , 26, 416-423	2.5	11
152	Study of the corrosion behaviors of 304 austenite stainless steel specimens exposed to static liquid lithium at 600 K. <i>Journal of Nuclear Materials</i> , 2016 , 480, 25-31	3.3	11
151	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. <i>Current Applied Physics</i> , 2018 , 18, 183-190	2.6	11
150	Development of the interatomic potentials for W-Ta system. <i>Computational Materials Science</i> , 2019 , 163, 91-99	3.2	10
149	Theoretical insights into nitrogen fixation on Ti ₂ C and Ti ₂ CO ₂ in a lithium–nitrogen battery. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 19950-19960	13	10
148	Diffusion properties of liquid lithium–lead alloys from atomistic simulation. <i>Computational Materials Science</i> , 2014 , 93, 74-80	3.2	10
147	Adsorption of hydrogen on palladium nanoparticle surfaces. <i>Surface and Interface Analysis</i> , 2009 , 41, 590-594	1.5	10
146	Atomistic simulation of helium bubble nucleation in palladium. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009 , 267, 3185-3188	1.2	10
145	First-principle study of the electronic structures and ferroelectric properties in BaZnF ₄ . <i>European Physical Journal B</i> , 2010 , 74, 447-450	1.2	10
144	Shock wave propagation, plasticity, and void collapse in open-cell nanoporous Ta. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 28039-28048	3.6	10
143	Mechanisms for interstitial dislocation loops to diffuse in BCC iron. <i>Nature Communications</i> , 2021 , 12, 225	17.4	10
142	Ab initio study of interstitial helium clusters in 3C-SiC. <i>Journal of Nuclear Materials</i> , 2019 , 521, 13-20	3.3	9
141	Ab initio solute–interstitial impurity interactions in vanadium alloys: the roles of vacancy. <i>RSC Advances</i> , 2016 , 6, 78621-78628	3.7	9
140	Development of a pair potential for Ni–Fe. <i>Journal of Nuclear Materials</i> , 2016 , 472, 105-109	3.3	9
139	Amorphization and thermal stability of aluminum-based nanoparticles prepared from the rapid cooling of nanodroplets: effect of iron addition. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 6511-22	3.6	9
138	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. <i>Fusion Engineering and Design</i> , 2017 , 117, 188-193	1.7	8
137	Effect of MCl ₃ (M=La, U or Sc) component on the local structures and transport properties of LiCl–MCl ₃ eutectic: A molecular dynamics study. <i>Electrochimica Acta</i> , 2019 , 306, 366-376	6.7	8
136	Dynamics diffusion behaviors of Pd small clusters on a Pd(1 1 1) surface. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 045010	2	8

- ¹³⁵ Self-diffusion dynamic behavior of atomic clusters on Re(0001) surface. *Applied Surface Science*, **2009**, 255, 8883-8889 6.7 8
- ¹³⁴ The Rh influence on the surface distribution of the ternary alloy PtPdRh. *Applied Surface Science*, **2007**, 253, 6074-6079 6.7 8
- ¹³³ Segregation and aggregation of rhenium in tungsten grain boundary: Energetics, configurations and strengthening effects. *Journal of Nuclear Materials*, **2020**, 528, 151867 3.3 8
- ¹³² A molecular dynamics study of the transport properties of LiF-BeF₂-ThF₄ molten salt. *Journal of Molecular Liquids*, **2017**, 234, 220-226 6 7
- ¹³¹ 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
- ¹³⁰ Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. *Journal of Nuclear Materials*, **2019**, 527, 151821 3.3 7
- ¹²⁹ Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. *Nuclear Fusion*, **2019**, 59, 076020 3.3 7
- ¹²⁸ 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
- ¹²⁷ 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
- ¹²⁶ 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
- ¹²⁵ First-principles study of nitrogen adsorption and dissociation on Uranium (001) surface. *RSC Advances*, **2014**, 4, 57308-57321 3.7 7
- ¹²⁴ First-principles study on the interaction of nitrogen atom with Uranium: From surface adsorption to bulk diffusion. *Journal of Applied Physics*, **2014**, 115, 164902 2.5 7
- ¹²³ Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. *Journal of Physical Chemistry C*, **2013**, 117, 17644-17649 3.8 7
- ¹²² Shock Waves Propagation and Phase Transition in Single Crystal Iron under Ramp Compression: Large Scale Parallel NEMD Simulations. *Procedia Engineering*, **2013**, 61, 122-129 7
- ¹²¹ Energetics and self-diffusion behavior of Zr atomic clusters on a Zr(0 0 0 1) surface. *Nuclear Instruments & Methods in Physics Research B*, **2009**, 267, 3267-3270 1.2 7
- ¹²⁰ Phase transition in nanocrystalline iron: Atomistic-level simulations. *International Journal of Materials Research*, **2010**, 101, 1361-1368 0.5 7
- ¹¹⁹ Magnetic properties in nitrogen-doped CeO₂ from first-principles calculations. *Physica B: Condensed Matter*, **2010**, 405, 4858-4862 2.8 7
- ¹¹⁸ First-principles study for the atomic structures and electronic properties of PbTiO₃ oxygen-vacancies (001) surface. *Surface Science*, **2007**, 601, 5412-5418 1.8 7

117	Surface segregation of AlPb immiscible alloy system with Monte Carlo simulation. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2003 , 98, 265-268	3.1	7
116	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. <i>Journal of Materials Research</i> , 2017 , 32, 1474-1483	2.5	6
115	Rectangular Tunnel-Structured Na _{0.4} MnO ₂ as a Promising Cathode Material Withstanding a High Cutoff Voltage for Na-Ion Batteries. <i>ChemElectroChem</i> , 2019 , 6, 1711-1721	4.3	6
114	Intrinsic strain-induced segregation in multiply twinned Cu-Pt icosahedra. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 4802-4809	3.6	6
113	Oxygen adsorption and diffusion on $\overline{1}10$ (0 0 1) surface: Effect of titanium. <i>Computational Materials Science</i> , 2018 , 144, 85-91	3.2	6
112	An ab initio study for probing iodization reactions on metallic anode surfaces of LiI ₂ batteries. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 7807-7814	1.3	6
111	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22351-22358	3.6	6
110	Effect of Re content on the $\overline{1}10$ interface: A Monte Carlo simulation. <i>Computational Materials Science</i> , 2014 , 89, 75-79	3.2	6
109	Simulation calculations of surface segregation for AuCu alloys using an analytic embedded atom model. <i>Physica Status Solidi A</i> , 2005 , 202, 2686-2699		6
108	Interatomic potentials and defect properties of FeCrAl alloys. <i>Journal of Nuclear Materials</i> , 2020 , 541, 152421	3.3	6
107	Atomistic simulation of mechanical properties and crack propagation of irradiated nickel. <i>Computational Materials Science</i> , 2016 , 120, 21-28	3.2	6
106	Retention and diffusion of transmutation H and He atoms in BeTi: first-principles calculations.. <i>RSC Advances</i> , 2018 , 8, 35735-35743	3.7	6
105	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. <i>Nano Letters</i> , 2021 , 21, 6875-6881	11.5	6
104	A better nanochannel tungsten film in releasing helium atoms. <i>Journal of Nuclear Materials</i> , 2020 , 532, 152044	3.3	5
103	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. <i>Computational Materials Science</i> , 2020 , 177, 109555	3.2	5
102	Double-Layer Honeycomb AlP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 2978-2986	3.8	5
101	Interatomic potentials of WMo and WMo ₂ binary systems for point defects studies. <i>Journal of Nuclear Materials</i> , 2020 , 531, 152020	3.3	5
100	Clustering of Fe atoms in liquid Li and its effect on the viscosity of liquid Li. <i>Nuclear Fusion</i> , 2016 , 56, 046004	3.3	5

99	Atomic simulation of helium trapping in displacement cascades. <i>RSC Advances</i> , 2016 , 6, 27113-27118	3.7	5
98	First-principles study of hydrogen-vacancy complexes in Be ₁₂ Ti. <i>Journal of Nuclear Materials</i> , 2019 , 525, 7-13	3.3	5
97	The alloying processes in solid-solid and liquid-solid Li-Pb interfaces with atomistic simulations. <i>Journal of Alloys and Compounds</i> , 2015 , 632, 467-472	5.7	5
96	Self-diffusion behaviors of Pd adatom and dimer on Pd(001) surface. <i>Computational Materials Science</i> , 2009 , 47, 501-505	3.2	5
95	Effect of transmutation elements Re and Ta on the vacancy formation and dissociation behaviors in W bulk. <i>Computational Materials Science</i> , 2020 , 179, 109624	3.2	5
94	Effect of tungsten on the vacancy behaviors in Ta-W alloys from first-principles calculations. <i>Solid State Communications</i> , 2020 , 306, 113767	1.6	5
93	Surface premelting/recrystallization governing the collapse of open-cell nanoporous Cu via thermal annealing. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16184-16192	3.6	5
92	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. <i>Journal of Alloys and Compounds</i> , 2018 , 763, 1-10	5.7	5
91	Development of a Ni-Mo interatomic potential for irradiation simulation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 045009	2	4
90	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. <i>Computational Materials Science</i> , 2020 , 183, 109845	3.2	4
89	Interactions of plasticity and phase transformation under shock in iron bicrystals. <i>Journal of Applied Physics</i> , 2019 , 126, 045901	2.5	4
88	Effect of voids on the tensile properties of vanadium nanowires. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 14-17	1.2	4
87	Helium diffusion behavior and its retention in LaNiAl alloy from molecular dynamic simulations. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2011 , 269, 1689-1692	1.2	4
86	Adsorption of hydrogen atoms on Pd (211), (311) and (511) stepped defective surfaces. <i>Transactions of Nonferrous Metals Society of China</i> , 2006 , 16, s820-s823	3.3	4
85	Boosting the charge transfer of LiTiSiO using nitrogen-doped carbon nanofibers: towards high-rate, long-life lithium-ion batteries. <i>Nanoscale</i> , 2020 , 12, 19702-19710	7.7	4
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