Huiqiu Deng

List of Publications by Year
in descending order

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249 papers	5,035 citations	109137 35 h-index	149479 56 g-index
250 all docs	250 docs citations	250 times ranked	4682 citing authors

#	Article	IF	Citations
1	Electroreduction of Carbon Dioxide Driven by the Intrinsic Defects in the Carbon Plane of a Single Feâ€“N₄ Site. Advanced Materials, 2021, 33, e2003238.	11.1	202
2	Size effect on alloying ability and phase stability of immiscible bimetallic nanoparticles. European Physical Journal B, 2006, 54, 479-484.	0.6	149
3	Dielectric Polarization in Inverse Spinelâ€Structured Mg₂TiO₄ Coating to Suppress Oxygen Evolution of Liâ€Rich Cathode Materials. Advanced Materials, 2020, 32, e2000496.	11.1	134
4	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. Acta Materialia, 2020, 196, 133-143.	3.8	124
5	Surface Segregation and Structural Features of Bimetallic Auâ^'Pt Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 11026-11032.	1.5	115
6	Shockwave generates < 100 > dislocation loops in bcc iron. Nature Communications, 2018, 9, 4880.	5.8	106
7	Auâ€“Ag Bimetallic Nanoparticles: Surface Segregation and Atomic-Scale Structure. Journal of Physical Chemistry C, 2011, 115, 11355-11363.	1.5	103
8	An atomic study on the shock-induced plasticity and phase transition for iron-based single crystals. International Journal of Plasticity, 2014, 59, 180-198.	4.1	97
9	Controlling magnetism of MoS2 sheets by embedding transition-metal atoms and applying strain. Physical Chemistry Chemical Physics, 2013, 15, 18464.	1.3	89
10	Dopant Segregation Boosting Highâ€Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. Advanced Materials, 2019, 31, e1904816.	11.1	89
11	Single-layered V2O5 a promising cathode material for rechargeable Li and Mg ion batteries: an ab initio study. Physical Chemistry Chemical Physics, 2013, 15, 8705.	1.3	84
12	A new Feâ€“He interatomic potential based on ab initio calculations in Î±-Fe. Journal of Nuclear Materials, 2011, 418, 115-120.	1.3	83
13	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.	10.8	77
14	Evaluating Pristine and Modified SnS₂ as a Lithium-Ion Battery Anode: A First-Principles Study. ACS Applied Materials & Interfaces, 2015, 7, 4000-4009.	4.0	75
15	Robust pseudo-capacitive Li-I2 battery enabled by catalytic, adsorptive N-doped graphene interlayer. Energy Storage Materials, 2018, 14, 129-135.	9.5	67
16	Point-defect properties in HCP rare earth metals with analytic modified embedded atom potentials. European Physical Journal B, 2003, 34, 429-440.	0.6	66
17	Temperature dependence of atomic relaxation and vibrations for the vicinal Ni(977) surface: a molecular dynamics study. Surface Science, 2004, 572, 439-448.	0.8	63
18	Nanochannel structures in W enhance radiation tolerance. Acta Materialia, 2018, 153, 147-155.	3.8	63

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19	Molecular dynamics simulation of fatigue crack propagation in bcc iron under cyclic loading. International Journal of Fatigue, 2014, 68, 253-259.	2.8	60
20	Comparison of Tetragonal and Cubic Tin as Anode for Mg Ion Batteries. ACS Applied Materials & Interfaces, 2014, 6, 6786-6789.	4.0	57
21	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. International Journal of Plasticity, 2015, 71, 218-236.	4.1	57
22	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	1.3	57
23	Modelling and simulation of electron-rich effect on Li diffusion in group IVA elements (Si, Ge and Sn) for Li ion batteries. Journal of Materials Chemistry A, 2014, 2, 13976-13982.	5.2	55
24	Wire-in-Wire TiO2/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.	14.4	55
25	In-situ TEM investigation of 30ÂkeV he+ irradiated tungsten: Effects of temperature, fluence, and sample thickness on dislocation loop evolution. Acta Materialia, 2021, 206, 116618.	3.8	47
26	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. Physical Review B, 2009, 79, .	1.1	45
27	Atomistic studies of nucleation of He clusters and bubbles in bcc iron. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 68-71.	0.6	45
28	Monte Carlo simulation of the surface segregation of Ptâ€“Pd and Ptâ€“Ir alloys with an analytic embedded-atom method. Surface Science, 2002, 517, 177-185.	0.8	44
29	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.	5.2	44
30	Hydrogen storage properties of destabilized MgH2â€“Li3AlH6 system. International Journal of Hydrogen Energy, 2010, 35, 8122-8129.	3.8	42
31	Diffusion of small He clusters in bulk and grain boundaries in Î±-Fe. Journal of Nuclear Materials, 2013, 442, S667-S673.	1.3	41
32	Modified analytic EAM potentials for the binary immiscible alloy systems. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2003, 355, 357-367.	2.6	40
33	Diffusion of Co, Ru and Re in Ni-based superalloys: A first-principles study. Journal of Alloys and Compounds, 2014, 588, 163-169.	2.8	40
34	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.	4.1	40
35	New Insight into the Confinement Effect of Microporous Carbon in Li/Se Battery Chemistry: A Cathode with Enhanced Conductivity. Small, 2020, 16, e2000266.	5.2	40
36	Surface Segregation and Chemical Ordering Patterns of Agâ€“Pd Nanoalloys: Energetic Factors, Nanoscale Effects, and Catalytic Implication. Journal of Physical Chemistry C, 2014, 118, 27850-27860.	1.5	36

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37	Molecular dynamics simulations of high-energy radiation damage in W and Wâ€“Re alloys. Journal of Nuclear Materials, 2019, 524, 9-20.	1.3	36
38	Chemical Ordering and Surface Segregation in Cuâ€“Pt Nanoalloys: The Synergetic Roles in the Formation of Multishell Structures. Journal of Physical Chemistry C, 2015, 119, 21515-21527.	1.5	33
39	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.	1.6	32
40	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.	1.3	32
41	Constructing a 3D compact sulfur host based on carbon-nanotube threaded defective Prussian blue nanocrystals for high performance lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2020, 8, 1154-1163.	5.2	32
42	First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys. Journal of Alloys and Compounds, 2016, 660, 55-61.	2.8	31
43	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. Journal of Alloys and Compounds, 2019, 775, 1184-1198.	2.8	30
44	Computer simulations of interstitial loop growth kinetics in irradiated bcc Fe. Journal of Nuclear Materials, 2012, 427, 259-267.	1.3	29
45	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.	1.3	29
46	Atomistic simulation of the segregation profiles in Moâ€“Re random alloys. Surface Science, 2003, 543, 95-102.	0.8	27
47	Ferromagnetic and metallic properties of the semihydrogenated GaN sheet. Physica Status Solidi (B): Basic Research, 2011, 248, 1442-1445.	0.7	27
48	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Naâ€“Se Batteries. ACS Applied Materials & Interfaces, 2019, 11, 4995-5002.	4.0	27
49	Firstâ€principles study of magnetic properties in Agâ€doped SnO₂. Physica Status Solidi (B): Basic Research, 2011, 248, 1961-1966.	0.7	26
50	Carbon monoxide adsorption and dissociation on Mn-decorated Rh(111) and Rh(553) surfaces: A first-principles study. Catalysis Today, 2011, 160, 228-233.	2.2	26
51	Morphology, dimension, and composition dependence of thermodynamically preferred atomic arrangements in Agâ€“Pt nanoalloys. Faraday Discussions, 2013, 162, 293.	1.6	26
52	Structure and electronic properties of transition metal dichalcogenide MX2 (MÂ=ÂMo, W, Nb; XÂ=ÂS, Se) monolayers with grain boundaries. Materials Chemistry and Physics, 2014, 147, 1068-1073.	2.0	26
53	Transition from ductilizing to hardening in tungsten: The dependence on rhenium distribution. Acta Materialia, 2019, 181, 110-123.	3.8	26
54	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	1.4	26

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55	Composition Dependence of Lithium Diffusion in Lithium Silicide: A Density Functional Theory Study. ChemElectroChem, 2015, 2, 1292-1297.	1.7	25
56	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	1.1	25
57	Tensile mechanical properties of Ni-based superalloy of nanophases using molecular dynamics simulation. Physica Status Solidi (B): Basic Research, 2016, 253, 726-732.	0.7	23
58	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. Computational Materials Science, 2016, 119, 114-119.	1.4	23
59	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. Computational Materials Science, 2016, 111, 203-208.	1.4	23
60	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. Fusion Engineering and Design, 2018, 128, 75-81.	1.0	23
61	Unraveling TM Migration Mechanisms in LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ by Modeling and Experimental Studies. Nano Letters, 2021, 21, 6875-6881.	4.5	23
62	Atomistic simulations of the Fe(001)â€“Li solidâ€“liquid interface. Fusion Engineering and Design, 2014, 89, 2894-2901.	1.0	22
63	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. Computational Materials Science, 2018, 141, 293-301.	1.4	22
64	Development of interatomic potentials for Fe-Cr-Al alloy with the particle swarm optimization method. Journal of Alloys and Compounds, 2019, 780, 881-887.	2.8	22
65	Mechanisms for <100> interstitial dislocation loops to diffuse in BCC iron. Nature Communications, 2021, 12, 225.	5.8	22
66	The stability and diffusion properties of foreign impurity atoms on the surface and in the bulk of vanadium: A first-principles study. Computational Materials Science, 2014, 81, 191-198.	1.4	21
67	Theoretical insights into nitrogen fixation on Ti₂C and Ti₂CO₂ in a lithiumâ€“nitrogen battery. Journal of Materials Chemistry A, 2019, 7, 19950-19960.	5.2	21
68	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. International Journal of Mechanical Sciences, 2022, 226, 107373.	3.6	21
69	Atomistic simulations of solid solution strengthening in Ni-based superalloy. Computational Materials Science, 2013, 68, 132-137.	1.4	20
70	First-principles calculation of self-diffusion coefficients in Ni3Al. Journal of Alloys and Compounds, 2014, 612, 361-364.	2.8	20
71	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. Physical Chemistry Chemical Physics, 2017, 19, 17607-17617.	1.3	20
72	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.	5.2	20

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73	Analytic embedded-atom method approach to studying the surface segregation of Alâ€“Mg alloys. Applied Surface Science, 2004, 221, 408-414.	3.1	19
74	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. Computational Materials Science, 2016, 122, 1-10.	1.4	19
75	Shock wave propagation, plasticity, and void collapse in open-cell nanoporous Ta. Physical Chemistry Chemical Physics, 2018, 20, 28039-28048.	1.3	19
76	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. Computational Materials Science, 2019, 156, 47-55.	1.4	19
77	Oxygen Deficiency and Defect Chemistry in Delithiated Spinel LiNi_{0.5}Mn_{1.5}O₄ Cathodes for Liâ€ion Batteries. ChemElectroChem, 2015, 2, 1182-1186.	1.7	18
78	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. Computational Materials Science, 2017, 137, 273-281.	1.4	18
79	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	1.3	18
80	Effect of MCl3 (M=La, U or Sc) component on the local structures and transport properties of LiClâ€“KClâ€“MCl3 eutectic: A molecular dynamics study. Electrochimica Acta, 2019, 306, 366-376.	2.6	18
81	Interatomic potentials and defect properties of Feâ€“Crâ€“Al alloys. Journal of Nuclear Materials, 2020, 541, 152421.	1.3	18
82	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. Computational Materials Science, 2020, 177, 109555.	1.4	18
83	Interatomic potentials of Wâ€“V and Wâ€“Mo binary systems for point defects studies. Journal of Nuclear Materials, 2020, 531, 152020.	1.3	18
84	Machine learning to predict aluminum segregation to magnesium grain boundaries. Scripta Materialia, 2021, 204, 114150.	2.6	18
85	Diffusion of tungsten clusters on tungsten (110) surface. European Physical Journal B, 2009, 68, 479-485.	0.6	17
86	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. Scripta Materialia, 2015, 100, 106-109.	2.6	17
87	A molecular dynamics study of helium diffusion and clustering in fcc nickel. Computational Materials Science, 2015, 107, 54-57.	1.4	17
88	Study of the corrosion behaviors of 304 austenite stainless steel specimens exposed to static liquid lithium at 600ÂK. Journal of Nuclear Materials, 2016, 480, 25-31.	1.3	17
89	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.	2.8	17
90	Theoretical Evaluation of MBenes as Catalysts for the CO₂ Reduction Reaction. Journal of Physical Chemistry C, 2021, 125, 19183-19189.	1.5	17

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91	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. Journal of Nuclear Materials, 2021, 556, 153162.	1.3	17
92	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. Journal of Nuclear Materials, 2015, 467, 398-405.	1.3	16
93	Atomic simulation of fatigue crack propagation in Ni3Al. Applied Physics A: Materials Science and Processing, 2015, 118, 1399-1406.	1.1	16
94	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. Computational Materials Science, 2018, 148, 242-248.	1.4	16
95	Orientation and grain-boundary dependence of shock-induced plasticity and transformation in nanocrystalline Ti. Physical Review B, 2019, 99, .	1.1	16
96	Segregation and aggregation of rhenium in tungsten grain boundary: Energetics, configurations and strengthening effects. Journal of Nuclear Materials, 2020, 528, 151867.	1.3	16
97	Strain-driven phase transition of molybdenum nanowire under uniaxial tensile strain. Computational Materials Science, 2010, 50, 373-377.	1.4	15
98	Gibbs free energy approach to calculate the thermodynamic properties of copper nanocrystals. Physica B: Condensed Matter, 2011, 406, 859-863.	1.3	15
99	First-principles study of nitrogen adsorption and dissociation on Î±-uranium (001) surface. RSC Advances, 2014, 4, 57308-57321.	1.7	15
100	Adsorption of hydrogen on palladium nanoparticle surfaces. Surface and Interface Analysis, 2009, 41, 590-594.	0.8	14
101	Orientation dependences of the Fe-Li solid-liquid interface properties: Atomistic simulations. Journal of Alloys and Compounds, 2016, 687, 875-884.	2.8	14
102	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. Journal of Materials Research, 2017, 32, 1474-1483.	1.2	14
103	In-situ TEM observation and MD simulation of the reaction and transformation of <100> loops in tungsten during H2+ & He+ dual-beam irradiation. Scripta Materialia, 2021, 204, 114154.	2.6	14
104	Atomic insight into iron corrosion exposed to supercritical water environment with an improved Fe-H2O reactive force field. Applied Surface Science, 2022, 580, 152300.	3.1	14
105	Self-diffusion of Al and Pb atoms in Alâ€“Pb immiscible alloy system. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 108, 253-257.	1.7	13
106	Atomic and molecular adsorption on RhMn alloy surface: A first principles study. Journal of Chemical Physics, 2008, 129, 244711.	1.2	13
107	Helium nanobubble release from Pd surface: An atomic simulation. Journal of Materials Research, 2011, 26, 416-423.	1.2	13
108	Thermodynamic properties of Li, Pb and Li 17 Pb 83 with molecular dynamics simulations. Fusion Engineering and Design, 2014, 89, 2946-2952.	1.0	13

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109	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. Fusion Engineering and Design, 2017, 117, 188-193.	1.0	13
110	Oxygen adsorption and diffusion on Î³-U(0â€¯0â€¯1) surface: Effect of titanium. Computational Materials Science, 2018, 144, 85-91.	1.4	13
111	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. Journal of Alloys and Compounds, 2018, 763, 1-10.	2.8	13
112	Effect of particle packing and density on shock response in ordered arrays of Ni + Al nanoparticles. Physical Chemistry Chemical Physics, 2019, 21, 7272-7280.	1.3	13
113	Molecular dynamics simulations of shock loading of nearly fully dense granular Niâ€“Al composites. Physical Chemistry Chemical Physics, 2019, 21, 20252-20261.	1.3	13
114	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. Journal of Nuclear Materials, 2019, 527, 151821.	1.3	13
115	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. Nuclear Fusion, 2019, 59, 076020.	1.6	13
116	First-principles study on the dissolution and diffusion behavior of hydrogen in carbide precipitates. International Journal of Hydrogen Energy, 2021, 46, 22030-22039.	3.8	13
117	First-principles approach to the properties of point defects and small helium-vacancy clusters in palladium. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3037-3040.	0.6	12
118	Atomic self-diffusion behaviors relevant to 2D homoepitaxy growth on stepped Pd(001) surface. Surface Science, 2014, 624, 89-94.	0.8	12
119	First-principles study on the interaction of nitrogen atom with Î±â€“uranium: From surface adsorption to bulk diffusion. Journal of Applied Physics, 2014, 115, .	1.1	12
120	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. Computational Materials Science, 2018, 149, 435-441.	1.4	12
121	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. Current Applied Physics, 2018, 18, 183-190.	1.1	12
122	Retention and diffusion of transmutation H and He atoms in Be₁₂Ti: first-principles calculations. RSC Advances, 2018, 8, 35735-35743.	1.7	12
123	Ab initio study of interstitial helium clusters in 3C-SiC. Journal of Nuclear Materials, 2019, 521, 13-20.	1.3	12
124	Evaluation of tungsten interatomic potentials for radiation damage simulations. Tungsten, 2020, 2, 3-14.	2.0	12
125	Diffusion properties of liquid lithiumâ€“lead alloys from atomistic simulation. Computational Materials Science, 2014, 93, 74-80.	1.4	11
126	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, 6511-6522.	1.3	11

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127	Ab initio soluteâ€“interstitial impurity interactions in vanadium alloys: the roles of vacancy. RSC Advances, 2016, 6, 78621-78628.	1.7	11
128	A molecular dynamics study of the transport properties of LiF-BeF 2 -ThF 4 molten salt. Journal of Molecular Liquids, 2017, 234, 220-226.	2.3	11
129	An ab initio study for probing iodization reactions on metallic anode surfaces of Liâ€“I₂ batteries. Journal of Materials Chemistry A, 2018, 6, 7807-7814.	5.2	11
130	Corrosion characteristics of copper in static liquid lithium under high vacuum. Journal of Nuclear Materials, 2019, 513, 282-292.	1.3	11
131	Effect of tungsten on the vacancy behaviors in Taâ€“W alloys from first-principles calculations. Solid State Communications, 2020, 306, 113767.	0.9	11
132	Chemistry of Defects in Crystalline Na₂Se: Implications for the Naâ€“Se Battery. Journal of Physical Chemistry C, 2020, 124, 27930-27936.	1.5	11
133	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. Fusion Engineering and Design, 2020, 159, 111850.	1.0	11
134	Double-Layer Honeycomb AlP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 2978-2986.	1.5	11
135	Finnisâ€“Sinclair-type potential for atomistic simulation of defects behaviour in V-Ti-Ta ternary system. Journal of Nuclear Materials, 2021, 557, 153231.	1.3	11
136	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.	4.1	11
137	Simulation calculations of surface segregation for Au-Cu alloys using an analytic embedded atom model. Physica Status Solidi A, 2005, 202, 2686-2699.	1.7	10
138	Atomistic simulation of helium bubble nucleation in palladium. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3185-3188.	0.6	10
139	First-principle study of the electronic structures and ferroelectric properties in BaZnF4. European Physical Journal B, 2010, 74, 447-450.	0.6	10
140	Development of a pair potential for Niâ€“He. Journal of Nuclear Materials, 2016, 472, 105-109.	1.3	10
141	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.	0.6	10
142	Compatibility of Molybdenum, Tungsten, and 304 Stainless Steel in Static Liquid Lithium Under High Vacuum. Plasma Physics Reports, 2018, 44, 671-677.	0.3	10
143	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. Energy Storage Materials, 2019, 17, 211-219.	9.5	10
144	Dynamics diffusion behaviors of Pd small clusters on a Pd(1â€‰1â€‰1) surface. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 045010.	0.8	9

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145	Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. Journal of Physical Chemistry C, 2013, 117, 17644-17649.	1.5	9
146	Does the Mgâ€“I₂ Battery Suffer Severe Shuttle Effect?. Journal of Physical Chemistry C, 2018, 122, 28518-28527.	1.5	9
147	Rectangular Tunnelâ€Structured Na 0.4 MnO 2 as a Promising Cathode Material Withstanding a High Cutoff Voltage for Naâ€Ion Batteries. ChemElectroChem, 2019, 6, 1711-1721.	1.7	9
148	Intrinsic strain-induced segregation in multiply twinned Cuâ€“Pt icosahedra. Physical Chemistry Chemical Physics, 2019, 21, 4802-4809.	1.3	9
149	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. Computational Materials Science, 2020, 173, 109412.	1.4	9
150	A better nanochannel tungsten film in releasing helium atoms. Journal of Nuclear Materials, 2020, 532, 152044.	1.3	9
151	Energetics and diffusional properties of helium in W-Ta systems studied by a new ternary potential. Journal of Nuclear Materials, 2021, 549, 152913.	1.3	9
152	Effect of transmutation elements Re and Ta on the vacancy formation and dissociation behaviors in W bulk. Computational Materials Science, 2020, 179, 109624.	1.4	9
153	Boosting the charge transfer of Li₂TiSiO₅ using nitrogen-doped carbon nanofibers: towards high-rate, long-life lithium-ion batteries. Nanoscale, 2020, 12, 19702-19710.	2.8	9
154	A First-Principles Study of MBene as Anode Material for Mg-Ion Battery. Journal of Electrochemical Energy Conversion and Storage, 2020, 17, .	1.1	9
155	First-principles study for the atomic structures and electronic properties of PbTiO3 oxygen-vacancies (001) surface. Surface Science, 2007, 601, 5412-5418.	0.8	8
156	The Rh influence on the surface distribution of the ternary alloy Ptâ€“Pdâ€“Rh. Applied Surface Science, 2007, 253, 6074-6079.	3.1	8
157	Self-diffusion dynamic behavior of atomic clusters on Re(0001) surface. Applied Surface Science, 2009, 255, 8883-8889.	3.1	8
158	Local identification of chemical ordering: Extension, implementation, and application of the common neighbor analysis for binary systems. Computational Materials Science, 2018, 143, 195-205.	1.4	8
159	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.	1.3	8
160	First-principles study of hydrogen-vacancy complexes in Be12Ti. Journal of Nuclear Materials, 2019, 525, 7-13.	1.3	8
161	Double-layer honeycomb AlP as a promising catalyst for Li-O2 and Na-O2 batteries. Applied Surface Science, 2021, 550, 149392.	3.1	8
162	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. Ceramics International, 2021, 47, 29386-29391.	2.3	8

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163	Shock-induced plasticity and phase transformation in single crystal magnesium: an interatomic potential and non-equilibrium molecular dynamics simulations. Journal of Physics Condensed Matter, 2022, 34, 115401.	0.7	8
164	Surface segregation of Alâ€“Pb immiscible alloy system with Monte Carlo simulation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2003, 98, 265-268.	1.7	7
165	Energetics and self-diffusion behavior of Zr atomic clusters on a Zr(0001) surface. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3267-3270.	0.6	7
166	Phase transition in nanocrystalline iron: Atomistic-level simulations. International Journal of Materials Research, 2010, 101, 1361-1368.	0.1	7
167	Magnetic properties in nitrogen-doped CeO2 from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 4858-4862.	1.3	7
168	Shock Waves Propagation and Phase Transition in Single Crystal Iron under Ramp Compression: Large Scale Parallel NEMD Simulations. Procedia Engineering, 2013, 61, 122-129.	1.2	7
169	Molecular Dynamics Simulation of the Displacement Cascades in Tungsten with Interstitial Helium Atoms. Fusion Science and Technology, 2014, 66, 112-117.	0.6	7
170	Atomistic simulation of mechanical properties and crack propagation of irradiated nickel. Computational Materials Science, 2016, 120, 21-28.	1.4	7
171	Clustering of Fe atoms in liquid Li and its effect on the viscosity of liquid Li. Nuclear Fusion, 2016, 56, 046004.	1.6	7
172	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.	0.6	7
173	Theoretical prediction of LiScO₂ nanosheets as a cathode material for Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2018, 20, 22351-22358.	1.3	7
174	Interactions of plasticity and phase transformation under shock in iron bicrystals. Journal of Applied Physics, 2019, 126, .	1.1	7
175	Suppressing/enhancing effect of rhenium on helium clusters evolution in tungsten: Dependence on rhenium distribution. Journal of Nuclear Materials, 2021, 543, 152545.	1.3	7
176	Revealing the hardening mechanisms of ion-irradiated nanostructured multilayers/substrate systems: A theoretical model. International Journal of Plasticity, 2021, 138, 102925.	4.1	7
177	On the relationship between potential of zero charge and solvent dynamics in the reversible hydrogen electrode. Journal of Catalysis, 2021, 398, 161-170.	3.1	7
178	Molecular dynamic simulations of displacement cascades in tungsten and tungstenâ€“rhenium alloys: Effects of grain boundary and/or Ïƒ phase. Journal of Nuclear Materials, 2022, 561, 153543.	1.3	7
179	Self-diffusion behaviors of Pd adatom and dimer on Pd(001) surface. Computational Materials Science, 2009, 47, 501-505.	1.4	6
180	Thermodynamic Properties of Nano-Silver and Alloy Particles. , 0, , .		6

#	Article	IF	Citations
181	Effect of voids on the tensile properties of vanadium nanowires. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 14-17.	0.6	6
182	Effect of Re content on the Î³/Î³â€² interface: A Monte Carlo simulation. Computational Materials Science, 2014, 89, 75-79.	1.4	6
183	Atomic simulation of helium trapping in displacement cascades. RSC Advances, 2016, 6, 27113-27118.	1.7	6
184	Surface premelting/recrystallization governing the collapse of open-cell nanoporous Cu via thermal annealing. Physical Chemistry Chemical Physics, 2018, 20, 16184-16192.	1.3	6
185	Ductile-brittle transition of open-cell nanoporous Cu in tension: A reliance of specific surface area. Scripta Materialia, 2020, 175, 43-48.	2.6	6
186	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. Computational Materials Science, 2020, 183, 109845.	1.4	6
187	Molecular dynamics simulation of shock wave propagation and spall failure in single crystal copper under cylindrical impact. Applied Physics Express, 2021, 14, 075504.	1.1	6
188	Phase transformation and mechanical stability of niobium aluminide (Nb3Al) induced by high pressures. Journal of Alloys and Compounds, 2021, 869, 159278.	2.8	6
189	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. Journal of Applied Physics, 2021, 130, .	1.1	6
190	Molecular dynamics simulation of the behavior of typical radiation defects under stress gradient field in tungsten. Journal of Applied Physics, 2021, 130, .	1.1	6
191	Molecular dynamics simulation study of helium bubble growth on W/Ta semi-coherent interface. Journal of Nuclear Materials, 2022, 558, 153340.	1.3	6
192	The mechanism of plasticity and phase transition in iron single crystals under cylindrically divergent shock loading. International Journal of Mechanical Sciences, 2022, 217, 107032.	3.6	6
193	Helium diffusion behavior and its retention in LaNiAl alloy from molecular dynamic simulations. Nuclear Instruments & Methods in Physics Research B, 2011, 269, 1689-1692.	0.6	5
194	The alloying processes in solidâ€“solid and liquidâ€“solid Liâ€“Pb interfaces with atomistic simulations. Journal of Alloys and Compounds, 2015, 632, 467-472.	2.8	5
195	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.	1.4	5
196	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.	1.1	5
197	Effect of symmetrical tilt grain boundary on the compatibility between copper and liquid lithium: Atomistic simulations. Journal of Alloys and Compounds, 2020, 835, 155212.	2.8	5
198	Unraveling the effects of anions in NixAy@CC (A=O, S, P) on Li-sulfur batteries. Materials Today Nano, 2021, 13, 100106.	2.3	5

#	Article	IF	Citations
199	Adsorption of hydrogen atoms on Pd (211), (311) and (511) stepped defective surfaces. Transactions of Nonferrous Metals Society of China, 2006, 16, s820-s823.	1.7	4
200	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.	0.3	4
201	Modified analytic embedded atom method potential for chromium. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065001.	0.8	4
202	Development of a Niâ€“Mo interatomic potential for irradiation simulation. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 045009.	0.8	4
203	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.	1.0	4
204	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. Metals, 2022, 12, 232.	1.0	4
205	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. Applied Physics Express, 2022, 15, 015503.	1.1	4
206	Effects of substitutional He atoms on the displacement cascades in Î±-Fe. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 72-74.	0.6	3
207	Stability and diffusion properties of Ti atom on Î±-uranium surfaces: A first-principles study. Computational Materials Science, 2015, 97, 201-208.	1.4	3
208	MD and OKMC simulations of the displacement cascades in nickel. Nuclear Science and Techniques/Hewuli, 2016, 27, 1.	1.3	3
209	Atomistic simulations of solidification process in B2-LiPb solid(0 0 1)-liquid system. Journal of Crystal Growth, 2017, 470, 113-121.	0.7	3
210	First-principles study of the adsorption properties of atoms and molecules on UN2 (001) surface. Journal of Nuclear Materials, 2017, 493, 124-131.	1.3	3
211	Simulation of radiation damages in molybdenum by combining molecular dynamics and OKMC. Nuclear Science and Techniques/Hewuli, 2017, 28, 1.	1.3	3
212	Investigation of wettability of Li on 316L SS surface and interfacial interactions for fusion device. Fusion Engineering and Design, 2018, 137, 420-426.	1.0	3
213	Effect of neon on the hydrogen behaviors in tungsten: AÂfirst-principles study. Journal of Nuclear Materials, 2018, 510, 492-498.	1.3	3
214	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.	0.8	3
215	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.	0.7	3
216	A First-Principles Study on Na and O Adsorption Behaviors on Mo (110) Surface. Metals, 2021, 11, 1322.	1.0	3

#	Article	IF	Citations
217	Formation mechanism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>âŒ©</mml:mo><mml:mn>111</mml:mn><mml:mo>〉 interstitial dislocation loops from irradiation-induced C15 clusters in tungsten. Physical Review Materials, 2021, 5, .	0.9	3
218	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Feâ€“10Niâ€“20Cr and Ni. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 075002.	0.8	3
219	Study of erosion and deposition characteristics of Li during liquid Li limiter experiment in HT-7. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 212801.	0.2	3
220	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.	0.8	3
221	Molecular Dynamics Simulations of Xe Behaviors at the Grain Boundary in UO2. Metals, 2022, 12, 763.	1.0	3
222	Monte carlo simulation of hydrogen adsorption on Ni surfaces. Frontiers of Physics in China, 2007, 2, 199-203.	1.0	2
223	Tungsten cluster migration on nanoparticles: minimum energy pathway and migration mechanism. European Physical Journal B, 2011, 80, 31-40.	0.6	2
224	Migration of defect clusters and xenon-vacancy clusters in uranium dioxide. International Journal of Modern Physics B, 2014, 28, 1450120.	1.0	2
225	Diffusion mechanisms at the Pb solidâ€“liquid interface: Atomic level point of view. Chemical Physics Letters, 2015, 634, 108-112.	1.2	2
226	Mesoscale elucidation of laser-assisted chemical deposition of Sn nanostructured electrodes. Journal of Applied Physics, 2015, 117, 214301.	1.1	2
227	Shock-induced migration of asymmetry tilt grain boundary in iron bicrystal: A case study of Î£3 [110]*. Chinese Physics B, 2019, 28, 126201.	0.7	2
228	DFT study on the nucleation of He bubbles in Pd: Effect of H and self-interstitial atoms. Journal of Nuclear Materials, 2021, 549, 152888.	1.3	2
229	A Mechanistic Study of Clustering and Diffusion of Molybdenum and Rhenium Atoms in Liquid Sodium. Metals, 2021, 11, 1430.	1.0	2
230	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. Metals, 2022, 12, 215.	1.0	2
231	Effect of nanopores on plasticity and their collapse mechanism in magnesium single crystal under shock loading. Journal of Applied Physics, 2022, 131, 055903.	1.1	2
232	Synergistically engineering of shell thickness and core ordering to boost the oxygen reduction performance. Physical Chemistry Chemical Physics, 0, , .	1.3	2
233	Investigation of the W/Y₂O₃ heterogeneous interface properties and its effect on hydrogen behavior using first-principles calculations. Nuclear Fusion, 2022, 62, 086015.	1.6	2
234	Monte Carlo simulations of strain-driven elemental depletion or enrichment in Cu95Al5 and Cu90Al10 alloys. Computational Materials Science, 2015, 106, 123-128.	1.4	1

#	Article	IF	Citations
235	Influence of hydrostatic strain on the behaviors of rhenium and osmium in tungsten. Journal of Nuclear Materials, 2019, 516, 111-117.	1.3	1
236	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.	0.8	1
237	Assessing Atomic-Phase Transitions and Ion Transport in Layered NaxNiO2 (x â‰ 0.67) Cathode Materials. Journal of Physical Chemistry C, 2021, 125, 4930-4937.	1.5	1
238	Modification of short-range repulsive interactions in ReaxFF reactive force field for Feâ€“Niâ€“Al alloy*. Chinese Physics B, 2021, 30, 086110.	0.7	1
239	Study on the relationship between surface and dislocation of nanoporous copper under cyclic shear loading. AIP Advances, 2022, 12, .	0.6	1
240	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.	1.0	1
241	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO2. Metals, 2022, 12, 789.	1.0	1
242	Preparation of titanium oxides films by CVD in O<inf>2</inf>-N<inf>2</inf> atmosphere. , 2011, , .		0
243	The interactions between nitrogen oxides and Î±-uranium surface. Nuclear Materials and Energy, 2021, 26, 100945.	0.6	0
244	Atomistic insights into interactions between oxygen and Î±â€“Zr (101-1) surface. Nuclear Materials and Energy, 2021, 27, 100974.	0.6	0
245	α-é“å'Œé''ä¸ºè•'ç¢°æ'žçš„å^†åå¨åŠ›å¦ æ¨¡æ‹Ÿç©¶. Zhongguo Kexue Jishu Kexue/Scientia Sinica Technologica,	0.8	0
246	The flow behavior of liquid Li in Cu micro-channels. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 104705.	0.2	0
247	Transition from Ductilizing to Hardening in Tungsten: The Dependence on Rhenium Distribution. SSRN Electronic Journal, 0, , .	0.4	0
248	Roles of triple and quadruple junctions on plasticity by phase-field crystal approach. Physica B: Condensed Matter, 2021, 626, 413449.	1.3	0
249	Ta concentration effect on nucleation of defects in W-Ta alloy from first-principles model. Materials Today Communications, 2022, 30, 103071.	0.9	0