Huiqiu Deng

List of Publications by Year
in descending order

249 papers	5,035 citations	109321 35 h-index	149698 56 g-index
250 all docs	250 docs citations	250 times ranked	4682 citing authors

#	Article	IF	Citations
1	Molecular dynamics simulation study of helium bubble growth on W/Ta semi-coherent interface. Journal of Nuclear Materials, 2022, 558, 153340.	2.7	6
2	Ta concentration effect on nucleation of defects in W-Ta alloy from first-principles model. Materials Today Communications, 2022, 30, 103071.	1.9	0
3	The mechanism of plasticity and phase transition in iron single crystals under cylindrically divergent shock loading. International Journal of Mechanical Sciences, 2022, 217, 107032.	6.7	6
4	Atomic insight into iron corrosion exposed to supercritical water environment with an improved Fe-H2O reactive force field. Applied Surface Science, 2022, 580, 152300.	6.1	14
5	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. Metals, 2022, 12, 232.	2.3	4
6	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. Applied Physics Express, 2022, 15, 015503.	2.4	4
7	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.	1.8	8
8	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. Metals, 2022, 12, 215.	2.3	2
9	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	2
10	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.	2.7	7
11	Study on the relationship between surface and dislocation of nanoporous copper under cyclic shear loading. AIP Advances, 2022, 12, .	1.3	1
12	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.	1.9	1
13	Molecular Dynamics Simulations of Xe Behaviors at the Grain Boundary in UO2. Metals, 2022, 12, 763.	2.3	3
14	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO2. Metals, 2022, 12, 789.	2.3	1
15	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.	8.8	11
16	Investigation of the W/Y₂O₃ heterogeneous interface properties and its effect on hydrogen behavior using first-principles calculations. Nuclear Fusion, 2022, 62, 086015.	3.5	2
17	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. International Journal of Mechanical Sciences, 2022, 226, 107373.	6.7	21
18	Unraveling the effects of anions in NixAy@CC (A=O, S, P) on Li-sulfur batteries. Materials Today Nano, 2021, 13, 100106.	4.6	5

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19	Electroreduction of Carbon Dioxide Driven by the Intrinsic Defects in the Carbon Plane of a Single Feâ€“N₄ Site. Advanced Materials, 2021, 33, e2003238.	21.0	202
20	Suppressing/enhancing effect of rhenium on helium clusters evolution in tungsten: Dependence on rhenium distribution. Journal of Nuclear Materials, 2021, 543, 152545.	2.7	7
21	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.	3.1	1
22	The interactions between nitrogen oxides and Î±-uranium surface. Nuclear Materials and Energy, 2021, 26, 100945.	1.3	0
23	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.	7.9	47
24	Revealing the hardening mechanisms of ion-irradiated nanostructured multilayers/substrate systems: A theoretical model. International Journal of Plasticity, 2021, 138, 102925.	8.8	7
25	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.	27.0	55
26	Energetics and diffusional properties of helium in W-Ta systems studied by a new ternary potential. Journal of Nuclear Materials, 2021, 549, 152913.	2.7	9
27	First-principles study on the dissolution and diffusion behavior of hydrogen in carbide precipitates. International Journal of Hydrogen Energy, 2021, 46, 22030-22039.	7.1	13
28	Atomistic insights into interactions between oxygen and Î±â€“Zr (101-1) surface. Nuclear Materials and Energy, 2021, 27, 100974.	1.3	0
29	On the relationship between potential of zero charge and solvent dynamics in the reversible hydrogen electrode. Journal of Catalysis, 2021, 398, 161-170.	6.2	7
30	DFT study on the nucleation of He bubbles in Pd: Effect of H and self-interstitial atoms. Journal of Nuclear Materials, 2021, 549, 152888.	2.7	2
31	Double-layer honeycomb AlP as a promising catalyst for Li-O2 and Na-O2 batteries. Applied Surface Science, 2021, 550, 149392.	6.1	8
32	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	6
33	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.	1.4	3
34	Phase transformation and mechanical stability of niobium aluminide (Nb3Al) induced by high pressures. Journal of Alloys and Compounds, 2021, 869, 159278.	5.5	6
35	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. Journal of Applied Physics, 2021, 130, .	2.5	6
36	A First-Principles Study on Na and O Adsorption Behaviors on Mo (110) Surface. Metals, 2021, 11, 1322.	2.3	3

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37	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.	9.1	23
38	Modification of short-range repulsive interactions in ReaxFF reactive force field for Feâ€“Niâ€“Al alloy*. Chinese Physics B, 2021, 30, 086110.	1.4	1
39	Theoretical Evaluation of MBenes as Catalysts for the CO₂ Reduction Reaction. Journal of Physical Chemistry C, 2021, 125, 19183-19189.	3.1	17
40	A Mechanistic Study of Clustering and Diffusion of Molybdenum and Rhenium Atoms in Liquid Sodium. Metals, 2021, 11, 1430.	2.3	2
41	Molecular dynamics simulation of the behavior of typical radiation defects under stress gradient field in tungsten. Journal of Applied Physics, 2021, 130, .	2.5	6
42	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>âŒ interstitial dislocation loops from irradiation-induced C15 clusters in tungsten. Physical Review Materials, 2021, 5, .	2.4	3
43	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. Ceramics International, 2021, 47, 29386-29391.	4.8	8
44	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.	5.2	14
45	Machine learning to predict aluminum segregation to magnesium grain boundaries. Scripta Materialia, 2021, 204, 114150.	5.2	18
46	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. Journal of Nuclear Materials, 2021, 556, 153162.	2.7	17
47	Finnisâ€“Sinclair-type potential for atomistic simulation of defects behaviour in V-Ti-Ta ternary system. Journal of Nuclear Materials, 2021, 557, 153231.	2.7	11
48	Mechanisms for <100> interstitial dislocation loops to diffuse in BCC iron. Nature Communications, 2021, 12, 225.	12.8	22
49	Roles of triple and quadruple junctions on plasticity by phase-field crystal approach. Physica B: Condensed Matter, 2021, 626, 413449.	2.7	0
50	Ductile-brittle transition of open-cell nanoporous Cu in tension: A reliance of specific surface area. Scripta Materialia, 2020, 175, 43-48.	5.2	6
51	Segregation and aggregation of rhenium in tungsten grain boundary: Energetics, configurations and strengthening effects. Journal of Nuclear Materials, 2020, 528, 151867.	2.7	16
52	Effect of tungsten on the vacancy behaviors in Taâ€“W alloys from first-principles calculations. Solid State Communications, 2020, 306, 113767.	1.9	11
53	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.	10.3	32
54	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. Computational Materials Science, 2020, 173, 109412.	3.0	9

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55	Interatomic potentials and defect properties of Feâ€“Crâ€“Al alloys. Journal of Nuclear Materials, 2020, 541, 152421.	2.7	18
56	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.	1.9	4
57	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.	10.3	44
58	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	5
59	Chemistry of Defects in Crystalline Na₂Se: Implications for the Naâ€“Se Battery. Journal of Physical Chemistry C, 2020, 124, 27930-27936.	3.1	11
60	Effect of symmetrical tilt grain boundary on the compatibility between copper and liquid lithium: Atomistic simulations. Journal of Alloys and Compounds, 2020, 835, 155212.	5.5	5
61	New Insight into the Confinement Effect of Microporous Carbon in Li/Se Battery Chemistry: A Cathode with Enhanced Conductivity. Small, 2020, 16, e2000266.	10.0	40
62	Dielectric Polarization in Inverse Spinelâ€Structured Mg₂TiO₄ Coating to Suppress Oxygen Evolution of Liâ€Rich Cathode Materials. Advanced Materials, 2020, 32, e2000496.	21.0	134
63	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. Computational Materials Science, 2020, 183, 109845.	3.0	6
64	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. Fusion Engineering and Design, 2020, 159, 111850.	1.9	11
65	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. Acta Materialia, 2020, 196, 133-143.	7.9	124
66	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.	2.0	1
67	A better nanochannel tungsten film in releasing helium atoms. Journal of Nuclear Materials, 2020, 532, 152044.	2.7	9
68	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. Computational Materials Science, 2020, 177, 109555.	3.0	18
69	Double-Layer Honeycomb AlP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 2978-2986.	3.1	11
70	Interatomic potentials of Wâ€“V and Wâ€“Mo binary systems for point defects studies. Journal of Nuclear Materials, 2020, 531, 152020.	2.7	18
71	Evaluation of tungsten interatomic potentials for radiation damage simulations. Tungsten, 2020, 2, 3-14.	4.8	12
72	Effect of transmutation elements Re and Ta on the vacancy formation and dissociation behaviors in W bulk. Computational Materials Science, 2020, 179, 109624.	3.0	9

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73	Boosting the charge transfer of Li₂TiSiO₅ using nitrogen-doped carbon nanofibers: towards high-rate, long-life lithium-ion batteries. Nanoscale, 2020, 12, 19702-19710.	5.6	9
74	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.	2.0	3
75	A First-Principles Study of MBene as Anode Material for Mg-Ion Battery. Journal of Electrochemical Energy Conversion and Storage, 2020, 17, .	2.1	9
76	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.	2.0	3
77	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. Energy Storage Materials, 2019, 17, 211-219.	18.0	10
78	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	3
79	Theoretical insights into nitrogen fixation on Ti₂C and Ti₂CO₂ in a lithiumâ€“nitrogen battery. Journal of Materials Chemistry A, 2019, 7, 19950-19960.	10.3	21
80	Interactions of plasticity and phase transformation under shock in iron bicrystals. Journal of Applied Physics, 2019, 126, .	2.5	7
81	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.	2.7	8
82	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.	20.2	77
83	First-principles study of hydrogen-vacancy complexes in Be12Ti. Journal of Nuclear Materials, 2019, 525, 7-13.	2.7	8
84	Transition from ductilizing to hardening in tungsten: The dependence on rhenium distribution. Acta Materialia, 2019, 181, 110-123.	7.9	26
85	Effect of particle packing and density on shock response in ordered arrays of Ni + Al nanoparticles. Physical Chemistry Chemical Physics, 2019, 21, 7272-7280.	2.8	13
86	Dopant Segregation Boosting Highâ€Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. Advanced Materials, 2019, 31, e1904816.	21.0	89
87	Shock-induced migration of asymmetry tilt grain boundary in iron bicrystal: A case study of Î£3 [110]*. Chinese Physics B, 2019, 28, 126201.	1.4	2
88	Molecular dynamics simulations of shock loading of nearly fully dense granular Niâ€“Al composites. Physical Chemistry Chemical Physics, 2019, 21, 20252-20261.	2.8	13
89	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. Journal of Nuclear Materials, 2019, 527, 151821.	2.7	13
90	Molecular dynamics simulations of high-energy radiation damage in W and Wâ€“Re alloys. Journal of Nuclear Materials, 2019, 524, 9-20.	2.7	36

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91	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.	2.7	32
92	Orientation and grain-boundary dependence of shock-induced plasticity and transformation in nanocrystalline Ti. Physical Review B, 2019, 99, .	3.2	16
93	Ab initio study of interstitial helium clusters in 3C-SiC. Journal of Nuclear Materials, 2019, 521, 13-20.	2.7	12
94	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. Nuclear Fusion, 2019, 59, 076020.	3.5	13
95	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.	5.2	18
96	Development of a Niâ€“Mo interatomic potential for irradiation simulation. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 045009.	2.0	4
97	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	3.0	26
98	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.	3.4	9
99	Intrinsic strain-induced segregation in multiply twinned Cuâ€“Pt icosahedra. Physical Chemistry Chemical Physics, 2019, 21, 4802-4809.	2.8	9
100	Corrosion characteristics of copper in static liquid lithium under high vacuum. Journal of Nuclear Materials, 2019, 513, 282-292.	2.7	11
101	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.	8.8	40
102	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.	8.0	27
103	Influence of hydrostatic strain on the behaviors of rhenium and osmium in tungsten. Journal of Nuclear Materials, 2019, 516, 111-117.	2.7	1
104	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. Journal of Alloys and Compounds, 2019, 775, 1184-1198.	5.5	30
105	Development of interatomic potentials for Fe-Cr-Al alloy with the particle swarm optimization method. Journal of Alloys and Compounds, 2019, 780, 881-887.	5.5	22
106	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. Computational Materials Science, 2019, 156, 47-55.	3.0	19
107	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. Fusion Engineering and Design, 2018, 128, 75-81.	1.9	23
108	Robust pseudo-capacitive Li-I2 battery enabled by catalytic, adsorptive N-doped graphene interlayer. Energy Storage Materials, 2018, 14, 129-135.	18.0	67

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109	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. Computational Materials Science, 2018, 148, 242-248.	3.0	16
110	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. Computational Materials Science, 2018, 149, 435-441.	3.0	12
111	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.	2.7	29
112	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	2.8	18
113	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	2.7	57
114	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	2.5	25
115	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.	10.3	20
116	Oxygen adsorption and diffusion on Î³-U(0â€¯0â€¯1) surface: Effect of titanium. Computational Materials Science, 2018, 144, 85-91.	3.0	13
117	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.	10.3	11
118	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. Computational Materials Science, 2018, 141, 293-301.	3.0	22
119	Local identification of chemical ordering: Extension, implementation, and application of the common neighbor analysis for binary systems. Computational Materials Science, 2018, 143, 195-205.	3.0	8
120	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. Current Applied Physics, 2018, 18, 183-190.	2.4	12
121	Shock wave propagation, plasticity, and void collapse in open-cell nanoporous Ta. Physical Chemistry Chemical Physics, 2018, 20, 28039-28048.	2.8	19
122	Retention and diffusion of transmutation H and He atoms in Be₁₂Ti: first-principles calculations. RSC Advances, 2018, 8, 35735-35743.	3.6	12
123	Shockwave generates < 100 > dislocation loops in bcc iron. Nature Communications, 2018, 9, 4880.	12.8	106
124	Does the Mgâ€“I₂ Battery Suffer Severe Shuttle Effect?. Journal of Physical Chemistry C, 2018, 122, 28518-28527.	3.1	9
125	Investigation of wettability of Li on 316L SS surface and interfacial interactions for fusion device. Fusion Engineering and Design, 2018, 137, 420-426.	1.9	3
126	Surface premelting/recrystallization governing the collapse of open-cell nanoporous Cu via thermal annealing. Physical Chemistry Chemical Physics, 2018, 20, 16184-16192.	2.8	6

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127	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. Journal of Alloys and Compounds, 2018, 763, 1-10.	5.5	13
128	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.	3.0	5
129	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.	0.9	4
130	Compatibility of Molybdenum, Tungsten, and 304 Stainless Steel in Static Liquid Lithium Under High Vacuum. Plasma Physics Reports, 2018, 44, 671-677.	0.9	10
131	Nanochannel structures in W enhance radiation tolerance. Acta Materialia, 2018, 153, 147-155.	7.9	63
132	Theoretical prediction of LiScO₂ nanosheets as a cathode material for Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2018, 20, 22351-22358.	2.8	7
133	Effect of neon on the hydrogen behaviors in tungsten: AÂfirst-principles study. Journal of Nuclear Materials, 2018, 510, 492-498.	2.7	3
134	Modified analytic embedded atom method potential for chromium. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065001.	2.0	4
135	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. Fusion Engineering and Design, 2017, 117, 188-193.	1.9	13
136	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.	5.5	17
137	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.	3.5	32
138	A molecular dynamics study of the transport properties of LiF-BeF 2 -ThF 4 molten salt. Journal of Molecular Liquids, 2017, 234, 220-226.	4.9	11
139	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. Journal of Materials Research, 2017, 32, 1474-1483.	2.6	14
140	Atomistic simulations of solidification process in B2-LiPb solid(0 0 1)-liquid system. Journal of Crystal Growth, 2017, 470, 113-121.	1.5	3
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.	1.4	10
142	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. Physical Chemistry Chemical Physics, 2017, 19, 17607-17617.	2.8	20
143	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. Computational Materials Science, 2017, 137, 273-281.	3.0	18
144	First-principles study of the adsorption properties of atoms and molecules on UN2 (001) surface. Journal of Nuclear Materials, 2017, 493, 124-131.	2.7	3

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145	Simulation of radiation damages in molybdenum by combining molecular dynamics and OKMC. Nuclear Science and Techniques/Hewuli, 2017, 28, 1.	3.4	3
146	Tensile mechanical properties of Ni-based superalloy of nanophases using molecular dynamics simulation. Physica Status Solidi (B): Basic Research, 2016, 253, 726-732.	1.5	23
147	MD and OKMC simulations of the displacement cascades in nickel. Nuclear Science and Techniques/Hewuli, 2016, 27, 1.	3.4	3
148	Atomistic simulation of mechanical properties and crack propagation of irradiated nickel. Computational Materials Science, 2016, 120, 21-28.	3.0	7
149	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. Computational Materials Science, 2016, 119, 114-119.	3.0	23
150	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.	2.7	17
151	Ab initio soluteâ€“interstitial impurity interactions in vanadium alloys: the roles of vacancy. RSC Advances, 2016, 6, 78621-78628.	3.6	11
152	Clustering of Fe atoms in liquid Li and its effect on the viscosity of liquid Li. Nuclear Fusion, 2016, 56, 046004.	3.5	7
153	Orientation dependences of the Fe-Li solid-liquid interface properties: Atomistic simulations. Journal of Alloys and Compounds, 2016, 687, 875-884.	5.5	14
154	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. Computational Materials Science, 2016, 122, 1-10.	3.0	19
155	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.	1.4	7
156	Development of a pair potential for Niâ€“He. Journal of Nuclear Materials, 2016, 472, 105-109.	2.7	10
157	Atomic simulation of helium trapping in displacement cascades. RSC Advances, 2016, 6, 27113-27118.	3.6	6
158	First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys. Journal of Alloys and Compounds, 2016, 660, 55-61.	5.5	31
159	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. Computational Materials Science, 2016, 111, 203-208.	3.0	23
160	The flow behavior of liquid Li in Cu micro-channels. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 104705.	0.5	0
161	Composition Dependence of Lithium Diffusion in Lithium Silicide: A Density Functional Theory Study. ChemElectroChem, 2015, 2, 1292-1297.	3.4	25
162	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.	3.4	18

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163	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. International Journal of Plasticity, 2015, 71, 218-236.	8.8	57
164	The alloying processes in solidâ€“solid and liquidâ€“solid Liâ€“Pb interfaces with atomistic simulations. Journal of Alloys and Compounds, 2015, 632, 467-472.	5.5	5
165	Evaluating Pristine and Modified SnS₂ as a Lithium-Ion Battery Anode: A First-Principles Study. ACS Applied Materials & Interfaces, 2015, 7, 4000-4009.	8.0	75
166	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. Scripta Materialia, 2015, 100, 106-109.	5.2	17
167	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.	2.8	11
168	Monte Carlo simulations of strain-driven elemental depletion or enrichment in Cu95Al5 and Cu90Al10 alloys. Computational Materials Science, 2015, 106, 123-128.	3.0	1
169	Diffusion mechanisms at the Pb solidâ€“liquid interface: Atomic level point of view. Chemical Physics Letters, 2015, 634, 108-112.	2.6	2
170	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. Journal of Nuclear Materials, 2015, 467, 398-405.	2.7	16
171	A molecular dynamics study of helium diffusion and clustering in fcc nickel. Computational Materials Science, 2015, 107, 54-57.	3.0	17
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