Wang-Yu Hu

List of Publications by Year
in descending order

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398	8,339	57631	95083
papers	citations	44 h-index	68 g-index

402	402	402	7213
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Highly effective Ru-based Heusler alloy catalysts for N2 activation: A theoretical study. Applied Surface Science, 2022, 575, 151658.	3.1	9
2	A hostâ€“guest self-assembly strategy to enhance Ï€-electron densities in ultrathin porous carbon nitride nanocages toward highly efficient hydrogen evolution. Chemical Engineering Journal, 2022, 430, 132880.	6.6	33
3	Crystallographic-orientation-dependence plasticity of niobium under shock compressions. International Journal of Plasticity, 2022, 150, 103195.	4.1	11
4	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
5	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. Metals, 2022, 12, 232.	1.0	4
6	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. Applied Physics Express, 2022, 15, 015503.	1.1	4
7	Highly efficient tree search algorithm for irreducible site-occupancy configurations. Physical Review B, 2022, 105, .	1.1	6
8	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
9	Critical structural invariant during high-pressure solidification of copper. MRS Communications, 2022, 12, 45-50.	0.8	2
10	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. Metals, 2022, 12, 215.	1.0	2
11	Synergistic Effects of Crystal Phase and Strain for N₂ Dissociation on Ru(0001) Surfaces with Multilayered Hexagonal Close-Packed Structures. ACS Omega, 2022, 7, 4492-4500.	1.6	4
12	Two-dimensional chromium phosphorus monolayer based gas sensors to detect NOx: A first-principles study. Results in Physics, 2022, 32, 105100.	2.0	10
13	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
14	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
15	Influence of orientation on crack propagation of aluminum by molecular dynamics. European Physical Journal B, 2022, 95, 1.	0.6	0
16	Atomistic simulation on the generation of defects in Cu/SiC composites during cooling. Journal of Materials Science and Technology, 2022, 123, 1-12.	5.6	6
17	Molecular dynamics study of fatigue behavior of nickel single-crystal under cyclic shear deformation and hyper-gravity condition. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 055006.	0.8	3
18	Pt-based intermetallic compounds with tunable activity and selectivity toward hydrogen production from formic acid. Applied Surface Science, 2022, 597, 153530.	3.1	7

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19	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO2. Metals, 2022, 12, 789.	1.0	1
20	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
21	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. International Journal of Mechanical Sciences, 2022, 226, 107373.	3.6	21
22	The Role of Grain Boundaries in the Corrosion Process of Fe Surface: Insights from ReaxFF Molecular Dynamic Simulations. Metals, 2022, 12, 876.	1.0	4
23	Analysis of fatigue crack propagation mechanism of Ni₃Al under supergravity at atomic size. AIP Advances, 2022, 12, 065223.	0.6	1
24	The Microstructural Evolution of Nickel Single Crystal under Cyclic Deformation and Hyper-Gravity Conditions: A Molecular Dynamics Study. Metals, 2022, 12, 1128.	1.0	3
25	Unraveling the mechanisms of aluminum solidification under hyper-gravity condition from molecular dynamics simulations. Journal of Applied Physics, 2022, 132, .	1.1	3
26	Unsaturated coordination polymer frameworks as multifunctional sulfur reservoir for fast and durable lithium-sulfur batteries. Nano Energy, 2021, 79, 105393.	8.2	37
27	A two-dimensional MoS2/SnS heterostructure for promising photocatalytic performance: First-principles investigations. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 126, 114453.	1.3	17
28	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
29	Strain and interfacial engineering to accelerate hydrogen evolution reaction of two-dimensional phosphorus carbide*. Chinese Physics B, 2021, 30, 027101.	0.7	2
30	The interactions between nitrogen oxides and Î±-uranium surface. Nuclear Materials and Energy, 2021, 26, 100945.	0.6	0
31	Highâ€Throughput Oneâ€Photon Excitation Pathway in 0D/3D Heterojunctions for Visibleâ€Light Driven Hydrogen Evolution. Advanced Functional Materials, 2021, 31, 2100816.	7.8	92
32	Effects of Se substitution on the Schottky barrier of a MoS _x Se_(2âˆ’x)/graphene heterostructure. Journal Physics D: Applied Physics, 2021, 54, 265302.	1.3	5
33	Oneâ€Photon Excitation Pathway: Highâ€Throughput Oneâ€Photon Excitation Pathway in 0D/3D Heterojunctions for Visibleâ€Light Driven Hydrogen Evolution (Adv. Funct. Mater. 18/2021). Advanced Functional Materials, 2021, 31, 2170125.	7.8	1
34	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
35	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
36	Atomistic insights into interactions between oxygen and Î±â€“Zr (101-1) surface. Nuclear Materials and Energy, 2021, 27, 100974.	0.6	0

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37	Amorphous B-doped graphitic carbon nitride quantum dots with high photoluminescence quantum yield of near 90% and their sensitive detection of Fe2+/Cd2+. Science China Materials, 2021, 64, 3037-3050.	3.5	17
38	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
39	Predicted Polymeric and Layered Covalent Networks in Transition Metal Pentazolate M(cyclo-N5)x Phases at Ambient and High Pressure: Up to 20 Nitrogen Atoms per Metal. Chemistry of Materials, 2021, 33, 5298-5307.	3.2	10
40	2D Amorphous CoO Incorporated gâ€C₃N₄ Nanotubes for Improved Photocatalytic Performance. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100254.	1.2	6
41	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. Journal of Applied Physics, 2021, 130, .	1.1	6
42	High-throughput computational design for 2D van der Waals functional heterostructures: Fragility of Anderson's rule and beyond. Applied Physics Letters, 2021, 119, .	1.5	24
43	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
44	Effects of electric field and strain on the Schottky barrier of the bilayer van der Waals heterostructures of graphene and pure/hydrogenated PC3 monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 133, 114785.	1.3	3
45	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
46	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>â interstitial dislocation loops from irradiation-induced C15 clusters in tungsten. Physical Review Materials, 2021, 5, .	0.9	3
47	Monolayer PtTe2: A promising candidate for NO2 sensor with ultrahigh sensitivity and selectivity. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 134, 114925.	1.3	11
48	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. Ceramics International, 2021, 47, 29386-29391.	2.3	8
49	Atomistic simulation of the surface configuration of the Niâ€“Re cluster. Thin Solid Films, 2021, 737, 138938.	0.8	1
50	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. Journal of Nuclear Materials, 2021, 556, 153162.	1.3	17
51	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
52	Generalized Synthetic Strategy for Amorphous Transition Metal Oxidesâ€Based 2D Heterojunctions with Superb Photocatalytic Hydrogen and Oxygen Evolution. Advanced Functional Materials, 2021, 31, 2009230.	7.8	97
53	Study on the effect of non-centrosymmetric orientation in shocked and ramp compressed Î± iron. Materials Today Communications, 2021, 29, 102893.	0.9	1
54	Dipole Engineering of Two-Dimensional van der Waals Heterostructures for Enhanced Power-Conversion Efficiency: The Case of Janus <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mrow><mml:mi>Se</mml:mi><mml:mi mathvariant="normal">S</mml:mi></mml:mrow></mml:math>. Physical Review Applied, 2021, 16, .	1.5	39

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55	In situ construction of hierarchical graphitic carbon nitride homojunction as robust bifunctional photoelectrocatalyst for overall water splitting. Journal of Chemical Technology and Biotechnology, 2020, 95, 758-769.	1.6	6
56	Interfacial charge modulation: carbon quantum dot implanted carbon nitride double-deck nanoframes for robust visible-light photocatalytic tetracycline degradation. Nanoscale, 2020, 12, 3135-3145.	2.8	45
57	Ultrahigh Sensitivity and Selectivity of Pentagonal SiC₂ Monolayer Gas Sensors: The Synergistic Effect of Composition and Structural Topology. Physica Status Solidi (B): Basic Research, 2020, 257, 1900445.	0.7	11
58	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. Computational Materials Science, 2020, 173, 109412.	1.4	9
59	Algorithm for generating irreducible site-occupancy configurations. Physical Review B, 2020, 102, .	1.1	16
60	Interatomic potentials and defect properties of Feâ€“Crâ€“Al alloys. Journal of Nuclear Materials, 2020, 541, 152421.	1.3	18
61	The phase transition of rapidly super-cooled Tungsten under 100 GPa. Chemical Physics Letters, 2020, 755, 137789.	1.2	2
62	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
63	Chemistry of Defects in Crystalline Na₂Se: Implications for the Naâ€“Se Battery. Journal of Physical Chemistry C, 2020, 124, 27930-27936.	1.5	11
64	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
65	Ultra-thin tubular graphitic carbon Nitride-Carbon Dot lateral heterostructures: One-Step synthesis and highly efficient catalytic hydrogen generation. Chemical Engineering Journal, 2020, 397, 125470.	6.6	72
66	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. Computational Materials Science, 2020, 183, 109845.	1.4	6
67	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. Fusion Engineering and Design, 2020, 159, 111850.	1.0	11
68	Dynamic self-diffusion behaviors of nickel adatoms on clusters with Wulff shape. International Journal of Modern Physics B, 2020, 34, 2050015.	1.0	2
69	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
70	Structural damage and phase stability of Al0.3CoCrFeNi high entropy alloy under high temperature ion irradiation. Acta Materialia, 2020, 188, 1-15.	3.8	83
71	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
72	Hierarchical Self-assembly of Well-Defined Louver-Like P-Doped Carbon Nitride Nanowire Arrays with Highly Efficient Hydrogen Evolution. Nano-Micro Letters, 2020, 12, 52.	14.4	45

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73	A comparative atomic simulation study of the configurations in M-Al (M = Mg, Ni, and Fe) nanoalloys: influence of alloying ability, surface energy, atomic radius, and atomic arrangement. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	3
74	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
75	From monolayer to lateral heterostructure of functionalized phosphorus carbide: Evolution of electronic properties. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 118, 113962.	1.3	6
76	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
77	A design rule for two-dimensional van der Waals heterostructures with unconventional band alignments. Physical Chemistry Chemical Physics, 2020, 22, 3037-3047.	1.3	19
78	Interatomic potentials of Wâ€“V and Wâ€“Mo binary systems for point defects studies. Journal of Nuclear Materials, 2020, 531, 152020.	1.3	18
79	Atomic simulation of mechanical properties of irradiated iron. International Journal of Modern Physics C, 2020, 31, 2050027.	0.8	1
80	Evaluation of tungsten interatomic potentials for radiation damage simulations. Tungsten, 2020, 2, 3-14.	2.0	12
81	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
82	Strain and Electric Field Controllable Schottky Barriers and Contact Types in Graphene-MoTe2 van der Waals Heterostructure. Nanoscale Research Letters, 2020, 15, 180.	3.1	15
83	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
84	Comparative investigation of microjetting from tin surface subjected to laser and plane impact loadings via molecular dynamics simulations. Mechanics of Materials, 2020, 148, 103479.	1.7	4
85	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
86	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
87	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
88	Interactions of plasticity and phase transformation under shock in iron bicrystals. Journal of Applied Physics, 2019, 126, .	1.1	7
89	Strategy to boost catalytic activity of polymeric carbon nitride: synergistic effect of controllable in situ surface engineering and morphology. Nanoscale, 2019, 11, 16393-16405.	2.8	45
90	Monolayer Phosphoreneâ€“Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. Nanoscale Research Letters, 2019, 14, 233.	3.1	10

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91	Steering charge kinetics boost the photocatalytic activity of graphitic carbon nitride: heteroatom-mediated spatial charge separation and transfer. Journal Physics D: Applied Physics, 2019, 53, 015502.	1.3	28
92	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
93	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
94	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
95	Assessment of van der Waals inclusive density functional theory methods for adsorption and selective dehydrogenation of formic acid on Pt(111) surface. Physical Chemistry Chemical Physics, 2019, 21, 21049-21056.	1.3	23
96	Influence of Irradiation on Mechanical Properties of Nickel. Advances in Materials Science and Engineering, 2019, 2019, 1-6.	1.0	0
97	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. Journal of Nuclear Materials, 2019, 527, 151821.	1.3	13
98	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
99	Chlorine doped graphitic carbon nitride nanorings as an efficient photoresponsive catalyst for water oxidation and organic decomposition. Journal of Materials Science and Technology, 2019, 35, 2288-2296.	5.6	61
100	Tunable Schottky barrier in van der Waals heterostructures of graphene and hydrogenated phosphorus carbide monolayer: first-principles calculations. Journal Physics D: Applied Physics, 2019, 52, 305104.	1.3	18
101	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
102	Doping-induced enhancement of crystallinity in polymeric carbon nitride nanosheets to improve their visible-light photocatalytic activity. Nanoscale, 2019, 11, 6876-6885.	2.8	128
103	Doping-Induced Hydrogen-Bond Engineering in Polymeric Carbon Nitride To Significantly Boost the Photocatalytic H₂ Evolution Performance. ACS Applied Materials & Interfaces, 2019, 11, 17341-17349.	4.0	71
104	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. Nuclear Fusion, 2019, 59, 076020.	1.6	13
105	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
106	Development of a Niâ€“Mo interatomic potential for irradiation simulation. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 045009.	0.8	4
107	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	1.4	26
108	Protonated supramolecular complex-induced porous graphitic carbon nitride nanosheets as bifunctional catalyst for water oxidation and organic pollutant degradation. Journal of Materials Science, 2019, 54, 7637-7650.	1.7	16

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109	Intrinsic strain-induced segregation in multiply twinned Cuâ€“Pt icosahedra. Physical Chemistry Chemical Physics, 2019, 21, 4802-4809.	1.3	9
110	Electrostatic Potential Anomaly in 2D Janus Transition Metal Dichalcogenides. Annalen Der Physik, 2019, 531, 1900369.	0.9	13
111	Penta-Graphene as a Potential Gas Sensor for NOx Detection. Nanoscale Research Letters, 2019, 14, 306.	3.1	52
112	Twoâ€Đimensional GaX/SnS₂ (Xâ€‰=â€‰S, Se) van der Waals Heterostructures for Photovoltaic Application: Heteroatom Doping Strategy to Boost Power Conversion Efficiency. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800565.	1.2	35
113	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
114	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
115	Isotype heterojunction g-C₃N₄/g-C₃N₄ nanosheets as 2D support to highly dispersed 0D metal oxide nanoparticles: Generalized self-assembly and its high photocatalytic activity. Journal Physics D: Applied Physics, 2019, 52, 025501.	1.3	46
116	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
117	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. Computational Materials Science, 2019, 156, 47-55.	1.4	19
118	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Twoâ€Đimensional WS₂/TX₂CO₂ (TXâ€‰=â€‰Ti, Zr) van der Waals Heterostructures. Physica Status Solidi (B): Basic Research, 2019, 256, 1800377.	0.7	2
119	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
120	Self-assembled hierarchical carbon/g-C₃N₄ composite with high photocatalytic activity. Journal Physics D: Applied Physics, 2018, 51, 135501.	1.3	12
121	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
122	Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B₂₀/Ag₃PO₄ van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 6151-6158.	1.5	7
123	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
124	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	1.3	18
125	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	1.3	57
126	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	1.1	25

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127	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
128	Oxygen adsorption and diffusion on Î³-U(0â€¯0â€¯1) surface: Effect of titanium. Computational Materials Science, 2018, 144, 85-91.	1.4	13
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	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. Computational Materials Science, 2018, 141, 293-301.	1.4	22
131	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
132	Interfacial Interactions in Monolayer and Fewâ€Layer SnS/CH₃NH₃PbI₃ Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. ChemPhysChem, 2018, 19, 291-299.	1.0	12
133	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. Current Applied Physics, 2018, 18, 183-190.	1.1	12
134	Does the Mgâ€“I₂ Battery Suffer Severe Shuttle Effect?. Journal of Physical Chemistry C, 2018, 122, 28518-28527.	1.5	9
135	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. Journal of Physical Chemistry C, 2018, 122, 28065-28074.	1.5	20
136	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
137	Facile in situ construction of mediator-free direct Z-scheme g-C₃N₄/CeO₂ heterojunctions with highly efficient photocatalytic activity. Journal Physics D: Applied Physics, 2018, 51, 275302.	1.3	110
138	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
139	Dispersive and covalent interactions in all-carbon heterostructures consisting of penta-graphene and fullerene: topological effect. Journal Physics D: Applied Physics, 2018, 51, 305301.	1.3	12
140	In-situ construction of 2D direct Z-scheme g-C3N4/g-C3N4 homojunction with high photocatalytic activity. Journal of Materials Science, 2018, 53, 15882-15894.	1.7	52
141	Substrate-induced magnetism and topological phase transition in silicene. Nanoscale, 2018, 10, 14667-14677.	2.8	10
142	Simultaneous dispersive and covalent monolayer MoS2/TiO2 cluster heterostructures: Insights into their enhanced photocatalytic activity. Superlattices and Microstructures, 2018, 121, 64-74.	1.4	0
143	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
144	Theoretical prediction of LiScO₂ nanosheets as a cathode material for Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2018, 20, 22351-22358.	1.3	7

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145	Effect of neon on the hydrogen behaviors in tungsten: AÂfirst-principles study. Journal of Nuclear Materials, 2018, 510, 492-498.	1.3	3
146	Surface segregation and alloying of immiscible Li-Cu and miscible Li-Pb nanoalloys investigated by basin-hopping Monte Carlo method. Computational Materials Science, 2018, 154, 371-379.	1.4	6
147	Modified analytic embedded atom method potential for chromium. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065001.	0.8	4
148	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. Fusion Engineering and Design, 2017, 117, 188-193.	1.0	13
149	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
150	Simultaneous covalent and noncovalent carbon nanotube/Ag₃PO₄ hybrids: new insights into the origin of enhanced visible light photocatalytic performance. Physical Chemistry Chemical Physics, 2017, 19, 7955-7963.	1.3	13
151	Construction of g-C 3 N 4 /CeO 2 /ZnO ternary photocatalysts with enhanced photocatalytic performance. Journal of Physics and Chemistry of Solids, 2017, 106, 1-9.	1.9	116
152	Hybrid TiO₂/graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. Catalysis Science and Technology, 2017, 7, 1423-1432.	2.1	20
153	Atomic simulations for configurations and solid-liquid interface of Li-Fe and Li-Cu icosahedra. Journal of Nanoparticle Research, 2017, 19, 1.	0.8	3
154	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
155	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. Journal of Materials Research, 2017, 32, 1474-1483.	1.2	14
156	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
157	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
158	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. Physical Chemistry Chemical Physics, 2017, 19, 17607-17617.	1.3	20
159	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. Computational Materials Science, 2017, 137, 273-281.	1.4	18
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