

Wang-Yu Hu

List of Publications by Year in descending order

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papers

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57631

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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	Insights into Enhanced Visible-Light Photocatalytic Hydrogen Evolution of g-C ₃ N ₄ and Highly Reduced Graphene Oxide Composite: The Role of Oxygen. Chemistry of Materials, 2015, 27, 1612-1621.	3.2	252
2	Size Effect on the Thermodynamic Properties of Silver Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 2359-2369.	1.5	194
3	Analytic modified embedded atom potentials for HCP metals. Journal of Physics Condensed Matter, 2001, 13, 1193-1213.	0.7	157
4	Hydroxyapatite/titania sol-gel coatings on titanium-zirconium alloy for biomedical applications. Acta Biomaterialia, 2007, 3, 403-410.	4.1	145
5	Two-Dimensional MoS ₂ -Graphene-Based Multilayer van der Waals Heterostructures: Enhanced Charge Transfer and Optical Absorption, and Electric-Field Tunable Dirac Point and Band Gap. Chemistry of Materials, 2017, 29, 5504-5512.	3.2	131
6	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
7	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
8	Point-defect properties in body-centered cubic transition metals with analytic EAM interatomic potentials. Computational Materials Science, 2002, 23, 175-189.	1.4	119
9	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
10	Surface Segregation and Structural Features of Bimetallic Au-Pt Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 11026-11032.	1.5	115
11	Facile <i>in situ</i> construction of mediator-free direct Z-scheme g-C ₃ N ₄ /CeO ₂ heterojunctions with highly efficient photocatalytic activity. Journal Physics D: Applied Physics, 2018, 51, 275302.	1.3	110
12	Au-Ag Bimetallic Nanoparticles: Surface Segregation and Atomic-Scale Structure. Journal of Physical Chemistry C, 2011, 115, 11355-11363.	1.5	103
13	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
14	Generalized Synthetic Strategy for Amorphous Transition Metal Oxides-Based 2D Heterojunctions with Superb Photocatalytic Hydrogen and Oxygen Evolution. Advanced Functional Materials, 2021, 31, 2009230.	7.8	97
15	High-Throughput One-Photon Excitation Pathway in 0D/3D Heterojunctions for Visible-Light Driven Hydrogen Evolution. Advanced Functional Materials, 2021, 31, 2100816.	7.8	92
16	Surface-area-difference model for thermodynamic properties of metallic nanocrystals. Journal Physics D: Applied Physics, 2005, 38, 1429-1436.	1.3	85
17	Structural damage and phase stability of Al _{0.3} CoCrFeNi high entropy alloy under high temperature ion irradiation. Acta Materialia, 2020, 188, 1-15.	3.8	83
18	Effects of Sr and Sn on microstructure and corrosion resistance of Mg-Zr-Ca magnesium alloy for biomedical applications. Materials & Design, 2012, 39, 379-383.	5.1	81

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19	Calculation of formation enthalpies and phase stability for Ru-Al alloys using an analytic embedded atom model. Journal of Alloys and Compounds, 1999, 287, 159-162.	2.8	75
20	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
21	Doping-Induced Hydrogen-Bond Engineering in Polymeric Carbon Nitride To Significantly Boost the Photocatalytic H ₂ Evolution Performance. ACS Applied Materials & Interfaces, 2019, 11, 17341-17349.	4.0	71
22	Oxidation behavior of sputter-deposited NiCrAlY coating. Surface and Coatings Technology, 2003, 165, 241-247.	2.2	68
23	Melting Behaviors of Nanocrystalline Ag. Journal of Physical Chemistry B, 2005, 109, 20339-20342.	1.2	68
24	First-principles study for vacancy-induced magnetism in nonmagnetic ferroelectric BaTiO ₃ . Physical Chemistry Chemical Physics, 2009, 11, 10934.	1.3	67
25	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
26	Melting evolution and diffusion behavior of vanadium nanoparticles. European Physical Journal B, 2005, 45, 547-554.	0.6	66
27	Sol-gel derived hydroxyapatite/titania biocoatings on titanium substrate. Materials Letters, 2006, 60, 1575-1578.	1.3	64
28	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
29	Calculation of thermodynamic properties of Mg-RE (RE = Sc, Y, Pr, Nd, Gd, Tb, Dy, Ho or Er) alloys by an analytic modified embedded atom method. Journal Physics D: Applied Physics, 2000, 33, 711-718.	1.3	61
30	First-principles study of the origin of magnetism induced by intrinsic defects in monolayer MoS ₂ . Applied Surface Science, 2016, 361, 199-205.	3.1	61
31	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
32	First-principles study of structural, electronic, and multiferroic properties in BiCoO ₃ . Journal of Chemical Physics, 2007, 126, 154708.	1.2	60
33	Molecular dynamics simulation of fatigue crack propagation in bcc iron under cyclic loading. International Journal of Fatigue, 2014, 68, 253-259.	2.8	60
34	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. International Journal of Plasticity, 2015, 71, 218-236.	4.1	57
35	Dual role of monolayer MoS ₂ in enhanced photocatalytic performance of hybrid MoS ₂ /SnO ₂ nanocomposite. Journal of Applied Physics, 2016, 119, .	1.1	57
36	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	1.3	57

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37	Magnetoelectric effect and critical thickness for ferroelectricity in Co/BaTiO ₃ /Co multiferroic tunnel junctions. Journal of Applied Physics, 2011, 109, .	1.1	53
38	In-situ construction of 2D direct Z-scheme g-C ₃ N ₄ /g-C ₃ N ₄ homojunction with high photocatalytic activity. Journal of Materials Science, 2018, 53, 15882-15894.	1.7	52
39	Penta-Graphene as a Potential Gas Sensor for NO _x Detection. Nanoscale Research Letters, 2019, 14, 306.	3.1	52
40	Hot Corrosion of a Single Crystal Ni-Base Superalloy by Na-Salts at 900°C. Oxidation of Metals, 2006, 65, 137-150.	1.0	50
41	First-principles study of electronic and magnetic properties in Co doped BaTiO ₃ . European Physical Journal B, 2015, 88, 1.	0.6	47
42	Isotype heterojunction g-C ₃ N ₄ /g-C ₃ N ₄ nanosheets as 2D support to highly dispersed OD metal oxide nanoparticles: Generalized self-assembly and its high photocatalytic activity. Journal Physics D: Applied Physics, 2019, 52, 025501.	1.3	46
43	Enhancement of the bioactivity of titanium oxide nanotubes by precalcification. Materials Letters, 2008, 62, 3035-3038.	1.3	45
44	Strategy to boost catalytic activity of polymeric carbon nitride: synergistic effect of controllable <i>in situ</i> surface engineering and morphology. Nanoscale, 2019, 11, 16393-16405.	2.8	45
45	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
46	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
47	Monte Carlo simulation of the surface segregation of Pt-Pd and Pt-Ir alloys with an analytic embedded-atom method. Surface Science, 2002, 517, 177-185.	0.8	44
48	Hydrogen storage properties of destabilized MgH ₂ -Li ₃ AlH ₆ system. International Journal of Hydrogen Energy, 2010, 35, 8122-8129.	3.8	42
49	Energy dissipation and defect generation in nanocrystalline silicon carbide. Physical Review B, 2010, 81, .	1.1	42
50	Diffusion of small He clusters in bulk and grain boundaries in δ -Fe. Journal of Nuclear Materials, 2013, 442, S667-S673.	1.3	41
51	The application of the analytic embedded atom potentials to alkali metals. Modelling and Simulation in Materials Science and Engineering, 2002, 10, 707-726.	0.8	40
52	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
53	Uniaxial strain-modulated conductivity in manganite superlattice (LaMnO ₃ /SrMnO ₃). Applied Physics Letters, 2011, 98, 031910.	1.5	40
54	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

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55	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
56	Acoustic-phonon transmission and thermal conductance in a double-bend quantum waveguide. Journal of Applied Physics, 2005, 98, 093524.	1.1	39
57	Dipole Engineering of Two-Dimensional van der Waals Heterostructures for Enhanced Power-Conversion Efficiency: The Case of Janus Ga_2Se_3 . Physical Review Applied, 2021, 16, .	1.5	39
58	Melting, melting competition, and structural transitions between shell-closed icosahedral and octahedral nickel nanoclusters. Physical Review B, 2006, 73, .	1.1	38
59	First-principles calculation of the elastic constants, the electronic density of states and the ductility mechanism of the intermetallic compounds: YAg, YCu and YRh. Physica B: Condensed Matter, 2008, 403, 3792-3797.	1.3	38
60	Critical thickness for ferroelectricity and magnetoelectric effect in multiferroic tunnel junction with symmetrical and asymmetrical electrodes. European Physical Journal B, 2013, 86, 1.	0.6	38
61	Long-Time Scale Molecular Dynamics Study of Diffusion Dynamics of Small Cu Clusters on Cu(111) Surface. Journal of Physical Chemistry C, 2008, 112, 2074-2078.	1.5	37
62	Unsaturated coordination polymer frameworks as multifunctional sulfur reservoir for fast and durable lithium-sulfur batteries. Nano Energy, 2021, 79, 105393.	8.2	37
63	Surface Segregation and Chemical Ordering Patterns of Ag-Pd Nanoalloys: Energetic Factors, Nanoscale Effects, and Catalytic Implication. Journal of Physical Chemistry C, 2014, 118, 27850-27860.	1.5	36
64	Molecular dynamics simulations of high-energy radiation damage in W and W-Re alloys. Journal of Nuclear Materials, 2019, 524, 9-20.	1.3	36
65	Melting temperature: From nanocrystalline to amorphous phase. Journal of Chemical Physics, 2006, 125, 184504.	1.2	35
66	Molecular dynamics simulation of polycrystalline molybdenum nanowires under uniaxial tensile strain: Size effects. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 3030-3036.	1.3	35
67	Two-Dimensional GaX/SnS_2 ($\text{X} = \text{S, Se}$) 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
68	Corrosion behavior in SBF for titania coatings on Mg-Ca alloy. Journal of Materials Science, 2011, 46, 2365-2369.	1.7	34
69	The improved electrochemical properties of novel La-Mg-Ni -based hydrogen storage composites. Electrochimica Acta, 2007, 52, 6700-6706.	2.6	33
70	Chemical Ordering and Surface Segregation in Cu-Pt Nanoalloys: The Synergetic Roles in the Formation of Multishell Structures. Journal of Physical Chemistry C, 2015, 119, 21515-21527.	1.5	33
71	A host-guest self-assembly strategy to enhance I^- -electron densities in ultrathin porous carbon nitride nanocages toward highly efficient hydrogen evolution. Chemical Engineering Journal, 2022, 430, 132880.	6.6	33
72	Electrochemical hydrogen storage properties of $\text{La}_{0.7}\text{Mg}_{0.3}\text{Ni}_{3.5}\text{Ti}_{0.17}\text{Zr}_{0.08}\text{V}_{0.35}\text{Cr}_{0.1}\text{Ni}_{0.3}\text{La}_{0.7}\text{Mg}_{0.3}\text{Ni}_{3.5}\text{Ti}_{0.17}\text{Zr}_{0.08}\text{V}_{0.35}\text{Cr}_{0.1}\text{Ni}_{0.3}$ composites. International Journal of Hydrogen Energy, 2008, 33, 755-761.	3.8	32

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73	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
74	Theoretical calculation of thermodynamic data for gold-rare earth alloys with the embedded-atom method. Journal of Alloys and Compounds, 2006, 420, 83-93.	2.8	31
75	Comparative study of microstructural evolution during melting and crystallization. Journal of Chemical Physics, 2006, 125, 014503.	1.2	31
76	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
77	Elastic constants and thermodynamic properties of Mg-Pr, Mg-Dy, Mg-Y intermetallics with atomistic simulations. Journal Physics D: Applied Physics, 2007, 40, 7584-7592.	1.3	30
78	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
79	First-principles study of pressure-induced metal-insulator transition in BiNiO ₃ . Applied Physics Letters, 2007, 91, 101901.	1.5	29
80	Thermal shock behavior of EB-PVD thermal barrier coatings. Surface and Coatings Technology, 2007, 201, 7387-7391.	2.2	29
81	Vacancy-induced magnetism in BaTiO ₃ (001) thin films based on density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 4738.	1.3	29
82	Discontinuity effect on the phonon transmission and thermal conductance in a dielectric quantum waveguide. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 336, 245-252.	0.9	28
83	Substrate Dependence of Growth Configurations for Co-Cu Bimetallic Clusters. Crystal Growth and Design, 2012, 12, 2978-2985.	1.4	28
84	Electronic properties and photoactivity of monolayer MoS ₂ /fullerene van der Waals heterostructures. RSC Advances, 2016, 6, 43228-43236.	1.7	28
85	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
86	Atomistic simulation of the segregation profiles in Mo-Re random alloys. Surface Science, 2003, 543, 95-102.	0.8	27
87	Sol-gel derived HA/TiO ₂ double coatings on Ti scaffolds for orthopaedic applications. Transactions of Nonferrous Metals Society of China, 2006, 16, s209-s216.	1.7	27
88	Diffusion and growth of nickel, iron and magnesium adatoms on the aluminum truncated octahedron: A molecular dynamics simulation. Surface Science, 2012, 606, 971-980.	0.8	27
89	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Na-Se Batteries. ACS Applied Materials & Interfaces, 2019, 11, 4995-5002.	4.0	27
90	Phase transition of iron-based single crystals under ramp compressions with extreme strain rates. International Journal of Plasticity, 2017, 96, 56-80.	4.1	27

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91	Ab initio study of structural and electronic properties of SrTiO ₃ (001) oxygen-vacancy surfaces. Journal of Chemical Physics, 2006, 124, 174701.	1.2	26
92	Morphology, dimension, and composition dependence of thermodynamically preferred atomic arrangements in Ag-Pt nanoalloys. Faraday Discussions, 2013, 162, 293.	1.6	26
93	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	1.4	26
94	Preparation and properties of HVOF NiAl nanostructured coatings. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 478, 1-8.	2.6	25
95	The calculation of surface free energy based on embedded atom method for solid nickel. Applied Surface Science, 2013, 265, 375-378.	3.1	25
96	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. Journal of Applied Physics, 2018, 123, .	1.1	25
97	Calculation of the cohesive energy of metallic nanoparticles by the Lennard-Jones potential. Materials Letters, 2004, 58, 1745-1749.	1.3	24
98	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
99	Melting temperature of Pb nanostructural materials from free energy calculation. Journal of Chemical Physics, 2008, 128, 074710.	1.2	23
100	Surface Self-Diffusion Behavior of a Pt Adatom on Wulff Polyhedral Clusters. Journal of Physical Chemistry C, 2009, 113, 21501-21505.	1.5	23
101	Gibbs free energy, surface stress and melting point of nanoparticle. Physica B: Condensed Matter, 2013, 425, 90-94.	1.3	23
102	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
103	Tunable synthesis of various ZnO architectural structures with enhanced photocatalytic activities. Materials Letters, 2016, 175, 68-71.	1.3	23
104	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. Computational Materials Science, 2016, 119, 114-119.	1.4	23
105	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. Computational Materials Science, 2016, 111, 203-208.	1.4	23
106	Noncovalent Functionalization of Monolayer MoS ₂ with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. Journal of Physical Chemistry C, 2017, 121, 21921-21929.	1.5	23
107	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. Fusion Engineering and Design, 2018, 128, 75-81.	1.0	23
108	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

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109	Unraveling TM Migration Mechanisms in $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ by Modeling and Experimental Studies. Nano Letters, 2021, 21, 6875-6881.	4.5	23
110	Shell and subshell periodic structures of icosahedral nickel nanoclusters. Journal of Chemical Physics, 2005, 122, 214501.	1.2	22
111	A comparative study of helium atom diffusion via an interstitial mechanism in nickel and palladium. Physica Status Solidi (B): Basic Research, 2006, 243, 579-583.	0.7	22
112	Atomistic simulations of the Fe(001)-Li solid-liquid interface. Fusion Engineering and Design, 2014, 89, 2894-2901.	1.0	22
113	Non-covalent functionalization of WS_2 monolayer with small fullerenes: tuning electronic properties and photoactivity. Dalton Transactions, 2016, 45, 13383-13391.	1.6	22
114	Enhanced photocatalytic performance of an Ag_3PO_4 photocatalyst via fullerene modification: first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 2878-2886.	1.3	22
115	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. Computational Materials Science, 2018, 141, 293-301.	1.4	22
116	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
117	Theoretical insights into nitrogen fixation on Ti_2C and Ti_2CO_2 in a lithium-nitrogen battery. Journal of Materials Chemistry A, 2019, 7, 19950-19960.	5.2	21
118	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. International Journal of Mechanical Sciences, 2022, 226, 107373.	3.6	21
119	Structure and crystallization of amorphous Fe-B alloys obtained by chemical plating. Physica B: Condensed Matter, 1991, 175, 396-400.	1.3	20
120	Electrical and Thermal Conductivities of Nickel-Zirconia Cermets. Journal of the American Ceramic Society, 1998, 81, 2209-2212.	1.9	20
121	A study of the behavior of helium atoms at Ni grain boundaries. Physica Status Solidi (B): Basic Research, 2006, 243, 2702-2710.	0.7	20
122	Atomistic behavior of helium-vacancy clusters in aluminum. Journal of Nuclear Materials, 2006, 350, 83-88.	1.3	20
123	Atomistic simulations of solid solution strengthening in Ni-based superalloy. Computational Materials Science, 2013, 68, 132-137.	1.4	20
124	First-principles calculation of self-diffusion coefficients in Ni_3Al . Journal of Alloys and Compounds, 2014, 612, 361-364.	2.8	20
125	Hybrid TiO_2 /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
126	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. Physical Chemistry Chemical Physics, 2017, 19, 17607-17617.	1.3	20

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127	A first-principles investigation of the ScO ₂ monolayer as the cathode material for alkali metal-ion batteries. Journal of Materials Chemistry A, 2018, 6, 3171-3180.	5.2	20
128	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. Journal of Physical Chemistry C, 2018, 122, 28065-28074.	1.5	20
129	Crystallization study of electroless Fe-Sn-B amorphous alloy deposits. Journal of Alloys and Compounds, 1999, 287, 234-238.	2.8	19
130	Synthesis and Characterization of Nanocrystalline Iron Aluminide Intermetallic Compounds. Materials Transactions, 2003, 44, 2678-2687.	0.4	19
131	Analytic embedded-atom method approach to studying the surface segregation of Al-Mg alloys. Applied Surface Science, 2004, 221, 408-414.	3.1	19
132	LATTICE THERMAL CONDUCTIVITY IN A HOLLOW SILICON NANOWIRE. International Journal of Modern Physics B, 2005, 19, 1017-1027.	1.0	19
133	Atomistic study of small helium bubbles in plutonium. Journal of Alloys and Compounds, 2007, 444-445, 300-304.	2.8	19
134	The alloying element dependence of the local lattice deformation and the elastic properties of Ni3Al: A molecular dynamics simulation. Journal of Applied Physics, 2014, 115, .	1.1	19
135	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. Computational Materials Science, 2016, 122, 1-10.	1.4	19
136	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. Computational Materials Science, 2019, 156, 47-55.	1.4	19
137	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
138	Microstructures and mechanical properties of as cast Mg-Zr-Ca alloys for biomedical applications. Materials Technology, 2012, 27, 52-54.	1.5	18
139	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. Computational Materials Science, 2017, 137, 273-281.	1.4	18
140	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithium-sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	1.3	18
141	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
142	Effect of MCl3 (M=La, U or Sc) component on the local structures and transport properties of LiCl-KCl-MCl3 eutectic: A molecular dynamics study. Electrochimica Acta, 2019, 306, 366-376.	2.6	18
143	Interatomic potentials and defect properties of Fe-Cr-Al alloys. Journal of Nuclear Materials, 2020, 541, 152421.	1.3	18
144	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

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145	Interatomic potentials of Wâ€“V and Wâ€“Mo binary systems for point defects studies. Journal of Nuclear Materials, 2020, 531, 152020.	1.3	18
146	Thermocyclic behavior of sputtered NiCrAlY/EB-PVD 7 wt.%Y2O3â€“ZrO2 thermal barrier coatings. Surface and Coatings Technology, 2006, 200, 3770-3774.	2.2	17
147	Microstructural changes and elemental diffusion of sputtered NiCrAlY coating on a Ni-base SC superalloy subjected to high temperature. Materials Letters, 2007, 61, 5169-5172.	1.3	17
148	Diffusion of tungsten clusters on tungsten (110) surface. European Physical Journal B, 2009, 68, 479-485.	0.6	17
149	Embedded-atom-method interatomic potentials from lattice inversion. Journal of Physics Condensed Matter, 2010, 22, 375503.	0.7	17
150	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. Scripta Materialia, 2015, 100, 106-109.	2.6	17
151	A molecular dynamics study of helium diffusion and clustering in fcc nickel. Computational Materials Science, 2015, 107, 54-57.	1.4	17
152	Study of the corrosion behaviors of 304 austenite stainless steel specimens exposed to static liquid lithium at 600ÅK. Journal of Nuclear Materials, 2016, 480, 25-31.	1.3	17
153	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
154	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
155	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
156	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. Journal of Nuclear Materials, 2021, 556, 153162.	1.3	17
157	Graded coatings prepared by plasma spraying with Ni-coated ZrO2 powders. Surface and Coatings Technology, 1998, 105, 102-108.	2.2	16
158	Molecular dynamics simulations of grain growth in nanocrystalline Ag. Journal of Crystal Growth, 2006, 286, 512-517.	0.7	16
159	The dynamic diffusion behaviors of 2D small Fe clusters on a Fe(110) surface. Journal of Physics Condensed Matter, 2007, 19, 446009.	0.7	16
160	Atomistic simulation of Pt trimer on Pt(1â€“1) surface. Applied Surface Science, 2007, 253, 8825-8829.	3.1	16
161	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. Journal of Nuclear Materials, 2015, 467, 398-405.	1.3	16
162	Atomic simulation of fatigue crack propagation in Ni3Al. Applied Physics A: Materials Science and Processing, 2015, 118, 1399-1406.	1.1	16

163	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
164	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
165	Algorithm for generating irreducible site-occupancy configurations. Physical Review B, 2020, 102, .	1.1	16
166	Strain-driven phase transition of molybdenum nanowire under uniaxial tensile strain. Computational Materials Science, 2010, 50, 373-377.	1.4	15
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