

# Wang-Yu Hu

## List of Publications by Citations

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388  
papers

6,195  
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39  
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58  
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402  
ext. papers

7,281  
ext. citations

3.6  
avg, IF

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L-index

#	Paper	IF	Citations
388	Insights into Enhanced Visible-Light Photocatalytic Hydrogen Evolution of g-C <sub>3</sub> N <sub>4</sub> and Highly Reduced Graphene Oxide Composite: The Role of Oxygen. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 1612-1621	9.6	219
387	Size Effect on the Thermodynamic Properties of Silver Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 2359-2369	3.8	156
386	Analytic modified embedded atom potentials for HCP metals. <i>Journal of Physics Condensed Matter</i> , <b>2001</b> , 13, 1193-1213	1.8	142
385	Hydroxyapatite/titania sol-gel coatings on titanium-zirconium alloy for biomedical applications. <i>Acta Biomaterialia</i> , <b>2007</b> , 3, 403-10	10.8	128
384	Surface Segregation and Structural Features of Bimetallic AuPt Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 11026-11032	3.8	106
383	Point-defect properties in body-centered cubic transition metals with analytic EAM interatomic potentials. <i>Computational Materials Science</i> , <b>2002</b> , 23, 175-189	3.2	106
382	Two-Dimensional MoS <sub>2</sub> -Graphene-Based Multilayer van der Waals Heterostructures: Enhanced Charge Transfer and Optical Absorption, and Electric-Field Tunable Dirac Point and Band Gap. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 5504-5512	9.6	99
381	Doping-induced enhancement of crystallinity in polymeric carbon nitride nanosheets to improve their visible-light photocatalytic activity. <i>Nanoscale</i> , <b>2019</b> , 11, 6876-6885	7.7	93
380	AuAg Bimetallic Nanoparticles: Surface Segregation and Atomic-Scale Structure. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 11355-11363	3.8	92
379	Construction of g-C <sub>3</sub> N <sub>4</sub> /CeO <sub>2</sub> /ZnO ternary photocatalysts with enhanced photocatalytic performance. <i>Journal of Physics and Chemistry of Solids</i> , <b>2017</b> , 106, 1-9	3.9	83
378	An atomic study on the shock-induced plasticity and phase transition for iron-based single crystals. <i>International Journal of Plasticity</i> , <b>2014</b> , 59, 180-198	7.6	80
377	Facile in situ construction of mediator-free direct Z-scheme g-C <sub>3</sub> N <sub>4</sub> /CeO <sub>2</sub> heterojunctions with highly efficient photocatalytic activity. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 275302	3	80
376	Surface-area-difference model for thermodynamic properties of metallic nanocrystals. <i>Journal Physics D: Applied Physics</i> , <b>2005</b> , 38, 1429-1436	3	76
375	Calculation of formation enthalpies and phase stability for RuAl alloys using an analytic embedded atom model. <i>Journal of Alloys and Compounds</i> , <b>1999</b> , 287, 159-162	5.7	71
374	Effects of Sr and Sn on microstructure and corrosion resistance of MgZrTi magnesium alloy for biomedical applications. <i>Materials &amp; Design</i> , <b>2012</b> , 39, 379-383		65
373	Point-defect properties in HCP rare earth metals with analytic modified embedded atom potentials. <i>European Physical Journal B</i> , <b>2003</b> , 34, 429-440	1.2	63
372	Temperature dependence of atomic relaxation and vibrations for the vicinal Ni(9 7 7) surface: a molecular dynamics study. <i>Surface Science</i> , <b>2004</b> , 572, 439-448	1.8	62

371	First-principles study for vacancy-induced magnetism in nonmagnetic ferroelectric BaTiO <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 10934-8	3.6	61
370	Melting evolution and diffusion behavior of vanadium nanoparticles. <i>European Physical Journal B</i> , <b>2005</b> , 45, 547-554	1.2	59
369	Sol-gel derived hydroxyapatite/titania biocoatings on titanium substrate. <i>Materials Letters</i> , <b>2006</b> , 60, 1575-1578	3.3	58
368	Oxidation behavior of sputter-deposited NiCrAlY coating. <i>Surface and Coatings Technology</i> , <b>2003</b> , 165, 241-247	4.4	58
367	First-principles study of the origin of magnetism induced by intrinsic defects in monolayer MoS <sub>2</sub> . <i>Applied Surface Science</i> , <b>2016</b> , 361, 199-205	6.7	52
366	First-principles study of structural, electronic, and multiferroic properties in BiCoO <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 154708	3.9	52
365	Melting behaviors of nanocrystalline Ag. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 20339-42	3.4	52
364	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. <i>Journal Physics D: Applied Physics</i> , <b>2000</b> , 33, 711-718	3	52
363	Dual role of monolayer MoS <sub>2</sub> in enhanced photocatalytic performance of hybrid MoS <sub>2</sub> /SnO <sub>2</sub> nanocomposite. <i>Journal of Applied Physics</i> , <b>2016</b> , 119, 205704	2.5	49
362	Magnetoelectric effect and critical thickness for ferroelectricity in Co/BaTiO <sub>3</sub> /Co multiferroic tunnel junctions. <i>Journal of Applied Physics</i> , <b>2011</b> , 109, 114107	2.5	48
361	Doping-Induced Hydrogen-Bond Engineering in Polymeric Carbon Nitride To Significantly Boost the Photocatalytic H Evolution Performance. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 17341-17349	9.5	46
360	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. <i>Acta Materialia</i> , <b>2020</b> , 196, 133-143	8.4	45
359	Generalized Synthetic Strategy for Amorphous Transition Metal Oxides-Based 2D Heterojunctions with Superb Photocatalytic Hydrogen and Oxygen Evolution. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2009230	15.6	45
358	Structural damage and phase stability of Al <sub>0.3</sub> CoCrFeNi high entropy alloy under high temperature ion irradiation. <i>Acta Materialia</i> , <b>2020</b> , 188, 1-15	8.4	42
357	First-principles study of electronic and magnetic properties in Co doped BaTiO <sub>3</sub> . <i>European Physical Journal B</i> , <b>2015</b> , 88, 1	1.2	41
356	Chlorine doped graphitic carbon nitride nanorings as an efficient photoresponsive catalyst for water oxidation and organic decomposition. <i>Journal of Materials Science and Technology</i> , <b>2019</b> , 35, 2288-2296	9.1	40
355	Enhancement of the bioactivity of titanium oxide nanotubes by precalcification. <i>Materials Letters</i> , <b>2008</b> , 62, 3035-3038	3.3	40
354	Monte Carlo simulation of the surface segregation of PtPd and PtNi alloys with an analytic embedded-atom method. <i>Surface Science</i> , <b>2002</b> , 517, 177-185	1.8	40

353	The application of the analytic embedded atom potentials to alkali metals. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2002</b> , 10, 707-726	2	40
352	High-Throughput One-Photon Excitation Pathway in 0D/3D Heterojunctions for Visible-Light Driven Hydrogen Evolution. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2100816	15.6	40
351	Uniaxial strain-modulated conductivity in manganite superlattice (LaMnO <sub>3</sub> /SrMnO <sub>3</sub> ). <i>Applied Physics Letters</i> , <b>2011</b> , 98, 031910	3.4	39
350	Hot Corrosion of a Single Crystal Ni-Base Superalloy by Na-Salts at 900°C. <i>Oxidation of Metals</i> , <b>2006</b> , 65, 137-150	1.6	39
349	Ultra-thin tubular graphitic carbon Nitride-Carbon Dot lateral heterostructures: One-Step synthesis and highly efficient catalytic hydrogen generation. <i>Chemical Engineering Journal</i> , <b>2020</b> , 397, 125470	14.7	38
348	Molecular dynamics simulation of fatigue crack propagation in bcc iron under cyclic loading. <i>International Journal of Fatigue</i> , <b>2014</b> , 68, 253-259	5	38
347	Coupling between plasticity and phase transition of polycrystalline iron under shock compressions. <i>International Journal of Plasticity</i> , <b>2015</b> , 71, 218-236	7.6	38
346	Melting, melting competition, and structural transitions between shell-closed icosahedral and octahedral nickel nanoclusters. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	37
345	Acoustic-phonon transmission and thermal conductance in a double-bend quantum waveguide. <i>Journal of Applied Physics</i> , <b>2005</b> , 98, 093524	2.5	37
344	Critical thickness for ferroelectricity and magnetoelectric effect in multiferroic tunnel junction with symmetrical and asymmetrical electrodes. <i>European Physical Journal B</i> , <b>2013</b> , 86, 1	1.2	36
343	Energy dissipation and defect generation in nanocrystalline silicon carbide. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	36
342	First-principles calculation of the elastic constants, the electronic density of states and the ductility mechanism of the intermetallic compounds: YAg, YCu and YRh. <i>Physica B: Condensed Matter</i> , <b>2008</b> , 403, 3792-3797	2.8	36
341	Modified analytic EAM potentials for the binary immiscible alloy systems. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , <b>2003</b> , 355, 357-367	5.3	36
340	Isotype heterojunction g-C <sub>3</sub> N <sub>4</sub> /g-C <sub>3</sub> N <sub>4</sub> nanosheets as 2D support to highly dispersed 0D metal oxide nanoparticles: Generalized self-assembly and its high photocatalytic activity. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 52, 025501	3	36
339	New interatomic potentials of W, Re and W-Re alloy for radiation defects. <i>Journal of Nuclear Materials</i> , <b>2018</b> , 502, 141-153	3.3	35
338	Hydrogen storage properties of destabilized MgH <sub>2</sub> □□3AlH <sub>6</sub> system. <i>International Journal of Hydrogen Energy</i> , <b>2010</b> , 35, 8122-8129	6.7	35
337	In-situ construction of 2D direct Z-scheme g-C <sub>3</sub> N <sub>4</sub> /g-C <sub>3</sub> N <sub>4</sub> homojunction with high photocatalytic activity. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 15882-15894	4.3	33
336	Strategy to boost catalytic activity of polymeric carbon nitride: synergistic effect of controllable in situ surface engineering and morphology. <i>Nanoscale</i> , <b>2019</b> , 11, 16393-16405	7.7	33

335	Long-Time Scale Molecular Dynamics Study of Diffusion Dynamics of Small Cu Clusters on Cu(111) Surface. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 2074-2078	3.8	33
334	Diffusion of Co, Ru and Re in Ni-based superalloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 588, 163-169	5.7	32
333	The improved electrochemical properties of novel LaMgNi-based hydrogen storage composites. <i>Electrochimica Acta</i> , <b>2007</b> , 52, 6700-6706	6.7	30
332	Diffusion of small He clusters in bulk and grain boundaries in Fe. <i>Journal of Nuclear Materials</i> , <b>2013</b> , 442, S667-S673	3.3	29
331	Comparative study of microstructural evolution during melting and crystallization. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 014503	3.9	29
330	Melting temperature: from nanocrystalline to amorphous phase. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 184504	3.9	29
329	Surface Segregation and Chemical Ordering Patterns of AgPd Nanoalloys: Energetic Factors, Nanoscale Effects, and Catalytic Implication. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 27850-27860	3.8	28
328	Electrochemical hydrogen storage properties of La <sub>0.7</sub> Mg <sub>0.3</sub> Ni <sub>3.5</sub> Ti <sub>0.17</sub> Zr <sub>0.08</sub> V <sub>0.35</sub> Cr <sub>0.1</sub> Ni <sub>0.3</sub> La <sub>0.7</sub> Mg <sub>0.3</sub> Ni <sub>3.5</sub> Ti <sub>0.17</sub> Zr <sub>0.08</sub> V <sub>0.35</sub> Cr <sub>0.1</sub> Ni <sub>0.3</sub> composites. <i>International Journal of Hydrogen Energy</i> , <b>2008</b> , 33, 755-761	6.7	28
327	Theoretical calculation of thermodynamic data for gold-rare earth alloys with the embedded-atom method. <i>Journal of Alloys and Compounds</i> , <b>2006</b> , 420, 83-93	5.7	28
326	Discontinuity effect on the phonon transmission and thermal conductance in a dielectric quantum waveguide. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2005</b> , 336, 245-252	2.3	28
325	Penta-Graphene as a Potential Gas Sensor for NO Detection. <i>Nanoscale Research Letters</i> , <b>2019</b> , 14, 306	5	28
324	Two-Dimensional GaX/SnS <sub>2</sub> (X = S, Se) van der Waals Heterostructures for Photovoltaic Application: Heteroatom Doping Strategy to Boost Power Conversion Efficiency. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2019</b> , 13, 1800565	2.5	27
323	Vacancy-induced magnetism in BaTiO <sub>3</sub> (001) thin films based on density functional theory. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 4738-45	3.6	26
322	Molecular dynamics simulation of polycrystalline molybdenum nanowires under uniaxial tensile strain: Size effects. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2008</b> , 40, 3030-3036	3	26
321	First-principles study of pressure-induced metal-insulator transition in BiNiO <sub>3</sub> . <i>Applied Physics Letters</i> , <b>2007</b> , 91, 101901	3.4	26
320	Elastic constants and thermodynamic properties of MgBr, MgDy, MgZr intermetallics with atomistic simulations. <i>Journal Physics D: Applied Physics</i> , <b>2007</b> , 40, 7584-7592	3	26
319	Electronic properties and photoactivity of monolayer MoS <sub>2</sub> /fullerene van der Waals heterostructures. <i>RSC Advances</i> , <b>2016</b> , 6, 43228-43236	3.7	26
318	Chemical Ordering and Surface Segregation in CuPt Nanoalloys: The Synergetic Roles in the Formation of Multishell Structures. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 21515-21527	3.8	25

3 <sup>17</sup>	First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 660, 55-61	5.7	25
3 <sup>16</sup>	Diffusion and growth of nickel, iron and magnesium adatoms on the aluminum truncated octahedron: A molecular dynamics simulation. <i>Surface Science</i> , <b>2012</b> , 606, 971-980	1.8	25
3 <sup>15</sup>	Substrate Dependence of Growth Configurations for CoCu Bimetallic Clusters. <i>Crystal Growth and Design</i> , <b>2012</b> , 12, 2978-2985	3.5	25
3 <sup>14</sup>	Hierarchical Self-assembly of Well-Defined Louver-Like P-Doped Carbon Nitride Nanowire Arrays with Highly Efficient Hydrogen Evolution. <i>Nano-Micro Letters</i> , <b>2020</b> , 12, 52	19.5	24
3 <sup>13</sup>	Ab initio study of structural and electronic properties of SrTiO <sub>3</sub> (001) oxygen-vacancy surfaces. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 174701	3.9	24
3 <sup>12</sup>	Atomistic simulation of the segregation profiles in MoRe random alloys. <i>Surface Science</i> , <b>2003</b> , 543, 95-102	1.8	24
3 <sup>11</sup>	Interfacial charge modulation: carbon quantum dot implanted carbon nitride double-deck nanoframes for robust visible-light photocatalytic tetracycline degradation. <i>Nanoscale</i> , <b>2020</b> , 12, 3135-3145	7.7	24
3 <sup>10</sup>	Atomistic studies of shock-induced plasticity and phase transition in iron-based single crystal with edge dislocation. <i>International Journal of Plasticity</i> , <b>2019</b> , 114, 215-226	7.6	24
3 <sup>09</sup>	Steering charge kinetics boost the photocatalytic activity of graphitic carbon nitride: heteroatom-mediated spatial charge separation and transfer. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 53, 015502	3	23
3 <sup>08</sup>	Corrosion behavior in SBF for titania coatings on MgCa alloy. <i>Journal of Materials Science</i> , <b>2011</b> , 46, 2365-2369	4.9	23
3 <sup>07</sup>	Enhanced photocatalytic performance of an Ag <sub>3</sub> PO <sub>4</sub> photocatalyst via fullerene modification: first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 2878-86	3.6	22
3 <sup>06</sup>	The calculation of surface free energy based on embedded atom method for solid nickel. <i>Applied Surface Science</i> , <b>2013</b> , 265, 375-378	6.7	22
3 <sup>05</sup>	Surface Self-Diffusion Behavior of a Pt Adatom on Wulff Polyhedral Clusters. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 21501-21505	3.8	22
3 <sup>04</sup>	Preparation and properties of HVOF NiAl nanostructured coatings. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , <b>2008</b> , 478, 1-8	5.3	22
3 <sup>03</sup>	Shell and subshell periodic structures of icosahedral nickel nanoclusters. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 214501	3.9	22
3 <sup>02</sup>	Tunable synthesis of various ZnO architectural structures with enhanced photocatalytic activities. <i>Materials Letters</i> , <b>2016</b> , 175, 68-71	3.3	22
3 <sup>01</sup>	Unsaturated coordination polymer frameworks as multifunctional sulfur reservoir for fast and durable lithium-sulfur batteries. <i>Nano Energy</i> , <b>2021</b> , 79, 105393	17.1	22
3 <sup>00</sup>	Morphology, dimension, and composition dependence of thermodynamically preferred atomic arrangements in Ag-Pt nanoalloys. <i>Faraday Discussions</i> , <b>2013</b> , 162, 293-306	3.6	21

299	Melting temperature of Pb nanostructural materials from free energy calculation. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 074710	3.9	21
298	Thermal shock behavior of EB-PVD thermal barrier coatings. <i>Surface and Coatings Technology</i> , <b>2007</b> , 201, 7387-7391	4.4	21
297	Sol-gel derived HA/TiO <sub>2</sub> double coatings on Ti scaffolds for orthopaedic applications. <i>Transactions of Nonferrous Metals Society of China</i> , <b>2006</b> , 16, s209-s216	3.3	21
296	Non-covalent functionalization of WS <sub>2</sub> monolayer with small fullerenes: tuning electronic properties and photoactivity. <i>Dalton Transactions</i> , <b>2016</b> , 45, 13383-91	4.3	20
295	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. <i>Journal of Applied Physics</i> , <b>2018</b> , 123, 045105	2.5	19
294	Noncovalent Functionalization of Monolayer MoS <sub>2</sub> with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 21921-21929	3.8	19
293	Atomistic study of small helium bubbles in plutonium. <i>Journal of Alloys and Compounds</i> , <b>2007</b> , 444-445, 300-304	5.7	19
292	A comparative study of helium atom diffusion via an interstitial mechanism in nickel and palladium. <i>Physica Status Solidi (B): Basic Research</i> , <b>2006</b> , 243, 579-583	1.3	19
291	Synthesis and Characterization of Nanocrystalline Iron Aluminide Intermetallic Compounds. <i>Materials Transactions</i> , <b>2003</b> , 44, 2678-2687	1.3	19
290	Analytic embedded-atom method approach to studying the surface segregation of AlMg alloys. <i>Applied Surface Science</i> , <b>2004</b> , 221, 408-414	6.7	19
289	Calculation of the cohesive energy of metallic nanoparticles by the Lennard-Jones potential. <i>Materials Letters</i> , <b>2004</b> , 58, 1745-1749	3.3	19
288	Electrical and Thermal Conductivities of Nickel-Zirconia Cermets. <i>Journal of the American Ceramic Society</i> , <b>2005</b> , 81, 2209-2212	3.8	19
287	Phase transition of iron-based single crystals under ramp compressions with extreme strain rates. <i>International Journal of Plasticity</i> , <b>2017</b> , 96, 56-80	7.6	19
286	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Na-Se Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 4995-5002	9.5	19
285	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 11713-11721	3.6	18
284	The stability and diffusion properties of foreign impurity atoms on the surface and in the bulk of vanadium: A first-principles study. <i>Computational Materials Science</i> , <b>2014</b> , 81, 191-198	3.2	18
283	Atomistic behavior of helium-vacancy clusters in aluminum. <i>Journal of Nuclear Materials</i> , <b>2006</b> , 350, 83-88	3.3	18
282	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. <i>Computational Materials Science</i> , <b>2016</b> , 111, 203-208	3.2	17

281	Hybrid TiO <sub>2</sub> /graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 1423-1432	5.5	17
280	Diffusion of tungsten clusters on tungsten (110) surface. <i>European Physical Journal B</i> , <b>2009</b> , 68, 479-485	1.2	17
279	A study of the behavior of helium atoms at Ni grain boundaries. <i>Physica Status Solidi (B): Basic Research</i> , <b>2006</b> , 243, 2702-2710	1.3	17
278	LATTICE THERMAL CONDUCTIVITY IN A HOLLOW SILICON NANOWIRE. <i>International Journal of Modern Physics B</i> , <b>2005</b> , 19, 1017-1027	1.1	17
277	Crystallization study of electroless Fe <sub>8</sub> N <sub>2</sub> B amorphous alloy deposits. <i>Journal of Alloys and Compounds</i> , <b>1999</b> , 287, 234-238	5.7	17
276	Structure and crystallization of amorphous Fe-B alloys obtained by chemical plating. <i>Physica B: Condensed Matter</i> , <b>1991</b> , 175, 396-400	2.8	17
275	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 775, 1184-1198	5.7	17
274	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. <i>Computational Materials Science</i> , <b>2019</b> , 156, 47-55	3.2	17
273	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 28065-28074	3.8	17
272	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. <i>Journal of Nuclear Materials</i> , <b>2019</b> , 522, 200-213	3.3	16
271	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. <i>Computational Materials Science</i> , <b>2018</b> , 141, 293-301	3.2	16
270	Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores. <i>Computational Materials Science</i> , <b>2016</b> , 122, 1-10	3.2	16
269	The alloying element dependence of the local lattice deformation and the elastic properties of Ni <sub>3</sub> Al: A molecular dynamics simulation. <i>Journal of Applied Physics</i> , <b>2014</b> , 115, 153507	2.5	16
268	Gibbs free energy, surface stress and melting point of nanoparticle. <i>Physica B: Condensed Matter</i> , <b>2013</b> , 425, 90-94	2.8	16
267	Atomistic simulation of Pt trimer on Pt(1 1 1) surface. <i>Applied Surface Science</i> , <b>2007</b> , 253, 8825-8829	6.7	16
266	Microstructural changes and elemental diffusion of sputtered NiCrAlY coating on a Ni-base SC superalloy subjected to high temperature. <i>Materials Letters</i> , <b>2007</b> , 61, 5169-5172	3.3	16
265	Thermocyclic behavior of sputtered NiCrAlY/EB-PVD 7 wt.%Y <sub>2</sub> O <sub>3</sub> /ZrO <sub>2</sub> thermal barrier coatings. <i>Surface and Coatings Technology</i> , <b>2006</b> , 200, 3770-3774	4.4	16
264	Assessment of van der Waals inclusive density functional theory methods for adsorption and selective dehydrogenation of formic acid on Pt(111) surface. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 21049-21056	3.6	15



263	A molecular dynamics study of helium diffusion and clustering in fcc nickel. <i>Computational Materials Science</i> , <b>2015</b> , 107, 54-57	3.2	15
262	A first-principles investigation of the ScO <sub>2</sub> monolayer as the cathode material for alkali metal-ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 3171-3180	13	15
261	Atomistic simulations of the Fe(001)/Li solid-liquid interface. <i>Fusion Engineering and Design</i> , <b>2014</b> , 89, 2894-2901	1.7	15
260	Atomistic simulations of solid solution strengthening in Ni-based superalloy. <i>Computational Materials Science</i> , <b>2013</b> , 68, 132-137	3.2	15
259	Effects of solute size on solid-solution hardening in vanadium alloys: A first-principles calculation. <i>Scripta Materialia</i> , <b>2015</b> , 100, 106-109	5.6	15
258	Embedded-atom-method interatomic potentials from lattice inversion. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 375503	1.8	15
257	Microstructures and mechanical properties of as cast Mg/Zr/Ca alloys for biomedical applications. <i>Materials Technology</i> , <b>2012</b> , 27, 52-54	2.1	15
256	Graded coatings prepared by plasma spraying with Ni-coated ZrO <sub>2</sub> powders. <i>Surface and Coatings Technology</i> , <b>1998</b> , 105, 102-108	4.4	15
255	Molecular dynamics simulations of grain growth in nanocrystalline Ag. <i>Journal of Crystal Growth</i> , <b>2006</b> , 286, 512-517	1.6	15
254	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17607-17617	3.6	14
253	Role of electrodes materials in determining the interfacial and magnetoelectric properties in BaTiO <sub>3</sub> -based multiferroic tunnel junctions. <i>European Physical Journal B</i> , <b>2017</b> , 90, 1	1.2	14
252	The dynamic diffusion behaviors of 2D small Fe clusters on a Fe(110) surface. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 446009	1.8	14
251	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. <i>Journal of Nuclear Materials</i> , <b>2015</b> , 467, 398-405	3.3	13
250	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. <i>Fusion Engineering and Design</i> , <b>2018</b> , 128, 75-81	1.7	13
249	Strain-driven phase transition of molybdenum nanowire under uniaxial tensile strain. <i>Computational Materials Science</i> , <b>2010</b> , 50, 373-377	3.2	13
248	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. <i>Computational Materials Science</i> , <b>2017</b> , 137, 273-281	3.2	12
247	Molecular dynamics simulations of high-energy radiation damage in W and WBe alloys. <i>Journal of Nuclear Materials</i> , <b>2019</b> , 524, 9-20	3.3	12
246	Atomic simulation of fatigue crack propagation in Ni <sub>3</sub> Al. <i>Applied Physics A: Materials Science and Processing</i> , <b>2015</b> , 118, 1399-1406	2.6	12

245	A design rule for two-dimensional van der Waals heterostructures with unconventional band alignments. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 3037-3047	3.6	12
244	Atomic self-diffusion behaviors relevant to 2D homoepitaxy growth on stepped Pd(001) surface. <i>Surface Science</i> , <b>2014</b> , 624, 89-94	1.8	12
243	First-principles approach to the properties of point defects and small helium-vacancy clusters in palladium. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2009</b> , 267, 3037-3040	1.2	12
242	Molecular dynamics simulation of helium-vacancy interaction in plutonium. <i>Journal of Nuclear Materials</i> , <b>2009</b> , 385, 75-78	3.3	12
241	Ab initio study of ruffled relaxation and core-level shift of barium titanate surface. <i>Surface Science</i> , <b>2007</b> , 601, 1345-1350	1.8	12
240	Self-diffusion of Al and Pb atoms in AlPb immiscible alloy system. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , <b>2004</b> , 108, 253-257	3.1	12
239	Crystallization of amorphous Ni <sub>7</sub> Cu <sub>3</sub> B alloys obtained by electroless plating. <i>Physica B: Condensed Matter</i> , <b>1995</b> , 212, 195-200	2.8	12
238	Tensile mechanical properties of Ni-based superalloy of nanophases using molecular dynamics simulation. <i>Physica Status Solidi (B): Basic Research</i> , <b>2016</b> , 253, 726-732	1.3	12
237	The wetting properties of Li droplet on Cu surfaces: A molecular dynamics study. <i>Computational Materials Science</i> , <b>2016</b> , 119, 114-119	3.2	12
236	Interfacial Interactions in Monolayer and Few-Layer SnS/CH <sub>3</sub> NH <sub>2</sub> PbI Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. <i>ChemPhysChem</i> , <b>2018</b> , 19, 291-299	3.2	12
235	The effects of interstitial impurities on the mechanical properties of vanadium alloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 701, 975-980	5.7	11
234	Simultaneous covalent and noncovalent carbon nanotube/AgPO hybrids: new insights into the origin of enhanced visible light photocatalytic performance. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 7955-7963	3.6	11
233	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. <i>Computational Materials Science</i> , <b>2018</b> , 148, 242-248	3.2	11
232	Orientation dependences of the Fe-Li solid-liquid interface properties: Atomistic simulations. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 687, 875-884	5.7	11
231	Thermodynamic properties of Li, Pb and Li <sub>17</sub> Pb <sub>83</sub> with molecular dynamics simulations. <i>Fusion Engineering and Design</i> , <b>2014</b> , 89, 2946-2952	1.7	11
230	First-principles calculation of self-diffusion coefficients in Ni <sub>3</sub> Al. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 612, 361-364	5.7	11
229	Atomistic simulation for the size effect on the mechanical properties of Ni/Ni <sub>3</sub> Al nanowire. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 094303	2.5	11
228	The mechanism of enhanced photocatalytic activity of SnO <sub>2</sub> through fullerene modification. <i>Current Applied Physics</i> , <b>2017</b> , 17, 1547-1556	2.6	11

227	Molecular dynamics simulations of point defects in plutonium grain boundaries. <i>Chinese Physics B</i> , <b>2012</b> , 21, 026103	1.2	11
226	Helium nanobubble release from Pd surface: An atomic simulation. <i>Journal of Materials Research</i> , <b>2011</b> , 26, 416-423	2.5	11
225	Surface melting of close-packed Mg(0001). <i>Solid State Communications</i> , <b>2007</b> , 143, 545-549	1.6	11
224	Study of the corrosion behaviors of 304 austenite stainless steel specimens exposed to static liquid lithium at 600 K. <i>Journal of Nuclear Materials</i> , <b>2016</b> , 480, 25-31	3.3	11
223	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. <i>Current Applied Physics</i> , <b>2018</b> , 18, 183-190	2.6	11
222	Tunable Schottky barrier in van der Waals heterostructures of graphene and hydrogenated phosphorus carbide monolayer: first-principles calculations. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 52, 305104	3	10
221	Development of the interatomic potentials for W-Ta system. <i>Computational Materials Science</i> , <b>2019</b> , 163, 91-99	3.2	10
220	Theoretical insights into nitrogen fixation on Ti <sub>2</sub> C and Ti <sub>2</sub> CO <sub>2</sub> in a lithium-nitrogen battery. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 19950-19960	13	10
219	Diffusion properties of liquid lithium-lead alloys from atomistic simulation. <i>Computational Materials Science</i> , <b>2014</b> , 93, 74-80	3.2	10
218	Strain driven enhancement of ferroelectricity and magnetoelectric effect in multiferroic tunnel junction. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 14770-6	3.6	10
217	Effect of incident energy on the configuration of FeAl nanoparticles, a molecular dynamics simulation of impact deposition. <i>RSC Advances</i> , <b>2014</b> , 4, 2155-2160	3.7	10
216	Material properties dependence of ballistic phonon transmission through two coupled nanocavities. <i>Journal of Applied Physics</i> , <b>2009</b> , 105, 124305	2.5	10
215	Adsorption of hydrogen on palladium nanoparticle surfaces. <i>Surface and Interface Analysis</i> , <b>2009</b> , 41, 590-594	1.5	10
214	Atomistic simulation of helium bubble nucleation in palladium. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2009</b> , 267, 3185-3188	1.2	10
213	First-principle study of the electronic structures and ferroelectric properties in BaZnF <sub>4</sub> . <i>European Physical Journal B</i> , <b>2010</b> , 74, 447-450	1.2	10
212	Strain and Electric Field Controllable Schottky Barriers and Contact Types in Graphene-MoTe van der Waals Heterostructure. <i>Nanoscale Research Letters</i> , <b>2020</b> , 15, 180	5	10
211	Dispersive and covalent interactions in all-carbon heterostructures consisting of penta-graphene and fullerene: topological effect. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 305301	3	10
210	High-throughput computational design for 2D van der Waals functional heterostructures: Fragility of Anderson's rule and beyond. <i>Applied Physics Letters</i> , <b>2021</b> , 119, 043102	3.4	10

209	Interfacial interaction in monolayer transition metal dichalcogenide/metal oxide heterostructures and its effects on electronic and optical properties: The case of MX <sub>2</sub> /CeO <sub>2</sub> . <i>Applied Physics Express</i> , <b>2017</b> , 10, 011201	2.4	9
208	Protonated supramolecular complex-induced porous graphitic carbon nitride nanosheets as bifunctional catalyst for water oxidation and organic pollutant degradation. <i>Journal of Materials Science</i> , <b>2019</b> , 54, 7637-7650	4.3	9
207	Self-assembled hierarchical carbon/g-C <sub>3</sub> N <sub>4</sub> composite with high photocatalytic activity. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 135501	3	9
206	Development of a pair potential for NiBe. <i>Journal of Nuclear Materials</i> , <b>2016</b> , 472, 105-109	3.3	9
205	Substrate-induced magnetism and topological phase transition in silicene. <i>Nanoscale</i> , <b>2018</b> , 10, 14667-14677	4.7	9
204	Amorphization and thermal stability of aluminum-based nanoparticles prepared from the rapid cooling of nanodroplets: effect of iron addition. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 6511-22	3.6	9
203	Compressive Properties of Hot-Rolled Mg-Zr-Ca Alloys for Biomedical Applications. <i>Advanced Materials Research</i> , <b>2011</b> , 197-198, 56-59	0.5	9
202	Computer Simulation of Helium Effects in Plutonium During the Aging Process of Self-Radiation Damage. <i>Communications in Computational Physics</i> , <b>2012</b> , 11, 1205-1225	2.4	9
201	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. <i>Fusion Engineering and Design</i> , <b>2017</b> , 117, 188-193	1.7	8
200	Effect of MCl <sub>3</sub> (M=La, U or Sc) component on the local structures and transport properties of LiCl <sub>2</sub> /MCl <sub>3</sub> eutectic: A molecular dynamics study. <i>Electrochimica Acta</i> , <b>2019</b> , 306, 366-376	6.7	8
199	Diffusion and growth of aluminum adatoms on magnesium clusters with hexahedral structure. <i>Physica B: Condensed Matter</i> , <b>2015</b> , 458, 144-148	2.8	8
198	Influence of solid-liquid interface on the thermal stability of LiBe nanoalloy with rhombohedral structure: A molecular dynamics study. <i>Thin Solid Films</i> , <b>2015</b> , 593, 137-143	2.2	8
197	The formation of Fe-core-Al-shell and Fe-shell-Al-core nanoparticles, a molecular dynamics simulation. <i>Computational Materials Science</i> , <b>2013</b> , 74, 160-164	3.2	8
196	Atomistic simulation for the $\beta$ -phase volume fraction dependence of the interfacial behavior of Ni-base superalloy. <i>Applied Surface Science</i> , <b>2013</b> , 264, 563-569	6.7	8
195	Dynamics diffusion behaviors of Pd small clusters on a Pd(1 1 1) surface. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2010</b> , 18, 045010	2	8
194	Self-diffusion dynamic behavior of atomic clusters on Re(0001) surface. <i>Applied Surface Science</i> , <b>2009</b> , 255, 8883-8889	6.7	8
193	Stress-induced phase transformation and strain rate effect in polycrystalline Mo nanowires. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2011</b> , 43, 1131-1139	3	8
192	Giant Magneto-Optical Kerr Effects in Ferromagnetic Perovskite BiNiO <sub>3</sub> with Half-Metallic State. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 16638-16642	3.8	8

191	Comparison of the Solid Solution Properties of Mg-RE (Gd, Dy, Y) Alloys with Atomistic Simulation. <i>Research Letters in Physics</i> , <b>2008</b> , 2008, 1-4		8
190	Comparative study of compact hexagonal cluster self-diffusion on Cu(111) and Pt(111). <i>Applied Surface Science</i> , <b>2008</b> , 255, 1736-1740	6.7	8
189	Electrostatic Potential Anomaly in 2D Janus Transition Metal Dichalcogenides. <i>Annalen Der Physik</i> , <b>2019</b> , 531, 1900369	2.6	8
188	A molecular dynamics study of the transport properties of LiF-BeF <sub>2</sub> -ThF <sub>4</sub> molten salt. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 234, 220-226	6	7
187	Molecular dynamics simulations of the structure evolutions of Cu-Zr metallic glasses under irradiation. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2017</b> , 393, 77-81	1.2	7
186	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. <i>Journal of Nuclear Materials</i> , <b>2019</b> , 527, 151821	3.3	7
185	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. <i>Nuclear Fusion</i> , <b>2019</b> , 59, 076020	3.3	7
184	Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B <sub>20</sub> /Ag <sub>3</sub> PO <sub>4</sub> van der Waals Heterostructure. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 6151-6158	3.8	7
183	The energy and stability of helium-related cluster in nickel: A study of molecular dynamics simulation. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2016</b> , 368, 75-80	1.2	7
182	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I <sub>2</sub> batteries. <i>Energy Storage Materials</i> , <b>2019</b> , 17, 211-219	19.4	7
181	Effect of particle packing and density on shock response in ordered arrays of Ni + Al nanoparticles. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 7272-7280	3.6	7
180	First-principles study of nitrogen adsorption and dissociation on Uranium (001) surface. <i>RSC Advances</i> , <b>2014</b> , 4, 57308-57321	3.7	7
179	First-principles study on the interaction of nitrogen atom with Uranium: From surface adsorption to bulk diffusion. <i>Journal of Applied Physics</i> , <b>2014</b> , 115, 164902	2.5	7
178	Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 17644-17649	3.8	7
177	Shock Waves Propagation and Phase Transition in Single Crystal Iron under Ramp Compression: Large Scale Parallel NEMD Simulations. <i>Procedia Engineering</i> , <b>2013</b> , 61, 122-129		7
176	Energetics and self-diffusion behavior of Zr atomic clusters on a Zr(0 0 0 1) surface. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2009</b> , 267, 3267-3270	1.2	7
175	Phase transition in nanocrystalline iron: Atomistic-level simulations. <i>International Journal of Materials Research</i> , <b>2010</b> , 101, 1361-1368	0.5	7
174	Surface self-diffusion of adatom on Pt cluster with truncated octahedron structure. <i>Thin Solid Films</i> , <b>2010</b> , 518, 4041-4045	2.2	7

173	Thermal expansion behavior of ZrO <sub>2</sub> -Y <sub>2</sub> O <sub>3</sub> -Ni cermets. <i>Materials Letters</i> , <b>1997</b> , 32, 59-62	3.3	7
172	First-principles study for the atomic structures and electronic properties of PbTiO <sub>3</sub> oxygen-vacancies (001) surface. <i>Surface Science</i> , <b>2007</b> , 601, 5412-5418	1.8	7
171	Influence of the coupling between the normal and lateral motions on surface states of a semi-infinite superlattice with a cap layer. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2004</b> , 325, 70-78	2.3	7
170	Determination of dynamic mechanical properties of metals from single pendulum scratch tests. <i>Tribology International</i> , <b>1999</b> , 32, 153-160	4.9	7
169	Microstructural Characterization and Mechanical Properties of Mg-Zr-Ca Alloys Prepared by Hot-Extrusion for Biomedical Applications. <i>Advanced Science Letters</i> , <b>2011</b> , 4, 2860-2863	0.1	7
168	A host-guest self-assembly strategy to enhance electron densities in ultrathin porous carbon nitride nanocages toward highly efficient hydrogen evolution. <i>Chemical Engineering Journal</i> , <b>2022</b> , 430, 132880	14.7	7
167	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. <i>Journal of Materials Research</i> , <b>2017</b> , 32, 1474-1483	2.5	6
166	Intrinsic strain-induced segregation in multiply twinned Cu-Pt icosahedra. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 4802-4809	3.6	6
165	Oxygen adsorption and diffusion on $\text{TiO}_2(001)$ surface: Effect of titanium. <i>Computational Materials Science</i> , <b>2018</b> , 144, 85-91	3.2	6
164	An ab initio study for probing iodization reactions on metallic anode surfaces of Li-I <sub>2</sub> batteries. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 7807-7814	13	6
163	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 22351-22358	3.6	6
162	Effect of Re content on the $\text{TiO}_2/\text{Ti}$ interface: A Monte Carlo simulation. <i>Computational Materials Science</i> , <b>2014</b> , 89, 75-79	3.2	6
161	Migration of Cr-vacancy clusters and interstitial Cr in $\alpha$ -Fe using the dimer method. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	6
160	The effect of vacancy created by ion irradiation on the ordering of FePt: A first-principle study. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2009</b> , 267, 3271-3273	1.2	6
159	Anharmonic effects on B <sub>2</sub> BeAl(110) surface: A molecular dynamics study. <i>Applied Surface Science</i> , <b>2007</b> , 254, 1475-1481	6.7	6
158	Simulation calculations of surface segregation for AuCu alloys using an analytic embedded atom model. <i>Physica Status Solidi A</i> , <b>2005</b> , 202, 2686-2699		6
157	Interatomic potentials and defect properties of FeCrAl alloys. <i>Journal of Nuclear Materials</i> , <b>2020</b> , 541, 152421	3.3	6
156	Atomistic simulation of mechanical properties and crack propagation of irradiated nickel. <i>Computational Materials Science</i> , <b>2016</b> , 120, 21-28	3.2	6

155	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. <i>Nano Letters</i> , <b>2021</b> , 21, 6875-6881	11.5	6
154	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. <i>Computational Materials Science</i> , <b>2020</b> , 177, 109555	3.2	5
153	Double-Layer Honeycomb AIP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 2978-2986	3.8	5
152	Interatomic potentials of W <sub>N</sub> and W <sub>Mo</sub> binary systems for point defects studies. <i>Journal of Nuclear Materials</i> , <b>2020</b> , 531, 152020	3.3	5
151	Dual functions of 2D WS <sub>2</sub> and MoS <sub>2</sub> /WS <sub>2</sub> monolayers coupled with a Ag <sub>3</sub> PO <sub>4</sub> photocatalyst. <i>Semiconductor Science and Technology</i> , <b>2016</b> , 31, 095013	1.8	5
150	Clustering of Fe atoms in liquid Li and its effect on the viscosity of liquid Li. <i>Nuclear Fusion</i> , <b>2016</b> , 56, 046004	3.3	5
149	Atomic simulation of helium trapping in displacement cascades. <i>RSC Advances</i> , <b>2016</b> , 6, 27113-27118	3.7	5
148	Temperature effects on growth configurations of Al atoms on an Fe rhombohedron: a molecular dynamics simulation. <i>Journal of Nanoparticle Research</i> , <b>2013</b> , 15, 1	2.3	5
147	The alloying processes in solid-solid and liquid-solid Li <sub>B</sub> interfaces with atomistic simulations. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 632, 467-472	5.7	5
146	Atomistic simulation for the size-dependent melting behaviour of vanadium nanowires. <i>Journal Physics D: Applied Physics</i> , <b>2012</b> , 45, 485304	3	5
145	Gibbs free energy approach to the prediction of melting points of isolated, supported, and embedded nanoparticles. <i>Journal of Applied Physics</i> , <b>2012</b> , 112, 014302	2.5	5
144	Self-diffusion behaviors of Pd adatom and dimer on Pd(001) surface. <i>Computational Materials Science</i> , <b>2009</b> , 47, 501-505	3.2	5
143	Force-sensitive resistor of carbon-filled liquid silicone rubber. <i>Journal of Applied Physics</i> , <b>1996</b> , 79, 866	2.5	5
142	The activation energy and the Avrami exponent for crystallization in amorphous Fe <sub>70.45</sub> W <sub>1.55</sub> Si <sub>3</sub> B <sub>25</sub> . <i>Physica B: Condensed Matter</i> , <b>1994</b> , 203, 147-150	2.8	5
141	Dipole Engineering of Two-Dimensional van der Waals Heterostructures for Enhanced Power-Conversion Efficiency: The Case of Janus Ga <sub>2</sub> SeTe/InS. <i>Physical Review Applied</i> , <b>2021</b> , 16,	4.3	5
140	In situ construction of hierarchical graphitic carbon nitride homojunction as robust bifunctional photoelectrocatalyst for overall water splitting. <i>Journal of Chemical Technology and Biotechnology</i> , <b>2020</b> , 95, 758-769	3.5	5
139	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 763, 1-10	5.7	5
138	Development of a Ni <sub>Mo</sub> interatomic potential for irradiation simulation. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2019</b> , 27, 045009	2	4

137	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. <i>Computational Materials Science</i> , <b>2020</b> , 183, 109845	3.2	4
136	From monolayer to lateral heterostructure of functionalized phosphorus carbide: Evolution of electronic properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2020</b> , 118, 113962	3	4
135	Surface segregation and alloying of immiscible Li-Cu and miscible Li-Pb nanoalloys investigated by basin-hopping Monte Carlo method. <i>Computational Materials Science</i> , <b>2018</b> , 154, 371-379	3.2	4
134	Interactions of plasticity and phase transformation under shock in iron bicrystals. <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 045901	2.5	4
133	Effect of voids on the tensile properties of vanadium nanowires. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2013</b> , 303, 14-17	1.2	4
132	The cluster-size dependence of self-diffusion behavior: A single Re adatom on a hexahedral surface. <i>Physica Status Solidi (B): Basic Research</i> , <b>2013</b> , 250, 1363-1369	1.3	4
131	Helium diffusion behavior and its retention in LaNiAl alloy from molecular dynamic simulations. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2011</b> , 269, 1689-1692	1.2	4
130	Surface self-diffusion behavior of individual tungsten adatoms on rhombohedral clusters. <i>Journal of Physics Condensed Matter</i> , <b>2011</b> , 23, 395004	1.8	4
129	Surface self-diffusion of a Pt adatom on cuboctahedral and truncated decahedral clusters, size dependence. <i>European Physical Journal B</i> , <b>2010</b> , 78, 315-321	1.2	4
128	Molecular dynamics simulation of surface melting behaviours of the V(110) plane. <i>Chinese Physics B</i> , <b>2008</b> , 17, 2633-2638	1.2	4
127	Melting mechanisms of Nb(111) plane with molecular dynamics simulations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2007</b> , 365, 161-165	2.3	4
126	Solid solution mechanism and thermodynamic properties of TiBe alloy system: Experiment and theory. <i>Intermetallics</i> , <b>2007</b> , 15, 1116-1121	3.5	4
125	Adsorption of hydrogen atoms on Pd (211), (311) and (511) stepped defective surfaces. <i>Transactions of Nonferrous Metals Society of China</i> , <b>2006</b> , 16, s820-s823	3.3	4
124	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. <i>Computational Materials Science</i> , <b>2020</b> , 173, 109412	3.2	4
123	Molecular dynamics simulation of the diffusion of self-interstitial atoms and interstitial loops under temperature gradient field in tungsten. <i>Journal of Applied Physics</i> , <b>2020</b> , 128, 065103	2.5	4
122	Atomic simulations for configurations and solid-liquid interface of Li-Fe and Li-Cu icosahedra. <i>Journal of Nanoparticle Research</i> , <b>2017</b> , 19, 1	2.3	3
121	Atomistic simulations of solidification process in B2-LiPb solid(0 0 1)-liquid system. <i>Journal of Crystal Growth</i> , <b>2017</b> , 470, 113-121	1.6	3
120	Simulation of radiation damages in molybdenum by combining molecular dynamics and OKMC. <i>Nuclear Science and Techniques/Hewuli</i> , <b>2017</b> , 28, 1	2.1	3



119	Molecular dynamics simulations of shock loading of nearly fully dense granular Ni-Al composites. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 20252-20261	3.6	3
118	Determination of thermodynamic and thermo-elastic properties for ductile B2-DyCu intermetallics using molecular dynamics simulations. <i>Physica B: Condensed Matter</i> , <b>2015</b> , 459, 69-73	2.8	3
117	Chemistry of Defects in Crystalline Na <sub>2</sub> Se: Implications for the NaBe Battery. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 27930-27936	3.8	3
116	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. <i>Fusion Engineering and Design</i> , <b>2020</b> , 159, 111850	1.7	3
115	Evaluation of tungsten interatomic potentials for radiation damage simulations. <i>Tungsten</i> , <b>2020</b> , 2, 3-14	4.6	3
114	Compatibility of Molybdenum, Tungsten, and 304 Stainless Steel in Static Liquid Lithium Under High Vacuum. <i>Plasma Physics Reports</i> , <b>2018</b> , 44, 671-677	1.2	3
113	Monolayer Phosphorene-Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. <i>Nanoscale Research Letters</i> , <b>2019</b> , 14, 233	5	3
112	The anisotropic character of Snoek relaxation in Fe <sub>3</sub> C system: A kinetic Monte Carlo and molecular dynamics simulation. <i>Physica Status Solidi (B): Basic Research</i> , <b>2015</b> , 252, 1382-1387	1.3	3
111	ANISOTROPY DIFFUSION DYNAMICS BEHAVIORS ON Pd(110) SURFACES: A MOLECULAR DYNAMICS STUDY. <i>Surface Review and Letters</i> , <b>2015</b> , 22, 1550013	1.1	3
110	Surface self-diffusion of Re adatom on the Re cluster with hexahedral structure. <i>Physica B: Condensed Matter</i> , <b>2013</b> , 414, 97-102	2.8	3
109	The effect of step thickness on the surface diffusion of a Pt adatom. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2009</b> , 17, 075004	2	3
108	Diffusion dynamics of vacancy on Re(0 0 0 1), compared with adatom. <i>Physica B: Condensed Matter</i> , <b>2009</b> , 404, 1546-1549	2.8	3
107	Ballistic phonon transmission in quasiperiodic acoustic nanocavities. <i>Journal of Applied Physics</i> , <b>2011</b> , 109, 084310	2.5	3
106	BALLISTIC PHONON TRANSPORT THROUGH GAUSSIAN ACOUSTIC NANOCAVITIES. <i>Modern Physics Letters B</i> , <b>2011</b> , 25, 1631-1642	1.6	3
105	Interaction between helium and vacancy in plutonium by embedded atom method. <i>Physica Status Solidi (B): Basic Research</i> , <b>2008</b> , 245, 1493-1497	1.3	3
104	Diffusion behaviors of helium atoms at two Pd grain boundaries. <i>Transactions of Nonferrous Metals Society of China</i> , <b>2006</b> , 16, s804-s807	3.3	3
103	Localized electronic states in $\alpha$ -layer-based superlattices with structural defects. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2005</b> , 28, 374-384	3	3
102	Shock-induced plasticity and phase transformation in single crystal magnesium: An interatomic potential and non-equilibrium molecular dynamics simulations.. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> ,	1.8	3

101	Ultrahigh Sensitivity and Selectivity of Pentagonal SiC <sub>2</sub> Monolayer Gas Sensors: The Synergistic Effect of Composition and Structural Topology. <i>Physica Status Solidi (B): Basic Research</i> , <b>2020</b> , 257, 1900445	1.3	3
100	Amorphous B-doped graphitic carbon nitride quantum dots with high photoluminescence quantum yield of near 90% and their sensitive detection of Fe <sup>2+</sup> /Cd <sup>2+</sup> . <i>Science China Materials</i> , <b>2020</b> , 13, 114453	7.1	3
99	Nucleation and solid-liquid interfacial energy of Li nanoparticles: A molecular dynamics study. <i>Physica Status Solidi (B): Basic Research</i> , <b>2016</b> , 253, 1941-1946	1.3	3
98	A two-dimensional MoS <sub>2</sub> /SnS heterostructure for promising photocatalytic performance: First-principles investigations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 126, 114453	3.3	3
97	Local identification of chemical ordering: Extension, implementation, and application of the common neighbor analysis for binary systems. <i>Computational Materials Science</i> , <b>2018</b> , 143, 195-205	3.2	3
96	Does the Mg <sup>2+</sup> Battery Suffer Severe Shuttle Effect?. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 28518-28527	3.5	3
95	The effect of solutes on the precipitate/matrix interface properties in the Vanadium alloys: A first-principles study. <i>Computational Materials Science</i> , <b>2018</b> , 153, 113-118	3.2	3
94	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. <i>Journal of Nuclear Materials</i> , <b>2021</b> , 556, 153162	3.3	3
93	Temperature effects on growth configurations for Al-Mg bimetallic nanoparticles. <i>Thin Solid Films</i> , <b>2017</b> , 626, 178-183	2.2	2
92	Diffusion mechanisms at the Pb solid-liquid interface: Atomic level point of view. <i>Chemical Physics Letters</i> , <b>2015</b> , 634, 108-112	2.5	2
91	Stability and diffusion properties of Ti atom on Uranium surfaces: A first-principles study. <i>Computational Materials Science</i> , <b>2015</b> , 97, 201-208	3.2	2
90	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. <i>Journal of Nanoparticle Research</i> , <b>2020</b> , 22, 1	2.3	2
89	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. <i>Computational Materials Science</i> , <b>2018</b> , 149, 435-441	3.2	2
88	Irradiation damage of helium-accumulated vanadium: atomic simulations. <i>RSC Advances</i> , <b>2016</b> , 6, 80939-80945	3.9	2
87	Effect of neon on the hydrogen behaviors in tungsten: A first-principles study. <i>Journal of Nuclear Materials</i> , <b>2018</b> , 510, 492-498	3.3	2
86	Modified analytic embedded atom method potential for chromium. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2018</b> , 26, 065001	2	2
85	Migration of defect clusters and xenon-vacancy clusters in uranium dioxide. <i>International Journal of Modern Physics B</i> , <b>2014</b> , 28, 1450120	1.1	2
84	Effects of substitutional He atoms on the displacement cascades in Fe. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2013</b> , 303, 72-74	1.2	2

83	Tungsten cluster migration on nanoparticles: minimum energy pathway and migration mechanism. <i>European Physical Journal B</i> , <b>2011</b> , 80, 31-40	1.2	2
82	Energetics and Properties of Vacancies, Anti-Sites, and Atomic Defects (B, C, and N) in Ductile B2-YM (M=Ag, Cu, Rh) Intermetallics. <i>Materials Science Forum</i> , <b>2011</b> , 689, 91-94	0.4	2
81	Molecular dynamics study of the hcpBcc phase transformation in nanocrystalline zirconium. <i>International Journal of Materials Research</i> , <b>2008</b> , 99, 626-631	0.5	2
80	Monte carlo simulation of hydrogen adsorption on Ni surfaces. <i>Frontiers of Physics in China</i> , <b>2007</b> , 2, 199-203		2
79	The Formation Energies and Binding Energies of Helium Vacancy Cluster: Comparative Study in Ni and Pd. <i>Journal of Physics: Conference Series</i> , <b>2006</b> , 29, 190-193	0.3	2
78	Anharmonic effects on Be(0001): A molecular dynamics study. <i>Computational Materials Science</i> , <b>2006</b> , 37, 607-612	3.2	2
77	Anharmonicity in Al vicinal surfaces of (1 0 0) with (1 1 1) step. <i>Applied Surface Science</i> , <b>2006</b> , 252, 4923-4930	0.7	2
76	The crystalline phases in rapidly solidified Al65Cu20Fe15 alloy powders. <i>Scripta Metallurgica Et Materialia</i> , <b>1995</b> , 32, 1325-1330		2
75	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. <i>Applied Physics Express</i> , <b>2022</b> , 15, 015503	2.4	2
74	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Fe10Ni20Cr and Ni. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2020</b> , 28, 075002	2	2
73	Effects of Se substitution on the Schottky barrier of a MoS <sub>2</sub> /graphene heterostructure. <i>Journal Physics D: Applied Physics</i> , <b>2021</b> , 54, 265302	3	2
72	First-principles study on the dissolution and diffusion behavior of hydrogen in carbide precipitates. <i>International Journal of Hydrogen Energy</i> , <b>2021</b> , 46, 22030-22039	6.7	2
71	Molecular dynamics simulation of shock wave propagation and spall failure in single crystal copper under cylindrical impact. <i>Applied Physics Express</i> , <b>2021</b> , 14, 075504	2.4	2
70	2D Amorphous CoO Incorporated g-C <sub>3</sub> N <sub>4</sub> Nanotubes for Improved Photocatalytic Performance. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2021</b> , 15, 2100254	2.5	2
69	Mechanism of enhanced photocatalytic activities on tungsten trioxide doped with sulfur: Dopant-type effects. <i>Modern Physics Letters B</i> , <b>2016</b> , 30, 1650340	1.6	2
68	Monolayer PtTe <sub>2</sub> : A promising candidate for NO <sub>2</sub> sensor with ultrahigh sensitivity and selectivity. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 134, 114925	3	2
67	First-principles study of the adsorption properties of atoms and molecules on UN <sub>2</sub> (001) surface. <i>Journal of Nuclear Materials</i> , <b>2017</b> , 493, 124-131	3.3	1
66	Monte Carlo simulations of strain-driven elemental depletion or enrichment in Cu <sub>95</sub> Al <sub>5</sub> and Cu <sub>90</sub> Al <sub>10</sub> alloys. <i>Computational Materials Science</i> , <b>2015</b> , 106, 123-128	3.2	1

65	Dynamic self-diffusion behaviors of nickel adatoms on clusters with Wulff shape. <i>International Journal of Modern Physics B</i> , <b>2020</b> , 34, 2050015	1.1	1
64	Carbide effects on tensile deformation behavior of [001] symmetric tilt grain boundaries in bcc Fe. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2020</b> , 28, 035006	2	1
63	Atomic simulation of mechanical properties of irradiated iron. <i>International Journal of Modern Physics C</i> , <b>2020</b> , 31, 2050027	1.1	1
62	A new embedded-atom method approach based on the pth moment approximation. <i>Journal of Physics Condensed Matter</i> , <b>2016</b> , 28, 505201	1.8	1
61	Interfacial structure, ferroelectric stability, and magnetoelectric effect of magnetoelectric junction FeCo/BaTiO <sub>3</sub> /FeCo with alloy electrode. <i>Journal of Materials Science</i> , <b>2016</b> , 51, 3297-3302	4.3	1
60	Shock-induced migration of asymmetry tilt grain boundary in iron bicrystal: A case study of $\Sigma$ [110]. <i>Chinese Physics B</i> , <b>2019</b> , 28, 126201	1.2	1
59	Molecular Dynamics Simulation of the Displacement Cascades in Tungsten with Interstitial Helium Atoms. <i>Fusion Science and Technology</i> , <b>2014</b> , 66, 112-117	1.1	1
58	Diffusion of Al dimers on the surface of Mg clusters. <i>European Physical Journal B</i> , <b>2017</b> , 90, 1	1.2	1
57	Site preference and elastic properties of ternary alloying additions in B2 YAg alloys by first-principles calculations. <i>Physica B: Condensed Matter</i> , <b>2012</b> , 407, 3749-3752	2.8	1
56	Effect of Gaussian acoustic nanocavities in a narrow constriction on ballistic phonon transmission. <i>Applied Physics A: Materials Science and Processing</i> , <b>2011</b> , 104, 635-642	2.6	1
55	Diffusion of Pt dimers on a Wulff polyhedral surface. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2011</b> , 54, 846-850	3.6	1
54	Effect of uniaxial strain on adatom diffusion across {111}-faceted step. <i>Applied Surface Science</i> , <b>2011</b> , 257, 3325-3330	6.7	1
53	Ballistic phonon transport through a Fibonacci array of acoustic nanocavities in a narrow constriction. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2011</b> , 375, 2000-2006	2.3	1
52	Calculation of Thermodynamic and Thermoelastic Properties for Ductile B2-YAg Intermetallics with Molecular Dynamics. <i>Advanced Materials Research</i> , <b>2012</b> , 550-553, 2814-2818	0.5	1
51	Atomistic simulations for the non-equilibrium surface premelting and melting of Nb(110) plane. <i>Current Applied Physics</i> , <b>2010</b> , 10, 436-443	2.6	1
50	Thermodynamic properties and elastic constants of NdMg intermetallics: a molecular dynamics study. <i>International Journal of Materials Research</i> , <b>2008</b> , 99, 42-49	0.5	1
49	Surface melting of close-packed Mg(0001), compared with Al(111). <i>Physica Status Solidi (B): Basic Research</i> , <b>2007</b> , 244, 1913-1924	1.3	1
48	Molecular dynamics simulation of thermal stability of nanocrystalline vanadium. <i>Science in China Series D: Earth Sciences</i> , <b>2006</b> , 49, 400-407		1

47	Synthesis of Zirconia-Nickel Cermets by a Powder Metallurgical Technique. <i>Materials and Manufacturing Processes</i> , <b>1998</b> , 13, 229-240	4.1	1
46	Synergistic Effects of Crystal Phase and Strain for N Dissociation on Ru(0001) Surfaces with Multilayered Hexagonal Close-Packed Structures.. <i>ACS Omega</i> , <b>2022</b> , 7, 4492-4500	3.9	1
45	Effect of nanopores on plasticity and their collapse mechanism in magnesium single crystal under shock loading. <i>Journal of Applied Physics</i> , <b>2022</b> , 131, 055903	2.5	1
44	Molecular dynamic simulations of displacement cascades in tungsten and tungsten-rhenium alloys: Effects of grain boundary and/or phase. <i>Journal of Nuclear Materials</i> , <b>2022</b> , 561, 153543	3.3	1
43	Comparative investigation of microjetting from tin surface subjected to laser and plane impact loadings via molecular dynamics simulations. <i>Mechanics of Materials</i> , <b>2020</b> , 148, 103479	3.3	1
42	The mechanism of plasticity and phase transition in iron single crystals under cylindrically divergent shock loading. <i>International Journal of Mechanical Sciences</i> , <b>2022</b> , 217, 107032	5.5	1
41	Highly effective Ru-based Heusler alloy catalysts for N <sub>2</sub> activation: A theoretical study. <i>Applied Surface Science</i> , <b>2021</b> , 151658	6.7	1
40	Algorithm for generating irreducible site-occupancy configurations. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	1
39	The phase transition of rapidly super-cooled Tungsten under 100 GPa. <i>Chemical Physics Letters</i> , <b>2020</b> , 755, 137789	2.5	1
38	Energetics and diffusional properties of helium in W-Ta systems studied by a new ternary potential. <i>Journal of Nuclear Materials</i> , <b>2021</b> , 549, 152913	3.3	1
37	MD and OKMC simulations of the displacement cascades in nickel. <i>Nuclear Science and Techniques/Hewuli</i> , <b>2016</b> , 27, 1	2.1	1
36	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Two-Dimensional WS <sub>2</sub> /TX <sub>2</sub> CO <sub>2</sub> (TX = Ti, Zr) van der Waals Heterostructures. <i>Physica Status Solidi (B): Basic Research</i> , <b>2019</b> , 256, 1800377	1.3	1
35	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. <i>Journal of Applied Physics</i> , <b>2021</b> , 130, 015107	2.5	1
34	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. <i>Ceramics International</i> , <b>2021</b> , 47, 29386-29391	5.1	1
33	FinnisSinclair-type potential for atomistic simulation of defects behaviour in V-Ti-Ta ternary system. <i>Journal of Nuclear Materials</i> , <b>2021</b> , 557, 153231	3.3	1
32	Pt-based intermetallic compounds with tunable activity and selectivity toward hydrogen production from formic acid. <i>Applied Surface Science</i> , <b>2022</b> , 153530	6.7	1
31	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO <sub>2</sub> . <i>Metals</i> , <b>2022</b> , 12, 789	2.3	1
30	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. <i>International Journal of Mechanical Sciences</i> , <b>2022</b> , 107373	5.5	1

29	The Role of Grain Boundaries in the Corrosion Process of Fe Surface: Insights from ReaxFF Molecular Dynamic Simulations. <i>Metals</i> , <b>2022</b> , 12, 876	2.3	1
28	Effect of symmetrical tilt grain boundary on the compatibility between copper and liquid lithium: Atomistic simulations. <i>Journal of Alloys and Compounds</i> , <b>2020</b> , 835, 155212	5.7	0
27	Clustering and dislocation loop punching induced by different noble gas bubbles in tungsten: a molecular dynamics study. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2019</b> , 27, 084002	2.0	0
26	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. <i>Metals</i> , <b>2022</b> , 12, 232	2.3	0
25	Critical structural invariant during high-pressure solidification of copper. <i>MRS Communications</i> , <b>2022</b> , 12, 45	2.7	0
24	Two-dimensional chromium phosphorus monolayer based gas sensors to detect NOx: A first-principles study. <i>Results in Physics</i> , <b>2022</b> , 32, 105100	3.7	0
23	Crystallographic-orientation-dependence plasticity of niobium under shock compressions. <i>International Journal of Plasticity</i> , <b>2022</b> , 150, 103195	7.6	0
22	Predicted Polymeric and Layered Covalent Networks in Transition Metal Pentazolate M(cyclo-N5) <sub>x</sub> Phases at Ambient and High Pressure: Up to 20 Nitrogen Atoms per Metal. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 5298-5307	9.6	0
21	Strain and interfacial engineering to accelerate hydrogen evolution reaction of two-dimensional phosphorus carbide*. <i>Chinese Physics B</i> , <b>2021</b> , 30, 027101	1.2	0
20	Effects of electric field and strain on the Schottky barrier of the bilayer van der Waals heterostructures of graphene and pure/hydrogenated PC3 monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 133, 114785	3	0
19	Molecular dynamics simulation of the behavior of typical radiation defects under stress gradient field in tungsten. <i>Journal of Applied Physics</i> , <b>2021</b> , 130, 125103	2.5	0
18	Atomistic simulation on the generation of defects in Cu/SiC composites during cooling. <i>Journal of Materials Science and Technology</i> , <b>2022</b> , 123, 1-12	9.1	0
17	Orientation dependence of shock-induced change of habit plane for the $\frac{1}{2}\langle 111 \rangle$ dislocation loop and plasticity in tungsten. <i>International Journal of Plasticity</i> , <b>2022</b> , 155, 103329	7.6	0
16	Influence of Irradiation on Mechanical Properties of Nickel. <i>Advances in Materials Science and Engineering</i> , <b>2019</b> , 2019, 1-6	1.5	
15	Simultaneous dispersive and covalent monolayer MoS <sub>2</sub> /TiO <sub>2</sub> cluster heterostructures: Insights into their enhanced photocatalytic activity. <i>Superlattices and Microstructures</i> , <b>2018</b> , 121, 64-74	2.8	
14	Composition and Size Dependence of Alloying in Ni <sub>3</sub> Al Nanoparticles With Icosahedral and Rhombohedral Configurations: An Atomic Simulation Study. <i>Physica Status Solidi (B): Basic Research</i> , <b>2017</b> , 254, 1700168	1.3	
13	Effects of contact shape on ballistic phonon transport in semiconductor nanowires. <i>Current Applied Physics</i> , <b>2012</b> , 12, 437-442	2.6	
12	Site Preference and Elastic Properties of 5d Transition Metals in Ductility YAg Alloys. <i>Advanced Materials Research</i> , <b>2012</b> , 472-475, 1397-1401	0.5	

11	Site Preference and Elastic Properties of 3d Transition Metals Alloying Addition in Ductility YAg Alloys. <i>Advanced Materials Research</i> , <b>2012</b> , 535-537, 1000-1004	0.5
10	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. <i>Metals</i> , <b>2022</b> , 12, 215	2.3
9	Influence of orientation on crack propagation of aluminum by molecular dynamics. <i>European Physical Journal B</i> , <b>2022</b> , 95, 1	1.2
8	Interaction between impurity elements (C, N and O) and hydrogen in hcp-Zr: a first-principles study. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2020</b> , 28, 085007	2
7	Study on the effect of non-centrosymmetric orientation in shocked and ramp compressed Iron. <i>Materials Today Communications</i> , <b>2021</b> , 29, 102893	2.5
6	The flow behavior of liquid Li in Cu micro-channels. <i>Wuli Xuebao/Acta Physica Sinica</i> , <b>2016</b> , 65, 104705	0.6
5	The interactions between nitrogen oxides and Uranium surface. <i>Nuclear Materials and Energy</i> , <b>2021</b> , 26, 100945	2.1
4	One-Photon Excitation Pathway: High-Throughput One-Photon Excitation Pathway in 0D/3D Heterojunctions for Visible-Light Driven Hydrogen Evolution (Adv. Funct. Mater. 18/2021). <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2170125	15.6
3	Atomistic insights into interactions between oxygen and Zr (101-1) surface. <i>Nuclear Materials and Energy</i> , <b>2021</b> , 27, 100974	2.1
2	Assessing Atomic-Phase Transitions and Ion Transport in Layered $\text{Na}_x\text{NiO}_2$ ( $x \in [0.67]$ ) Cathode Materials. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 4930-4937	3.8
1	Atomistic simulation of the surface configuration of the NiBe cluster. <i>Thin Solid Films</i> , <b>2021</b> , 737, 138938	2.2