

Efficient iterative schemes for a set

Physical Review B

54, 11169-11186

DOI: [10.1103/physrevb.54.11169](https://doi.org/10.1103/physrevb.54.11169)

Citation Report

#	ARTICLE	IF	CITATIONS
3	Molecular Precursors in the Dissociative Adsorption of O ₂ on Pt(111). <i>Physical Review Letters</i> , 1997, 79, 4481-4484.	2.9	309
4	Role of silicon vacancies in yttrium-disilicide compounds from ab initio calculations. <i>Physical Review B</i> , 1997, 55, 13479-13484.	1.1	30
5	An Introduction to Ab-Initio Molecular Dynamics Schemes. <i>Molecular Simulation</i> , 1997, 20, 63-77.	0.9	7
6	Application of Ab Initio Methods to Secondary Lithium Batteries. <i>Materials Research Society Symposia Proceedings</i> , 1997, 496, 65.	0.1	3
7	Transitory Metastable Phases in Refractory Metals-Based Systems Solidified by Drop-Tube Processing: A First-Principles Approach. <i>Materials Research Society Symposia Proceedings</i> , 1997, 481, 27.	0.1	0
8	Ab INITIO CALCULATION OF THE Li _x CoO ₂ PHASE DIAGRAM. <i>Materials Research Society Symposia Proceedings</i> , 1997, 496, 121.	0.1	5
9	First principles calculations on crystalline and liquid iron at Earth's core conditions. <i>Faraday Discussions</i> , 1997, 106, 205-218.	1.6	106
10	Ab initio simulation of molecular processes on oxide surfaces. <i>Faraday Discussions</i> , 1997, 106, 135-154.	1.6	69
11	Ab initio density functional studies of transition-metal sulphides: II. Electronic structure. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 11107-11140.	0.7	109
12	Ab initio density functional studies of transition-metal sulphides: I. Crystal structure and cohesive properties. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 11085-11106.	0.7	118
13	H ₂ dissociative adsorption on Pd(111). <i>Physical Review B</i> , 1997, 56, 15396-15403.	1.1	151
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20	The electrochemical stability of lithium-metal oxides against metal reduction. <i>Solid State Ionics</i> , 1998, 109, 151-157.	1.3	17

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8286	Atomic transport in ordered compounds mediated by local disorder: Diffusion in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{B} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Ni} \langle \text{mml:mtext} \rangle \text{ and formation of oxide islands on Be(0001): An atomistic model for metal oxidation. Physical Review B, 2010, 81, .$	1.1	21
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8291	Structure and energetics of ferroelectric domain walls in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{LiNbO} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{ atomic-level simulations. Physical Review B, 2010, 82, .$	1.1	45
8292	$\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{BaCu} \langle \text{mml:mtext} \rangle \langle \text{mml:mi} \rangle \text{C} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{h} \langle \text{mml:mi} \rangle \langle \text{mml:mtext} \rangle \text{F} \langle \text{mml:mtext} \rangle \text{ and scanning tunneling microscopy study of an indium-terminated GaAs(100) surface: An indium-induced surface reconstruction change in the} \langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{c} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 8 \langle \text{mml:mn} \rangle \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle$	1.1	23
8293	<i>Ab initio</i> study of low-dimensional quantum spin systems $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Sr} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Sr} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Sr} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Sr} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle$	1.1	25
8294	Pathways for thermal phosphorus desorption from the silicon (001) surface. Physical Review B, 2010, 82, .	1.1	4
8295	Phase transformation in Si from semiconducting diamond to metallic $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \hat{I}^2 \langle \text{mml:mi} \rangle \langle \text{mml:mtext} \rangle \text{-Sn} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{ phase} \langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \hat{I}^2 \langle \text{mml:mi} \rangle \langle \text{mml:mtext} \rangle \text{-Sn} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{ phase}$	1.1	65
8296	Structure of the (010) surface of the orthorhombic complex metallic alloy $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{T} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{-Al} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{-Al} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle$	1.1	22
8297	Tailoring perpendicular magnetic anisotropy in ultrathin Co/Pt multilayers coupled to NiO. Physical Review B, 2010, 81, .	1.1	8
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8300	Hydrogen interaction with point defects in tungsten. <i>Physical Review B</i> , 2010, 82, .	1.1	216
8301	Extrinsic point defects in aluminum antimonide. <i>Physical Review B</i> , 2010, 81, .	1.1	21
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11209	$\text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"}\ \text{display}=\text{"inline"}\ >\ <\text{mml:msub}\ <\text{mml:mrow}$		

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12791	(xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" style="color: yellow;"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>		

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12864	First-principles investigation of the Al–Si–Sr ternary system: Ground state determination and mechanical properties. <i>Intermetallics</i> , 2012, 21, 31-44.	1.8	19
12865	First-principles investigation on shear deformation of a TiAl/Ti ₃ Al interface and effects of oxygen. <i>Intermetallics</i> , 2012, 22, 41-46.	1.8	21
12866	First-principles investigations of elastic, electronic and thermodynamic properties of Al ₁₂ X (X=Mo, W) Tj ETQq1 1.8 0.7843 14 rgBT / 17	1.8	14

#	ARTICLE	IF	CITATIONS
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12879	First principles investigation of temperature and pressure dependent elastic properties of ZrC and ZrN using Debye–Grüneisen theory. <i>Journal of Alloys and Compounds</i> , 2012, 540, 94-99.	2.8	33
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12884	The structure and electronic properties of AlN/SrTiO ₃ (111) interfaces. <i>Journal of Crystal Growth</i> , 2012, 353, 134-139.	0.7	7

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14844			

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18058	First-principles study of the phonon dispersion and dielectric properties of wurtzite InP: Role of In d electrons. <i>Physical Review B</i> , 2014, 89, 085411.		

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20083	Structural and electronic properties of germanene/MoS ₂ monolayer and silicene/MoS ₂ monolayer superlattices. <i>Nanoscale Research Letters</i> , 2014, 9, 110.	3.1	69
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28071	A Comprehensive Set of High-Quality Point Charges for Simulations of Metal-Organic Frameworks. <i>Chemistry of Materials</i> , 2016, 28, 785-793.	3.2	140
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28798	Novel superhard B ⁺ C ⁻ O phases predicted from first principles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1859-1863.	1.3	44
28799	Covalent pathways in engineering h-BN supported graphene. <i>Carbon</i> , 2016, 98, 449-456.	5.4	8
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28801	Theoretical investigation of Chevrel phase materials for cathodes accommodating Ca ²⁺ ions. <i>Journal of Power Sources</i> , 2016, 306, 431-436.	4.0	58
28802	Stability and nucleation of Ir _n (n = 1-5) clusters on different β -Al ₂ O ₃ surfaces: A density functional theory study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 718-725.	0.9	8
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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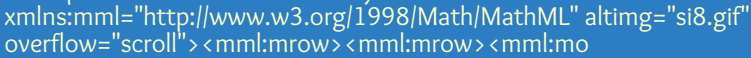
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#	ARTICLE	IF	CITATIONS
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31356	Solution-based synthesis and processing of Sn- and Bi-doped Cu ₃ SbSe ₄ nanocrystals, nanomaterials and ring-shaped thermoelectric generators. <i>Journal of Materials Chemistry A</i> , 2017, 5, 2592-2602.	5.2	73
31357	Anisotropic intrinsic lattice thermal conductivity of borophane from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2843-2849.	1.3	40
31358	Electronic and optical properties of oxygen vacancies in amorphous Ta ₂ O ₅ from first principles. <i>Nanoscale</i> , 2017, 9, 1120-1127.	2.8	45
31359	How covalence breaks adsorption-energy scaling relations and solvation restores them. <i>Chemical Science</i> , 2017, 8, 124-130.	3.7	145
31360	Band alignment of two-dimensional lateral heterostructures. <i>2D Materials</i> , 2017, 4, 015038.	2.0	80
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31370	Quasimolecules in Compressed Lithium. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 972-975.	7.2	32

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31386	Aluminum nitride nanotubes. <i>Chemical Papers</i> , 2017, 71, 881-893.	1.0	51
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#	ARTICLE	IF	CITATIONS
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31409	Hybrid Palladium Nanoparticles for Direct Hydrogen Peroxide Synthesis: The Key Role of the Ligand. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 1775-1779.	7.2	78
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#	ARTICLE	IF	CITATIONS
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32158	I_2 I_3 I^2		

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#	ARTICLE	IF	CITATIONS
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34336	Doubly Screened Hybrid Functional: An Accurate First-Principles Approach for Both Narrow- and Wide-Gap Semiconductors. Journal of Physical Chemistry Letters, 2018, 9, 2338-2345.	2.1	37
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34354	Improving visible-light-driven photocatalytic NO oxidation over BiOBr nanoplates through tunable oxygen vacancies. <i>Chinese Journal of Catalysis</i> , 2018, 39, 779-789.	6.9	57
34355	Evaluation of dry reforming reaction catalysts via computational screening. <i>Catalysis Today</i> , 2018, 312, 23-34.	2.2	8
34356	Inducing skyrmions in ultrathin Fe films by hydrogen exposure. <i>Nature Communications</i> , 2018, 9, 1571.	5.8	40
34357	Toxicity assessment and mechanistic investigation of engineered monoclinic VO ₂ nanoparticles. <i>Nanoscale</i> , 2018, 10, 9736-9746.	2.8	14
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34382	A One-Dimensional Model for Photoemission Calculations from Plane-Wave Band Structure Codes. <i>E-Journal of Surface Science and Nanotechnology</i> , 2018, 16, 49-52.	0.1	1
34383	Structural Analysis of Self-Assembled Platinum-Silicide Nanostructures on Si(001) Using Ion Scattering Spectroscopy. <i>E-Journal of Surface Science and Nanotechnology</i> , 2018, 16, 66-71.	0.1	0
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#	ARTICLE	IF	CITATIONS
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34447	Mechanism of Phosphorus Transport Through Silicon Oxide During Phosphonic Acid Monolayer Doping. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10088-10095.	1.5	16
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34477	Anti-site defected MoS ₂ sheet for catalytic application. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	1
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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36011	A theoretical perspective of the enhanced photocatalytic properties achieved by forming tetragonal ZnS/ZnSe hetero-bilayer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9950-9956.	1.3	14
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36109	Photocatalytic Activity of Phosphorene Derivatives: Coverage, Electronic, Optical, and Excitonic Properties. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7194-7202.	1.5	9
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36119	Anisotropic vacancy-mediated phonon mode softening in Sm and Gd doped ceria. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10048-10059.	1.3	10
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36138	Metal-organic framework-derived porous shuttle-like vanadium oxides for sodium-ion battery application. <i>Nano Research</i> , 2018, 11, 449-463.	5.8	108
36139	Superior catalytic performance of Mn-Mullite over Mn-Perovskite for NO oxidation. <i>Catalysis Today</i> , 2018, 310, 195-201.	2.2	52
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36143	Tunable Magnetic Interaction of Mn-Doped MoS ₂ /SiC van der Waals Heterostructures Under Normal Strain. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 449-453.	0.8	1
36144	Strain and different edge terminations modulated electronic and magnetic properties of armchair AlN/SiC nanoribbons: first-principles study. <i>Canadian Journal of Physics</i> , 2018, 96, 30-35.	0.4	0
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36147	Surface Termination of Fe ₃ O ₄ (111) Films Studied by CO Adsorption Revisited. <i>Journal of Physical Chemistry B</i> , 2018, 122, 527-533.	1.2	46
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36158	Interaction of Pd single atoms with different CeO ₂ crystal planes: A first-principles study. <i>Applied Surface Science</i> , 2018, 433, 1036-1048.	3.1	17
36159	Heterolytic dissociative adsorption state of dihydrogen favored by interfacial defects. <i>Applied Surface Science</i> , 2018, 433, 862-868.	3.1	9
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#	ARTICLE	IF	CITATIONS
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36306	Geometric structure and photovoltaic properties of mixed halide germanium perovskites from theoretical view. <i>Organic Electronics</i> , 2018, 53, 50-56.	1.4	74
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36309	Tuning the electronic properties of bilayer group-IV monochalcogenides by stacking order, strain and an electric field: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 214-220.	1.3	32
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36312	First principles calculations for iodine atom diffusion in SiC with point defects. <i>Computational Materials Science</i> , 2018, 142, 427-436.	1.4	3
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36314	Theoretical study on the photocatalytic properties of graphene oxide with single Au atom adsorption. <i>Surface Science</i> , 2018, 669, 71-78.	0.8	18
36315	Reactivity of CO ₂ on the surfaces of magnetite (Fe ₃ O ₄), greigite (Fe ₃ S ₄) and mackinawite (FeS). <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2018, 376, 20170065.	1.6	27

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36317	First-Principles Study on the Tensile Properties and Failure Mechanism of the CoSb ₃ /Ti Interface. <i>Journal of Electronic Materials</i> , 2018, 47, 3210-3217.	1.0	3
36318	Crystal structure of Th ₂ B ₂ C ₃ with unique mixed B-C structural units. <i>Acta Materialia</i> , 2018, 144, 484-495.	3.8	7
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36320	Effects of rare-earth doping on the ionic conduction of CeO ₂ in solid oxide fuel cells. <i>Ceramics International</i> , 2018, 44, 3707-3711.	2.3	30
36321	The effect of B on solid solution structure and preferred orientation of vapor-deposited Al-B thin film: A first-principles study. <i>Computational Materials Science</i> , 2018, 142, 325-331.	1.4	4
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36323	Impact of bi-axial strain on the structural, electronic and optical properties of photo-catalytic bulk bismuth oxyhalides. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 103-111.	1.3	18
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36330	Spin-orbit coupling effect on structural and magnetic properties of Co Rh ₁₃ (n ⁻ =13) clusters. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 451, 360-367.	1.0	11
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36332	Graphene Oxide Epoxy (GO _{xy}): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities. <i>Advanced Materials Interfaces</i> , 2018, 5, 1700657.	1.9	19
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36336	Strain-modulated magnetic behavior in Li-doped WS ₂ monolayer. <i>Optik</i> , 2018, 157, 827-832.	1.4	2
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36338	Dynamic imaging of metastable reaction pathways in lithiated cobalt oxide electrodes. <i>Nano Energy</i> , 2018, 44, 15-22.	8.2	24
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36343	Confined Li ion migration in the silicon-graphene complex system: An ab initio investigation. <i>Applied Surface Science</i> , 2018, 436, 505-510.	3.1	14
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36350	Theoretical design and exploration of novel high energy density materials based on silicon. <i>Journal of Energetic Materials</i> , 2018, 36, 291-301.	1.0	4
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36356	Brush-Like Cobalt Nitride Anchored Carbon Nanofiber Membrane: Current Collector-Catalyst Integrated Cathode for Long Cycle O_2 Batteries. <i>ACS Nano</i> , 2018, 12, 128-139.	7.3	230
36357	Pressure-Induced Polymerization of CO_2 in Lithium-Carbon Dioxide Phases. <i>Journal of the American Chemical Society</i> , 2018, 140, 413-422.	6.6	11
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36362	Remarkable enhancement in thermoelectric performance of BiCuSeO through biaxial strain modulation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 97, 392-400.	1.3	11
36363	Intrinsic sources of high thermal conductivity of CdSiP_2 determined by first-principle anharmonic calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1568-1574.	1.3	8
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36367	Support effects in single atom iron catalysts on adsorption characteristics of toxic gases (NO_2 , NH_3). <i>Tj ETQq1 1 0,784314 rgBT /Ove</i>	3.1	81
36368	<i>Ab initio</i> dynamical stability of tungsten at high pressures and high temperatures. <i>Computational Materials Science</i> , 2018, 144, 32-35.	1.4	10
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#	ARTICLE	IF	CITATIONS
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36371	Two-dimensional silicon crystals with sizable band gaps and ultrahigh carrier mobility. <i>Nanoscale</i> , 2018, 10, 1265-1271.	2.8	28
36372	Bandgap engineering and charge separation in two-dimensional GaS-based van der Waals heterostructures for photocatalytic water splitting. <i>Applied Surface Science</i> , 2018, 439, 374-379.	3.1	36
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36375	Characterization of lattice defects in metallic materials by positron annihilation spectroscopy: A review. <i>Journal of Materials Science and Technology</i> , 2018, 34, 577-598.	5.6	127
36376	Debye temperature for binary alloys and its relationship with cohesive energy. <i>Physica B: Condensed Matter</i> , 2018, 531, 95-101.	1.3	9
36377	Chemical Origin of Sodium Phosphate Interactions on Iron and Iron Oxide Surfaces by First Principle Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 635-647.	1.5	29
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36384	Electronic structure engineering in silicene via atom substitution and a new two-dimensional Dirac structure Si ₃ C. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 98, 39-44.	1.3	11
36385	Ferromagnetism and antiferromagnetism coexistence in Sr _{1-x} La _x RuO ₃ induced by La-doping. <i>Solid State Communications</i> , 2018, 270, 119-123.	0.9	7
36386	The Rich Solid-State Phase Behavior of dl-Aminoheptanoic Acid: Five Polymorphic Forms and Their Phase Transitions. <i>Crystal Growth and Design</i> , 2018, 18, 242-252.	1.4	11
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#	ARTICLE	IF	CITATIONS
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36389	Enhancing Ferroelectric Dipole Ordering in Organicâ€“Inorganic Hybrid Perovskite CH ₃ NH ₃ PbI ₃ : Strain and Doping Engineering. <i>Journal of Physical Chemistry C</i> , 2018, 122, 177-184.	1.5	35
36390	Band Structure Engineering of Cs ₂ AgBiBr ₆ Perovskite through Orderâ€“Disordered Transition: A First-Principle Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 31-35.	2.1	121
36391	Tunneling Hot Spots in Ferroelectric SrTiO ₃ . <i>Nano Letters</i> , 2018, 18, 491-497.	4.5	30
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36397	Exploring the charge localization and band gap opening of borophene: a first-principles study. <i>Nanoscale</i> , 2018, 10, 1403-1410.	2.8	77
36398	Influence of a Confined Methanol Solvent on the Reactivity of Active Sites in UiOâ€“66. <i>ChemPhysChem</i> , 2018, 19, 420-429.	1.0	17
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36403	Potential Semiconducting and Superconducting Metastable Si ₃ C Structures under Pressure. <i>Chemistry of Materials</i> , 2018, 30, 421-427.	3.2	5
36404	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metalâ€“Organic Frameworks for Adsorption Applications. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 365-376.	2.3	18
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36407	In situ surface stress measurement and computational analysis examining the oxygen reduction reaction on Pt and Pd. <i>Electrochimica Acta</i> , 2018, 260, 400-406.	2.6	14
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36409	First principle calculation of helium in La ₂ Zr ₂ O ₇ : Effects on structural, electronic properties and radiation tolerance. <i>Journal of Nuclear Materials</i> , 2018, 500, 72-80.	1.3	18
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36411	Unusual Ferroelectricity in Two-Dimensional Perovskite Oxide Thin Films. <i>Nano Letters</i> , 2018, 18, 595-601.	4.5	41
36412	Ultralow and anisotropic thermal conductivity in semiconductor As ₂ Se ₃ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1809-1816.	1.3	16
36413	Orthorhombic Ti ₂ O ₃ : A Polymorph-Dependent Narrow-Bandgap Ferromagnetic Oxide. <i>Advanced Functional Materials</i> , 2018, 28, 1705657.	7.8	36
36414	Phase, hardness, and deformation slip behavior in mixed Hf _x Ta _{1-x} C. <i>Acta Materialia</i> , 2018, 145, 142-153.	3.8	81
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36418	Diffusion Kinetics of Gold and Copper Atoms on Pristine and Reduced Rutile TiO ₂ (110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3824-3837.	1.5	12
36419	Enhancing Intermolecular Interaction by Cyano Substitution in Copper Phthalocyanine. <i>Journal of Physical Chemistry C</i> , 2018, 122, 429-437.	1.5	8
36420	Controllable dissociation of H ₂ O on a CeO ₂ (111) surface. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1575-1582.	1.3	10
36421	Atomic-scale mechanisms of defect- and light-induced oxidation and degradation of InSe. <i>Journal of Materials Chemistry C</i> , 2018, 6, 518-525.	2.7	43
36422	A combined theoretical and experimental approach of a new ternary metal oxide in molybdate composite for hybrid energy storage capacitors. <i>APL Materials</i> , 2018, 6, .	2.2	26
36423	First-principles study of SnS electronic properties using LDA, PBE and HSE06 functionals. <i>Philosophical Magazine</i> , 2018, 98, 710-726.	0.7	16

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36425	Highly efficient catalytic scavenging of oxygen free radicals with graphene-encapsulated metal nanoshields. <i>Nano Research</i> , 2018, 11, 2821-2835.	5.8	31
36426	Design lateral heterostructure of monolayer ZrS ₂ and HfS ₂ from first principles calculations. <i>Applied Surface Science</i> , 2018, 436, 919-926.	3.1	33
36427	Validation of inter-atomic potential for WS ₂ and WSe ₂ crystals through assessment of thermal transport properties. <i>Computational Materials Science</i> , 2018, 144, 92-98.	1.4	36
36428	Predicting two-dimensional carbon phosphide compounds: C ₂ P ₄ by the global optimization method. <i>Computational Materials Science</i> , 2018, 144, 70-75.	1.4	21
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36430	Exploring the properties of carbazole-based derivatives as hole transport materials from first principle and MD simulation. <i>Organic Electronics</i> , 2018, 54, 14-20.	1.4	18
36431	Origin of n-type conductivity in two-dimensional InSe: In atoms from surface adsorption and van der Waals gap. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 98, 66-73.	1.3	8
36432	Comparative DFT+U and HSE Study of the Oxygen Evolution Electrocatalysis on Perovskite Oxides. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1135-1147.	1.5	46
36433	Carboxylic Acid Group-Induced Oxygen Vacancy Migration on an Anatase (101) Surface. <i>Langmuir</i> , 2018, 34, 546-552.	1.6	11
36434	A new pnictidehalide with van der Waals host-guest interactions exhibiting both geometric spin frustration and resistive humidity sensitivity. <i>New Journal of Chemistry</i> , 2018, 42, 1787-1795.	1.4	1
36435	Electronic properties of topological insulator candidate CaAgAs. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 045501.	0.7	18
36436	Stable structures of exohedrally decorated C ₆₀ -fullerenes. <i>Carbon</i> , 2018, 129, 847-853.	5.4	27
36437	Understanding All-Solid Frustrated-Lewis-Pair Sites on CeO ₂ from Theoretical Perspectives. <i>ACS Catalysis</i> , 2018, 8, 546-554.	5.5	135
36438	The truth is out there: the metal- π interactions in crystal of Cr(CO) ₃ (pcp) as revealed by the study of vibrational smearing of electron density. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 317-336.	0.4	7
36439	First-principles studies on the electronic and optical properties of Fe-doped potassium dihydrogen phosphate crystal. <i>Computational Materials Science</i> , 2018, 143, 398-402.	1.4	16
36440	First principles study on interface between dual-channel anchorable organic dyes and TiO ₂ for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2018, 149, 908-914.	2.0	22
36441	Atomistic simulation of cubic and tetragonal phases of U-Mo alloy: Structure and thermodynamic properties. <i>Journal of Nuclear Materials</i> , 2018, 499, 451-463.	1.3	47

#	ARTICLE	IF	CITATIONS
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36443	Charge and strain induced magnetism in monolayer MoS ₂ with S vacancy. Journal of Magnetism and Magnetic Materials, 2018, 451, 520-525.	1.0	23
36444	Edge orientations of mechanically exfoliated anisotropic two-dimensional materials. Journal of the Mechanics and Physics of Solids, 2018, 112, 157-168.	2.3	22
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#	ARTICLE	IF	CITATIONS
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38068	Strain induced electronic structure variation in methyl-ammonium lead iodide perovskite. <i>Scientific Reports</i> , 2018, 8, 7760.	1.6	53
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38357	Grain Boundaries Are Benign and Suppress Nonradiative Electron-Hole Recombination in Monolayer Black Phosphorus: A Time-Domain Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3856-3862.	2.1	54
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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40998	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>x</mml:mi></mml:math><mml:math type="doping"></mml:math><mml:mi>Mn</mml:mi><mml:msub></mml:msub></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnGeN</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and	1.1	8
40999	Robust circular polarization of indirect Q-K transitions in bilayer xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn></mml:mrow><mml:mi>R</mml:mi><mml:mo>â”ˆ</mml:mo></mml:mrow></mml:math> mathvariant="normal">W</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>.	1.1	11
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42409	Possible emergence of a skyrmion phase in ferroelectric xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>GaM</mml:mi><mml:mn>2</mml:mn></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>o</mml:mi><mml:mn>4</mml:mn></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mn>8</mml:mn></mml:mrow></mml:math>.	1.1	18
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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46605	Carbon vacancy in C ₃ N ₄ nanotube: Electronic structure, photocatalysis mechanism and highly enhanced activity. <i>Applied Catalysis B: Environmental</i> , 2020, 262, 118281.	10.8	162
46606	Insight to unprecedented catalytic activity of double-nitrogen defective metal-free catalyst: Key role of coal gangue. <i>Applied Catalysis B: Environmental</i> , 2020, 263, 118316.	10.8	51
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46610	Low Lying Magnetic States of the Mixed Valence Cobalt Ludwigite. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900298.	0.7	3
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47205	Tight-Binding Parameterizations of Ti and Ba Oxides and Their Application for the Prediction of 2D Phases. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900634.	0.7	2
47206	Influence of oxide support on Pd properties: A gain for O diffusion versus minor impact for CH ₄ dissociation. <i>Catalysis Today</i> , 2020, 357, 368-379.	2.2	4
47207	BOPcat software package for the construction and testing of tight-binding models and bond-order potentials. <i>Computational Materials Science</i> , 2020, 173, 109455.	1.4	6
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47209	Nanoscale Pd catalysts decorated WO ₃ -SnO ₂ heterojunction nanotubes for highly sensitive and selective acetone sensing. <i>Sensors and Actuators B: Chemical</i> , 2020, 306, 127575.	4.0	63
47210	Insight into the Characteristics of 4f-Related Electronic Transitions for Rare-Earth-Doped KLuS ₂ Luminescent Materials through First-Principles Calculation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 932-938.	1.5	8
47211	Radiation-Induced Evolution of Tungsten Carbide in Fusion Reactors: Accommodation of Defect Clusters and Transmutation Elements. <i>ACS Applied Energy Materials</i> , 2020, 3, 868-878.	2.5	16
47212	Q-Carbon: A New Carbon Allotrope with a Low Degree of s-p Orbital Hybridization and Its Nucleation Lithiation Process in Lithium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 619-626.	4.0	16
47213	Origin of the Flat Band in Heavily Cs-Doped Graphene. <i>ACS Nano</i> , 2020, 14, 1055-1069.	7.3	28
47214	Enhancing Chemical Interaction of Polysulfide and Carbon through Synergetic Nitrogen and Phosphorus Doping. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 806-813.	3.2	11
47215	Induced magnetism in oxygen-decorated N-doped graphene. <i>Carbon</i> , 2020, 159, 102-109.	5.4	7
47216	Evidence for bandwidth-control metal-insulator transition in Ti ₃ O ₅ . <i>Computational Materials Science</i> , 2020, 173, 109435.	1.4	7
47217	Zintl phase crystal assembled by magic Al ₆ CNa ₄ cluster. <i>Chemical Physics Letters</i> , 2020, 739, 137026.	1.2	0
47218	Band inversion induced multiple electronic valleys for high thermoelectric performance of SnTe with strong lattice softening. <i>Nano Energy</i> , 2020, 69, 104395.	8.2	80
47219	Modulation of spin-valley splitting in a two-dimensional MnPSe ₃ /CrBr ₃ van der Waals heterostructure. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 125104.	1.3	13
47220	Structural, mechanical and electronic properties of two-dimensional chlorine-terminated transition metal carbides and nitrides. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 135302.	0.7	18
47221	The feasibility analysis of growing the modified borophene on substrates: First-principles calculation. <i>Applied Surface Science</i> , 2020, 507, 144154.	3.1	2

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47223	Experimental and ab Initio Studies of Deep-Bulk Traps in Doped Rare-Earth Oxide Thick Films. <i>Journal of Physical Chemistry C</i> , 2020, 124, 997-1007.	1.5	7
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47225	Modified Generalized Stacking Fault Energy Surface of II-VI Ionic Crystals from Excess Electrons and Holes. <i>ACS Applied Electronic Materials</i> , 2020, 2, 56-65.	2.0	3
47226	Size-Controlled Pd Nanoparticles Loaded on Co ₃ O ₄ Nanoparticles by Calcination for Enhanced CO Oxidation. <i>ACS Applied Nano Materials</i> , 2020, 3, 486-495.	2.4	26
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47233	TensorAlloy: An automatic atomistic neural network program for alloys. <i>Computer Physics Communications</i> , 2020, 250, 107057.	3.0	8
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47238	Defect Engineering of Iron-Rich Orthosilicate Cathode Materials with Enhanced Lithium-Ion Intercalation Capacity and Kinetics. <i>ACS Applied Energy Materials</i> , 2020, 3, 675-686.	2.5	3
47239	A Flexible Potassium-Ion Hybrid Capacitor with Superior Rate Performance and Long Cycling Life. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 2424-2431.	4.0	59

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47259	The effects of dilute concentrations of substitutional Re or Os on the thermodynamics and kinetics of oxygen in tungsten. <i>Physica B: Condensed Matter</i> , 2020, 580, 411937.	1.3	1
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47261	Lattice-Strain Control of Flexible Janus Indium Chalcogenide Monolayers for Photocatalytic Water Splitting. <i>Journal of Physical Chemistry C</i> , 2020, 124, 167-174.	1.5	30
47262	Promotional Effect of La in the Three-Way Catalysis of La-Loaded Al_2O_3 -Supported Pd Catalysts ($\text{Pd/La/Al}_2\text{O}_3$). <i>ACS Catalysis</i> , 2020, 10, 1010-1023.	5.5	46
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47264	Effect of IT-M doping on charge transfer and ultrafast carrier dynamics of ternary organic solar cell materials. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 095103.	1.3	4
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47266	New Family of Anisotropic Zinc-Based Semiconductors in a Shallow Energy Landscape. <i>Chemistry of Materials</i> , 2020, 32, 326-332.	3.2	7
47267	Synthesis of orthogonally assembled 3D cross-stacked metal oxide semiconducting nanowires. <i>Nature Materials</i> , 2020, 19, 203-211.	13.3	172
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47271	Facile CO Oxidation on Oxygen-Functionalized MXenes via the Mars-van Krevelen Mechanism. <i>ChemCatChem</i> , 2020, 12, 1007-1012.	1.8	7
47272	Influence of defects and dopants on the sensitivity of arsenene towards HCN. <i>Applied Surface Science</i> , 2020, 506, 144936.	3.1	61
47273	Structural and electrochemical studies of Fe-doped $\text{Na}_3\text{Mn}_2\text{P}_3\text{O}_{11}$ cathode materials for sodium-ion batteries. <i>Journal of Alloys and Compounds</i> , 2020, 821, 153206.	2.8	12
47274	Phase stability, magnetic and elastic properties of Co_2NiGa alloy: A first-principles calculation. <i>Materials Today Communications</i> , 2020, 22, 100810.	0.9	7
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47283	DFT study of Pt sub-monolayer adsorption on the positive BiFeO ₃ (0001) surface. Surface Science, 2020, 693, 121553.	0.8	0
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47285	Proton irradiation of Ni-Cr alloy: Understanding the evolution of the damage microstructure. Journal of Alloys and Compounds, 2020, 815, 152408.	2.8	4
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47298	Experimental and ab initio study of the Ag–Li system for energy storage and high-temperature solders. <i>Journal of Alloys and Compounds</i> , 2020, 817, 152811.	2.8	10
47299	A general rule for transition metals doping on magnetic properties of Fe-based metallic glasses. <i>Journal of Alloys and Compounds</i> , 2020, 819, 153062.	2.8	10
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47302	Hydrogen induced AFM to FM magnetic transition in $\hat{\mu}$ -FeHx. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 498, 166147.	1.0	1
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47304	Thermodynamic stability analysis of Bi-containing III-V quaternary alloys and the effect of epitaxial strain. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 138, 109245.	1.9	6
47305	Electronic and magnetic properties of Fe-doped narrow zigzag boron nitride nanoribbons. <i>Materials Today Communications</i> , 2020, 22, 100753.	0.9	5
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47308	d-orbital-frustration-induced ferromagnetic monolayer Cu ₃ O ₂ . <i>Physica B: Condensed Matter</i> , 2020, 577, 411826.	1.3	3
47309	Cu-doping impact on the electronic and magnetic properties of Co ₂ ZrSn. <i>Physica B: Condensed Matter</i> , 2020, 580, 411836.	1.3	6
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#	ARTICLE	IF	CITATIONS
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47313	Core effect of local atomic configuration and design principles in Al _x CoCrFeNi high-entropy alloys. <i>Scripta Materialia</i> , 2020, 178, 181-186.	2.6	29
47314	Electronic structures of new layered hexaboron Cr ^α B compounds from first principles. <i>Solid State Sciences</i> , 2020, 99, 106069.	1.5	2
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47316	Nano-patterned honeycomb structure of monolayer copper selenide on Cu(111). <i>Thin Solid Films</i> , 2020, 693, 137709.	0.8	4
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47319	Shining Emitter in a Stable Host: Design of Halide Perovskite Scintillators for X-ray Imaging from Commercial Concept. <i>ACS Nano</i> , 2020, 14, 5183-5193.	7.3	205
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47321	Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain. <i>Nanotechnology</i> , 2020, 31, 115701.	1.3	4
47322	Non-chemical fluorination of hexagonal boron nitride by high-energy ion irradiation. <i>Nanotechnology</i> , 2020, 31, 125705.	1.3	5
47323	Oxygen Evolution on Metal ^α Oxy ^β Hydroxides: Beneficial Role of Mixing Fe, Co, Ni Explained via Bifunctional Edge/acceptor Route. <i>ChemCatChem</i> , 2020, 12, 1436-1442.	1.8	21
47324	A decohesion pathway for hydrogen embrittlement in nickel: Mechanism and quantitative prediction. <i>Acta Materialia</i> , 2020, 185, 98-109.	3.8	55
47325	stretchy="false">[</mml:mo><mml:mn>1</mml:mn><mml:mover accent="true"><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:mover></mml:math> tilt grain boundary in BCC Fe.	1.4	37
47326	A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 135901.	0.7	9
47327	Rotation Tunable Photocatalytic Properties of ZnO/GaN Heterostructures. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900663.	0.7	11
47328	First-Principles Study of Structural, Elastic, and Thermodynamic Properties of PdSn ₄ with Ni Addition. <i>Journal of Electronic Materials</i> , 2020, 49, 1435-1444.	1.0	6
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47331	Exploring the effect of dopant (Si, P, S, Ge, Se, and Sb) in arsenene: A DFT study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126146.	0.9	8
47332	Band alignment engineering: ultrabroadband photodetection with SnX ₂ (X = S, Se)/ZnS heterostructures. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 115703.	0.7	15
47333	The Systematic Refinement for the Phase Change and Conversion Reactions Arising from the Lithiation of Magnetite Nanocrystals. <i>Advanced Functional Materials</i> , 2020, 30, 1907337.	7.8	8
47334	PBCF@Graphene: A 2D Hybridized Honeycomb Carbon Allotrope with a Direct Band Gap. <i>ChemNanoMat</i> , 2020, 6, 139-147.	1.5	54
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47336	Electronic structure and morphology of thin surface alloy layers formed by deposition of Sn on Au(111). <i>Applied Surface Science</i> , 2020, 506, 144606.	3.1	13
47337	High conductivity Ni ₂ P nanowires as high-rate electrode material for battery-supercapacitor hybrid devices. <i>Chemical Engineering Journal</i> , 2020, 392, 123661.	6.6	78
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47339	Electrochemical CO ₂ Reduction Reaction on M@Cu(211) Bimetallic Single-Atom Surface Alloys: Mechanism, Kinetics, and Catalyst Screening. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 210-222.	3.2	86
47340	Rational Synthesis for a Noble Metal Carbide. <i>Journal of the American Chemical Society</i> , 2020, 142, 1247-1253.	6.6	15
47341	Ag-modified Fe ₂ O ₃ nanoparticles on a carbon cloth as an anode material for high-performance supercapacitors. <i>Nanotechnology</i> , 2020, 31, 125405.	1.3	4
47342	Recent Progress in Two-Dimensional Ferroelectric Materials. <i>Advanced Electronic Materials</i> , 2020, 6, 1900818.	2.6	236
47343	Atomic Self-Reconstruction of Catalyst Dominated Growth Mechanism of Graphite Structures. <i>ChemCatChem</i> , 2020, 12, 1316-1324.	1.8	6
47344	Iron-doping induced multiferroic in two-dimensional In ₂ Se ₃ . <i>Science China Materials</i> , 2020, 63, 421-428.	3.5	30
47345	In situ no-slot joint integration of half-metallic C(CN) ₃ cocatalyst into g-C ₃ N ₄ scaffold: An absolute metal-free in-plane heterosystem for efficient and selective photoconversion of CO ₂ into CO. <i>Applied Catalysis B: Environmental</i> , 2020, 264, 118470.	10.8	41
47346	Thickness effect on the structural, electronic and energetic properties of the cubic KMgF ₃ surfaces: A first-principles study. <i>Applied Surface Science</i> , 2020, 506, 144678.	3.1	4
47347	Ohmic contact formation mechanisms of TiN film on 4H-SiC. <i>Ceramics International</i> , 2020, 46, 7142-7148.	2.3	3

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48285	Temperature-dependent electronic structure in a higher-order topological insulator candidate $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" \rangle \langle \text{mml:mrow} \langle \text{mml:mi} \rangle \text{Eu} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{In} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$	1.1	30
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51012	Ultrafast band-gap renormalization and build-up of optical gain in monolayer <math xmlns:mml="http://www.w3.org/1998/Math/MathML" > < mml:msub > < mml:mi > MoTe </ mml:mi > < mml:mn > 2 </ mml:mn > </ mml:msub > </ math> Physical Review B, 2020, 101, .	1.1	22
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53157	Thermodynamic stability, phase separation and Ag grading in (Ag,Cu)(In,Ga)Se ₂ solar absorbers. <i>Journal of Materials Chemistry A</i> , 2020, 8, 8740-8751.	5.2	29
53158	Identifying Raman modes of Sb ₂ Se ₃ and their symmetries using angle-resolved polarised Raman spectra. <i>Journal of Materials Chemistry A</i> , 2020, 8, 8337-8344.	5.2	62
53159	Long-lifespan lithium metal batteries obtained using a perovskite intercalation layer to stabilize the lithium electrode. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9137-9145.	5.2	4
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53166	Exploring the landscape of Buckingham potentials for silica by machine learning: Soft vs hard interatomic forcefields. <i>Journal of Chemical Physics</i> , 2020, 152, 051101.	1.2	14
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53168	Possible monoclinic distortion of Mo ₂ GaC under high pressure. <i>Journal of Applied Physics</i> , 2020, 127, 145103.	1.1	2
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53171	Strain-tunable electronic, elastic, and optical properties of Ca ₂ monolayer: first-principles study. <i>Philosophical Magazine</i> , 2020, 100, 1982-2000.	0.7	8
53172	Kohn anomaly and van Hove singularity in IV ^B and V ^B group transition metals nitrides and carbides. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 075401.	0.7	0

#	ARTICLE	IF	CITATIONS
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53192	Phase Transformations in Ni(Co)–Mn(Cr,C)–(In,Sn) Alloys: An Ab Initio Study. <i>Physics of Metals and Metallography</i> , 2020, 121, 202-209.	0.3	4
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#	ARTICLE	IF	CITATIONS
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53226	Cu-Al spinel-oxide catalysts for selective hydrogenation of furfural to furfuryl alcohol. <i>Catalysis Today</i> , 2021, 367, 177-188.	2.2	25

#	ARTICLE	IF	CITATIONS
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53239	Synergy of copper doping and oxygen vacancies in porous CoOOH nanoplates for efficient water oxidation. <i>Chemical Engineering Journal</i> , 2021, 405, 126198.	6.6	38
53240	Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26380.	1.0	15
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53244	High-Pressure Structural and Electronic Properties of Potassium-Based Green Primary Explosives. <i>Journal of Electronic Materials</i> , 2021, 50, 1581-1590.	1.0	3

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53246	Promoting effect of acid sites on NH ₃ -SCO activity with water vapor participation for Pt-Fe/ZSM-5 catalyst. <i>Catalysis Today</i> , 2021, 376, 311-317.	2.2	23
53247	First Principles Study of Structure, Alloying and Electronic Properties of Mg-doped CuAg Nanoalloys. <i>Journal of Cluster Science</i> , 2021, 32, 719-725.	1.7	1
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53249	Microstructure and mechanical properties of CoCrNi-Mo medium entropy alloys: Experiments and first-principle calculations. <i>Journal of Materials Science and Technology</i> , 2021, 62, 25-33.	5.6	64
53250	Adsorption and diffusion of oxygen on metal surfaces studied by first-principle study: A review. <i>Journal of Materials Science and Technology</i> , 2021, 62, 180-194.	5.6	78
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53262	Structure, thermal stability, optoelectronic and electrophysical properties of Mg- and Na-codoped bismuth niobate pyrochlores: Experimental and theoretical study. <i>Journal of Alloys and Compounds</i> , 2021, 858, 157742.	2.8	12

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53280	CCS: A software framework to generate two-body potentials using Curvature Constrained Splines. <i>Computer Physics Communications</i> , 2021, 258, 107602.	3.0	5

#	ARTICLE	IF	CITATIONS
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53282	Insights into electrochemical nitrogen reduction reaction mechanisms: Combined effect of single transition-metal and boron atom. <i>Journal of Energy Chemistry</i> , 2021, 58, 577-585.	7.1	66
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53284	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. <i>Advanced Functional Materials</i> , 2021, 31, 2008056.	7.8	97
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53288	Surface excess free energies and equilibrium Wulff shapes in variable chemical environments at finite temperatures. <i>Applied Surface Science</i> , 2021, 540, 148383.	3.1	10
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53292	Tribological properties of V ₂ O ₅ studied via reactive molecular dynamics simulations. <i>Tribology International</i> , 2021, 154, 106750.	3.0	6
53293	Strain engineering the electronic and photocatalytic properties of WS ₂ /blue phosphene van der Waals heterostructures. <i>Catalysis Science and Technology</i> , 2021, 11, 179-190.	2.1	12
53294	Atomic Co/Ni active sites assisted MOF-derived rich nitrogen-doped carbon hollow nanocages for enhanced lithium storage. <i>Chemical Engineering Journal</i> , 2021, 420, 127583.	6.6	36
53295	Computational screening of dopants for mitigating degradation behaviors in sodium-ion layered oxide cathode material. <i>Journal of Alloys and Compounds</i> , 2021, 859, 157785.	2.8	5
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53298	AMMCR: Ab initio model for mobility and conductivity calculation by using Rode Algorithm. <i>Computer Physics Communications</i> , 2021, 259, 107697.	3.0	8

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53303	Synthesis and photoluminescence properties of a novel red emitting Ba ₃ ZnTa ₂ O ₉ : Eu ³⁺ phosphor. <i>Journal of Molecular Structure</i> , 2021, 1224, 129075.	1.8	14
53304	HCOOH Decomposition on Sub-Nanometer Pd ₆ Cluster Catalysts: The Effect of Defective Boron Nitride Supports Through First Principles. <i>Applied Catalysis B: Environmental</i> , 2021, 280, 119392.	10.8	19
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53306	First steps of blue phosphorene growth on Au(1 1 1). <i>Materials Today: Proceedings</i> , 2021, 39, 1153-1156.	0.9	4
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53308	Nanoscale surface modification of P2-type Na _{0.65} [Mn _{0.70} Ni _{0.16} Co _{0.14}]O ₂ cathode material for high-performance sodium-ion batteries. <i>Chemical Engineering Journal</i> , 2021, 404, 126446.	6.6	32
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53327	Enhanced photocatalytic water oxidation by hierarchical 2D-Bi ₂ MoO ₆ @2D-MXene Schottky junction nanohybrid. <i>Chemical Engineering Journal</i> , 2021, 403, 126328.	6.6	94
53328	Orbital symmetry matching: Achieving superior nitrogen reduction reaction over single-atom catalysts anchored on Mxene substrates. <i>Chinese Journal of Catalysis</i> , 2021, 42, 288-296.	6.9	41
53329	Turning chemistry into information for heterogeneous catalysis. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26382.	1.0	9
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53334	Enhanced photocatalytic degradation of organic contaminants over CaFe ₂ O ₄ under visible LED light irradiation mediated by peroxymonosulfate. <i>Journal of Materials Science and Technology</i> , 2021, 62, 34-43.	5.6	78

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#	ARTICLE	IF	CITATIONS
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53750	The thermal and electrical transport properties of layered LaCuOSe under high pressure. <i>Journal of Alloys and Compounds</i> , 2021, 861, 157984.	2.8	15
53751	Theoretical insight into oxidation catalysis of chromite spinel MCr ₂ O ₄ (M = Mg, Co, Cu, and Zn): Volcano plot for oxygen-vacancy formation and catalytic activity. <i>Journal of Catalysis</i> , 2021, 393, 30-41.	3.1	11
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53754	One-step synthesis of oxygen doped g-C ₃ N ₄ for enhanced visible-light photodegradation of Rhodamine B. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 151, 109900.	1.9	64
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53762	Gate tunable self-powered few-layer black phosphorus broadband photodetector. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 399-404.	1.3	2
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53766	Mo ₂ B ₂ MBene-supported single-atom catalysts as bifunctional HER/OER and OER/ORR electrocatalysts. <i>Journal of Materials Chemistry A</i> , 2021, 9, 433-441.	5.2	175

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53775	Improved H ₂ detection performance of GaN sensor with Pt/Sulfide treatment of porous active layer prepared by metal electroless etching. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 4614-4625.	3.8	8
53776	Insights on alkylidene formation on Mo ₂ C: A potential overlap between direct deoxygenation and olefin metathesis. <i>Journal of Catalysis</i> , 2021, 393, 381-389.	3.1	3
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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57222	The effects of heteroatoms-doping on the stability, electronic and magnetic properties of CH ₃ NH ₃ PbI ₃ perovskite. <i>Surfaces and Interfaces</i> , 2021, 24, 101027.	1.5	6
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57225	Single Metal Atom Supported on N-Doped 2D Nitride Black Phosphorus: An Efficient Electrocatalyst for the Oxygen Evolution and Oxygen Reduction Reactions. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12541-12550.	1.5	24
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57228	Determination of Thermal Expansion, Defect Formation Energy, and Defect-Induced Strain of Î±-U Via ab Initio Molecular Dynamics. <i>Frontiers in Materials</i> , 2021, 8, .	1.2	10
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57232	A dual strategy for synthesizing carbon/defect comodified polymeric carbon nitride porous nanotubes with boosted photocatalytic hydrogen evolution and synchronous contaminant degradation. <i>Applied Catalysis B: Environmental</i> , 2021, 287, 119995.	10.8	66
57233	The strain-induced excellent thermoelectric performance of PbTe. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 130, 114685.	1.3	18
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#	ARTICLE	IF	CITATIONS
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59822	The modulating effect of N coordination on single-atom catalysts researched by Pt-N-C model through both experimental study and DFT simulation. <i>Journal of Materials Science and Technology</i> , 2021, 91, 160-167.	5.6	27
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59827	Tunable electronic structure and magnetic anisotropy of two dimensional Mn ₂ CFCl/MoSSe van der Waals heterostructures by electric field and biaxial strain. <i>Applied Surface Science</i> , 2021, 566, 150683.	3.1	14
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59834	An efficient and durable trifunctional electrocatalyst for zinc-air batteries driven overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120405.	10.8	127
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59841	Modulating CoFe ₂ O ₄ nanocube with oxygen vacancy and carbon wrapper towards enhanced electrocatalytic nitrogen reduction to ammonia. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120452.	10.8	42
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59845	Orientation independent heat transport characteristics of diamond/copper interface with ion beam bombardment. <i>Acta Materialia</i> , 2021, 220, 117283.	3.8	8
59846	Half-metallicity and Curie temperature enhancement of CrI ₃ through boron atoms adsorption. <i>Superlattices and Microstructures</i> , 2021, 159, 107054.	1.4	7
59847	Electronic, magnetic and optical properties of various surfaces of TiHfIrZ (Z=Al and Ga) quaternary Heusler alloy. <i>Thin Solid Films</i> , 2021, 737, 138952.	0.8	1
59848	Effect of the projector augmented wave potentials on the simulation of thermodynamic properties of vanadium. <i>Matter and Radiation at Extremes</i> , 2021, 6, .	1.5	2
59849	Manipulating selenium molecular configuration in N/O dual-doped porous carbon for high performance potassium-ion storage. <i>Journal of Energy Chemistry</i> , 2021, 62, 581-589.	7.1	19
59850	Electronic, mechanical and thermodynamic properties of ZrC, HfC and their solid solutions studied by first-principles calculation. <i>Solid State Communications</i> , 2021, 338, 114481.	0.9	9
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59852	Vacancy-cluster and off-lattice metal-atom diffusion mechanisms in transition metal carbides. <i>Computational Materials Science</i> , 2021, 199, 110713.	1.4	3
59853	Interactions and electronic properties of adatom/Gra/adatom sandwich complexes. <i>Materials Chemistry and Physics</i> , 2021, 272, 125013.	2.0	0
59854	Magnetism and topological Hall effect in antiferromagnetic Ru ₂ MnSn-based Heusler compounds. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 537, 168104.	1.0	5
59855	Electronic and magnetic properties of metal-organic polymers with 4d and 5d-transition metal ions. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 537, 168183.	1.0	6
59856	Dual-doped carbon hollow nanospheres achieve boosted pseudocapacitive energy storage for aqueous zinc ion hybrid capacitors. <i>Energy Storage Materials</i> , 2021, 42, 705-714.	9.5	96
59857	A first-principles study of thiadiazole and dimercapto-thiadiazole adsorption on copper and silver surfaces. <i>Materials Chemistry and Physics</i> , 2021, 273, 125057.	2.0	6
59858	Bridging the gap between simulated and experimental ionic conductivities in lithium superionic conductors. <i>Materials Today Physics</i> , 2021, 21, 100463.	2.9	43
59859	Effect and Mechanism of Hydrogen-Assisted Sulfur Intercalation for Decoupling Graphene from Cu(1 1) Tj ETQq1 1,0,784314,rgBT /Ove	3.1	2
59860	Dual active site tandem catalysis of metal hydroxyl oxides and single atoms for boosting oxygen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120451.	10.8	44
59861	Cadmium copper selenite chloride, CdCu ₂ (SeO ₃) ₂ Cl ₂ , an insulating spin gap system. <i>Journal of Solid State Chemistry</i> , 2021, 303, 122518.	1.4	0

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59863	Symmetrical dehalogenation of 2, 7-dibromopyrene on Cu(1 1 1) with tunable intermediates and reaction paths. <i>Applied Surface Science</i> , 2021, 566, 150663.	3.1	3
59864	Theoretical insights on the exsolved behavior of ruthenium atom in titanate perovskite. <i>Applied Surface Science</i> , 2021, 566, 150641.	3.1	5
59865	Effects of transition metal doping on surface properties and resistance to Cl ⁻ adsorption of γ -Al ₂ O ₃ . <i>Surface Science</i> , 2021, 713, 121909.	0.8	6
59866	DFT investigation of mechanical and vibrational properties of CuTe. <i>Physica B: Condensed Matter</i> , 2021, 620, 413214.	1.3	2
59867	High-throughput approach for estimation of intrinsic barriers in FCC structures for alloy design. <i>Scripta Materialia</i> , 2021, 204, 114126.	2.6	6
59868	Interfacial polymerized copolymers of aniline and phenylenediamine with tunable magnetoresistance and negative permittivity. <i>Materials Today Physics</i> , 2021, 21, 100502.	2.9	34
59869	Trifunctional Pt coupled with NiFe hydroxide synthesized via corrosion engineering to boost the cleavage of water molecule for alkaline water-splitting. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120395.	10.8	109
59870	Functional group tuning of two-dimensional carbon nanosheets for boosting oxygen reduction electrocatalysis. <i>Carbon</i> , 2021, 185, 395-403.	5.4	10
59871	A systematic analysis of phase stability in refractory high entropy alloys utilizing linear and non-linear cluster expansion models. <i>Acta Materialia</i> , 2021, 220, 117269.	3.8	10
59872	Point defects in VS ₂ monolayer towards NH ₃ synthesis. <i>Materials and Design</i> , 2021, 209, 110006.	3.3	5
59873	Micro-alloying effects of Co on structural and dynamic properties of CeAlCu glass-forming melts by ab initio molecular dynamics simulations. <i>Journal of Non-Crystalline Solids</i> , 2021, 572, 121109.	1.5	2
59874	Bridging the miscibility gap towards higher thermoelectric performance of PbS. <i>Acta Materialia</i> , 2021, 220, 117337.	3.8	17
59875	Combined density functional theory/kinetic Monte Carlo investigation of surface morphology during cycling of Li-Cu electrodes. <i>Electrochimica Acta</i> , 2021, 397, 139272.	2.6	3
59876	Intensified solar thermochemical CO ₂ splitting over iron-based redox materials via perovskite-mediated dealloying-exsolution cycles. <i>Chinese Journal of Catalysis</i> , 2021, 42, 2049-2058.	6.9	13
59877	The impact of atomic defects on high-temperature stability and electron transport properties in Sr ₂ Mg _{1-x} Ni _x MoO ₆ solid solutions. <i>Journal of Alloys and Compounds</i> , 2021, 883, 160821.	2.8	2
59878	Enhanced singlet oxygen production over a photocatalytic stable metal organic framework composed of porphyrin and Ag. <i>Journal of Colloid and Interface Science</i> , 2021, 602, 300-306.	5.0	15
59879	Adsorption mechanism of CO ₂ on the single atom doped or promoted Li ₄ SiO ₄ (0 1 0) surface from first principles. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113424.	1.1	7

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59899	First-principles study on electronic structure, optical properties and doping-induced half metallicity in double perovskite Bi ₂ CuCrO ₆ . <i>Journal of Solid State Chemistry</i> , 2021, 303, 122521.	1.4	4
59900	Variation of structural disorder in Zr substituted Y ₂ Sn ₂ O ₇ : Its impact on photocatalysis. <i>Journal of Solid State Chemistry</i> , 2021, 303, 122472.	1.4	4
59901	Experimental and theoretical investigation of the mechanical characteristics of sillenite compound: Bi ₁₂ GeO ₂₀ . <i>Journal of Alloys and Compounds</i> , 2021, 882, 160686.	2.8	4
59902	Equiatomic quaternary Heusler compounds TiVFeZ (Z=Al, Si, Ge): Half-metallic ferromagnetic materials. <i>Journal of Alloys and Compounds</i> , 2021, 883, 160869.	2.8	27
59903	A strongly interactive adatom/substrate interface for dendrite-free and high-rate Li metal anodes. <i>Journal of Energy Chemistry</i> , 2021, 62, 179-190.	7.1	22
59904	Two-dimensional SiM ₄ (M=Ge, Sn) monolayers as visible-light-driven photocatalyst of hydrogen production. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120013.	2.0	8
59905	Designing artificial carbon clusters using Ge ₂ Sb ₂ Te ₅ /C superlattice-like structure for phase change applications. <i>Journal of Alloys and Compounds</i> , 2021, 882, 160695.	2.8	13
59906	A novel hard superconductor obtained in di-molybdenum carbide (Mo ₂ C) with Mo ⁴⁺ C octahedral structure. <i>Journal of Alloys and Compounds</i> , 2021, 881, 160631.	2.8	8
59907	First-principles-based high-throughput computation for high entropy alloys with short range order. <i>Journal of Alloys and Compounds</i> , 2021, 882, 160776.	2.8	17
59908	Anomalous temperature and symmetry-dependent electronic excitations in Gd ₆ B ₆ . <i>Journal of Alloys and Compounds</i> , 2021, 881, 160507.	2.8	0
59909	Magnetocrystalline anisotropy regulations in bulk L1 ₀ -MnGa alloys by tailoring the tetragonal lattice parameter c: Selectively alloying Al and C atoms. <i>Journal of Alloys and Compounds</i> , 2021, 881, 160646.	2.8	2
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59912	Resistive switching characteristics of epitaxial NiO thin films affected by lattice strains and external forces. <i>Applied Surface Science</i> , 2021, 566, 150685.	3.1	5
59913	Coupled Sn/Mo ₂ C nanoparticles wrapped in carbon nanofibers by electrospinning as high-performance electrocatalyst for hydrogen evolution reaction. <i>Applied Surface Science</i> , 2021, 566, 150754.	3.1	22
59914	Addressing electrocatalytic activity and stability of LnBaCo ₂ O ₅₊ perovskites for hydrogen evolution reaction by structural and electronic features. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120403.	10.8	30
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59916	Short-range ordering governs brittleness and ductility in W-Ta solid solution: Insights from Pugh's shear-to-bulk modulus ratio. <i>Scripta Materiala</i> , 2021, 204, 114136.	2.6	21
59917	Piezotronic-enhanced photocatalytic performance of heterostructured BaTiO ₃ /SrTiO ₃ nanofibers. <i>Nano Energy</i> , 2021, 89, 106391.	8.2	70
59918	First-principles calculations of precursor adsorption on substrate during atomic layer deposition: The example of SiO ₂ deposition using tris(dimethylamino)silane. <i>Current Applied Physics</i> , 2021, 31, 228-231.	1.1	1
59919	Multi-objective optimization of alkali/alkaline earth metals doped graphyne for ultrahigh-performance CO ₂ capture and separation over N ₂ /CH ₄ . <i>Materials Today Physics</i> , 2021, 21, 100539.	2.9	4
59920	Janus WSe monolayer adsorbed with transition-metal atoms (Fe, Co and Ni): excellent performance for gas sensing and CO catalytic oxidation. <i>Applied Surface Science</i> , 2021, 565, 150558.	3.1	17
59921	First-Principle study of lithium polysulfide adsorption on heteroatom doped graphitic carbon nitride for Lithium-Sulfur batteries. <i>Applied Surface Science</i> , 2021, 565, 150378.	3.1	24
59922	Transition metal single-atom anchored g-CN monolayer for constructing high-activity multifunctional electrocatalyst. <i>Applied Surface Science</i> , 2021, 565, 150547.	3.1	28
59923	Atomic layer deposited boron nitride nanoscale films act as high temperature hydrogen barriers. <i>Applied Surface Science</i> , 2021, 565, 150428.	3.1	9
59924	Effects of atom-to-defect ratio on the thermostability of dispersed Au atoms on reduced TiO ₂ (1 0 1) surface. <i>Applied Surface Science</i> , 2021, 565, 150519.	3.1	2
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59926	Multi-level phase-change memory with ultralow power consumption and resistance drift. <i>Science Bulletin</i> , 2021, 66, 2217-2224.	4.3	41
59927	Triggering in-plane defect cluster on MoS ₂ for accelerated dinitrogen electroreduction to ammonia. <i>Journal of Energy Chemistry</i> , 2021, 62, 359-366.	7.1	40
59928	Anomalous Hall and Nernst Conductivities in Co ₂ NbGa: A first principles study. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 538, 168303.	1.0	6
59929	Structure, magnetism, electronic properties and high magnetic-field-induced stability of alloy carbide M ₇ C ₃ . <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 538, 168263.	1.0	9
59930	Boosting oxygen evolution reaction by enhanced intrinsic activity in Ruddlesden-Popper iridate oxides. <i>Chemical Engineering Journal</i> , 2021, 423, 130185.	6.6	13
59931	Atomically dispersed Ni on Mo ₂ C embedded in N, P co-doped carbon derived from polyoxometalate supramolecule for high-efficiency hydrogen evolution electrocatalysis. <i>Applied Catalysis B: Environmental</i> , 2021, 296, 120336.	10.8	58
59932	Recording the Pt-beyond hydrogen production electrocatalysis by dirhodium phosphide with an overpotential of only 4.3 mV in alkaline electrolyte. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120457.	10.8	15
59933	Regulation of Nb ³⁺ , Sb ³⁺ and V ³⁺ doping on the photo-induced ferroelectricity of KTaO ₃ . <i>Physica B: Condensed Matter</i> , 2021, 620, 413248.	1.3	1

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59936	Internal and external electric field tunable electronic structures for photocatalytic water splitting: Janus transition-metal chalcogenides/C ₃ N ₄ van der Waals heterojunctions. Applied Surface Science, 2021, 566, 150639.	3.1	12
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59940	Behavior of copper under high pressure: Experimental and theoretical analyses. Current Applied Physics, 2021, 31, 93-98.	1.1	4
59941	Bct-C5: A new body-centered tetragonal carbon allotrope. Diamond and Related Materials, 2021, 119, 108571.	1.8	6
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59951	V ₂ C MXene synergistically coupling FeNi LDH nanosheets for boosting oxygen evolution reaction. Applied Catalysis B: Environmental, 2021, 297, 120474.	10.8	106

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59953	Organic nanocrystals induced surface passivation towards high-efficiency and stable perovskite solar cells. <i>Nano Energy</i> , 2021, 89, 106445.	8.2	19
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59961	Selective adsorption of glucose towards itaconic acid on amorphous silica surfaces: Insights from density functional theory calculations. <i>Journal of Molecular Liquids</i> , 2021, 343, 117586.	2.3	5
59962	Realization of all-in-one hydrogen-evolving photocatalysts via selective atomic substitution. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120518.	10.8	49
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59966	Theoretical study on thermal properties of molybdenum disulfide/silicon heterostructures. <i>Computational Materials Science</i> , 2021, 200, 110835.	1.4	2
59967	Interfacing 2D VS ₂ with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. <i>Applied Surface Science</i> , 2021, 570, 151129.	3.1	4
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60012	Field-induced half-metallic phase in epitaxial TcO ₂ bilayer on rutile TiO ₂ surface. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 540, 168478.	1.0	0
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60158	Multi-dimensional hybrid flexible films promote uniform lithium deposition and mitigate volume change as lithium metal anodes. <i>Journal of Energy Chemistry</i> , 2022, 65, 583-591.	7.1	6
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60161	Effect of Li and Li-RE co-doping on structure, stability, optical and electrical properties of bismuth magnesium niobate pyrochlore. <i>Materials Research Bulletin</i> , 2022, 145, 111520.	2.7	6
60162	A comprehensive study of structure and properties of nanocrystalline zinc peroxide. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 160, 110318.	1.9	6
60163	Conductive Fe ₂ N/N-rGO composite boosts electrochemical redox reactions in wide temperature accommodating lithium-sulfur batteries. <i>Chemical Engineering Journal</i> , 2022, 427, 131622.	6.6	12
60164	Niobium carbide (MXene) reduces UHMWPE particle-induced osteolysis. <i>Bioactive Materials</i> , 2022, 8, 435-448.	8.6	38
60165	WloopPHI: A tool for ab initio characterization of Weyl semimetals. <i>Computer Physics Communications</i> , 2022, 270, 108147.	3.0	5
60166	Ga doping enables superior alkaline hydrogen evolution reaction performances of CoP. <i>Chemical Engineering Journal</i> , 2022, 429, 132012.	6.6	25
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60169	Enhanced phosphate removal from practical wastewater via in situ assembled dimension-engineered MOF@carbon heterostructures. <i>Chemical Engineering Journal</i> , 2022, 428, 132536.	6.6	40
60170	Topological tuning of Two-Dimensional polytriazine imides by halide anions for selective lead removal from wastewater. <i>Separation and Purification Technology</i> , 2021, 278, 119595.	3.9	5
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60177	Fluorine-doped graphene oxide prepared by direct plasma treatment for supercapacitor application. <i>Chemical Engineering Journal</i> , 2022, 428, 132086.	6.6	41
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60180	Deposition kinetics and mechanism of pyrocarbon for electromagnetic-coupling chemical vapor infiltration process. <i>Journal of Materials Science and Technology</i> , 2022, 101, 118-127.	5.6	3
60181	A novel Fe-Co double-atom catalyst with high low-temperature activity and strong water-resistant for O ₃ decomposition: A theoretical exploration. <i>Journal of Hazardous Materials</i> , 2022, 421, 126639.	6.5	16
60182	Ab initio study on magnetism of SnO ₂ (110) surface with non-metallic elements doping. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106194.	1.9	5
60183	Ferromagnetism in \hat{I}^2 -Ag ₂ Se topological semimetal. <i>Journal of Alloys and Compounds</i> , 2022, 891, 162025.	2.8	1
60184	Morphology optimization strategy of flower-like CoNi ₂ S ₄ /Co ₉ S ₈ @MoS ₂ core@shell nanocomposites to achieve extraordinary microwave absorption performances. <i>Journal of Colloid and Interface Science</i> , 2022, 606, 1128-1139.	5.0	22
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#	ARTICLE	IF	CITATIONS
60186	Spatial carrier separation in cobalt phosphate deposited ZnIn ₂ S ₄ nanosheets for efficient photocatalytic hydrogen evolution. <i>Journal of Colloid and Interface Science</i> , 2022, 606, 317-327.	5.0	27
60187	Confined Pd clusters with dynamic structure for highly efficient Cascade-type catalysis. <i>Chemical Engineering Journal</i> , 2022, 429, 132128.	6.6	5
60188	A new thermodynamically stable Nb ₂ Ni intermetallic compound phase revealed by peritectoid transition within binary Nb-Ni alloy system. <i>Journal of Materials Science and Technology</i> , 2022, 100, 246-253.	5.6	28
60189	Correlating structure and orbital occupation with the stability and mechanical properties of 3d transition metal carbides. <i>Journal of Alloys and Compounds</i> , 2022, 891, 161866.	2.8	12
60190	1 T-MoSe ₂ monolayer supported single Pd atom as a highly-efficient bifunctional catalyst for ORR/OER. <i>Journal of Colloid and Interface Science</i> , 2022, 605, 155-162.	5.0	55
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60192	Rational design of honeycomb Ni-Co LDH/graphene composite for remarkable supercapacitor via ultrafast microwave synthesis. <i>Applied Surface Science</i> , 2022, 571, 151322.	3.1	62
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60195	Vacancy ordered phases of nonstoichiometric hafnium carbide from evolutionary crystal structure predictions. <i>Journal of Alloys and Compounds</i> , 2022, 891, 162063.	2.8	5
60196	Small-scale analysis of brittle-to-ductile transition behavior in pure tungsten. <i>Journal of Materials Science and Technology</i> , 2022, 105, 242-258.	5.6	15
60197	ElaTool: An automated toolkit for elastic constants calculation. <i>Computer Physics Communications</i> , 2022, 270, 108180.	3.0	17
60198	Enhanced electronic interaction in hemin@Ni(OH) ₂ composite for efficient electrocatalytic oxygen evolution. <i>Journal of Alloys and Compounds</i> , 2022, 892, 161780.	2.8	6
60199	Phase transformation of ZrO ₂ by Si incorporation and catalytic activity for isopropyl alcohol dehydration and dehydrogenation. <i>Chemical Engineering Journal</i> , 2022, 428, 131766.	6.6	16
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60201	Processing bulk insulating CaTiO ₃ into a high-performance thermoelectric material. <i>Chemical Engineering Journal</i> , 2022, 428, 131121.	6.6	12
60202	Suppression of Co-Cr antisite defect and robust half metallicity in CoM ₂ CrAl (M = Mn, Fe) Heusler alloys. <i>Journal of Alloys and Compounds</i> , 2022, 891, 161856.	2.8	4
60203	Influence of alkaline species on the high temperature lubrication of molten carbonate. <i>Tribology International</i> , 2022, 165, 107257.	3.0	1

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60204	Directionally maximizing CO selectivity to near-unity over cupric oxide with indium species for electrochemical CO ₂ reduction. <i>Chemical Engineering Journal</i> , 2022, 427, 131654.	6.6	18
60205	Carbon-coated MoS ₂ nanosheets@CNTs-Ti ₃ C ₂ MXene quaternary composite with the superior rate performance for sodium-ion batteries. <i>Journal of Materials Science and Technology</i> , 2022, 100, 101-109.	5.6	29
60206	Monoclinic Cu ₃ (OH) ₂ V ₂ O ₇ ·2H ₂ O nanobelts/reduced graphene oxide: A novel high-capacity and long-life composite for potassium-ion battery anodes. <i>Journal of Energy Chemistry</i> , 2022, 66, 140-151.	7.1	7
60207	Modulating the stability, electronic and reactivity properties of single-atom catalyst anchored graphene by coordination environments. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114975.	1.3	5
60208	An integrated strategy based on Schiff base reactions to construct unique two-dimensional nanostructures for intrinsic pseudocapacitive sodium/lithium storage. <i>Chemical Engineering Journal</i> , 2022, 429, 132339.	6.6	12
60209	In-depth understanding of the crystal-facet effect of La ₂ O ₂ CO ₃ for low-temperature oxidative coupling of methane. <i>Fuel</i> , 2022, 308, 121848.	3.4	10
60210	In-situ vulcanization synthesis of honeycomb-like SnS/C nanocomposites as anode materials for lithium-ion batteries. <i>Journal of Alloys and Compounds</i> , 2022, 891, 162051.	2.8	7
60211	Charge induced reconstruction of glide partial dislocations and electronic properties in GaN. <i>Scripta Materialia</i> , 2022, 207, 114276.	2.6	3
60212	Compression tuned crystalline and amorphous phases of Gd ₂ Si ₂ O ₇ : Raman spectroscopic and first-principles studies. <i>Journal of Alloys and Compounds</i> , 2022, 890, 161864.	2.8	0
60213	Existence of spin-polarized Dirac cone in $\text{Sr}_2\text{NiM}_2\text{O}_{10}$ CrB^2	1.3	4
60214	Theoretical insights into the adsorption mechanism of Cd(II) on the basal surfaces of kaolinite. <i>Journal of Hazardous Materials</i> , 2022, 422, 126795.	6.5	15
60215	Phase transformations in Al-Ti-Mg powders consolidated by high-pressure torsion: Experiments and first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2021, 889, 161815.	2.8	8
60216	A theoretical study of the twinned ZnO nanostructures. <i>Applied Surface Science</i> , 2022, 571, 151295.	3.1	0
60217	Intrinsic vacancy suppression and band convergence to enhance thermoelectric performance of (Ge, Tl) ETQq1 1 0.784314 rgBT /Overlo	6.6	21
60218	Theoretical insight into surface structures of pentlandite toward hydrogen evolution. <i>Journal of Colloid and Interface Science</i> , 2022, 607, 645-654.	5.0	13
60219	2D XBiSe ₃ (X=Ga, In, Tl) monolayers with high carrier mobility and enhanced visible-light absorption. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120309.	2.0	7
60220	Phase stability and mechanical properties of carbide solid solutions with 2d principal metals. <i>Computational Materials Science</i> , 2022, 201, 110869.	1.4	20
60221	Oxygen-containing groups and P doped porous carbon nitride nanosheets towards enhanced photocatalytic activity. <i>Chemosphere</i> , 2022, 287, 132399.	4.2	9

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60222	Correlation between precipitates evolution and mechanical properties of Al-Sc-Zr alloy with Er additions. <i>Journal of Materials Science and Technology</i> , 2022, 99, 61-72.	5.6	32
60223	Heat capacity of a MnFe(P,Si,B) compound with first-order magnetic transition. <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 541, 168513.	1.0	2
60224	Effect of dimensional expansion on carrier transport behaviors of the hexagonal Bi-based perovskite crystals. <i>Journal of Energy Chemistry</i> , 2022, 66, 459-465.	7.1	16
60225	Molecule functionalization to facilitate electrocatalytic oxygen reduction on graphdiyne. <i>Journal of Energy Chemistry</i> , 2022, 65, 141-148.	7.1	11
60226	Visible-light deposition of CrO cocatalyst on TiO ₂ : Cr valence regulation for superior photocatalytic CO ₂ reduction to CH ₄ . <i>Journal of Energy Chemistry</i> , 2022, 64, 103-112.	7.1	25
60227	Role of H-bond along with oxygen and zinc vacancies in the enhancement of ferromagnetic behavior of ZnO films: An experimental and first principle-based study. <i>Journal of Alloys and Compounds</i> , 2021, 889, 161663.	2.8	16
60228	Combined Schottky junction and doping effect in Cd _x Zn _{1-x} S@Au/BiVO ₄ Z-Scheme photocatalyst with boosted carriers charge separation for CO ₂ reduction by H ₂ O. <i>Journal of Colloid and Interface Science</i> , 2022, 606, 1469-1476.	5.0	32
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60230	Fabrication of ultra-thin MgAl layered double oxide by cellulose templating and its immobilization effect toward heavy metal ions: cation-exchange and deposition mechanism. <i>Chemical Engineering Journal</i> , 2022, 427, 132017.	6.6	36
60231	Chelating effect between uranyl and pyridine N containing covalent organic frameworks: A combined experimental and DFT approach. <i>Journal of Colloid and Interface Science</i> , 2022, 606, 1617-1626.	5.0	18
60232	Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. <i>Chemosphere</i> , 2022, 287, 132232.	4.2	12
60233	Effects of electric field on Schottky barrier in graphene and hexagonal boron phosphide heterostructures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114973.	1.3	4
60234	The formation of atomic and sub-nano scale pores under tensile strain in oxide films on Zr alloys: A first-principles study. <i>Applied Surface Science</i> , 2022, 571, 151316.	3.1	2
60235	Large-scale defect-rich iron/nitrogen co-doped graphene-based materials as the excellent bifunctional electrocatalyst for liquid and flexible all-solid-state zinc-air batteries. <i>Journal of Colloid and Interface Science</i> , 2022, 607, 1201-1214.	5.0	49
60236	Theoretical study on the formation of diamond germanium vacancy color center. <i>Surface Science</i> , 2022, 715, 121950.	0.8	2
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60238	Taming the challenges of activity and selectivity in catalysts for electrochemical N ₂ fixation via single metal atom supported on WS ₂ . <i>Applied Surface Science</i> , 2022, 571, 151357.	3.1	16
60239	Structural, electronic, and optic properties of Se nanotubes. <i>Physica B: Condensed Matter</i> , 2022, 624, 413417.	1.3	4

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60259	Nanostructure Shape-Effects in ZnO heterogeneous photocatalysis. <i>Journal of Colloid and Interface Science</i> , 2022, 606, 588-599.	5.0	32
60260	Monolayer MoSi ₂ N ₄ as promising electrocatalyst for hydrogen evolution reaction: A DFT prediction. <i>Journal of Materials Science and Technology</i> , 2022, 99, 215-222.	5.6	31
60261	Experimental and density functional theory studies on Cu/Ba-coimpregnated γ -Al ₂ O ₃ for low-temperature NO storage and adsorbent regeneration. <i>Chemical Engineering Journal</i> , 2022, 429, 132112.	6.6	7
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60265	Substitutional doping effect of C ₃ N anode material: A first principles calculations study. <i>Applied Surface Science</i> , 2022, 571, 151330.	3.1	11
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60267	Deep learning for mapping element distribution of high-entropy alloys in scanning transmission electron microscopy images. <i>Computational Materials Science</i> , 2022, 201, 110905.	1.4	8
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60274	<i>Ab initio</i> study of metal carbide hydrides in the 2.25Cr1Mo0.25V steel. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5199-5206.	1.3	2
60275	Cesium Lead Bromides Structural, Electronic and Optical Properties. <i>Minerals, Metals and Materials Series</i> , 2021, , 3-14.	0.3	0

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60278	All inorganic lead free solar cell material Cs ₂ PdI ₆ : a first-principles study. Applied Physics Express, 2021, 14, 021005.	1.1	3
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60281	First-principles study of pristine and metal decorated blue phosphorene for sensing toxic H ₂ S, SO ₂ and NO ₂ molecules. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	5
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60491	A photo-induced spin crossover based molecular switch and spin filter operating at room temperature. <i>Dalton Transactions</i> , 2021, 50, 6578-6587.	1.6	4
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60505	Modifying Electronic and Elastic Properties of 2-Dimensional [110] Diamond by Nitrogen Substitution. <i>Journal of Carbon Research</i> , 2021, 7, 8.	1.4	8
60506	First-principles investigation of electronic, mechanical and thermoelectric properties of graphene-like XB ₁ (X = Si, Ge, Sn) monolayers. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12471-12478.	1.3	16
60507	Ultra-smooth and robust graphene-based hybrid anode for high-performance flexible organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 2106-2114.	2.7	12
60508	Novel Polymorph of Favipiravir—An Antiviral Medication. <i>Pharmaceutics</i> , 2021, 13, 139.	2.0	17
60509	High partial thermal conductivity of luminescence sites: a crucial factor for reducing the heat-induced lowering of the luminescence efficiency. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14439-14443.	2.7	4
60510	Lithiation mechanism of W18O ₄₉ anode material for lithium-ion batteries: Experiment and first-principles calculations. <i>Journal of Electroanalytical Chemistry</i> , 2021, 880, 114885.	1.9	10
60511	A theoretical study of de-charging excitations of the NV-center in diamond involving a nitrogen donor [*] . <i>New Journal of Physics</i> , 2020, 22, 123042.	1.2	6

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60513	Exploring promising gas sensing and highly active catalysts for CO oxidation: transition-metal (Fe, Co) Tj ETQq1 1 0,784314 rgBT /Overl	1.3	4
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60518	Emerging flat bands in large-angle twisted bi-layer graphene under pressure. <i>Nanoscale</i> , 2021, 13, 9264-9269.	2.8	6
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60522	Production of C, N Alternating 2D Materials Using Covalent Modification and Their Electroluminescence Performance. <i>Small Science</i> , 2021, 1, 2000042.	5.8	9
60523	Crystalline red phosphorus for selective photocatalytic reduction of CO ₂ into CO. <i>Journal of Materials Chemistry A</i> , 2021, 9, 338-348.	5.2	38
60524	<i>Ab Initio</i> Local-Energy and Local-Stress Calculations for Materials Science and Engineering. <i>Materials Transactions</i> , 2021, 62, 1-15.	0.4	12
60525	Ni/NiO heterostructures encapsulated in oxygen-doped graphene as multifunctional electrocatalysts for the HER, UOR and HMF oxidation reaction. <i>Catalysis Science and Technology</i> , 2021, 11, 2480-2490.	2.1	50
60526	Evolutionary exploration of polytypism in lead halide perovskites. <i>Chemical Science</i> , 2021, 12, 12165-12173.	3.7	11
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60528	Spontaneous flexoelectricity and band engineering in MS ₂ (M = Mo, W) nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20574-20582.	1.3	7
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60537	First-Principles Study on Redox Magnetism and Electrochromism of Cyclometalated Triarylamine-Core Triruthenium Complex. <i>Crystals</i> , 2021, 11, 57.	1.0	1
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60543	Experimental and theoretical evidence of charge transfer in multi-component alloys – how chemical interactions reduce atomic size mismatch. <i>Materials Chemistry Frontiers</i> , 2021, 5, 5746-5759.	3.2	14
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60559	Modulating the thermal and structural stability of gallene via variation of atomistic thickness. <i>Nanoscale Advances</i> , 2021, 3, 499-507.	2.2	10
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60564	Selective catalytic reduction of NO over Cu-AFX zeolites: mechanistic insights from in situ operando spectroscopic and DFT studies. <i>Catalysis Science and Technology</i> , 2021, 11, 4459-4470.	2.1	6
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60567	Core-shell nanoparticles with tensile strain enable highly efficient electrochemical ethanol oxidation. <i>Journal of Materials Chemistry A</i> , 2021, 9, 15373-15380.	5.2	26
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60573	High-throughput systematic topological generation of low-energy carbon allotropes. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	14
60574	CO ₂ Photoelectrochemical Reduction Catalyzed by a GaP(001) Photoelectrode. <i>ACS Catalysis</i> , 2021, 11, 1233-1241.	5.5	15
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60576	Nonuniversal structure of point defects in face-centered cubic metals. <i>Physical Review Materials</i> , 2021, 5, .	0.9	14
60577	Reply to "Comment on "Structural characterization, reactivity, and vibrational properties of silver clusters: A new global minimum for Ag ₁₆ " by P. V. Nhat, N. T. Si, L. V. Duong and M. T. Nguyen, <i>Phys. Chem. Chem. Phys.</i> , 2021, 23, DOI: D1CP00646K. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12904-12906.	1.3	1
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60579	Substantial and stable magnetoresistance and spin conductance in phosphorene-based spintronic devices with Co electrodes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10573-10579.	1.3	6
60580	Microstructure and defect characteristics of lithium niobate with different Li concentrations. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 4006-4013.	3.0	18
60581	C-H Bond Activation of Methane through Electronic Interaction with Pd(110). <i>Journal of Physical Chemistry C</i> , 2021, 125, 1368-1377.	1.5	8
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60583	Tunable electronic and magnetic properties of transition-metal atoms doped CrBr ₃ monolayer. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 247401.	0.2	2

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60606	Ultrafast Charge Transfer Coupled to Quantum Proton Motion at Molecule/Metal Oxide Interface. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
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60617	Can Electron Transport through a Blue-Copper Azurin Be Coherent? An Ab Initio Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1693-1702.	1.5	25
60618	Direct aryl-aryl coupling of pentacene on Au(110). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22155-22159.	1.3	0
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60621	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. <i>Nanoscale</i> , 2021, 13, 5479-5488.	2.8	61
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60623	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	62
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60631	The MLIP package: moment tensor potentials with MPI and active learning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 025002.	2.4	181
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60635	Regulation of nitrogen configurations and content in 3D porous carbons for improved lithium storage. <i>Dalton Transactions</i> , 2021, 50, 14390-14399.	1.6	2
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60642	Hydrogen generation from ammonia borane hydrolysis catalyzed by ruthenium nanoparticles supported on Co-Ni layered double oxides. <i>Sustainable Energy and Fuels</i> , 2021, 5, 2301-2312.	2.5	17
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61162	Vibrational Frequencies of Cerium-Oxide-Bound CO: A Challenge for Conventional DFT Methods. Physical Review Letters, 2020, 125, 256101.	2.9	13
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61249	$\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle T \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle a \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle O \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle 5 \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle$	0.9	19
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61255	perovskite compounds by combining machine learning and density functional theory. <i>Physical Review Materials</i> , 2018, 2, .	0.9	127
61256	$\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle B \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle i \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle 2 \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle S \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle$	0.9	4
61257	Antiferromagnetic ground state in the $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{MnGa} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle 4 \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant="normal"} \rangle$ compound. <i>Physical Review Materials</i> , 2018, 2, .	0.9	12
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61277	Plasmon spectroscopy: Robust metallicity of Au wires on Si(557) upon oxidation. Physical Review Materials, 2018, 2, .	0.9	10
61278	Non-Heisenberg covalent magnetism in iron oxide clusters. Physical Review Materials, 2018, 2, .	0.9	6
61279	Effect of fluoropolymer composition on topochemical synthesis of SrMnF_3 oxyfluoride films. Physical Review Materials, 2018, 2, .	0.9	1
61280	Ab initio calculation of thermal expansion with application to understanding Invar behavior in gum metal. Physical Review Materials, 2018, 2, .	0.9	2

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61281	Finite-temperature structure of the MAPbI_3 perovskite. Comparing density functional approximations and force fields to experiment. <i>Physical Review Materials</i> , 2018, 2, .	0.9	31
61282	Crystallography and substitution patterns in the ZrO_2 system. <i>Physical Review Materials</i> , 2018, 2, .	0.9	10
61283	Unusual composition dependence of transformation temperatures in Ti-Ta-X shape memory alloys. <i>Physical Review Materials</i> , 2018, 2, .	0.9	11
61284	Precipitate-induced nonlinearities of diffusion along grain boundaries in Al-based alloys. <i>Physical Review Materials</i> , 2018, 2, .	0.9	13
61285	$\text{Al}_x\text{Ga}_{1-x}$ crystals with direct 2 eV band gaps from computational alchemy. <i>Physical Review Materials</i> , 2018, 2, .	0.9	17
61286	Topological band crossings in hexagonal materials. <i>Physical Review Materials</i> , 2018, 2, .	0.9	35
61287	Relativistic $\text{GW}+\text{BSE}$ study of the optical properties of Ruddlesden-Popper iridates. <i>Physical Review Materials</i> , 2018, 2, .	0.9	40
61288	Nontrivial strength of van der Waals epitaxial interaction in soft perovskites. <i>Physical Review Materials</i> , 2018, 2, .	0.9	40
61289	Systematic search for two-dimensional ferromagnetic materials. <i>Physical Review Materials</i> , 2018, 2, .	0.9	81
61290	Combined ab initio and empirical model of the thermal conductivity of uranium, uranium-zirconium, and uranium-molybdenum. <i>Physical Review Materials</i> , 2018, 2, .	0.9	9
61291	First-principles insights on phase stability of titanium interstitial alloys. <i>Physical Review Materials</i> , 2018, 2, .	0.9	10
61292	Minimizing vibrational energy on the concentrations of oxygen interstitial clusters and uranium vacancies in nonstoichiometric UO_2 . <i>Physical Review Materials</i> , 2018, 2, .	0.9	15
61293	Magnetic properties of transition metal dichalcogenides-Fe/Ir(111) interfaces from first principles. <i>Physical Review Materials</i> , 2018, 2, .	0.9	4
61294	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. <i>Physical Review Materials</i> , 2018, 2, .	0.9	21
61295	Room-temperature ferrimagnetic multiferroic BiFeO_3 . <i>Physical Review Materials</i> , 2018, 2, .	0.9	12
61296	Structural and magnetic transitions accompanied by large responses in epitaxial $\text{Sr}_{0.5}\text{Ba}_{0.5}\text{MnO}_3$ films. <i>Physical Review Materials</i> , 2018, 2, .	0.9	5
61297	Magnetocrystalline anisotropy in ZrCo_5 compounds from first-principles real-space pseudopotentials calculations. <i>Physical Review Materials</i> , 2018, 2, .	0.9	4
61298	Real-space pseudopotential method for calculating magnetocrystalline anisotropy. <i>Physical Review Materials</i> , 2018, 2, .	0.9	7

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61299	Properties of mixed transition metal oxides: M^M corundum-type structures		

#	ARTICLE	IF	CITATIONS
61317	Beyond thermodynamic defect models: A kinetic simulation of arsenic activation in CdTe. <i>Physical Review Materials</i> , 2018, 2, .	0.9	21
61318	Automated construction of symmetrized Wannier-like tight-binding models from <i>ab initio</i> calculations. <i>Physical Review Materials</i> , 2018, 2, .	0.9	32
61319	Highly crystalline synthesis of tellurene sheets on two-dimensional surfaces: Control over helical chain direction of tellurene. <i>Physical Review Materials</i> , 2018, 2, .	0.9	27
61320	Monolayer C : Negative Poisson's ratio and unconventional two-dimensional emergent fermions. <i>Physical Review Materials</i> , 2018, 2, .	0.9	36
61321	Type-II Dirac line node in strained NaN . <i>Physical Review Materials</i> , 2018, 2, .	0.9	33
61322	Relationship between crystal structure and multiferroic orders in orthorhombic perovskite manganites. <i>Physical Review Materials</i> , 2018, 2, .	0.9	16
61323	Magnetic structural unit with convex geometry: A building block hosting an exchange-striction-driven magnetoelectric coupling. <i>Physical Review Materials</i> , 2018, 2, .	0.9	13
61324	Polymorphism in Bi-based perovskite oxides: A first-principles study. <i>Physical Review Materials</i> , 2018, 2, .	0.9	10
61325	Surface reconstructions and modified surface states in L_aC .	0.9	7
61326	Chemical nature of the anion adsorbate in dilute phosphide $GaAs_{1-x}Mn_x$ alloy grown at low temperature. <i>Physical Review Materials</i> , 2018, 2, .	0.9	10
61327	Effect of temperature and configurational disorder on the electronic band gap of boron carbide from first principles. <i>Physical Review Materials</i> , 2018, 2, .	0.9	2
61328	Towards bipolar tin monoxide: Revealing unexplored dopants. <i>Physical Review Materials</i> , 2018, 2, .	0.9	9
61329	Influence of I^- -conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. <i>Physical Review Materials</i> , 2018, 2, .	0.9	24
61330	Interface-driven thermal rectification in nanoscale systems. <i>Physical Review Materials</i> , 2018, 2, .	0.9	6
61331	Metalorganic vapor phase epitaxy of large size CdTe grains on mica through chemical and van der Waals interactions. <i>Physical Review Materials</i> , 2018, 2, .	0.9	12
61332	First-principles study of phase stability of bcc $XCZn$.	0.9	10
61333	Geometries of edge and mixed dislocations in bcc Fe from first-principles calculations. <i>Physical Review Materials</i> , 2018, 2, .	0.9	18
61334	Autonomous efficient experiment design for materials discovery with Bayesian model averaging. <i>Physical Review Materials</i> , 2018, 2, .	0.9	58

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61336	An example of exploring the hidden Cairo tessellation in the pyrite structure for discovering novel two-dimensional materials. Physical Review Materials. 2018. 2, .	0.9	14
61337	Refrigeration in 2D: Electrostaticcaloric effect in monolayer materials. Physical Review Materials, 2018, 2, .	0.9	5
61338	Evolution of electronic structure and electron-phonon coupling in ultrathin tetragonal CoSe films. Physical Review Materials, 2018, 2, .	0.9	7
61339	Electronic structure of monolayer antimonene nanoribbons under out-of-plane and transverse bias. Physical Review Materials, 2018, 2, .	0.9	3
61340	Universal superconductivity phase diagram for pressurized tetradymite topological insulators. Physical Review Materials, 2018, 2, .	0.9	8
61341	Topological phonons and thermoelectricity in triple-point metals. Physical Review Materials, 2018, 2, .	0.9	76
61342	Stoichiometry control and electronic and transport properties of pyrochlore	0.9	7
61343	Charged domain walls in improper ferroelectric hexagonal manganites and gallates. Physical Review Materials, 2018, 2, .	0.9	29
61344	Role of interstitial hydrogen in antiferromagnetic insulator. Physical Review Materials, 2018, 2, .	0.9	7
61345	Structural dynamics in hybrid halide perovskites: Bulk Rashba splitting, spin texture, and carrier localization. Physical Review Materials, 2018, 2, .	0.9	19
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61347	Nematicity and superconductivity in orthorhombic superconductor		

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61354	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	24
61355	Strain-engineered Peierls instability in layered perovskite $\text{LaO}_{7-x}\text{F}_x$ from first principles. Physical Review Materials, 2018, 2, .	0.9	10
61356	Polar metallic behavior of strained antiperovskites ACNi_3 (A=Mg,Zn,and Cd) from first principles. Physical Review Materials, 2018, 2, .	0.9	14
61357	Presence of water at elevated temperatures, structural transition, and thermal expansion behavior in $\text{LaP}_4\text{O}_{12}$. Physical Review Materials, 2018, 2, .	0.9	4
61358	Protective layer enhanced the stability and superconductivity of tailored antimonene bilayer. Physical Review Materials, 2018, 2, .	0.9	13
61359	New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. Physical Review Materials, 2019, 3, .	0.9	44
61360	Strain-induced heteronuclear charge disproportionation in EuMnO_3 . Physical Review Materials, 2019, 3, .	0.9	2
61361	Hybrid functional study of nonlinear elasticity and internal strain in zinc-blende III-V materials. Physical Review Materials, 2019, 3, .	0.9	10
61362	Universality of point defect structure in body-centered cubic metals. Physical Review Materials, 2019, 3, .	0.9	53
61363	First-principles study on the grain boundary embrittlement of bcc-Fe by Mn segregation. Physical Review Materials, 2019, 3, .	0.9	23
61364	Deciphering structural and magnetic disorder in the chiral skyrmion host materials $\text{Co}_x\text{Mn}_{1-x}$.		

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61371	Remarkable thermoelectric performance in BaPdS_2 via pudding-mold band structure, band convergence, and ultralow lattice thermal conductivity. Physical Review Materials, 2019, 3, .	0.9	11
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61373	Temperature-induced phase transition and Li self-diffusion in Li_2C_2 : A first-principles study. Physical Review Materials, 2019, 3, .	0.9	3
61374	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	0.9	299
61375	Theoretical study of scattering in graphene ribbons in the presence of structural and atomistic edge roughness. Physical Review Materials, 2019, 3, .	0.9	9
61376	Computational design of flexible electrides with nontrivial band topology. Physical Review Materials, 2019, 3, .	0.9	18
61377	High-throughput screening for spin-gapless semiconductors in quaternary Heusler compounds. Physical Review Materials, 2019, 3, .	0.9	79
61378	Effect of N interstitial complexes on the electronic properties of GaAs_3N alloys from first principles. Physical Review Materials, 2019, 3, .	0.9	3
61379	Towards understanding the special stability of $\text{SrCoO}_{2.5}$ and $\text{HSrCoO}_{2.5}$. Physical Review Materials, 2019, 3, .	0.9	8
61380	Insights into the electronic structure of OsO_2 using soft and hard x-ray photoelectron spectroscopy in combination with density functional theory. Physical Review Materials, 2019, 3, .	0.9	9
61381	Diffusion-driven ultralow thermal conductivity in amorphous Nb_2O_5 thin films. Physical Review Materials, 2019, 3, .	0.9	18
61382	Computational evaluation of new lithium-3 garnets for lithium-ion battery applications as anodes, cathodes, and solid-state electrolytes. Physical Review Materials, 2019, 3, .	0.9	13
61383	Phonons, magnons, and lattice thermal transport in antiferromagnetic semiconductor MnTe. Physical Review Materials, 2019, 3, .	0.9	25
61384	Ferroelectricity in [111]-oriented epitaxially strained SrTiO_3 from first principles. Physical Review Materials, 2019, 3, .	0.9	11
61385	First-principles calculations of solute transport in zirconium: Vacancy-mediated diffusion with metastable states and interstitial diffusion. Physical Review Materials, 2019, 3, .	0.9	12
61386	First-principles study of phonon anharmonicity and negative thermal expansion in ScF_3 . Physical Review Materials, 2019, 3, .	0.9	6
61387	Density functional study of self-diffusion along an isolated screw dislocation in fcc Ni. Physical Review Materials, 2019, 3, .	0.9	4
61388	Dislocation core structures in Ni-based superalloys computed using a density functional theory based flexible boundary condition approach. Physical Review Materials, 2019, 3, .	0.9	11

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61389	Thermal properties of disordered $\text{Li}_x\text{M}_2\text{O}_3$: An <i>ab initio</i> study. Physical Review Materials, 2019, 3, .	0.9	4
61390	Influence of strain and chemical substitution on the magnetic anisotropy of antiferromagnetic Cr_2O_3 : An	0.9	18
61391	Computationally driven high-throughput identification of CaTe and $\text{Li}_3\text{M}_2\text{O}_3$ as promising candidates for high-mobility p -type transparent conducting materials. Physical Review Materials, 2019, 3, .	0.9	16
61392	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. Physical Review Materials, 2019, 3, .	0.9	41
61393	Reduced thermal conductivity of epitaxial GaAs on Si due to symmetry-breaking biaxial strain. Physical Review Materials, 2019, 3, .	0.9	20
61394	Enabling visible-light absorption and p -type doping in In_2O_3 by adding Bi. Physical Review Materials, 2019, 3, .	0.9	7
61395	Giant power output in lead-free ferroelectrics by shock-induced phase transition. Physical Review Materials, 2019, 3, .	0.9	29
61396	Ternary mixed-anion semiconductors with tunable band gaps from machine-learning and crystal structure prediction. Physical Review Materials, 2019, 3, .	0.9	16
61397	Influence of lattice dynamics on lithium-ion conductivity: A first-principles study. Physical Review Materials, 2019, 3, .	0.9	45
61398	Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties. Physical Review Materials, 2019, 3, .	0.9	16
61399	Symmetry-broken self-interstitial defects in chromium, molybdenum, and tungsten. Physical Review Materials, 2019, 3, .	0.9	28
61400	Ultralow shear modulus of incommensurate SnSe layers synthesized by the method of modulated elemental reactants. Physical Review Materials, 2019, 3, .	0.9	5
61401	<i>Ab initio</i> investigation of structural stability and exfoliation energies in transition metal dichalcogenides based on Ti-, V-, and Mo-group elements. Physical Review Materials, 2019, 3, .	0.9	44
61402	Electronic structure of a monoatomic Cu_2Si layer on a Si(111) substrate. Physical Review Materials, 2019, 3, .	0.9	15
61403	Pressure tuning of the electrical transport properties in the Weyl semimetal TaP. Physical Review Materials, 2019, 3, .	0.9	4
61404	High-pressure lithium as an elemental topological semimetal. Physical Review Materials, 2019, 3, .	0.9	7
61405	Magnetic order effects on the electronic structure of KMn_2S_4 with the first-principles study of self-trapped holes and acceptor impurities in MnS .	0.9	5
61406	First-principles study of self-trapped holes and acceptor impurities in O_3M_2 polymorphs. Physical Review Materials, 2019, 3, .	0.9	80

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61426	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	0.9	65
61427	van der Waals forces stabilize low-energy polymorphism in B_2O_3 . Implications for the crystallization anomaly. Physical Review Materials, 2019, 3, .	0.9	9
61428	Three-dimensional subnanoscale imaging of unit cell doubling due to octahedral tilting and cation modulation in strained perovskite thin films. Physical Review Materials, 2019, 3, .	0.9	12
61429	Stochastic replica voting machine prediction of stable cubic and double perovskite materials and binary alloys. Physical Review Materials, 2019, 3, .	0.9	10
61430	Atomic-resolution visualization and doping effects of complex structures in intercalated bilayer graphene. Physical Review Materials, 2019, 3, .	0.9	10
61431	Topological semimetal features in the multiferroic hexagonal manganites. Physical Review Materials, 2019, 3, .	0.9	9
61432	Orbital magnetic moments of phonons. Physical Review Materials, 2019, 3, .	0.9	80
61433	High-pressure synthesis of the $BiVO_3$ perovskite. Physical Review Materials, 2019, 3, .	0.9	7
61434	Influence of antiphase boundary of the $MnAl_2$ phase on the energy product. Physical Review Materials, 2019, 3, .	0.9	1
61435	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the G_0W_0 plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	0.9	61
61436	A -site cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. Physical Review Materials, 2019, 3, .	0.9	7
61437	Role of the exchange-correlation functional on the structural, electronic, and optical properties of cubic and tetragonal $SrTiO_3$ including many-body effects. Physical Review Materials, 2019, 3, .	0.9	13
61438	Hyperbolic dispersion and negative refraction in a metal-organic framework Cu-BHT. Physical Review Materials, 2019, 3, .	0.9	9
61439	Finite temperature optoelectronic properties of BAs from first principles. Physical Review Materials, 2019, 3, .	0.9	13
61440	Marked enhancement of the photoresponsivity and minority-carrier lifetime of BaS_2 passivated with atomic hydrogen. Physical Review Materials, 2019, 3, .	0.9	20
61441	Dimensionality reduction and band quantization induced by potassium intercalation in $TmTe_2$. Physical Review Materials, 2019, 3, .	0.9	20
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61444	Mechanistic insights in phosphorene degradation. <i>Physical Review Materials</i> , 2019, 3, .	0.9	3
61445	Magnetic order in single crystals of Na_3O_3 with a honeycomb arrangement of d^7 . <i>Physical Review Materials</i> , 2019, 3, .	0.9	49
61446	Evidence of a second-order Peierls-driven metal-insulator transition in crystalline NbO_2 . <i>Physical Review Materials</i> , 2019, 3, .	0.9	18
61447	Machine-learning-based interatomic potential for phonon transport in perfect crystalline Si and crystalline Si with vacancies. <i>Physical Review Materials</i> , 2019, 3, .	0.9	40
61448	Role of point defects in the electrical and optical properties of In_2O_3 . <i>Physical Review Materials</i> , 2019, 3, .	0.9	37
61449	Effects of oxygen stoichiometry on the phase stability of sputter-deposited C_d . <i>Physical Review Materials</i> , 2019, 3, .	0.9	8
61450	Energy level alignment of Cu^{I} absorber compounds with ZnO . <i>Physical Review Materials</i> , 2019, 3, .	0.9	18
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61452	Parametrization of LSDA for noncollinear magnetic configurations: Multipolar magnetism in UO_2 . <i>Physical Review Materials</i> , 2019, 3, .	0.9	35
61453	Formation of graphene atop a Si adlayer on the C-face of SiC. <i>Physical Review Materials</i> , 2019, 3, .	0.9	3
61454	Transferable screened range-separated hybrids for layered materials: The cases of MoS_2 and h-BN. <i>Physical Review Materials</i> , 2019, 3, .	0.9	20
61455	Two-dimensional nodal-loop half-metal in monolayer MnN. <i>Physical Review Materials</i> , 2019, 3, .	0.9	55
61456	Enhanced ferroelectricity in perovskite oxysulfides. <i>Physical Review Materials</i> , 2019, 3, .	0.9	4
61457	<i>ab initio</i> phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. <i>Physical Review Materials</i> , 2019, 3, .	0.9	18
61458	Segregation tendency of Heusler alloys. <i>Physical Review Materials</i> , 2019, 3, .	0.9	12
61459	Persistent spin helix in Rashba-Dresselhaus ferroelectric $\text{CsBiNb}_3\text{O}_{10}$. <i>Physical Review Materials</i> , 2019, 3, .	0.9	41
61460	Machine-learning-assisted prediction of magnetic double perovskites. <i>Physical Review Materials</i> , 2019, 3, .	0.9	28

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61463	Thermal conductivity for III-V and II-VI semiconductor wurtzite and zinc-blende polytypes: The role of anharmonicity and phase space. Physical Review Materials, 2019, 3, .	0.9	14
61464	Strain tuning of plasma frequency in vanadate, niobate, and molybdate perovskite oxides. Physical Review Materials, 2019, 3, .	0.9	18
61465	Role of short- and long-range ordering on diffusion in Ni-Al alloys. Physical Review Materials, 2019, 3, .	0.9	11
61466	Atomic energy mapping of neural network potential. Physical Review Materials, 2019, 3, .	0.9	24
61467	Anharmonic thermodynamics of vacancies using a neural network potential. Physical Review Materials, 2019, 3, .	0.9	14
61468	<i>Ab initio</i> study of magnetic nanopatterning of a hybrid transition metal dichalcogenides/Ir(111) system via magnetic clusters. Physical Review Materials, 2019, 3, .	0.9	4
61469	New kagome prototype materials: discovery of KV_3 , and CsV_3 . Physical Review Materials, 2019, 3, .	0.9	398
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61471	Atomically thin oxide layer on the elemental superconductor Ta(001) surface. Physical Review Materials, 2019, 3, .	0.9	2
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61474	van der Waals heterostructure for photocatalysis: Graphitic carbon nitride and Janus transition-metal dichalcogenides. Physical Review Materials, 2019, 3, .	0.9	14
61475	Discovery of Ti-Ta_x -free high-temperature Ti-Ta-X shape memory alloys from first-principles calculations. Physical Review Materials, 2019, 3, .	0.9	7
61476	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	0.9	10
61477	Towards predictive band gaps for halide perovskites: Lessons from one-shot and eigenvalue self-consistent GW . Physical Review Materials, 2019, 3, .	0.9	39
61478	Topological band crossings in epitaxial strained SnTe. Physical Review Materials, 2019, 3, .	0.9	6

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61480	Magnetic frustration control through tunable stereochemically driven disorder in entropy-stabilized oxides. Physical Review Materials, 2019, 3, .	0.9	29
61481	Structural and electronic properties of lithiated Si nanowires: An <i>ab initio</i> study. Physical Review Materials, 2019, 3, .	0.9	3
61482	Computational prediction of nanostructured alloys with enhanced thermoelectric properties. Physical Review Materials, 2019, 3, .	0.9	3
61483	Visualizing the metal- S contacts in two-dimensional field-effect transistors with atomic resolution. Physical Review Materials, 2019, 3, .	0.9	25
61484	In-plane hexagonal antiferromagnet in the Cu-Mn-As system. Physical Review Materials, 2019, 3, .	0.9	0.82
61485	Finite-temperature simulation of anharmonicity and octahedral tilting transitions in halide perovskites. Physical Review Materials, 2019, 3, .	0.9	28
61486	Materials synthesis, neutron powder diffraction, and first-principles calculations of Mo . Physical Review Materials, 2019, 3, .	0.9	11
61487	Intrinsic ductility of random substitutional alloys from nonlinear elasticity theory. Physical Review Materials, 2019, 3, .	0.9	9
61488	Dynamics of graphene/Al interfaces using COMB3 potentials. Physical Review Materials, 2019, 3, .	0.9	7
61489	Electronic, magnetic, and thermodynamic properties of the kagome layer compound FeSn. Physical Review Materials, 2019, 3, .	0.9	49
61490	Stabilization of small polarons in $BaTiO_3$ by local distortions. Physical Review Materials, 2019, 3, .	0.9	13
61491	High-density electron doping of $SmNiO_3$ from first principles. Physical Review Materials, 2019, 3, .	0.9	24
61492	Boosting ionic conductivity in antiperovskite Li_3OCl via defect engineering: Interstitial versus vacancy. Physical Review Materials, 2019, 3, .	0.9	11
61493	Understanding phonon properties in isorecticular metal-organic frameworks from first principles. Physical Review Materials, 2019, 3, .	0.9	16
61494	Interlayer dielectric function of a type-II van der Waals semiconductor: The HfS_2 heterobilayer. Physical Review Materials, 2019, 3, .	0.9	5
61495	Group-IV monochalcogenide monolayers: Two-dimensional ferroelectrics with weak intralayer bonds and a phosphorenelike monolayer dissociation energy. Physical Review Materials, 2019, 3, .	0.9	19
61496	Unusual valence state in the antiperovskites Sr_3SnO and Sr_3PbO revealed by x-ray photoelectron spectroscopy. Physical Review Materials, 2019, 3, .	0.9	12

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61497	Symmetry-enforced band crossings in trigonal materials: Accordion states and Weyl nodal lines. Physical Review Materials, 2019, 3, .	0.9	20
61498	Magneto-optic response of the metallic antiferromagnet Fe_2O_3 to ultrafast temperature excursions. Physical Review Materials, 2019, 3, .		
61499	Structural, electronic, and magnetic properties of bulk and epitaxial LaCoO_3 through diffusion Monte Carlo. Physical Review Materials, 2019, 3, .	0.9	13
61500	Dopability of divalent tin containing phosphates for p -type transparent conductors. Physical Review Materials, 2019, 3, .	0.9	5
61501	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	0.9	20
61502	Predicting copper gallium diselenide and band structure engineering through order-disordered transition. Physical Review Materials, 2019, 3, .	0.9	5
61503	Influence of crystalline order and defects on the absolute work functions and electron affinities of TiO_2 - and SrO -terminated TiO_2	0.9	17
61504	Large-scale interlayer rotations and Te grain boundaries in SrTiO_3 thin films. Physical Review Materials, 2020, 4, .	0.9	10
61505	Insights into the elastic properties of RE- i -MAX phases and their potential exfoliation into two-dimensional RE- i -MXenes. Physical Review Materials, 2020, 4, .	0.9	18
61506	Atomistic description of self-diffusion in molybdenum: A comparative theoretical study of non-Arrhenius behavior. Physical Review Materials, 2020, 4, .	0.9	14
61507	Thickness dependence of transport behaviors in SrRuO_3 superlattices. Physical Review Materials, 2020, 4, .	0.9	11
61508	Unveiling the mechanism of abnormal magnetic behavior of FeNiCoMnCu high-entropy alloys through a joint experimental-theoretical study. Physical Review Materials, 2020, 4, .	0.9	18
61509	Investigation of the band gaps and bowing parameter of $\text{InAs}_{1-x}\text{Sb}_x$ alloys using the modified Becke-Johnson potential. Physical Review Materials, 2020, 4, .	0.9	2
61510	Possible high-potential ilmenite-type NaM_3O_7	0.9	2
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62233	Two-dimensional conducting states in infinite-layer oxide/perovskite oxide hetero-structures. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 035003.		

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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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64204	Prediction of superconductivity in bilayer borophenes. <i>RSC Advances</i> , 2021, 11, 40220-40227.	1.7	9
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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64378	Formation of metastable aluminum silicide as intermediate stage of Al-Si alloy crystallization. <i>Scripta Materialia</i> , 2022, 210, 114481.	2.6	3
64379	Density functional theory and Monte Carlo study of electronic, magnetic and magnetocaloric properties of Fe ₃ CoN and FeCo ₃ N antiperovskites. <i>Journal of Crystal Growth</i> , 2022, 581, 126497.	0.7	12
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64381	Ta concentration effect on nucleation of defects in W-Ta alloy from first-principles model. <i>Materials Today Communications</i> , 2022, 30, 103071.	0.9	0
64382	Coexistence of a self-interstitial atom with light impurities in a tungsten grain boundary. <i>Journal of Nuclear Materials</i> , 2022, 560, 153481.	1.3	5
64383	Unlocking the origin of triggering hysteretic oxygen capacity in divalent species incorporated O-type sodium layered-oxide cathodes. <i>Energy Storage Materials</i> , 2022, 45, 432-441.	9.5	7
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64386	Controllable synthesis of Si-based GeSn quantum dots with room-temperature photoluminescence. <i>Applied Surface Science</i> , 2022, 579, 152249.	3.1	3
64387	Computational evaluation of FeMo heteroatom coeffect induced high electroreduction activity of N ₂ -to-NH ₃ . <i>Applied Surface Science</i> , 2022, 579, 152214.	3.1	15
64388	Thermodynamic assessment of the Ga-La and Ga-Pr systems supported by ab-initio calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 76, 102387.	0.7	3
64389	Identification of active sites available for hydrogen evolution of Single-Atom Ni ¹ /TiO ₂ catalysts. <i>Applied Surface Science</i> , 2022, 579, 152139.	3.1	11
64390	Correlating the dispersion of Li@Mn ₆ superstructure units with the oxygen activation in Li-rich layered cathode. <i>Energy Storage Materials</i> , 2022, 45, 422-431.	9.5	23
64391	The new stable phases of Fe ₂ Pd crystal alloy and their properties. <i>Computational Materials Science</i> , 2022, 204, 111183.	1.4	1
64392	Flexible Si ₃ C monolayer: A superior anode for high-performance non-lithium ion batteries. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 637, 128238.	2.3	17
64393	Insights into CrS ₂ monolayer and CrS ₂ /HfN ₂ interface for low-power digital and analog nanoelectronics. <i>Applied Surface Science</i> , 2022, 579, 152211.	3.1	14
64394	First-principle investigation on the thermoelectric properties of XCoGe (X = V, Nb, and Ta) half-Heusler compounds. <i>Materials Science in Semiconductor Processing</i> , 2022, 140, 106387.	1.9	9

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64396	Surface functionalization of Ta ₄ C ₃ MXene for broadband ultrafast photonics in the near-infrared region. <i>Applied Materials Today</i> , 2022, 26, 101341.	2.3	17
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64398	Chromium doping: A new approach to regulate electronic structure of cobalt carbonate hydroxide for oxygen evolution improvement. <i>Journal of Colloid and Interface Science</i> , 2022, 609, 414-422.	5.0	14
64399	Surface Termination of BaTiO ₃ (1 1 1) Single Crystal: A Combined DFT and XPS Study. <i>Applied Surface Science</i> , 2022, 578, 152018.	3.1	20
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64408	3D cubic framework of fluoride perovskite SEI inducing uniform lithium deposition for air-stable and dendrite-free lithium metal anodes. <i>Chemical Engineering Journal</i> , 2022, 431, 134266.	6.6	17
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64411	Thermodynamic assessment of the Fe-Ni-Rh-Ti system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 76, 102386.	0.7	0
64412	Excited state charge transfer promoted Raman enhancement of copper phthalocyanine by twisted bilayer graphenes. <i>Carbon</i> , 2022, 188, 305-314.	5.4	1

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64418	Group three nitride clusters as promising components for nanoelectronics. <i>Materials Today Chemistry</i> , 2022, 23, 100751.	1.7	2
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64420	Studying GPI zones in Al-Zn-Mg alloys by 4D-STEM. <i>Materials Characterization</i> , 2022, 185, 111675.	1.9	14
64421	Structure of PtRu/Ru(O ₂) and AgPd/Pd(111) surface alloys: A kinetic Monte Carlo study. <i>Chemical Physics</i> , 2022, 555, 111428.	0.9	4
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64432	A highly efficient narrow-band blue phosphor of Bi ³⁺ -activated cubic borate Ba ₃ Lu ₂ B ₆ O ₁₅ towards backlight display applications. <i>Chemical Engineering Journal</i> , 2022, 432, 134265.	6.6	28
64433	The effect of W and Mo modification on arsenic adsorption over Cu ²⁺ -Al ₂ O ₃ catalyst: Experimental and theoretical analysis. <i>Chemical Engineering Journal</i> , 2022, 432, 134376.	6.6	11
64434	The high piezoelectricity, flexibility and electronic properties of new Janus ZnXY ₂ (X = Ge, Sn, Si and Tl) and Y = S, Se, Te. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 138, 115116.	3.1	9
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64436	Au adsorption on stepped Si(hhk)-Au surfaces. <i>Surface Science</i> , 2022, 718, 122010.	0.8	0
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64438	Single transition metal atom anchored on VSe ₂ as electrocatalyst for nitrogen reduction reaction. <i>Applied Surface Science</i> , 2022, 580, 152272.	3.1	15
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64442	Structure and lattice thermal conductivity of grain boundaries in silicon by using machine learning potential and molecular dynamics. <i>Computational Materials Science</i> , 2022, 204, 111137.	1.4	9
64443	Double charge polarity switching in Sb-doped SnSe for enhanced thermo-electric power generation. <i>Journal of Alloys and Compounds</i> , 2022, 899, 163269.	2.8	4
64444	DFT insights into competitive adsorption and reaction mechanism of benzothiophene and naphthalene on Fe-doped Ni ₂ P catalyst. <i>Fuel</i> , 2022, 314, 123114.	3.4	3
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64459	Starburst configured imidazole-arylamine organic sensitizers for DSSC applications. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 426, 113735.	2.0	5
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64483	The role of Dy doping on cyclic oxidation behavior of Al-Si coating on new cobalt-based In^3/In^2 superalloy. Corrosion Science, 2022, 197, 110077.	3.0	1
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64488	Boosting CO ₂ hydrogenation performance for light olefin synthesis over GaZrOx combined with SAPO-34. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121042.	10.8	30
64489	Roles of optical phonons and logarithmic profile of electron-phonon coupling integration in superconducting Sc _{0.5} Y _{0.5} H ₆ superhydride under pressures. <i>Journal of Alloys and Compounds</i> , 2022, 901, 163524.	2.8	11
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64495	Coordination-tuned Fe single-atom catalyst for efficient CO ₂ electroreduction: The power of B atom. <i>Chemical Engineering Journal</i> , 2022, 433, 134270.	6.6	29
64496	Ultrasonic-assisted soldering of Mg alloy joints using Cu-foam/Sn composite solder foils. <i>Journal of Advanced Joining Processes</i> , 2022, 5, 100092.	1.5	0
64497	Anode-cathode interchangeable strategy for in situ reviving electrocatalysts' critical active sites for highly stable methanol upgrading and hydrogen evolution reactions. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121082.	10.8	21
64498	A novel tunable two dimensional ferroelectric material SbAs(CH ₂ OCH ₃) ₂ with topological and valley polarized properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 138, 115123.	1.3	1
64499	Phase-dependent catalytic performance of MnO ₂ for solvent-free oxidation of ethylbenzene with molecular oxygen. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121050.	10.8	25
64500	First-principles-based multiscale modelling of heterogeneous CoO oxidation kinetics in high-temperature thermochemical energy storage. <i>Fuel Processing Technology</i> , 2022, 228, 107164.	3.7	7
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64504	Capture and recycling of toxic selenite anions by cobalt-based metal-organic-frameworks for electrocatalytic overall water splitting. <i>Chemical Engineering Journal</i> , 2022, 433, 134553.	6.6	16
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64507	Confinement effect induced conformation change of one-dimensional phosphorus chains filled in carbon nanotubes. <i>Carbon</i> , 2022, 189, 467-473.	5.4	10
64508	Reducing the high hydrogen binding strength of vanadium carbide MXene with atomic Pt confinement for high activity toward HER. <i>Applied Catalysis B: Environmental</i> , 2022, 304, 120989.	10.8	58
64509	Ultrafine Co-MoS ₂ monolayer catalyst derived from oil-soluble single-molecule polyoxometalates for slurry phase hydrocracking. <i>Fuel</i> , 2022, 315, 123134.	3.4	11
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64512	Tailoring interphase structure to enable high-rate, durable sodium-ion battery cathode. <i>Journal of Energy Chemistry</i> , 2022, 68, 564-571.	7.1	22
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64979	Tuning the Carrier Scattering Mechanism by Rare-Earth Element Doping for High Average $\langle i \rangle zT \langle /i \rangle$ in $Mg_{3Sb_{2}}$ -Based Compounds. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 7022-7029.	4.0	16
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64981	Compressed superhydrides: the road to room temperature superconductivity. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 173001.	0.7	12
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64983	Two Nonlinear Optical Thiophosphates $Cu_{5}Hg_{0.5}P_{2}S_{8}$ and $AgHg_{3}PS_{6}$ Activated by Their Tetrahedra-Stacking Architecture. <i>Inorganic Chemistry</i> , 2022, 61, 1620-1626.	1.9	8
64984	Spatially Confined Synthesis of SnSe Spheres Encapsulated in N, Se Dual-Doped Carbon Networks toward Fast and Durable Sodium Storage. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 4230-4241.	4.0	43
64985	High-Pressure $Mg\hat{c}H$ Phase Diagram and Its Superconductivity from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2747-2755.	1.5	17
64986	$\langle i \rangle$ In silico $\langle /i \rangle$ design of dual-doped nitrogenated graphene ($C_{2}N$) employed in electrocatalytic reduction of carbon monoxide to ethylene. <i>Journal of Materials Chemistry A</i> , 2022, 10, 4703-4710.	5.2	12
64987	Ab initio Study of Atomic Structure and Electronic Properties of Different Phases of Polymorphic $Ag_{2}S$. <i>Physica Status Solidi (B): Basic Research</i> , 0, , 2100617.	0.7	0
64988	N-Doped Graphene Supported Cu Single Atoms: Highly Efficient Recyclable Catalyst for Enhanced $C\hat{c}N$ Coupling Reactions. <i>ACS Nano</i> , 2022, 16, 1142-1149.	7.3	36
64989	Type-II quadratic and cubic Weyl fermions. <i>Physical Review B</i> , 2022, 105, .	1.1	6
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64991	Deformation and Failure Mechanisms of Thermoelectric Type-I Clathrate $Ba_{8}Au_{6}Ge_{40}$. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 4326-4334.	4.0	1
64992	Air-grown hybrid copper($\langle scp \rangle i \langle /scp \rangle$) halide single crystals: structural transformations and ultraviolet-pumped photoluminescence applications. <i>Materials Advances</i> , 2022, 3, 2447-2455.	2.6	16
64993	Impact of the dopant-induced ensemble structure of hetero-double atom catalysts in electrochemical NH_{3} production. <i>Journal of Materials Chemistry A</i> , 2022, 10, 6216-6230.	5.2	11
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67019	Study of vacancy, voids, atom adsorption and domain substitution in hexagonal gallium nitride monolayer. Surfaces and Interfaces, 2022, 30, 101898.	1.5	1
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67023	Determination of thermodynamic growth conditions for a high-efficiency Cu		

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67034	Thermodynamic re-modelling of the Cu-Nb-Sn system: Integrating the nausite phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 77, 102409.	0.7	4
67035	Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries. <i>Nano Energy</i> , 2022, 96, 107066.	8.2	29
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67039	Local atomic ordering strategy for high strength Mg alloy design by first-principle calculations. <i>Journal of Alloys and Compounds</i> , 2022, 907, 164491.	2.8	10
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67041	The SiPb monolayer with high thermoelectric performance at room temperature. <i>Surfaces and Interfaces</i> , 2022, 30, 101831.	1.5	1
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67046	Carbon-rehybridization-induced templated growth of metal nanoclusters on graphene moiré patterns. <i>Carbon</i> , 2022, 192, 295-300.	5.4	6
67047	Investigating the role of ultrasound in improving the photocatalytic ability of CQD decorated boron-doped g-C ₃ N ₄ for tetracycline degradation and first-principles study of nitrogen-vacancy formation. <i>Carbon</i> , 2022, 192, 405-417.	5.4	68
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67049	Property changes in two-dimensional electride bilayers through compression, sliding, and twisting. <i>Applied Surface Science</i> , 2022, 586, 152596.	3.1	4
67050	Controllable carrier polarity in 2D HfS ₂ (1-x)Te _{2x} for short-wave infrared photodiodes. <i>Infrared Physics and Technology</i> , 2022, 123, 104139.	1.3	2

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67054	Thermally-induced spin transition in Fe(4,4'-Azopyridine)[Fe(CN)5NO]. <i>Journal of Solid State Chemistry</i> , 2022, 310, 123054.	1.4	12
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67059	Effect of hybridization in PdAlY-(Ni/Au/Ir) metallic glasses thin films on electrical resistivity. <i>Scripta Materialia</i> , 2022, 214, 114681.	2.6	0
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67072	Atomic site occupancy of alloying elements and Laves phase stability in $\hat{\Gamma}^3\text{-}\hat{\Gamma}^3\hat{\Gamma}^2$ Co-base superalloys. <i>Journal of Alloys and Compounds</i> , 2022, 906, 164261.	2.8	4
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67078	Single noble metals (Pd, Pt and Ir) anchored Janus MoSSe monolayers: Efficient oxygen reduction/evolution reaction bifunctional electrocatalysts and harmful gas detectors. <i>Journal of Colloid and Interface Science</i> , 2022, 616, 177-188.	5.0	10
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67080	Effect of selected dopants on conductivity and moisture stability of Li ₃ PS ₄ sulfide solid electrolyte: a first-principles study. <i>Materials Today Chemistry</i> , 2022, 24, 100837.	1.7	4
67081	Could $\hat{\Gamma}^3\text{-Ti}_3\text{O}_5$ with lamellar and channel microstructure characteristics determine the excellent properties of LIBs? The first-principles study of $\hat{\Gamma}^3\text{-Ti}_3\text{O}_5$ lithiation mechanism. <i>Materials Today Communications</i> , 2022, 31, 103332.	0.9	1
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67085	Transverse electronic transport through nucleobase-pairs of a DNA wire. <i>Materials Today Chemistry</i> , 2022, 24, 100834.	1.7	2
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#	ARTICLE	IF	CITATIONS
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67088	Surface stability of WN ultrathin films under O ₂ and H ₂ O exposure: A first-principles study. <i>Applied Surface Science</i> , 2022, 588, 152940.	3.1	5
67089	Thermodynamically driven Al migration across ultrathin Ag layered electrodes without thermal loading. <i>Applied Surface Science</i> , 2022, 588, 152907.	3.1	3
67090	Polyether sulfone and Li _{6.4} La ₃ Zr _{1.4} Ta _{0.6} O ₁₂ based polymer-in-ceramic electrolyte with enhanced conductivity at low temperature for solid state lithium batteries. <i>Applied Materials Today</i> , 2022, 27, 101447.	2.3	4
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67093	Nitrobenzene inarched carbon nitride nanotube drives efficient directional carriers separation for superior photocatalytic hydrogen production. <i>Journal of Colloid and Interface Science</i> , 2022, 616, 691-700.	5.0	15
67094	Persistent luminescence ratiometric thermometry. <i>Chemical Engineering Journal</i> , 2022, 438, 135573.	6.6	24
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67096	Possible topological states in two dimensional Kagome ferromagnet MnGe. <i>Journal of Alloys and Compounds</i> , 2022, 907, 164389.	2.8	5
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67098	Enhancing cycling stability in Li-rich Mn-based cathode materials by solid-liquid-gas integrated interface engineering. <i>Nano Energy</i> , 2022, 97, 107201.	8.2	17
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67100	The spin-state transition in ACo ₂ O ₄ spinels (A=Be, Mg, Ca, Cd, Zn). <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 552, 169206.	1.0	1
67101	Predicted crystal structures of AlN ₄ at high pressure. <i>Solid State Communications</i> , 2022, 348-349, 114745.	0.9	0
67102	Tailoring the structural stability, electrochemical performance and CO ₂ tolerance of aluminum doped SrFeO ₃ . <i>Separation and Purification Technology</i> , 2022, 290, 120843.	3.9	10
67103	Sustainable Fe ³⁺ reduction by Fe ₃ O ₄ @tourmaline in Fenton-like system. <i>Chemical Engineering Journal</i> , 2022, 437, 135480.	6.6	23
67104	Computational insights into structural, electronic and optical properties of Al _{0.5} Ga _{0.5} N nanowire with different diameters. <i>Chemical Physics Letters</i> , 2022, 797, 139597.	1.2	0

#	ARTICLE	IF	CITATIONS
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67106	First-principles study of CO gas adsorption on pristine and Fe-doped H<math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1723" altimg="si98.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mn><mml:mo>,</mml:mo><mml:mn>4</mml:mn></mml:mn><mml:mo>,</mml:mo><mml:mn>4</mml:mn></mml:mn></math> Applied Surface Science, 2022, 586, 152749.	3.1	5
67107	Quantitative calculations of thermal-expansion coefficient in Fe-Ni alloys: First-principles approach. <i>Current Applied Physics</i> , 2022, 38, 76-80.	1.1	3
67108	Extreme structure and spontaneous lift of spin degeneracy in doped perforated bilayer graphenes. <i>Carbon</i> , 2022, 192, 61-70.	5.4	6
67109	A graphdiyne analogue for dendrite-free lithium metal anode. <i>Electrochimica Acta</i> , 2022, 416, 140286.	2.6	2
67110	Using tetramethylammonium hydroxide electrolyte to inhibit corrosion of Mg-based amorphous alloy anodes: A route for promotion energy density of Ni-MH battery. <i>Journal of Alloys and Compounds</i> , 2022, 907, 164293.	2.8	5
67111	Li- and Na-doped bismuth titanate pyrochlores: From the point of view ab initio calculation and experiment. <i>Solid State Ionics</i> , 2022, 379, 115904.	1.3	0
67112	Trade-off effect of 3d transition metal doped boron nitride on anchoring polysulfides towards application in lithium-sulfur battery. <i>Journal of Colloid and Interface Science</i> , 2022, 616, 886-894.	5.0	4
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67115	CoP/Cu ₃ P heterostructured nanoplates for high-rate supercapacitor electrodes. <i>Chemical Engineering Journal</i> , 2022, 437, 135352.	6.6	66
67116	Hydrogen absorption and diffusion behaviors in cube-shaped palladium nanoparticles revealed by ambient-pressure X-ray photoelectron spectroscopy. <i>Applied Surface Science</i> , 2022, 587, 152797.	3.1	7
67117	An ab initio simulation and experimental studies of the glass-forming ability and properties of Al ₈₆ Ni _(14-x) Zr _x (x=1/47) alloys. <i>Journal of Non-Crystalline Solids</i> , 2022, 586, 121566.	1.5	8
67118	Hydrogen localization and cluster formation in $\hat{1}\pm$ -Zr from first-principles investigations. <i>Computational Materials Science</i> , 2022, 209, 111384.	1.4	3
67119	First principles study of the structural, electronic, magnetic and optical properties of the Fe doped CoS ₂ thin films. <i>Thin Solid Films</i> , 2022, 751, 139228.	0.8	1
67120	Ordered and disordered two-dimensional tellurium-selenium binary compounds from swarm intelligence and first principles. <i>Materials Today Communications</i> , 2022, 31, 103409.	0.9	0
67121	First-principles study of the effect of aluminum content on the elastic properties of Cu-Al alloys. <i>Materials Today Communications</i> , 2022, 31, 103399.	0.9	5
67122	Micro-mechanism of multi-pathway activation peroxy monosulfate by copper-doped cobalt silicate: The dual role of copper. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121276.	10.8	45

#	ARTICLE	IF	CITATIONS
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67124	One-pot synthesis of novel porous carbon adsorbents derived from poly vinyl chloride for high methane adsorption uptake. <i>Chemical Engineering Journal</i> , 2022, 440, 135867.	6.6	9
67125	Au decorated Pd nanowires for methane oxidation to liquid C ₁ products. <i>Applied Catalysis B: Environmental</i> , 2022, 308, 121223.	10.8	20
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67127	Nano gold coupled black titania composites with enhanced surface plasma properties for efficient photocatalytic alkyne reduction. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121222.	10.8	11
67128	The flexible Janus X ₂ PAs (X=Si, Ge and Sn) monolayers with in-plane and out-of-plane piezoelectricity. <i>Applied Surface Science</i> , 2022, 589, 152999.	3.1	23
67129	Electrochemical reforming of ethanol with acetate Co-Production on nickel cobalt selenide nanoparticles. <i>Chemical Engineering Journal</i> , 2022, 440, 135817.	6.6	19
67130	Two-dimensional Sc ₂ CCl ₂ /SiS ₂ van der Waals heterostructure with high solar power conversion efficiency. <i>Applied Surface Science</i> , 2022, 591, 153232.	3.1	8
67131	Type-II CdS/PtS ₂ heterostructures used as highly efficient water-splitting photocatalysts. <i>Applied Surface Science</i> , 2022, 589, 152931.	3.1	59
67132	Influence of Co and Co-F co-doping on defect-induced intrinsic ferromagnetic properties of PbPdO ₂ nanoparticles. <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 553, 169240.	1.0	2
67133	Electron redistribution of ruthenium-tungsten oxides Mott-Schottky heterojunction for enhanced hydrogen evolution. <i>Applied Catalysis B: Environmental</i> , 2022, 308, 121229.	10.8	69
67134	A new Sc-doped La _{0.5} Sr _{0.5} MnO _{3-δ} cathode allows high performance for proton-conducting solid oxide fuel cells. <i>Sustainable Materials and Technologies</i> , 2022, 32, e00409.	1.7	13
67135	CdS/ethylenediamine nanowires 3D photocatalyst with rich sulfur vacancies for efficient syngas production from CO ₂ photoreduction. <i>Applied Catalysis B: Environmental</i> , 2022, 308, 121227.	10.8	59
67136	How do the products in methane dehydroaromatization impact the distinct stages of the reaction?. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121274.	10.8	15
67137	Amorphous NiSb ₂ O ₆ nanofiber: A d-/p-block Janus electrocatalyst toward efficient NH ₃ synthesis through boosted N ₂ adsorption and activation. <i>Applied Catalysis B: Environmental</i> , 2022, 308, 121225.	10.8	12
67138	Outstanding stability of Gd-doped UO ₂ against surface oxidation: First-principles study. <i>Applied Surface Science</i> , 2022, 589, 152955.	3.1	1
67139	Large enhancement of thermoelectric properties of CoSb ₃ tuned by uniaxial strain. <i>Journal of Alloys and Compounds</i> , 2022, 908, 164404.	2.8	1
67140	Exploring the structural stability, electronic and thermal attributes of synthetic 2D materials and their heterostructures. <i>Applied Surface Science</i> , 2022, 590, 153131.	3.1	15

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67142	Electric field tunable electronic properties of antimonene/graphyne van der Waals heterostructure. <i>Journal of Alloys and Compounds</i> , 2022, 909, 164653.	2.8	7
67143	Growth and Electrical Properties of Polymorphs of Mo-Te Crystals. <i>Materials Research Bulletin</i> , 2022, 151, 111796.	2.7	1
67144	Construction of dual active sites on diatomic metal (FeCo ^x N/C-x) catalysts for enhanced Fenton-like catalysis. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121256.	10.8	40
67145	Density functional theory screening of thiophene adsorbents and study of adsorption mechanism. <i>Surface Science</i> , 2022, 721, 122069.	0.8	3
67146	Subtle modulation on electronic properties of platinum by Cu-N _x containing carbon support for highly efficient electrocatalytic hydrogen evolution. <i>Applied Surface Science</i> , 2022, 591, 153057.	3.1	7
67147	An emerging direct monolayer $\hat{\Gamma}$ -AlP ₃ : High stability, desirable carrier mobility, NO ₂ -sensitive sensing performance, and superior catalytic properties toward the nitrogen reduction reaction. <i>Applied Surface Science</i> , 2022, 591, 153191.	3.1	11
67148	Element segregation and thermal stability of Ni ²⁺ /Rh nanoparticles. <i>Journal of Solid State Chemistry</i> , 2022, 311, 123096.	1.4	8
67149	Insights into enhanced O ₃ adsorption on Ti/ anatase TiO ₂ (1 0 1) surfaces by positive electric Fields: A theoretical exploration. <i>Chemical Engineering Journal</i> , 2022, 440, 135665.	6.6	8
67150	A combined first-principles and machine-learning investigation on the stability, electronic, optical, and mechanical properties of novel C ₆ N ₇ -based nanoporous carbon nitrides. <i>Carbon</i> , 2022, 194, 230-239.	5.4	24
67151	Heterogeneous interface in hollow ferroferric oxide/ iron phosphide@carbon spheres towards enhanced Li storage. <i>Journal of Colloid and Interface Science</i> , 2022, 617, 442-453.	5.0	15
67152	Optimal surface/diffusion-controlled kinetics of bimetallic selenide nanotubes for hybrid supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2022, 617, 304-314.	5.0	18
67153	Theoretical insights into the CO/NO oxidation mechanisms on single-atom catalysts anchored H ₄ ,4,4-graphyne and H ₄ ,4,4-graphyne/graphene sheets. <i>Fuel</i> , 2022, 319, 123810.	3.4	8
67154	Density functional theory study of CH ₄ dissociation and C C coupling on W-terminated WC(0001) surface. <i>Applied Surface Science</i> , 2022, 591, 153128.	3.1	5
67155	Unveiling the promotion of intermediates transport kinetics on the N/S co-doping 3D structure titanium carbide aerogel for high-performance supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2022, 618, 161-172.	5.0	8
67156	Peroxy monosulfate activation by black TiO ₂ nanotube arrays under solar light: Switching the activation mechanism and enhancing catalytic activity and stability. <i>Journal of Hazardous Materials</i> , 2022, 433, 128796.	6.5	24
67157	Design strategy of bifunctional catalysts for CO oxidation. <i>Fuel</i> , 2022, 320, 123909.	3.4	10
67158	Anomalous elasticity of talc at high pressures: Implications for subduction systems. <i>Geoscience Frontiers</i> , 2022, 13, 101381.	4.3	4

#	ARTICLE	IF	CITATIONS
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67160	Tandem catalysis on adjacent active motifs of copper grain boundary for efficient CO ₂ electroreduction toward C ₂ products. <i>Journal of Energy Chemistry</i> , 2022, 70, 219-223.	7.1	29
67161	Dangling bonds on the Cl- and Br-terminated Si(100) surfaces. <i>Applied Surface Science</i> , 2022, 591, 153080.	3.1	7
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68281	2D spin transport through graphene- MnBi_2Te_4 heterojunction. Nanotechnology, 2022, , .	1.3	2
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68320	Electrochemically induced amorphous-to-rock-salt phase transformation in niobium oxide electrode for Li-ion batteries. <i>Nature Materials</i> , 2022, 21, 795-803.	13.3	69
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68357	Computational design of ternary NiO/MPt interface active sites for H ₂ O dissociation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 20040-20048.	3.8	2
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69405	Effect of iron vacancies on magnetic order and spin dynamics of the spin ladder $\langle \text{mml:math} \text{xmlns:mml}=\text{http://www.w3.org/1998/Math/MathML} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant}=\text{normal} \rangle \text{BaFe} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{S} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 1.5 \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{mathvariant}=\text{normal} \rangle \text{Se} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 1.5 \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Physical Review B, 2022, 105, .}$	1.1	11

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69675	In-situ formation of Are-MXY (M = Mo, W; (X % Y) = S, Se, Te) van der Waals heterostructure. <i>Journal of Solid State Chemistry</i> , 2022, 313, 123284.	1.4	2
69676	$\frac{1}{5} \times \frac{1}{4} = \frac{1}{20}$	1.3	1

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69684	The spatially separated active sites for holes and electrons boost the radicals generation for toluene degradation. <i>Journal of Hazardous Materials</i> , 2022, 437, 129329.	6.5	9
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69687	Enhanced thermoelectric performance of the AlN/GaN bilayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 143, 115333.	1.3	2
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69689	Pumpkin-like MoP-MoS ₂ @ <i>Aspergillus niger</i> spore-derived N-doped carbon heterostructure for enhanced potassium storage. <i>Journal of Energy Chemistry</i> , 2022, 72, 479-486.	7.1	14
69690	New method of atomistic modeling of $\hat{\mu}$ $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e340" altimg="si168.svg"} \rangle \langle \text{mml:mrow} \langle \text{mml:mi} \rangle \hat{\mu} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \text{linebreak="goodbreak" linebreakstyle="after"} \rangle \hat{\mu} \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \hat{\mu} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle \hat{\epsilon}^2 \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ phase transition in Fe $\hat{\epsilon}$ Cr alloy with effective accounting for vibrational entropy. <i>Computational Materials Science</i> , 2022, 212, 111563.	1.4	1
69691	Insight into ideal shear strength of Ni-based dilute alloys using first-principles calculations and correlational analysis. <i>Computational Materials Science</i> , 2022, 212, 111564.	1.4	1
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69693	Enabling deep conversion reactions by weakening molybdenum-oxygen bonds through K ⁺ pre-intercalation. <i>Electrochimica Acta</i> , 2022, 425, 140694.	2.6	0
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69702	Evolution of the structure and properties of (Zr _{1-x} Hf _x)B ₂ solid solution ceramics from first-principle theory. <i>Vacuum</i> , 2022, 203, 111283.	1.6	4
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70003			

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70323	Interface chemistry effects in nanofluids: Experimental and computational study of oil-based nanofluids with gold nanoplates. <i>Journal of Molecular Liquids</i> , 2022, 362, 119762.	2.3	3
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73427	Investigation of interfacial interaction of graphene oxide and Ti ₃ C ₂ T _x (MXene) via atomic force microscopy. <i>Applied Surface Science</i> , 2023, 609, 155303.	3.1	4
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74162	Synthesis and high-temperature ferromagnetism of Fe-doped SiGe diluted magnetic semiconductor thin films. <i>Nanoscale</i> , 2023, 15, 2206-2213.	2.8	6
74163	A new high capacity cathode material for Li/Na-ion batteries: dihafnium sulfide (Hf ₂ S). <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1114-1122.	1.3	1
74164	Strain engineering the electronic properties of the type-II CdO/MoS ₂ van der Waals heterostructure. <i>Thin Solid Films</i> , 2023, 764, 139626.	0.8	7
74165	Ultralow lattice thermal conductivity and promising thermoelectric properties of a new 2D MoW ₃ Te ₈ membrane. <i>Results in Physics</i> , 2023, 44, 106136.	2.0	2
74166	Exploring coverage-dependent chain-growth mechanisms on Ru(111) for Fischer-Tropsch synthesis. <i>Catalysis Science and Technology</i> , 2023, 13, 437-456.	2.1	2
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74169	Electron density and thermal motion of diamond at elevated temperatures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2023, 79, 41-50.	0.0	2
74170	Thermophysical properties in the Al-Cu-Ag system: A combined CALPHAD and first-principles study. <i>Journal of Molecular Liquids</i> , 2023, 370, 121001.	2.3	1
74171	Bandgap widening through doping for improving the photocatalytic oxidation ability of narrow-bandgap semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2022, 25, 255-261.	1.3	2
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74173	A computational study on CO ₂ electrochemical reduction on two dimensional metal-1,2,3,4,5,6,7,8,9,10,11,12-perthiolated coronene frameworks. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
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74175	Advanced materials based on montmorillonite modified with poly(ethylenimine) and poly(2-methyl-2-oxazoline): Experimental and DFT study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 659, 130784.	2.3	3

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74195	Strain-enhanced properties of Janus Si ₂ PA _s monolayer as a promising photocatalyst for the splitting of water: Insights from first-principles calculations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 659, 130782.	2.3	10
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74197	Strain effect on the defect formation and diffusion in Ti ₂ AlC and Ti ₃ AlC ₂ : A first-principles study. <i>Computational Materials Science</i> , 2023, 218, 111946.	1.4	1
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74199	A phase-field study of stainless-steel oxidation from high-temperature carbon dioxide exposure. <i>Computational Materials Science</i> , 2023, 218, 111996.	1.4	1
74200	Coupled effect of Cr and Al on interactions between a prismatic interstitial dislocation loop and an edge dislocation line in Fe-Cr-Al alloy. <i>Acta Materialia</i> , 2023, 245, 118651.	3.8	7
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74202	MgO promoted by Fe ₂ O ₃ and nitrate molten salt for fast and enhanced CO ₂ capture: Experimental and DFT investigation. <i>Separation and Purification Technology</i> , 2023, 307, 122766.	3.9	7
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74206	The structure and mechanical properties of NbHfTaW refractory high-entropy alloy: A combined theoretical and experimental study. <i>International Journal of Refractory Metals and Hard Materials</i> , 2023, 111, 106067.	1.7	3
74207	A dispersion-corrected DFT method for zeolite-based CO ₂ /N ₂ separation: Assessment and application. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109052.	3.3	2
74208	Effect of transition metals on the crystal field in CeCo _{0.4} Fe _{0.6} Ge ₃ . <i>Intermetallics</i> , 2023, 153, 107776.	1.8	1
74209	Exploring the relationship between the accelerated austenite reversion and two-steps solution treatment in a Cr-Ni-Mo cryogenic maraging stainless steel. <i>Materials Characterization</i> , 2023, 196, 112581.	1.9	3
74210	Molecular dynamics of electric-field driven ionic systems using a universal neural-network potential. <i>Computational Materials Science</i> , 2023, 218, 111955.	1.4	2
74211	Enhancing the thermal stability of n-type Mg _{3+x} Sb _{1.5} Bi _{0.49} Te _{0.01} by defect manipulation. <i>Nano Energy</i> , 2023, 106, 108036.	8.2	7

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74213	Density functional theory study of formation and diffusion of hydrogen, deuterium, and tritium in Pd-V intermetallic compounds. Computational Materials Science, 2023, 218, 111976.	1.4	2
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74216	Accurate Fe-He machine learning potential for studying He effects in BCC-Fe. Journal of Nuclear Materials, 2023, 574, 154183.	1.3	1
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74222	Nanosized LaInO3 perovskite for efficient electrocatalytic reduction of CO2 to formate. Journal of CO2 Utilization, 2023, 68, 102342.	3.3	6
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74228	A novel Co1.29Ni1.71O4/glycerolate-derived oxygen-vacancies-containing TiO2 composite for highly efficient photocatalytic hydrogen evolution. Journal of Environmental Chemical Engineering, 2023, 11, 109142.	3.3	4
74229	Development of GD-containing austenitic stainless steel. Journal of Nuclear Materials, 2023, 574, 154197.	1.3	3

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74231	Ab-initio study of vacancy-defective aluminium nitride nanosheets as trifluoroacetonitrile gas sensor. Applied Surface Science, 2023, 612, 155803.	3.1	2
74232	Role of lattice thermal conductivity in thermoelectric properties of chalcopyrite-type antimonides XSiSb ₂ (X = Mg, Be): A DFT insight. Materials Chemistry and Physics, 2023, 295, 127190.	2.0	3
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74268	Adsorption behavior of small molecule on monolayered SiAs and sensing application for NO2 toxic gas. <i>Applied Surface Science</i> , 2023, 613, 156010.	3.1	7
74269	Exploration of threshold and resistive-switching behaviors in MXene/BaFe12O19 ferroelectric memristors. <i>Applied Surface Science</i> , 2023, 613, 155956.	3.1	13
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74274	Interfacial charge transfer and electronic structure of diamond/c-BN heterointerface. <i>Computational Materials Science</i> , 2023, 218, 111947.	1.4	2
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74276	The intrinsic high ductility in B2 intermetallic compound YAg: Causality clarified by ab initio study. <i>Materials Today Communications</i> , 2023, 34, 105177.	0.9	0
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74283	A unified framework of slip controlled bending and rippled superlattice design of few-layer graphene. <i>Applied Surface Science</i> , 2023, 613, 155979.	3.1	2

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74287	Synthesis, crystal structure and ¹⁹ F NMR parameters modelling of CaTiF ₆ (H ₂ O) ₂ yielding to a revision of the bond-valence parameters for the Ti ⁴⁺ /F ²⁻ ion pair. <i>Journal of Solid State Chemistry</i> , 2023, 319, 123793.	1.4	1
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74289	Revisiting the origin of ORR and HER activities of N-doped ¹³ C-graphdiyne from the perspective of edge effects. <i>Applied Surface Science</i> , 2023, 613, 156084.	3.1	4
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74291	Strain-regulated magnetic phase transition and perpendicular magnetic anisotropy in CrSBr monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 147, 115590.	1.3	1
74292	A DFT study of Mn ₃ O ₄ Hausmannite thin films supported on coinage metals. <i>Applied Surface Science</i> , 2023, 612, 155920.	3.1	4
74293	Two novel phases of germa-graphene: Prediction, electronic and transport applications. <i>Applied Surface Science</i> , 2023, 614, 156107.	3.1	5
74294	Optical and thermoelectric properties of square lattice phases of alkali halide compounds. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 174, 111142.	1.9	1
74295	First-principles study of impurity diffusion coefficients in Niobium. <i>Vacuum</i> , 2023, 209, 111739.	1.6	0
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74297	Two-dimensional interface superstructures assembled by well-ordered solute atoms. <i>Journal of Materials Science and Technology</i> , 2023, 142, 253-259.	5.6	2
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74304	Theoretical exploration of the structural evolution of sodium sulfide clusters in Na-S batteries. <i>Applied Surface Science</i> , 2023, 613, 155906.	3.1	4
74305	Electronic structures of defects in bottom-up N-doped graphene nanoribbons: Experiment and theory. <i>Applied Surface Science</i> , 2023, 612, 155874.	3.1	0
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74309	Tailored Pd/C bifunctional catalysts for styrene production under an ethylbenzene oxidative dehydrogenation assisted direct dehydrogenation scheme. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122205.	10.8	6
74310	Mechanochemical localization of vanadia on titania to prepare a highly sulfur-resistant catalyst for low-temperature NH ₃ -SCR. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122290.	10.8	4
74311	Atomically dispersed cerium sites in carbon-doped boron nitride for photodriven CO ₂ reduction: Local polarization and mechanism insight. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122235.	10.8	9
74312	Highly selective nitrate reduction to ammonia on CoO/Cu foam via constructing interfacial electric field to tune adsorption of reactants. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122201.	10.8	21
74313	Adjustable heterointerface-vacancy enhancement effect in RuO ₂ @Co ₃ O ₄ electrocatalysts for efficient overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122294.	10.8	38
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74317	Efficient carbon monoxide electroreduction on two-dimensional transition metal phosphides: A computational study. <i>Applied Surface Science</i> , 2023, 613, 156025.	3.1	2
74318	A comparative analysis of different van der Waals treatments for molecular adsorption on the basal plane of 2H-MoS ₂ . <i>Surface Science</i> , 2023, 729, 122226.	0.8	5
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75433	Atomic scale simulations of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si12.svg" display="inline" id="d1e2335"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mo} \rangle \{ \langle \text{mml:mo} \rangle \langle \text{mml:mn} \rangle 112 \langle \text{mml:mn} \rangle \langle \text{mml:mo} \rangle \} \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ symmetric incoherent twin boundaries in gold. <i>Materialia</i> , 2023, 27, 101678.	1.3	0
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75437	Catalytic active interfacial B-C bonds of boron nanosheet/reduced graphene oxide heterostructures for efficient oxygen reduction reaction. <i>Composites Part B: Engineering</i> , 2023, 252, 110496.	5.9	3
75438	Sb and O dual doping of Chlorine-rich lithium argyrodite to improve air stability and lithium compatibility for all-solid-state batteries. <i>Journal of Power Sources</i> , 2023, 559, 232659.	4.0	48
75439	Bulk and monolayer thermoelectric and optical properties of anisotropic NbS ₂ $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si61.svg" display="inline" id="d1e859"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle \text{Cl} \langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si61.svg" display="inline" id="d1e867"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$	0.9	0
75440	Remarkable reactivity of Fe modified Cu(100) surface towards CO2 decomposition: A DFT study. <i>Materials Today Communications</i> , 2023, 34, 105395.	0.9	3
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75801

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76070	Adsorption Tuning of Polarity and Magnetism in AgCr ₂ S ₄ Monolayer. <i>Materials</i> , 2023, 16, 3058.	1.3	1

#	ARTICLE	IF	CITATIONS
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76073	The effects of electric field and strain on the BP/GeTe van der Waals heterojunction. <i>Journal Physics D: Applied Physics</i> , 2023, 56, 315102.	1.3	1
76074	Cooperative roles of water and metal-support interfaces in the selective hydrogenation of cinnamaldehyde over cobalt boride catalysts. <i>Cell Reports Physical Science</i> , 2023, 4, 101367.	2.8	1
76075	A pressure-induced high-pressure metallic GeTe phase. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
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76077	The Facet Dependence of CO_{2} Electroreduction Selectivity on a Pd_{3}Au Bimetallic Catalyst: A DFT Study. <i>Molecules</i> , 2023, 28, 3169.	1.7	1
76078	Magnetic field effects and excitonic selection rules in monolayer palladium diselenide as a large-gap quantum spin Hall insulator. <i>Physical Review B</i> , 2023, 107, .	1.1	0
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76080	Enhancing the accuracy of density functional tight binding models through ChIMES many-body interaction potentials. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	3
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76082	Predicted the structural diversity and electronic properties of Pt^{N} compounds under high pressure. <i>Journal of Physics Condensed Matter</i> , 2023, 35, 285501.	0.7	0
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76084	Effect of Surface Termination on Carrier Dynamics of Metal Halide Perovskites: Ab Initio Quantum Dynamics Study. <i>Electronic Materials Letters</i> , 0, .	1.0	0
76085	Electron deficiency modulates hydrogen adsorption strength of Ru single-atomic catalyst for efficient hydrogen evolution. <i>Renewable Energy</i> , 2023, 210, 258-268.	4.3	3
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76088	Electronic Modulation of Metal-Organic Frameworks Caused by Atomically Dispersed Ru for Efficient Hydrogen Evolution. <i>Small</i> , 2023, 19, .	5.2	8
76089	Dynamic catalysis of sub-nanometer metal clusters in oxygen dissociation. , 2023, , 100002.		0

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76092	Characterizing and Overcoming Surface Paramagnetism in Magnetolectric Antiferromagnets. <i>Physical Review Letters</i> , 2023, 130, .	2.9	2
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76098	Competing spin fluctuations in $SrRu_2O_4$ and their tuning through epitaxial strain. <i>Physical Review B</i> , 2023, 107, .	1.1	0
76099	Surface engineering of carbon fiber via upcycling of waste gases generated during carbon fiber production: A sustainable approach towards high-performance composites. <i>Composites Part B: Engineering</i> , 2023, 255, 110624.	5.9	2
76100	Optimization of Ti with modified SiC ceramics for electromagnetic absorption properties. <i>Materials Characterization</i> , 2023, 198, 112761.	1.9	10
76101	In-situ construction of hierarchical 2D MoS ₂ /1D Te hybrid for supercapacitor applications. <i>Journal of Energy Storage</i> , 2023, 60, 106703.	3.9	9
76102	First-principles design of highly active and durable Ti ₅₅ Cx@Pt ₉₂ nanocatalyst for oxygen reduction reaction through charge control at nanointerfaces. <i>Applied Surface Science</i> , 2023, 618, 156685.	3.1	1
76103	Hollow macroporous CeO ₂ /Bi ₂ O ₃ heterostructure sphere via one-step spray solution combustion synthesis for efficient photocatalysis. <i>Applied Surface Science</i> , 2023, 619, 156718.	3.1	8
76104	Facet effects on bimetallic ZnSn hydroxide microcrystals for selective electrochemical CO ₂ reduction. <i>Green Energy and Environment</i> , 2023, , .	4.7	1
76105	Concentration Phase Separation of Substitutionally Doped Atoms in TMDCs Monolayer. <i>Small</i> , 2023, 19, .	5.2	5
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76109	Promoter not inhibitor: The antidotal effects of arsenic on lead-poisoning V ₂ O ₅ ~WO ₃ /TiO ₂ catalyst for selective catalytic reduction of NO with NH ₃ . <i>Journal of Cleaner Production</i> , 2023, 397, 136621.	4.6	3
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76116	Energetic and configurational mechanisms to facilitate mica nanosheets synthesis by organo-ammonium cation intercalation. <i>Computational Materials Science</i> , 2023, 224, 112162.	1.4	1
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76119	Theoretical study of the mechanism of the hydrogen evolution reaction on the V ₂ C MXene: Thermodynamic and kinetic aspects. <i>Journal of Catalysis</i> , 2023, 421, 252-263.	3.1	11
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76121	Vacancy defects in nitrogen doped diamond. <i>Physica B: Condensed Matter</i> , 2023, 655, 414769.	1.3	0
76122	Anomalous temperature dependence of self-interstitial diffusivity in metallic lithium and sodium. <i>Materialia</i> , 2023, 28, 101718.	1.3	0
76123	First-principle studies of oxidation effects on grain boundary strength in nickel. <i>Materialia</i> , 2023, 28, 101745.	1.3	2
76124	Insight into B S ratio model and surface atom interactions of co-doping diamond: First-principles studies. <i>Diamond and Related Materials</i> , 2023, 135, 109824.	1.8	2
76125	Enhanced strength and plasticity in a Nb ₂ MoWC _{0.5} alloy via eutectic dilute carbide. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2023, 872, 144920.	2.6	1

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76127	Directed synthesis of nylon 5X key monomer cadaverine with alkaline metal modified Ru@FAU catalysts. <i>Applied Catalysis A: General</i> , 2023, 658, 119172.	2.2	2
76128	Micro-kinetics of ethylene and methane oxidation on platinum. <i>Chemical Engineering Journal</i> , 2023, 464, 142608.	6.6	3
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76134	Transfer learning aided high-throughput computational design of oxygen evolution reaction catalysts in acid conditions. <i>Journal of Energy Chemistry</i> , 2023, 80, 744-757.	7.1	7
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76137	First-principles study of the native defects with charge states in ZrSe $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si10.svg" display="inline" id="d1e937"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$. <i>Solid State Communications</i> , 2023, 365, 115138.	0.9	2
76138	Magnetic nano-size normal spinel-ZnFe ₂ O ₄ and inverse spinel-MnFe ₂ O ₄ for catalytic ozonation: Performance and mechanism. <i>Separation and Purification Technology</i> , 2023, 313, 123535.	3.9	1
76139	Phase transformation and radiation resistance of B-site high entropy pyrochlores. <i>Scripta Materialia</i> , 2023, 229, 115367.	2.6	6
76140	Electron-rich platinum single sites anchored on sulfur-doped covalent organic frameworks for boosting anti-Markovnikov hydrosilylation of alkenes. <i>Chemical Engineering Journal</i> , 2023, 463, 142255.	6.6	6
76141	Effects of magnetic ordering on structural stability and phonon transport in monolayer Td-VX ₂ (X=Se, I). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2023, 469, 128746.	0.9	2
76142	Reduced MgFe hydroxalcite efficiently catalyzes the aerobic oxidation of alkylarenes. <i>Applied Catalysis A: General</i> , 2023, 657, 119143.	2.2	2
76143	Adjacent diatomic Cu ₁ N ₃ /Mo ₁ S ₂ entities decorated carbon nitride for markedly enhanced photocatalytic hydrogen generation. <i>Chemical Engineering Journal</i> , 2023, 463, 142470.	6.6	2

#	ARTICLE	IF	CITATIONS
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76145	Carbon-confined Cu-Pd alloy nanoparticles as high-performance catalysts for acetylene selective hydrogenation. <i>Chemical Engineering Journal</i> , 2023, 464, 142609.	6.6	7
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76151	Prediction of mechanical properties of AlTiCrVNb high entropy alloys with B2 ordered structure. <i>Journal of Materials Research and Technology</i> , 2023, 24, 440-448.	2.6	2
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76160	Phonon thermal transport in two-dimensional PbTe monolayers via extensive molecular dynamics simulations with a neuroevolution potential. <i>Materials Today Physics</i> , 2023, 34, 101066.	2.9	2
76161	States of Pt/CeO ₂ catalysts for CO oxidation below room temperature. <i>Journal of Catalysis</i> , 2023, 421, 285-299.	3.1	9

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76164	Enhancement in the thermoelectric performance of ZrNiSn-based alloys through extra Zr-rich nanoprecipitates with superstructures. <i>Chemical Engineering Journal</i> , 2023, 464, 142531.	6.6	2
76165	Theoretical studies of sliding ferroelectricity, magnetoelectric couplings, and piezo-multiferroicity in two-dimensional magnetic materials. <i>Chemical Physics Letters</i> , 2023, 818, 140430.	1.2	8
76166	Selective oxidation of vanadium from vanadium slag by CO ₂ during CaCO ₃ roasting treatment. <i>Separation and Purification Technology</i> , 2023, 312, 123407.	3.9	7
76167	Charge localization induced by Fe doping in porous Bi ₅ O ₇ Micro-flower for enhanced photoreduction of CO ₂ to CO. <i>Separation and Purification Technology</i> , 2023, 312, 123379.	3.9	16
76168	Revealing active edge sites induced by oriented lattice bending of Co-CeO ₂ nanosheets for boosting auto-exhaust soot oxidation. <i>Journal of Catalysis</i> , 2023, 421, 351-364.	3.1	11
76169	Prediction of new stable crystal structures for ternary ErAgTe ₂ and YAgTe ₂ semiconductors: Ab initio study. <i>Solid State Sciences</i> , 2023, 139, 107160.	1.5	1
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76178	First principles study of oxygen diffusion in plutonium dioxide, sesquioxide, and their interface under activated conditions. <i>Journal of Nuclear Materials</i> , 2023, 578, 154348.	1.3	4
76179	Atomic and electronic structure of grain boundaries in α-Al ₂ O ₃ : A combination of machine learning, first-principles calculation and electron microscopy. <i>Scripta Materialia</i> , 2023, 229, 115368.	2.6	3

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76181	Syngas-to-C ₂ oxygenates over the inverse Mo ₆ C ₄ /Cu catalyst: Identifying the role of synergistic effect. <i>Applied Surface Science</i> , 2023, 619, 156746.	3.1	0
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76183	Theoretical insights into the removal pathways of adsorbed oxygen on the surface of $\sqrt{3}\times\sqrt{3}$ -Fe ₅ C ₂ (5 1 0). <i>Chemical Engineering Science</i> , 2023, 271, 118576.	1.9	4
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76186	Strongly enhanced infrared absorption of HfSe ₂ monolayer by lanthanide doping: A first-principles study. <i>Results in Physics</i> , 2023, 48, 106415.	2.0	3
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76188	The effect of B/P/S doping on Li ⁺ charge transfer during ion transport along the H-diamond surface: A first-principles calculation. <i>Diamond and Related Materials</i> , 2023, 135, 109846.	1.8	1
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76193	Exploring the basal/prismatic slip transfer at grain boundaries in magnesium: A molecular dynamic simulation. <i>Vacuum</i> , 2023, 212, 111995.	1.6	2
76194	Tuning the UV absorbing ability of CeO ₂ nanoparticles with F [•] doping. <i>FlatChem</i> , 2023, 39, 100494.	2.8	6
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76199	CO oxidation mechanism on surfaces of B-site doped SrFeO ₃ -based perovskite materials for thermochemical water splitting. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114109.	1.1	0
76200	Insight into the effect of Li/P co-doping on the electronic structure and photocatalytic performance of g-C ₃ N ₄ by the first principle. <i>Applied Surface Science</i> , 2023, 623, 157031.	3.1	13
76201	Indirect interactions between the ionic liquid and Cu surface in 0.5 Å HCl: a novel mechanism explaining cathodic corrosion inhibition. <i>Corrosion Science</i> , 2023, 216, 111100.	3.0	12
76202	Dual MOF-derived Fe/N/P-tridoped carbon nanotube as high-performance oxygen reduction catalysts for zinc-air batteries. <i>Applied Catalysis B: Environmental</i> , 2023, 327, 122469.	10.8	58
76203	Structural construction of Bi-anchored honeycomb N-doped porous carbon catalyst for efficient CO ₂ conversion. <i>Chemical Engineering Journal</i> , 2023, 464, 142672.	6.6	5
76204	Anisotropic and high thermal conductivity in monolayer quasi-hexagonal fullerene: A comparative study against bulk phase fullerene. <i>International Journal of Heat and Mass Transfer</i> , 2023, 206, 123943.	2.5	18
76205	On the enhanced performance of Pt-based high-entropy alloys catalyst during water-gas shift reaction: A density functional theory study. <i>Applied Surface Science</i> , 2023, 623, 157023.	3.1	3
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76207	An anti Si/Zr-poisoning strategy of Al grain refinement by the evolving effect of doped complex. <i>Acta Materialia</i> , 2023, 249, 118812.	3.8	14
76208	Symmetry-breaking of LiMn ₆ hexatomic-ring in grain surface of Li ₂ MnO ₃ . <i>Journal of Energy Chemistry</i> , 2023, 81, 110-117.	7.1	1
76209	A dual-halogen electrolyte for protective-layer-free all-solid-state lithium batteries. <i>Journal of Power Sources</i> , 2023, 568, 232992.	4.0	7
76210	Phase equilibria and non-transformable tetragonal zirconia in ZrO ₂ -RETaO ₄ systems and their stabilization mechanism: Experiments and calculations. <i>Ceramics International</i> , 2023, 49, 15969-15978.	2.3	2
76211	Breakdown of the correlation between oxidation states and core electron binding energies at the sub-nanoscale. <i>Applied Surface Science</i> , 2023, 619, 156755.	3.1	1
76212	Structure and stability investigation of oxygen interaction with Fe in bcc-Fe. <i>Vacuum</i> , 2023, 212, 112005.	1.6	1
76213	Defective 1T $\bar{5}$ -MoX ₂ (X = S, Se, Te) monolayers for electrocatalytic ammonia synthesis: Steric and electronic effects on the catalytic activity. <i>Fuel</i> , 2023, 342, 127779.	3.4	1
76214	Phase transformation induced transitional twin boundary in body-centered cubic metals. <i>Acta Materialia</i> , 2023, 249, 118815.	3.8	10
76215	Development of TaC-based transition metal carbide superlattices via compound target magnetron sputtering. <i>International Journal of Refractory Metals and Hard Materials</i> , 2023, 113, 106165.	1.7	4

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76217	High temperature elastic properties of sub-stoichiometric yttrium dihydrides. <i>Materials Today Communications</i> , 2023, 35, 105879.	0.9	0
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76219	Predicting formation of chemically graded metal/ceramic interfaces. <i>Computational Materials Science</i> , 2023, 224, 112155.	1.4	0
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76221	Machine learning insight into h-BN growth on Pt(111) from atomic states. <i>Applied Surface Science</i> , 2023, 621, 156893.	3.1	4
76222	Molecular dynamics simulations of CaCl ₂ -NaCl molten salt based on the machine learning potentials. <i>Solar Energy Materials and Solar Cells</i> , 2023, 254, 112275.	3.0	3
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76224	Atomic-scale de-passivation mechanisms of anatase TiO ₂ induced by corrosive halides based on density-functional theory. <i>Applied Surface Science</i> , 2023, 621, 156859.	3.1	1
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76226	Interfacial properties of In-plane monolayer 2H-MoTe ₂ /1T'-WTe ₂ heterostructures. <i>Applied Surface Science</i> , 2023, 623, 157022.	3.1	1
76227	Correlation between stabilizing and strengthening effects due to grain boundary segregation in iron-based alloys: Theoretical models and first-principles calculations. <i>Acta Materialia</i> , 2023, 251, 118899.	3.8	6
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76231	Record volumetric activities of oxygen electroreduction in partly packing graphene/AgTCNQ electrodes. <i>Carbon Trends</i> , 2023, 11, 100254.	1.4	0
76232	Nitrogen-doped or boron-doped twin T-graphene as advanced and reversible hydrogen storage media. <i>Applied Surface Science</i> , 2023, 622, 156895.	3.1	11
76233	Theoretical study on surface stability, distortion and oxygen adsorption behavior of TiZrHfNb high entropy alloys. <i>Surface Science</i> , 2023, 732, 122273.	0.8	0

#	ARTICLE	IF	CITATIONS
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76236	Structural, electronic, elastic and thermal properties of Cr-doped U ₃ Si ₂ : A DFT study. <i>Journal of Nuclear Materials</i> , 2023, 579, 154388.	1.3	1
76237	Microstructural and magnetic properties of Mn ₂ FeSi and Mn ₂ FeAl alloys prepared in bulk form. <i>Journal of Alloys and Compounds</i> , 2023, 947, 169672.	2.8	6
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76240	Small-data-based machine learning interatomic potentials for graphene grain boundaries enabled by structural unit model. <i>Carbon Trends</i> , 2023, 11, 100260.	1.4	1
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76242	Synthesis of large-size bulk hierarchically graphene-structured porous carbon and its versatile applications as hosts of sulfur and lithium for Li-S full cells and electrocatalyst for water splitting. <i>Journal of Alloys and Compounds</i> , 2023, 947, 169587.	2.8	0
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76246	Construction of strong built-in electric field in binary metal sulfide heterojunction to propel high-loading lithium-sulfur batteries. <i>Journal of Energy Chemistry</i> , 2023, 81, 492-501.	7.1	10
76247	Calculation of tunable electronic and optical properties of AlP/InSe heterostructure based on first principles. <i>Materials Science in Semiconductor Processing</i> , 2023, 160, 107443.	1.9	0
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76250	One-dimensional $\hat{\Gamma}$ -Al ₂ O ₃ growth from the oxidation of NiAl. <i>Corrosion Science</i> , 2023, 216, 111069.	3.0	5
76251	First principles investigation on electronic structure, elasticity, thermodynamic properties of $\hat{\Gamma}$ -Cu ₂ As ₂ O ₇ . <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2023, 292, 116371.	1.7	0

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76253	Red anatase TiO ₂ microspheres with exposed major {0 0 1} facets and boron-stabilized hydrogen-occupied oxygen vacancies for visible-light-responsive water oxidation. <i>Journal of Colloid and Interface Science</i> , 2023, 640, 211-219.	5.0	2
76254	Strain tuning of the electronic structure and optical properties of novel Janus MgBrI monolayer: Insights from first-principles calculations. <i>Computational Condensed Matter</i> , 2023, 35, e00802.	0.9	1
76255	Construction of diluted magnetic semiconductor to endow nonmagnetic semiconductor with spin-regulated photocatalytic performance. <i>Nano Energy</i> , 2023, 110, 108381.	8.2	14
76256	VTAnDeM: A python toolkit for simultaneously visualizing phase stability, defect energetics, and carrier concentrations of materials. <i>Computer Physics Communications</i> , 2023, 287, 108691.	3.0	1
76257	First-principles calculations integrated with experimental optical and electronic properties for MoS ₂ -graphene heterostructures and MoS ₂ -graphene-Au heterointerfaces. <i>Applied Surface Science</i> , 2023, 623, 156948.	3.1	3
76258	Theoretical study on mechanical and electronic properties of ternary diborides Sc _{0.5} V _{0.5} B ₂ , Sc _{0.5} Nb _{0.5} B ₂ and Sc _{0.5} Ta _{0.5} B ₂ . <i>Materials Today Communications</i> , 2023, 35, 105760.	0.9	1
76259	Single 1:7H solid-solution phase achieving in iron-rich Sm-Co-Fe-Cu-Zr magnets. <i>Journal of Alloys and Compounds</i> , 2023, 945, 169373.	2.8	3
76260	Design of molecular M N C dual-atom catalysts for nitrogen reduction starting from surface state analysis. <i>Journal of Colloid and Interface Science</i> , 2023, 640, 983-989.	5.0	3
76261	Ab initio prediction of temperature-dependent stability of heterogeneous B19â€² phase in TiNi alloy using atomistically informed Eshelbyâ€™s ellipsoidal inclusion. <i>Materials Today Communications</i> , 2023, 35, 105861.	0.9	1
76262	Surface Gibbs free energy analyses of Sr segregation in lanthanum strontium iron oxide. <i>Surface Science</i> , 2023, 732, 122268.	0.8	0
76263	Design and development of low density, high strength ZrNbAlVTi high entropy alloy for high temperature applications. <i>International Journal of Refractory Metals and Hard Materials</i> , 2023, 113, 106222.	1.7	7
76264	The effects of mixing non-metal atoms in the B1 structured transition metal carbo-nitrides on their structure and mechanical properties: HfC ₁ -N. <i>Open Ceramics</i> , 2023, 14, 100356.	1.0	0
76265	Zr ⁴⁺ and Bi ³⁺ codoped Cs ₂ Ag _{0.3} Na _{0.7} InCl ₆ double perovskite for single-composition white-light emitting phosphors and multimodal optical anti-counterfeiting. <i>Journal of Luminescence</i> , 2023, 258, 119783.	1.5	9
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76268	Efficiently electrochemical CO ₂ reduction on molybdenum-nitrogen-carbon catalysts with optimized p-block axial ligands. <i>Chemical Engineering Science</i> , 2023, 273, 118638.	1.9	2
76269	Designing layered V ₂ O ₃ @C with stable oxygen defects via UV-curing technology for highâ€™performance Zn-ion hybrid supercapacitors. <i>Applied Surface Science</i> , 2023, 622, 156951.	3.1	7

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76276	First-principles investigation of structural, electronic, and energetic properties of BaSnO ₃ (001) surfaces. Vacuum, 2023, 212, 111977.	1.6	5
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76325	Unraveling the role of Fe ₅ C ₂ in CH ₄ formation during CO ₂ hydrogenation over hydrophobic iron catalysts. <i>Applied Catalysis B: Environmental</i> , 2023, 327, 122449.	10.8	7
76326	Theoretical study of the influence of H-SAPO-34 modified with Zn ²⁺ on the formation of butadiene. <i>Chemical Engineering Science</i> , 2023, 273, 118652.	1.9	0
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76328	New insights into the co-adsorption behavior of H ₂ O and H ₂ on defective PuH ₂ (100), (110), and (111) surfaces from first-principles study. <i>Vacuum</i> , 2023, 212, 112044.	1.6	1
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76331	The hinge morphology of SnO ₂ as multifunctional semiconductor: What we can learn from simulations, theory, and experiments. <i>Applied Surface Science</i> , 2023, 622, 156904.	3.1	3
76332	Structure, vibrations and electronic transport in silicon suboxides: Application to physical unclonable functions. <i>Journal of Non-Crystalline Solids: X</i> , 2023, 18, 100179.	0.5	1
76333	Theoretical study on structural transformation and mechanical properties of Ni ₃ Ti _{1-x} Nb _x . <i>Results in Materials</i> , 2023, 18, 100387.	0.9	0
76334	First-principles study of Xe behavior in $\hat{\Gamma}$ -UZr ₂ . <i>Journal of Nuclear Materials</i> , 2023, 579, 154387.	1.3	1
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76336	Activation of basal-plane sulfur sites on MoS ₂ @Ni ₃ S ₂ nanorods by Zr plasma ion implantation for bifunctional electrocatalysts. <i>Journal of Alloys and Compounds</i> , 2023, 947, 169448.	2.8	5
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76339	Surpassing Pt hydrogen production from {200} facet-riched polyhedral Rh ₂ P nanoparticles by one-step synthesis. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122645.	10.8	4
76340	Two-dimensional van der Waals layered VSi ₂ N ₄ as anode materials for alkali metal (Li, Na and K) ion batteries. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 178, 111339.	1.9	3
76341	Uncertainty quantification of predicting stable structures for high-entropy alloys using Bayesian neural networks. <i>Journal of Energy Chemistry</i> , 2023, 81, 118-124.	7.1	2

#	ARTICLE	IF	CITATIONS
76342	2D/2D Z-scheme-based Fe_2O_3 @NGr heterojunction implanted with Pt single-atoms for remarkable photocatalytic hydrogen evolution. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122586.	10.8	15
76343	Atomistic mechanism of Fe^{TM} -to- Fe^{I} transformation in Al-Zn-Mg-Cu alloys. <i>Scripta Materialia</i> , 2023, 231, 115474.	2.6	6
76344	CO_2 electroreduction on single atom catalysts: Is water just a solvent?. <i>Journal of Catalysis</i> , 2023, 422, 1-11.	3.1	10
76345	Significance of different dopamine species as reducing agents of graphene oxide: Fundamental aspects. <i>Surface Science</i> , 2023, 732, 122285.	0.8	1
76346	Defect engineered Janus MoSiGeN_4 as highly efficient electrocatalyst for hydrogen evolution reaction. <i>Applied Surface Science</i> , 2023, 622, 156894.	3.1	9
76347	DFT study of superlight ambient temperature reversible H_2 storage media based on Li decorated on new planar BCN. <i>Applied Surface Science</i> , 2023, 622, 156947.	3.1	9
76348	Efficient biobased carboxylic acids synthesis by synergistic electrocatalysis of multi-active sites on bimetallic Cu-Co oxide/oxyhydroxide. <i>Applied Catalysis B: Environmental</i> , 2023, 331, 122709.	10.8	8
76349	Amorphous quantum dots co-catalyst: Defect level induced solar-to-hydrogen production. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122583.	10.8	8
76350	Dual functional effect of oxygen vacancies and depolarity shield embedded NiCo_2O_4 cathode in lithium sulfur battery. <i>Applied Surface Science</i> , 2023, 622, 156939.	3.1	3
76351	Novel dual-photoelectrode photoelectrocatalytic system based on TiO_2 nanoneedle arrays photoanode and nitrogen-doped carbon dots/ Co_3O_4 photocathode for efficient water purification at low/no applied voltage. <i>Applied Catalysis B: Environmental</i> , 2023, 331, 122676.	10.8	6
76352	Ion diffusion, and hysteresis of magnesium hydride conversion electrode materials. <i>Journal of Materials Science and Technology</i> , 2023, 155, 47-53.	5.6	2
76353	Free Ca^{2+} -templated synthesis of N^{doped} PtCu porous hollow nanospheres for efficient ethanol oxidation and oxygen reduction reactions. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122602.	10.8	8
76354	Effect of flue gas components on the removal of cadmium pollutants by transition metal-modified activated carbon: Density functional theory and thermodynamic study. <i>Fuel</i> , 2023, 343, 128011.	3.4	7
76355	Precisely optimizing polysulfides adsorption and conversion by local coordination engineering for high-performance Li-S batteries. <i>Nano Energy</i> , 2023, 110, 108353.	8.2	20
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76357	Design of bifunctional TiO_2 -SSZ-13 mixed supports for potassium-resistant vanadia catalysts for NH_3 -SCR. <i>Fuel</i> , 2023, 342, 127804.	3.4	3
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76359	Ab initio study of pressure-dependent phonon heat conduction in cubic boron nitride. <i>International Journal of Heat and Mass Transfer</i> , 2023, 208, 124092.	2.5	3

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76363	Systemic analysis to reveal the improved stability of LiNi _{0.6} Co _{0.2} Mn _{0.2} O ₂ electrode-electrolyte interface modulated by N-methylpyrrolidone. Chinese Journal of Analytical Chemistry, 2023, 51, 100250.	0.9	1
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76366	Stable Li deposition of 3D highstrength-lithiophilicity-porous CuZn current collector with gradient structure. Journal of Alloys and Compounds, 2023, 951, 169953.	2.8	4
76367	Nonlinear optical crystals KPb ₃ (3-C ₅ H ₄ NCOO) ₂ Br ₅ and KPb ₃ (3-C ₅ H ₄ NCOO) ₂ Cl ₃ Br ₂ with new Pb-centered nitrogen-halide polyhedrons obtained by the halide anionic substitution. Journal of Alloys and Compounds, 2023, 951, 169945.	2.8	0
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76369	Boron pretreatment promotes phosphorization of FeNi catalysts for oxygen evolution. Applied Catalysis B: Environmental, 2023, 330, 122598.	10.8	20
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76372	Observation of low thermal expansion behavior and weak thermal anisotropy in M3A2C phases. Journal of Materials Science and Technology, 2023, 154, 210-216.	5.6	2
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77925	xmins:mml="http://www.w3.org/1998/Math/MathML" altimg="si0033.svg"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mn>1</mml:mn><mml:mover>Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 307 Td (accent="true" Li ₂ N ₂ Battery for Ammonia Synthesis and Computational Insight. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 19032-19042.	4.0	1
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