

# Special points for Brillouin-zone integrations

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Self-consistent numerical-basis-set linear-combination-of-atomic-orbitals model for the study of solids in the local density formalism. Physical Review B, 1977, 15, 4716-4737.	1.1	137
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12105	Adsorption of ammonia on vanadium-antimony mixed oxides. <i>Applied Surface Science</i> , 2012, 258, 3617-3623.	3.1	10
12106	Reaction mechanism for CO oxidation on Cu(311): A density functional theory study. <i>Applied Surface Science</i> , 2012, 258, 3980-3985.	3.1	7
12107	Nitric oxide adsorption on Nb(110) surface. <i>Applied Surface Science</i> , 2012, 258, 4428-4435.	3.1	10
12108	Tuning of CeO <sub>2</sub> buffer layers for coated superconductors through doping. <i>Applied Surface Science</i> , 2012, 260, 32-35.	3.1	29
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12141	Nanoporous PtCo and PtNi alloy ribbons for methanol electrooxidation. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 10489-10498.	3.8	125
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12998	Doping and temperature dependence of thermoelectric properties of AgGaTe <sub>2</sub> : First principles investigations. <i>Chemical Physics Letters</i> , 2012, 537, 62-64.	1.2	25
12999	Boron nitride substrate-induced reversible hydrogen storage in bilayer solid matrix via interlayer spacing. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 9677-9687.	3.8	13
13000	Structural, electronic and thermodynamic properties of Al- and Si-doped $\hat{1}\pm$ , $\hat{1}^3$ , and $\hat{1}^2$ -MgH <sub>2</sub> : Density functional and hybrid density functional calculations. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 9112-9122.	3.8	27
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13004	Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (111). <i>Journal of Catalysis</i> , 2012, 286, 88-94.	3.1	146
13005	Performance, structure, and mechanism of CeO <sub>2</sub> in HCl oxidation to Cl <sub>2</sub> . <i>Journal of Catalysis</i> , 2012, 286, 287-297.	3.1	185
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13007	Solvent effects in the hydrogenation of 2-butanone. <i>Journal of Catalysis</i> , 2012, 289, 30-41.	3.1	140
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13010	The electric double layer on graphite. <i>Electrochimica Acta</i> , 2012, 71, 82-85.	2.6	53
13011	Decomposition of methylamine on Mo(100) surface: A DFT study. <i>Journal of Natural Gas Chemistry</i> , 2012, 21, 132-137.	1.8	8
13012	Thermodynamic properties of (Mg,Fe <sub>2+</sub> )SiO <sub>3</sub> perovskite at the lower-mantle pressures and temperatures: an internally consistent LSDA+ <i>i</i> study. <i>Geophysical Journal International</i> , 2012, 190, 310-322.	1.0	40
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13014	Minimizing the Kohn-Sham total energy for periodic systems. <i>Linear Algebra and Its Applications</i> , 2012, 436, 2764-2779.	0.4	0

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13017	Visible-light photocatalytic activity of Ni-doped TiO <sub>2</sub> from ab initio calculations. <i>Materials Chemistry and Physics</i> , 2012, 133, 746-750.	2.0	35
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13023	Generalized stacking fault energy in magnesium alloys: Density functional theory calculations. <i>Scripta Materialia</i> , 2012, 66, 219-222.	2.6	157
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13041	Ab initio lattice dynamics and thermodynamic properties of SrO under pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2012, 73, 129-135.	1.9	25
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13147	Structural, electronic and vibrational properties of InN under high pressure. <i>Physica B: Condensed Matter</i> , 2012, 407, 1008-1013.	1.3	19
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13803	Shock-induced phase transformations in gallium single crystals by atomistic methods. <i>Physical Review B</i> , 2013, 88, .	1.1	15
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14006	DFT study of interaction of O, O <sub>2</sub> , and OH with unreconstructed Pt(hkl) (h, k, l = 0, 1) surfaces—similarities, differences, and universalities. <i>Russian Journal of Physical Chemistry A</i> , 2013, 87, 2214-2218.	0.1	7
14007	Lithium Adsorption on Hexagonal Boron Nitride Nanosheet Using Dispersion-Corrected Density Functional Theory Calculations. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 06GG08.	0.8	20
14008	First-principle calculations on the structural stability and electronic properties of superhard B <sub>x</sub> C <sub>y</sub> compounds. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 425502.	0.7	8
14009	Electronic and phononic properties of V <sub>2</sub> AlC via first principles. <i>Canadian Journal of Physics</i> , 2013, 91, 822-825.	0.4	5
14010	Design of Shallow Acceptors in GaN through Zinc—Magnium Codoping: First-Principles Calculation. <i>Applied Physics Express</i> , 2013, 6, 042104.	1.1	5
14011	Comparative study on the performance of exchange and correlation in wide-gap semiconductors: the case of BeS, BeSe, and BeTe. <i>Journal of Materials Science</i> , 2013, 48, 5499-5508.	1.7	6
14012	Semiconducting layered technetium dichalcogenides: insights from first-principles. <i>Dalton Transactions</i> , 2013, 42, 15288.	1.6	23
14013	Band structure, shape controllable synthesis and luminescence properties of the precursor and final product Lu <sub>6</sub> O <sub>5</sub> F <sub>8</sub> :Eu/Tb/Ce/Dy nano/microstructures. <i>Journal of Materials Chemistry C</i> , 2013, 1, 7952.	2.7	11
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14015	Formamide adsorption over the TiO <sub>2</sub> (110) surface: a theoretical study. <i>RSC Advances</i> , 2013, 3, 16829.	1.7	3
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14017	Strain effects on hydrogen storage in Ti decorated pyridinic N-doped graphene. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12757.	1.3	14
14018	Relative contributions of quantum and double layer capacitance to the supercapacitor performance of carbon nanotubes in an ionic liquid. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19741-19747.	1.3	68
14019	Room-temperature proton transport and its effect on thermopower in a solid ionic semiconductor, TTF <sub>2</sub> COONH <sub>4</sub> . <i>Journal of Materials Chemistry A</i> , 2013, 1, 5089.	5.2	5
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14021	Water and ammonia on Cu{110}: comparative structure and bonding. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4785.	1.3	14
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14029	A theoretical analysis of the role of defects in the adsorption of hydrogen sulfide on graphene. <i>AIP Advances</i> , 2013, 3, .	0.6	21
14030	Theoretical perspective of photocatalytic properties of single-layer $\text{SnS}_2$ . <i>Physical Review B</i> , 2013, 88, .	1.1	215
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14037	Stability and superconductivity of Ca-B phases at ambient and high pressure. <i>Physical Review B</i> , 2013, 88, .	1.1	32
14038	First-principles study of the structural, electronic, and optical properties of Y-doped $\text{SrSi}_2$ . <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	3
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14042	Molecular adsorption on silicon (001): A systematic evaluation of size effects in slab and cluster models. <i>AIP Advances</i> , 2013, 3, 042117.	0.6	13
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14053	Local surface structure effect on reactivity of molecules confined between metallic surfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1647-1654.	1.3	9
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14055	Phonon-mediated superconductivity in silicene predicted by first-principles density functional calculations. <i>Europhysics Letters</i> , 2013, 104, 36001.	0.7	55
14056	CO <sub>2</sub> capture properties of lithium silicates with different ratios of Li <sub>2</sub> O/SiO <sub>2</sub> : an ab initio thermodynamic and experimental approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13538.	1.3	100
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14060	Structural and electronic properties of $\text{Li}_8\text{ZrO}_6$ and its $\text{CO}_2$ capture capabilities: an ab initio thermodynamic approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9752.	1.3	36
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14078	Single-crystal adsorption calorimetry and density functional theory of CO chemisorption on fcc Co{110}. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4059.	1.3	20
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14083	Polymerization of nitrogen in lithium azide. <i>Journal of Chemical Physics</i> , 2013, 139, 164710.	1.2	69
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14086	Tuning the electronic and magnetic properties of zigzag silicene nanoribbons by edge hydrogenation and doping. <i>RSC Advances</i> , 2013, 3, 24075.	1.7	63
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14091	Ab initio and cluster expansion study of surface alloys of Fe and Au on Ru(0001) and Mo(110): Importance of magnetism. <i>Physical Review B</i> , 2013, 88, .	1.1	4
14092	Topological phase transitions in (Bi<math>x</math>Sb<math>1-x</math>)<math>2</math>Te<math>3</math>. <i>Physical Review B</i> , 2013, 88, .	1.1	45
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14117	Electronic changes at the Pt(111) interface induced by the adsorption of OH species. <i>Catalysis Today</i> , 2013, 202, 120-127.	2.2	9
14118	Inhibition of water dissociation on a pitted Pt(111) surface: First principles study. <i>Catalysis Today</i> , 2013, 202, 163-167.	2.2	9
14119	Modeling of the symmetry factor of electrochemical proton discharge via the Volmer reaction. <i>Catalysis Today</i> , 2013, 202, 168-174.	2.2	16
14120	Hydrogen oxidation on ordered intermetallic phases of platinum and tin - A combined experimental and theoretical study. <i>Catalysis Today</i> , 2013, 202, 191-196.	2.2	13
14121	Atomic ensemble effects on formic acid oxidation on PdAu electrode studied by first-principles calculations. <i>Journal of Power Sources</i> , 2013, 224, 241-249.	4.0	58
14122	Synthesis and crystal structure of Mg <sub>0.5</sub> NbO <sub>2</sub> : An ion-exchange reaction with Mg <sup>2+</sup> between trigonal [NbO <sub>2</sub> ] <sup>2-</sup> layers. <i>Journal of Solid State Chemistry</i> , 2013, 197, 471-474.	1.4	4
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14124	Hybrid functional calculation of electronic and phonon structure of BaSnO. <i>Journal of Solid State Chemistry</i> , 2013, 197, 134-138.	1.4	42
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14127	First-principle calculations of thermodynamic properties of ZrC and ZrN at high pressures and high temperatures. <i>Physica B: Condensed Matter</i> , 2013, 410, 57-62.	1.3	22
14128	Growth, properties and first-principles study of mid-IR nonlinear optical crystal LiInS <sub>2</sub> . <i>Journal of Crystal Growth</i> , 2013, 362, 271-275.	0.7	9
14129	Na-Si Clathrates Are High-Pressure Phases: A Melt-Based Route to Control Stoichiometry and Properties. <i>Crystal Growth and Design</i> , 2013, 13, 303-307.	1.4	75
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14133	First-principles calculations of vibrational and thermodynamical properties of rare-earth diborides. Computational Materials Science, 2013, 68, 307-313.	1.4	4
14134	Exfoliated graphene-supported Pt and Pt-based alloys as electrocatalysts for direct methanol fuel cells. Carbon, 2013, 52, 595-604.	5.4	117
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14146	Hydrogen Dissociation Catalyzed by Carbon-Coated Nickel Nanoparticles: Experiment and Theory. ChemPhysChem, 2013, 14, 381-385.	1.0	26
14147	Band offsets and heterostructures of two-dimensional semiconductors. Applied Physics Letters, 2013, 102, .	1.5	1,361
14148	Orthorhombic $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle A \langle /mml:mi \rangle B \langle /mml:mi \rangle C \langle /mml:mi \rangle \langle /mml:math \rangle$ Semiconductors as Antiferroelectrics. Physical Review Letters, 2013, 110, 017603.	2.9	59



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14150	Formation and structure of inhibitive molecular film of imidazole on iron surface. <i>Corrosion Science</i> , 2013, 68, 195-203.	3.0	87
14151	Synthesis and Structure Determination of CaSi <sub>1/3</sub> B <sub>2/3</sub> O <sub>8/3</sub> : A New Calcium Borosilicate. <i>Inorganic Chemistry</i> , 2013, 52, 4250-4258.	1.9	31
14152	Method of preparation and thermodynamic properties of transparent Y <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> nanoceramics. <i>Journal of Thermal Analysis and Calorimetry</i> , 2013, 111, 289-294.	2.0	5
14153	<i>Ab initio</i> study of edge effect on relative motion of walls in carbon nanotubes. <i>Journal of Chemical Physics</i> , 2013, 138, 024703.	1.2	22
14154	The role of van der Waals forces in water adsorption on metals. <i>Journal of Chemical Physics</i> , 2013, 138, 024708.	1.2	173
14155	Comparative studies on total energetics of nonequivalent hexagonal polytypes for group IV semiconductors and group III nitrides. <i>Journal of Materials Research</i> , 2013, 28, 7-16.	1.2	5
14156	Dissociation and reconstruction of O <sub>2</sub> on Al (111) studied by First-principles. <i>Applied Surface Science</i> , 2013, 264, 247-254.	3.1	15
14157	Formation of n-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations. <i>Journal of Catalysis</i> , 2013, 299, 146-149.	3.1	10
14158	A density functional theory study of CO oxidation on Pd-Ni alloy with sandwich structure. <i>Applied Catalysis A: General</i> , 2013, 451, 79-85.	2.2	35
14159	Structural and elastic properties of ternary metal nitrides TixTa <sub>1-x</sub> N alloys: First-principles calculations versus experiments. <i>Surface and Coatings Technology</i> , 2013, 215, 199-208.	2.2	39
14160	Structure, hydrogen bond network and proton conductivity of new benzimidazole compounds with dicarboxylic acids. <i>CrystEngComm</i> , 2013, 15, 1950.	1.3	30
14161	The electronic and optical properties of MB <sub>12</sub> (M = Zr, Hf, Y, Lu) dodecaboride compounds. <i>Physica Scripta</i> , 2013, 87, 015702.	1.2	6
14162	Structural, elastic and electronic properties of equiatomic PtTi as potential high-temperature shape memory alloy. <i>Intermetallics</i> , 2013, 33, 27-32.	1.8	37
14163	Structural, magnetic, multiferroic and electronic properties of Sr <sub>2</sub> ZrMnO <sub>6</sub> double perovskite. <i>Journal of Molecular Structure</i> , 2013, 1034, 233-237.	1.8	19
14164	Trivalent Actinide and Lanthanide Complexation of 5,6-Dialkyl-2,6-bis(1,2,4-triazin-3-yl)pyridine (RBTP; R =) <i>Tj ETQq1 1 0.784314 rgBT</i> <i>Inorganic Chemistry</i> , 2013, 52, 761-776.	1.9	18
14165	N- and Mo-doping Bi <sub>2</sub> WO <sub>6</sub> in photocatalytic water splitting. <i>Computational Materials Science</i> , 2013, 67, 88-92.	1.4	39
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14169	First-principles studies on lattice constants and local lattice distortions in solid solution aluminum alloys. <i>Computational Materials Science</i> , 2013, 67, 1-10.	1.4	121
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14171	Band gap change induced by defect complexes in Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>Thin Solid Films</i> , 2013, 535, 265-269.	0.8	91
14172	Ab initio study of ZnCoO diluted magnetic semiconductor and its magnetic properties. <i>Journal of Alloys and Compounds</i> , 2013, 551, 306-311.	2.8	19
14173	Electronic, elastic, thermodynamic properties and structure disorder of $\hat{\Gamma}^3$ -AlON solid solution from ab initio calculations. <i>Journal of Alloys and Compounds</i> , 2013, 548, 228-234.	2.8	14
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14175	Structural phase transition of CdTe: an ab initio study. <i>Journal of Molecular Modeling</i> , 2013, 19, 421-426.	0.8	3
14176	The Oxygen Reduction Reaction on Nitrogen-Doped Graphene. <i>Catalysis Letters</i> , 2013, 143, 58-60.	1.4	69
14177	Electronic and optical properties of (Al <sub>x</sub> Ga <sub>1-x</sub> ) <sub>1-y</sub> Mn <sub>y</sub> As single crystal: a new candidate for integrated optical isolators and spintronics. <i>Journal of Materials Science</i> , 2013, 48, 758-764.	1.7	11
14178	The effect of the phase transition on the elasticity of cubic platinum carbide. <i>Journal of Materials Science</i> , 2013, 48, 1660-1668.	1.7	4
14179	P-type reduced graphene oxide membranes induced by iodine doping. <i>Journal of Materials Science</i> , 2013, 48, 2284-2289.	1.7	28
14180	Pb <sub>2</sub> B <sub>5</sub> O <sub>9</sub> Cl: a chloride borate with second harmonic generation effect. <i>Journal of Materials Science</i> , 2013, 48, 2590-2596.	1.7	33
14181	Electronic and Phonon Structures of BaFe <sub>2</sub> As <sub>2</sub> Superconductor by Ab-initio Density Functional Theory. <i>Journal of Superconductivity and Novel Magnetism</i> , 2013, 26, 93-100.	0.8	10
14182	Mechanism of Alcohol–Water Separation in Metal–Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4124-4130.	1.5	33
14183	Electric-Field Dependence of the Effective Dielectric Constant in Graphene. <i>Nano Letters</i> , 2013, 13, 898-902.	4.5	181
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14188	Ab Initio Based conformational study of the crystalline $\alpha$ -chitin. Biopolymers, 2013, 99, 22-34.	1.2	27
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14192	First principles calculation of electronic structure, chemical bonding and elastic properties of ultra-incompressible Re <sub>2</sub> P. Transactions of Nonferrous Metals Society of China, 2013, 23, 3400-3404.	1.7	2
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14213	Energetic and structural analysis of N <sub>2</sub> H <sub>4</sub> BH <sub>3</sub> inorganic solid and its modified material for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 6718-6725.	3.8	7
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14220	Theoretical study on optoelectronic properties of Ga <sub>0.75</sub> Al <sub>0.25</sub> N (001) reconstruction surfaces. <i>Applied Surface Science</i> , 2013, 287, 1-7.	3.1	5

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14226	Interactions of lead with carboxyl and hydroxyl-decorated(10, 0) single-walled carbon nanotubes: First-principle calculations. <i>Applied Surface Science</i> , 2013, 285, 198-204.	3.1	12
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14235	The electronic and optical properties of Cu doped CdI <sub>2</sub> . <i>Optik</i> , 2013, 124, 3230-3234.	1.4	6
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14277	Knock-on damage in bilayer graphene: Indications for a catalytic pathway. <i>Physical Review B</i> , 2013, 88, .	1.1	19
14278	Insights into the atomic and electronic structure triggered by ordered nitrogen vacancies in CrN. <i>Physical Review B</i> , 2013, 87, .	1.1	22
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14280	Free energies of (Co, Fe, Ni, Zn)Fe <sub>2</sub> O <sub>4</sub> spinels and oxides in water at high temperatures and pressure from density functional theory: results for stoichiometric NiO and NiFe <sub>2</sub> O <sub>4</sub> surfaces. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 445008.	1.1	53
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14869	Manipulation of surface energy anisotropy in iron using surface segregation of phosphorus: An atomistic simulation. <i>Scripta Materialia</i> , 2013, 68, 329-332.	2.6	13



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14870	Magnetic behavior of (MnN) <sub>1</sub> /(AlN) <sub>1</sub> , (MnN) <sub>1</sub> /(GaN) <sub>1</sub> , and (MnN) <sub>1</sub> /(InN) <sub>1</sub> superlattices. <i>Superlattices and Microstructures</i> , 2013, 53, 16-23.	1.4	10
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14883	Digitized Charge Transfer Magnitude Determined by Metal-Organic Coordination Number. <i>ACS Nano</i> , 2013, 7, 2814-2819.	7.3	36
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17405	Methanol synthesis by CO and CO <sub>2</sub> hydrogenation on Cu/Al <sub>2</sub> O <sub>3</sub> surface in liquid paraffin solution. <i>Applied Surface Science</i> , 2014, 290, 398-404.	3.1	25
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17409	Ab initio calculations of mechanical stability of bcc Cu under pressure. <i>Solid State Communications</i> , 2014, 184, 25-28.	0.9	4
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24051	Quantitative and Atomic-Scale View of CO-Induced Pt Nanoparticle Surface Reconstruction at Saturation Coverage via DFT Calculations Coupled with <i>in Situ</i> TEM and IR. <i>Journal of the American Chemical Society</i> , 2017, 139, 4551-4558.	6.6	186
24052	To address surface reaction network complexity using scaling relations machine learning and DFT calculations. <i>Nature Communications</i> , 2017, 8, 14621.	5.8	399
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24876	In situ intercalation polymerization approach to polyamide-6/graphite nanoflakes for enhanced thermal conductivity. <i>Composites Part B: Engineering</i> , 2017, 117, 165-173.	5.9	92
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25020	Graphene-family nanomaterials assembled with cobalt oxides and cobalt nanoparticles as hybrid supercapacitive electrodes and enzymeless glucose detection platforms. <i>Journal of Materials Research</i> , 2017, 32, 301-322.	1.2	25
25021	A new carbon allotrope: Penta-graphene as a metal-free catalyst for CO oxidation. <i>Carbon</i> , 2017, 114, 465-472.	5.4	91
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25031	The work function of few-layer graphene. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 035003.	0.7	56
25032	From Active Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation. <i>ChemCatChem</i> , 2017, 9, 1594-1600.	1.8	15
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25036	The influence of carbon on the seismic properties of solid iron. <i>Geophysical Research Letters</i> , 2017, 44, 128-134.	1.5	15
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25038	Hydrodeoxygenation of acrylic acid using Mo <sub>2</sub> C/Al <sub>2</sub> O <sub>3</sub> . <i>Applied Catalysis A: General</i> , 2017, 531, 69-78.	2.2	22
25039	Mechanistic study for enhanced CO oxidation activity on (Mn,Fe) co-doped CeO <sub>2</sub> (111). <i>Catalysis Today</i> , 2017, 293-294, 82-88.	2.2	32
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25042	A first-principles study of Sc-decorated graphene with pyridinic-N defects for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 3106-3113.	3.8	47
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25055	BN-schwarzite: novel boron nitride spongy crystals. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1167-1173.	1.3	8
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25100	Partial-Redox-Promoted Mn Cycling of Mn(II)-Doped Heterogeneous Catalyst for Efficient H <sub>2</sub> O <sub>2</sub> -Mediated Oxidation. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 371-380.	4.0	31
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26882	The intrinsic interface properties of the top and edge 1T/2H <i>MoS</i> <sub>2</sub> contact: A first-principles study. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	19
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26886	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 16911-16917.	4.0	25
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26888	Metal-organic framework-derived integrated nanoarrays for overall water splitting. <i>Journal of Materials Chemistry A</i> , 2018, 6, 9009-9018.	5.2	74
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26893	Unveiling Hidden Catalysts for the Oxidative Coupling of Methane based on Combining Machine Learning with Literature Data. <i>ChemCatChem</i> , 2018, 10, 3223-3228.	1.8	62
26894	Combined DFT and Differential Electrochemical Mass Spectrometry Investigation of the Effect of Dopants in Secondary Zinc-Air Batteries. <i>ChemSusChem</i> , 2018, 11, 1933-1941.	3.6	23
26895	Planar metallic carbon allotrope from graphene-like nanoribbons. <i>Carbon</i> , 2018, 135, 21-28.	5.4	55
26896	<i>Beryllium-Free Nonlinear-Optical Crystals</i> A <sub>3</sub> Ba <sub>3</sub> Li <sub>2</sub> Ga <sub>4</sub> B <sub>6</sub> O <sub>20</sub> F (A = K) Tj ETQq1 1 0.784314 rgB	1.9	23
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27150	A photoemission moments model using density functional and transfer matrix methods applied to coating layers on surfaces: Theory. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	15
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27999	Elastic properties and plastic deformation of TiC- and VC-based pseudobinary alloys. <i>Acta Materialia</i> , 2018, 144, 376-385.	3.8	45
28000	Protomene: A new carbon allotrope. <i>Carbon</i> , 2018, 126, 574-579.	5.4	28
28001	First-Principles Study of MoO <sub>3</sub> /Graphene Composite as Cathode Material for High-Performance Lithium-Ion Batteries. <i>Applied Surface Science</i> , 2018, 433, 1083-1093.	3.1	27
28002	Thermoelectric power factor of La <sub>0.9</sub> M <sub>0.1</sub> FeO <sub>3</sub> (M=Ca and Ba) system: Structural, band gap and electrical transport evaluations. <i>Physica B: Condensed Matter</i> , 2018, 529, 1-8.	1.3	13
28003	Electronic and Magnetic Investigations of Rare-Earth Tm-doped AlGa <sub>N</sub> Ternary Alloy. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 1767-1771.	0.8	28
28004	Reaction mechanism for oxygen evolution on RuO <sub>2</sub> , IrO <sub>2</sub> , and RuO <sub>2</sub> @IrO <sub>2</sub> core-shell nanocatalysts. <i>Journal of Electroanalytical Chemistry</i> , 2018, 819, 296-305.	1.9	141
28005	Structural, electronic, elastic, vibrational and thermodynamic properties of U <sub>3</sub> Si <sub>2</sub> : A comprehensive study using DFT. <i>Journal of Alloys and Compounds</i> , 2018, 732, 160-166.	2.8	35
28006	Strengthening mechanism of aluminum on elastic properties of NbVTiZr high-entropy alloys. <i>Intermetallics</i> , 2018, 92, 7-14.	1.8	44
28007	Structural, elastic, electronic and vibrational properties of BaRh <sub>2</sub> P <sub>2</sub> and SrIr <sub>2</sub> As <sub>2</sub> superconductors: A DFT study. <i>Journal of Alloys and Compounds</i> , 2018, 740, 754-765.	2.8	27
28008	First-principles study of mechanical, thermodynamic, transport and superconducting properties of Sr <sub>3</sub> SnO. <i>Journal of Alloys and Compounds</i> , 2018, 730, 279-283.	2.8	18
28009	Elucidating the unintentional p-type nature of spinel Co <sub>3</sub> O <sub>4</sub> : A defect study using ab-initio calculation. <i>Journal of the European Ceramic Society</i> , 2018, 38, 629-635.	2.8	10
28010	Strained noble metal di chalcogenides PtX <sub>2</sub> (X = S, Se) mono-layer: Ab initio study of electronic and lattice dynamic properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 139-143.	1.3	16
28011	Electronic and optical properties of ultra-thin 2D tungsten disulfide for photovoltaic applications. <i>Solar Energy Materials and Solar Cells</i> , 2018, 174, 370-379.	3.0	80
28012	High Temperature Stability of BaZrO <sub>3</sub> : An Ab Initio Thermodynamic Study. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700398.	0.7	4
28013	Analytical modeling of electron energy loss spectroscopy of graphene: Ab initio study versus extended hydrodynamic model. <i>Ultramicroscopy</i> , 2018, 184, 134-142.	0.8	13
28014	Honeycomb BeO monolayer on the Mo(112) surface: LEED and DFT study. <i>Applied Surface Science</i> , 2018, 428, 815-818.	3.1	17
28015	A new insight into the theoretical design of highly dispersed and stable ceria supported metal nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2018, 512, 775-783.	5.0	8



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28017	Electronic structure and H <sub>2</sub> S adsorption property of Pt <sub>3</sub> cluster decorated (8, 0) SWCNT. <i>Applied Surface Science</i> , 2018, 428, 82-88.	3.1	30
28018	Adsorption and reaction of CO and H <sub>2</sub> O on WC(0001) surface: A first-principles investigation. <i>Applied Surface Science</i> , 2018, 428, 579-585.	3.1	8
28019	Computational study of Mn-doped GaN polar and non-polar surfaces. <i>Computational Materials Science</i> , 2018, 141, 68-74.	1.4	8
28020	The grain refinement performance of B-doped TiC on Zr-containing Al alloys. <i>Journal of Alloys and Compounds</i> , 2018, 731, 774-783.	2.8	22
28021	First-Principles Study of Pressure Dependence of Optical Spectra of MnS. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 1643-1647.	0.8	11
28022	Ferromagnetism and Half-Metallicity in a High-Band-Gap Hexagonal Boron Nitride System. <i>ChemPhysChem</i> , 2018, 19, 153-161.	1.0	10
28023	Defect structure of oxygen-vacancy clusters in O <sub>18</sub> and self ion implanted Fe(100) crystal by ion channeling and ab-initio study. <i>Acta Materialia</i> , 2018, 143, 198-204.	3.8	2
28024	Adsorption of bentazon on CAT and CARBOPAL activated carbon: Experimental and computational study. <i>Applied Surface Science</i> , 2018, 433, 487-501.	3.1	9
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28026	High-pressure phase transition and thermodynamic properties from first-principles calculations: Application to cubic copper iodide. <i>Materials Chemistry and Physics</i> , 2018, 203, 362-373.	2.0	15
28027	First-principles investigation of graphitic carbon nitride monolayer with embedded Fe atom. <i>Surface Science</i> , 2018, 667, 112-120.	0.8	20
28028	Effects of an electric field on the adsorption of water molecules on the Cd(0001) surface. <i>Surface Science</i> , 2018, 668, 1-6.	0.8	3
28029	Theoretical investigations of group IV alloys in the Lonsdaleite phase. <i>Journal of Materials Science</i> , 2018, 53, 2785-2801.	1.7	31
28030	Structure and transport properties of AgI-AgCl-CsCl glasses: molecular dynamics study. <i>Ionics</i> , 2018, 24, 1371-1376.	1.2	6
28031	Formation of carbon composite structures on the Ge(110) surfaces. <i>Current Applied Physics</i> , 2018, 18, 96-101.	1.1	2
28032	Chromium-vacancy clusters in dilute bcc Fe-Cr alloys: An ab initio study. <i>Journal of Nuclear Materials</i> , 2018, 499, 613-621.	1.3	12
28033	A DFT study for adsorption of CO on Ni, Pd and Pt atoms doped (7, 0) boron nitride nanotube. <i>Molecular Physics</i> , 2018, 116, 204-211.	0.8	10

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28035	A novel aluminum dual-ion battery. <i>Energy Storage Materials</i> , 2018, 11, 91-99.	9.5	123
28036	First-principles study of the electronic transport properties of a 1,3-diazabicyclo[3.1.0]hex-3-ene molecular optical switch. <i>Optik</i> , 2018, 153, 135-143.	1.4	14
28037	Molecular-level insights into mercury removal mechanism by pyrite. <i>Journal of Hazardous Materials</i> , 2018, 344, 104-112.	6.5	138
28038	The role of the anionic and cationic pt sites in the adsorption site preference of water and ethanol on defected Pt <sub>4</sub> /Pt(111) substrates: A density functional theory investigation within the D3 van der waals corrections. <i>Surface Science</i> , 2018, 667, 84-91.	0.8	6
28039	Band structure and optical properties of polyaniline polymer material. <i>Polymer Bulletin</i> , 2018, 75, 3023-3033.	1.7	36
28040	Doped phosphorene for hydrogen capture: A DFT study. <i>Applied Surface Science</i> , 2018, 433, 249-255.	3.1	48
28041	Oxygen vacancy chain and conductive filament formation in hafnia. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	34
28042	Physical Properties of Superhard Diamond-Like BC <sub>5</sub> from a First-Principles Study. <i>Journal of Electronic Materials</i> , 2018, 47, 272-284.	1.0	5
28043	Simultaneous Detection and Removal of Formaldehyde at Room Temperature: Janus Au@ZnO@ZIF-8 Nanoparticles. <i>Nano-Micro Letters</i> , 2018, 10, 4.	14.4	84
28044	Layered heterostructures based on graphene, hexagonal zinc oxide and molybdenum disulfide: Modeling of geometry and electronic properties. <i>Computational Materials Science</i> , 2018, 142, 32-37.	1.4	7
28045	Magnetic behavior study of samarium nitride using density functional theory. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 448, 186-191.	1.0	11
28046	Defect pair formation in fluorine and nitrogen codoped TiO <sub>2</sub> . <i>Journal of Applied Physics</i> , 2018, 123, 161510.	1.1	9
28047	Accurate Bandgap of Zr x Al <sup>1-x</sup> N Using Modified Becke-Johnson (mBJ) Exchange Potential. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 1545-1548.	0.8	1
28048	Anion-Codoped Monolayer MoS <sub>2</sub> for Visible Light Photocatalysis. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700413.	0.7	9
28049	Ab Initio Investigation on Electronic, Magnetic, Mechanical, and Thermodynamic Properties of AMO <sub>3</sub> (A) Tj ETQq1 1,0,784314 rgBT /Ov	0,8	14
28050	Effects of dopant separation on electronic states and magnetism in monolayer MoS <sub>2</sub> . <i>Applied Surface Science</i> , 2018, 428, 226-232.	3.1	16
28051	DFT study on the interaction of TiO <sub>2</sub> (001) surface with HCHO molecules. <i>Applied Surface Science</i> , 2018, 428, 954-963.	3.1	25

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28053	DFT study on structural, electronic, and optical properties of cubic and monoclinic CuO. <i>Journal of Computational Electronics</i> , 2018, 17, 21-28.	1.3	29
28054	Asymmetric hydrogenation-induced ferromagnetism in stanene nanoribbons considering electric field and strain effects. <i>Journal of Materials Science</i> , 2018, 53, 657-666.	1.7	3
28055	Electronic structure and relative stability of the coherent and semi-coherent HfO <sub>2</sub> /III-V interfaces. <i>Applied Surface Science</i> , 2018, 427, 243-252.	3.1	6
28056	Density functional theory calculations of biomolecules adsorption on phosphorene for biomedical applications. <i>Applied Surface Science</i> , 2018, 427, 1227-1234.	3.1	32
28057	Stability enhancement and electronic tunability of two-dimensional SbIV compounds via surface functionalization. <i>Applied Surface Science</i> , 2018, 427, 363-368.	3.1	8
28058	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. <i>Applied Surface Science</i> , 2018, 427, 609-612.	3.1	79
28059	Electronic structure and optical properties of BiOI {001} monolayer under biaxial strain. <i>Journal of Materials Science</i> , 2018, 53, 708-715.	1.7	9
28060	First-principles calculations of high-pressure iron-bearing monoclinic dolomite and single-cation carbonates with internally consistent Hubbard U. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 293-302.	0.3	11
28061	The location of excess electrons on H <sub>2</sub> O/TiO <sub>2</sub> (110) surface and its role in the surface reactions. <i>Molecular Physics</i> , 2018, 116, 171-178.	0.8	7
28062	Underpotential deposition and involved alloy formation of cadmium on silver particles modified HOPG substrates. <i>Journal of Solid State Electrochemistry</i> , 2018, 22, 193-202.	1.2	2
28063	Theoretical investigation of thermoelectric and elastic properties of intermetallic compounds ScTM (TM = Cu, Ag, Au and Pd). <i>International Journal of Modern Physics B</i> , 2018, 32, 1850004.	1.0	7
28064	Theoretical and experimental investigations of mercury adsorption on hematite surfaces. <i>Journal of the Air and Waste Management Association</i> , 2018, 68, 39-53.	0.9	13
28065	Electronic structure and thermoelectric properties of narrow-band-gap intermetallic compound Al <sub>2</sub> Fe <sub>3</sub> Si <sub>3</sub> . <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 131, 281-287.	2.0	20
28066	Ab Initio Prediction of the Structural, Electronic, Elastic, and Thermoelectric Properties of Half-Heusler Ternary Compounds TiIrX (X=As and Sb). <i>Journal of Electronic Materials</i> , 2018, 47, 196-204.	1.0	25
28067	High-metallic-phase-concentration Mo <sub>1-x</sub> W <sub>x</sub> S <sub>2</sub> nanosheets with expanded interlayers as efficient electrocatalysts. <i>Nano Research</i> , 2018, 11, 1687-1698.	5.8	37
28068	Influences of Electrode Potential on Mechanism of Oxygen Reduction Reaction on Pd-Skin/Pd <sub>3</sub> Fe(111) Electrocatalyst: Insights from DFT-Based Calculations. <i>Electrocatalysis</i> , 2018, 9, 10-21.	1.5	4
28069	Efficient defect-controlled photocatalytic hydrogen generation based on near-infrared Cu-In-Zn-S quantum dots. <i>Nano Research</i> , 2018, 11, 1379-1388.	5.8	41

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28071	Theoretical Evidence behind Bifunctional Catalytic Activity in Pristine and Functionalized Al <sub>2</sub> C Monolayers. <i>ChemPhysChem</i> , 2018, 19, 148-152.	1.0	11
28072	Electrical contacts in monolayer blue phosphorene devices. <i>Nano Research</i> , 2018, 11, 1834-1849.	5.8	55
28073	Elastic properties and thermal expansion of lead-free halide double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . <i>Computational Materials Science</i> , 2018, 141, 49-58.	1.4	87
28074	Understanding the synergistic effects, optical and electronic properties of ternary Fe/C/S-doped TiO <sub>2</sub> anatase within the DFT + U approach. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25505.	1.0	12
28075	Self-supported CoMoS <sub>4</sub> nanosheet array as an efficient catalyst for hydrogen evolution reaction at neutral pH. <i>Nano Research</i> , 2018, 11, 2024-2033.	5.8	147
28076	DFT study on the adsorption sensitivity of graphane doped with Cr and Mn toward H <sub>2</sub> CO molecule. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 16-21.	1.3	35
28077	Atomic and molecular adsorption on Fe(110). <i>Surface Science</i> , 2018, 667, 54-65.	0.8	49
28078	Phase transformations in the relaxor Na <sub>1/2</sub> Bi <sub>1/2</sub> TiO <sub>3</sub> studied by means of density functional theory calculations. <i>Journal of the American Ceramic Society</i> , 2018, 101, 472-482.	1.9	10
28079	Investigation of the structural and electronic properties of CdS under high pressure: an ab initio study. <i>Canadian Journal of Physics</i> , 2018, 96, 216-224.	0.4	20
28080	Comparison of standard DFT and Hubbard-DFT methods in structural and electronic properties of TiO <sub>2</sub> polymorphs and H-titanate ultrathin sheets for DSSC application. <i>Applied Surface Science</i> , 2018, 428, 118-123.	3.1	50
28081	Effects of alloying elements on relative phase stability and elastic properties of L12 Co <sub>3</sub> V from first-principles calculations. <i>Journal of Materials Science</i> , 2018, 53, 1204-1216.	1.7	8
28082	First-Principle Predictions of Electronic Properties and Half-Metallic Ferromagnetism in Vanadium-Doped Rock-Salt SrO. <i>Journal of Electronic Materials</i> , 2018, 47, 449-456.	1.0	27
28083	Phase stability, elastic, anisotropic properties, lattice dynamical and thermodynamic properties of B12M (M=Th, U, Np, Pu) dodecaborides. <i>Ceramics International</i> , 2018, 44, 128-135.	2.3	33
28084	Adsorption characteristics of DNA nucleobases, aromatic amino acids and heterocyclic molecules on silicene and germanene monolayers. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2713-2720.	4.0	56
28085	Effect of tetravalent dopants on hematite nanostructure for enhanced photoelectrochemical water splitting. <i>Applied Surface Science</i> , 2018, 427, 1203-1212.	3.1	51
28086	Enhanced catalytic performance by oxygen vacancy and active interface originated from facile reduction of OMS-2. <i>Chemical Engineering Journal</i> , 2018, 331, 626-635.	6.6	100
28087	Insights into the photocatalytic mechanism of mediator-free direct Z-scheme g-C <sub>3</sub> N <sub>4</sub> /Bi <sub>2</sub> MoO <sub>6</sub> (010) and g-C <sub>3</sub> N <sub>4</sub> /Bi <sub>2</sub> WO <sub>6</sub> (010) heterostructures: A hybrid density functional theory study. <i>Applied Surface Science</i> , 2018, 427, 487-498.	3.1	125

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28089	Controlling phenolic hydrodeoxygenation by tailoring metal–O bond strength via specific catalyst metal type and particle size selection. <i>Comptes Rendus Chimie</i> , 2018, 21, 155-163.	0.2	30
28090	Predicted MAX Phase $\text{Sc}_2\text{InC}$ : Dynamical Stability, Vibrational and Optical Properties. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700235.	0.7	39
28091	Combined theoretical and experimental study on alcoholysis of amides on $\text{CeO}_2$ surface: A catalytic interplay between Lewis acid and base sites. <i>Catalysis Today</i> , 2018, 303, 256-262.	2.2	13
28092	$\text{CH}_4$ dissociation in the early stage of graphene growth on $\text{Fe}/\text{Cu}(100)$ surface: Theoretical insights. <i>Applied Surface Science</i> , 2018, 427, 953-960.	3.1	11
28093	Sodium storage mechanism of N, S co-doped nanoporous carbon: Experimental design and theoretical evaluation. <i>Energy Storage Materials</i> , 2018, 11, 274-281.	9.5	112
28094	Initial Stages in the Formation of Nickel Phosphides. <i>Journal of Physical Chemistry B</i> , 2018, 122, 672-678.	1.2	12
28095	Synthesis and characterization of rhodium nanoclusters on $\text{TiO}_2(110)$ surface using organometallic compounds. <i>Surface Science</i> , 2018, 667, 38-44.	0.8	2
28096	New Polymorph Form of Dexamethasone Acetate. <i>Journal of Pharmaceutical Sciences</i> , 2018, 107, 672-681.	1.6	8
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28098	High Lithium Insertion Voltage Single-Crystal $\text{Hf}_2\text{Ti}_{12}\text{O}_{25}$ Nanorods as a High-Capacity and High-Rate Lithium-Ion Battery Anode Material. <i>ChemSusChem</i> , 2018, 11, 299-310.	3.6	18
28099	Substitution behavior of Si atoms in the $\text{Ti}_2\text{AlC}$ ceramics. <i>Acta Materialia</i> , 2018, 144, 543-551.	3.8	26
28100	Role of the X and n factors in ion-irradiation induced phase transformations of $\text{Mn}_n\text{AlX}_n$ phases. <i>Acta Materialia</i> , 2018, 144, 432-446.	3.8	21
28101	Fluorine-graphite intercalation compound $(\text{C}_4\text{F})_n$ at high pressure: Experimental and theoretical study. <i>Carbon</i> , 2018, 127, 384-391.	5.4	12
28102	Efficient hydrogen evolution electrocatalysis in alkaline medium using Pd-modified zeolite X. <i>Electrochimica Acta</i> , 2018, 259, 882-892.	2.6	27
28103	Equilibrium nickel isotope fractionation in nickel sulfide minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 222, 1-16.	1.6	24
28104	Variation of the $z$ factor of $\text{SnSe}$ with doping: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2018, 732, 536-546.	2.8	9
28105	Prediction of novel stable Fe-V-Si ternary phase. <i>Journal of Alloys and Compounds</i> , 2018, 732, 567-572.	2.8	4

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28106	Search for New Half-Metallic Ferromagnets in Quaternary Diamond-Like Compounds $II_2IV_2VI_4$ and $II_2IV_2VI_4$ (I = Cu; II = Mn, Fe, Co; III = In; IV = Ge, Sn; VI = S, Se, Te). <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 1941-1947.	0.8	18
28107	Adsorption of alkylamine cations on montmorillonite (001) surface: A density functional theory study. <i>Applied Clay Science</i> , 2018, 152, 249-258.	2.6	47
28108	Mechanistic insight into the synergetic catalytic effect of Pd and MnO <sub>2</sub> for high-performance Li-O <sub>2</sub> cells. <i>Energy Storage Materials</i> , 2018, 12, 8-16.	9.5	23
28109	Electronic and magnetic behavior of transition metal-doped cubic gallium nitride: first-principles calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 451, 295-299.	1.0	10
28110	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
28111	Morphological Changes in Electrografted Aryl-Based Thin Films Induced by using Diazonium Salts or Aryl Iodides. <i>ChemElectroChem</i> , 2018, 5, 464-470.	1.7	7
28112	Ab-initio study of electronic and elastic properties of Mg(BH <sub>4</sub> )(NH <sub>2</sub> ) complex hydride. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 1587-1595.	3.8	3
28113	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
28114	Discovery of 2D Anisotropic Dirac Cones. <i>Advanced Materials</i> , 2018, 30, 1704025.	11.1	91
28115	Hydrostatic pressure and temperature effect on the Raman spectra of the molecular crystal 2-amine-1,3,4-thiadiazole. <i>Journal of Molecular Structure</i> , 2018, 1156, 127-135.	1.8	4
28116	Ab initio study of structural and electronic properties of copper and nickel tungstate. <i>Computational Materials Science</i> , 2018, 143, 301-307.	1.4	9
28117	Effect of the Mechanism of H <sub>2</sub> S on Elemental Mercury Removal Using the MnO <sub>2</sub> Sorbent during Coal Gasification. <i>Energy &amp; Fuels</i> , 2018, 32, 4453-4460.	2.5	44
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28119	Theoretical study of the structural and electronic properties of novel stanene-based buckled nanotubes and their adsorption behaviors. <i>Applied Surface Science</i> , 2018, 435, 733-742.	3.1	22
28120	Dislocation nucleation facilitated by atomic segregation. <i>Nature Materials</i> , 2018, 17, 56-63.	13.3	99
28121	A first-principles study on the interaction of biogas with noble metal (Rh, Pt, Pd) decorated nitrogen doped graphene as a gas sensor: A DFT study. <i>Applied Surface Science</i> , 2018, 435, 1199-1212.	3.1	66
28122	Water dissociation and CO oxidation over Au/anatase catalyst. A DFT-D2 study. <i>Applied Surface Science</i> , 2018, 435, 1168-1173.	3.1	10
28123	Revisiting intrinsic brittleness and deformation behavior of B <sub>2</sub> NiAl intermetallic compound: A first-principles study. <i>Journal of Materials Science and Technology</i> , 2018, 34, 620-626.	5.6	16

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28124	Pressure effect of magnetic and electronic properties of Mn <sub>2</sub> PtGa Heusler alloy. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 224-230.	0.9	9
28125	Stress and strain effects on the electronic structure and optical properties of ScN monolayer. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 339-345.	0.9	22
28126	Origin of enhanced Brønsted acidity of NiF-modified synthetic mica montmorillonite clay. <i>Catalysis Science and Technology</i> , 2018, 8, 244-251.	2.1	8
28127	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
28128	Jacob's Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 395-403.	2.3	60
28129	Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS(001), (011), and (111) Surfaces: A Dispersion-Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 359-370.	1.5	24
28130	Co-doped phosphorene: Enhanced sensitivity of CO gas sensing. <i>International Journal of Modern Physics B</i> , 2018, 32, 1850068.	1.0	10
28131	Mapping the relationship among composition, stacking fault energy and ductility in Nb alloys: A first-principles study. <i>Acta Materialia</i> , 2018, 144, 853-861.	3.8	32
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28133	Influence of nearest neighbor atoms and coordination polyhedron on atomic volume of sigma phases. <i>Computational Materials Science</i> , 2018, 143, 308-315.	1.4	3
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29246	Theoretical and experimental evidences of defects in LiMgPO <sub>4</sub> . <i>Journal of Alloys and Compounds</i> , 2018, 766, 626-636.	2.8	27
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29261	Calculation of strained BaTiO <sub>3</sub> with different exchange correlation functionals examined with criterion by Ginzburg-Landau theory, uncovering expressions by crystallographic parameters. <i>Journal of Chemical Physics</i> , 2018, 148, 194702.	1.2	9
29262	A DFT perspective analysis of optical properties of defected germanene mono-layer. <i>Physical Sciences Reviews</i> , 2018, 3, .	0.8	1
29263	Probing Quantum Confinement and Electronic Structure at Polar Oxide Interfaces. <i>Advanced Science</i> , 2018, 5, 1800242.	5.6	9
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29266	Electronic and mechanical properties of MgN compound: Prediction of stable half-metallic ferromagnet in NaCl and ZB phases. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 466, 28-37.	1.0	5
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29268	Pure CO <sub>2</sub> electrolysis over an Ni/YSZ cathode in a solid oxide electrolysis cell. <i>Journal of Materials Chemistry A</i> , 2018, 6, 13661-13667.	5.2	77
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29271	Pressure-Induced Sublattice Disorder in SnO <sub>2</sub> : Invasive Selective Percolation. <i>Physical Review Letters</i> , 2018, 120, 265702.	2.9	11
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29275	Ab-initio based search for late blooming phase compositions in iron alloys. <i>Journal of Nuclear Materials</i> , 2018, 509, 225-236.	1.3	14
29276	Mechanical anisotropy and ideal strength of ThBC. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 122, 203-209.	1.9	5
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29820	and $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msubsup} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Mn} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Al}$ <i>Optical Materials</i> , 2018, 85, 162-166.	1.7	12
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29972	Sub-5 nm Monolayer Arsenene and Antimonene Transistors. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 22363-22371.	4.0	77
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29974	Selecting electrode materials for monolayer ReS <sub>2</sub> with an Ohmic contact. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6764-6770.	2.7	34
29975	Magnetic properties of X-C <sub>2</sub> N (X=Cl, Br and I) monolayers: A first-principles study. <i>AIP Advances</i> , 2018, 8, 055333.	0.6	4
29976	Diffusion quantum Monte Carlo and density functional calculations of the structural stability of bilayer arsenene. <i>Journal of Chemical Physics</i> , 2018, 148, 214706.	1.2	23
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30390	Building egg-tray-shaped graphenes that have superior mechanical strength and band gap. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	19
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31215	Elementary kinetics of nitrogen electroreduction to ammonia on late transition metals. <i>Catalysis Science and Technology</i> , 2019, 9, 174-181.	2.1	47
31216	A dimer path for CO dissociation on PtSn. <i>Catalysis Science and Technology</i> , 2019, 9, 695-701.	2.1	9
31217	Molecular or dissociative adsorption of water on clean and oxygen pre-covered Ni(111) surfaces. <i>Catalysis Science and Technology</i> , 2019, 9, 199-212.	2.1	9
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31220	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers <i>via</i> biaxial straining. <i>Nanoscale</i> , 2019, 11, 2335-2342.	2.8	80
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31225	Carrier density control in Cu <sub>2</sub> HgGeTe <sub>4</sub> and discovery of Hg <sub>2</sub> GeTe <sub>4</sub> phase boundary mapping. <i>Journal of Materials Chemistry A</i> , 2019, 7, 621-631.	5.2	27

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31499	Controlling the magnetocrystalline anisotropy of $\mu\text{-Fe}_2\text{O}_3$ . <i>AIP Advances</i> , 2019, 9, 035231.	0.6	3
31500	External strain-enhanced cysteine enantiomeric separation ability on alloyed stepped surfaces. <i>Journal of Chemical Physics</i> , 2019, 150, 154701.	1.2	4
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31502	Thermal expansion of energetic material TEX obtained from x-ray diffraction and first principles calculations. <i>Journal of Molecular Structure</i> , 2019, 1195, 859-862.	1.8	6
31503	Efficient band structure engineering and visible-light response in $\text{ZrS}_2/\text{GaS}$ heterobilayer by electrical field or external strains. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 2969-2973.	0.9	8
31504	<i>Ab initio</i> calculations of $\text{CaZrO}_3$ , $\text{BaZrO}_3$ , $\text{PbTiO}_3$ and $\text{SrTiO}_3$ (001), (011) and (111) surfaces as well as their (001) interfaces. <i>Integrated Ferroelectrics</i> , 2019, 196, 7-15.	0.3	10
31505	Structural stability of MoB up to 25 GPa: experiment and computation. <i>Materials Research Express</i> , 2019, 6, 096502.	0.8	4
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31508	Reliable thermodynamic estimators for screening caloric materials. <i>Journal of Alloys and Compounds</i> , 2019, 802, 712-722.	2.8	22
31509	First-principles study of dopant stability and related optical properties in $\text{CdSiP}_2$ crystal. <i>Journal of Alloys and Compounds</i> , 2019, 802, 310-317.	2.8	2
31510	Giant Magnetoelectric Coupling and Two-Dimensional Electron Gas Regulated by Polarization in $\text{BiFeO}_3/\text{LaFeO}_3$ Heterostructures. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16393-16399.	1.5	18
31511	Trace doping of multiple elements enables stable battery cycling of $\text{LiCoO}_2$ at 4.6%V. <i>Nature Energy</i> , 2019, 4, 594-603.	19.8	572
31512	Anisotropic thermoelectric properties of Weyl semimetal $\text{NbX}$ ( $X = \text{P}$ and $\text{As}$ ): a potential thermoelectric material. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15167-15176.	1.3	31
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31514	Micromachining of ferrous metal with an ion implanted diamond cutting tool. <i>Carbon</i> , 2019, 152, 598-608.	5.4	27
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31524	Stable, one-dimensional suspended and supported monatomic chains of pnictogens: a metal–insulator framework. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14832-14845.	1.3	9
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32188	Monopole mining method for high-throughput screening for Weyl semimetals. <i>Physical Review B</i> , 2019, 99, .	1.1	10
32189	Static subspace approximation for the evaluation of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{G} / \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 0.1 / \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ quasiparticle energies within a sum-over-bands approach. <i>Physical Review B</i> , 2019, 99, .		
32190	High-pressure structural phase transitions, electronic properties, and intermediate states of CaSe. <i>Canadian Journal of Physics</i> , 2019, 97, 797-802.	0.4	2
32191	Study of thermo-elastic and lattice dynamics properties of half-Heusler compounds $\text{XMgAl}$ ( $X = \text{Li}, \text{Na}$ ) by computational investigations. <i>Modern Physics Letters B</i> , 2019, 33, 1950093.	1.0	8
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32197	Morphology evolution of fcc Ru nanoparticles under hydrogen atmosphere. <i>Nanoscale</i> , 2019, 11, 8037-8046.	2.8	18
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32200	Phase stability of three-dimensional bulk and two-dimensional monolayer $\text{As}_{1-x}\text{Sb}_x$ solid solutions from first principles. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 245702.	0.7	6
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32203	Microstructural Evolution and Mechanical Properties of Intermetallics at the CuW/Al Interface with a Ni Interlayer. <i>Advanced Engineering Materials</i> , 2019, 21, 1801273.	1.6	4
32204	Vibrational and Thermodynamical Properties of MgO Nanosheets of (111) and (100) Facets by Density Functional Theory. <i>Journal of Electronic Materials</i> , 2019, 48, 3816-3822.	1.0	14
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32215	Experimental and Computational Design of Highly Active Ce <sup>4+</sup> /ZrO <sub>2</sub> /GO Photocatalyst for Eosin Yellow Dye Degradation: The Role of Interface and Ce <sup>3+</sup> Ion. <i>Catalysis Letters</i> , 2019, 149, 1633-1650.	1.4	18
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32231	A synergistic reinforcement of Re and W for ideal shear strengths of $\beta$ -Ni <sub>3</sub> Al phases. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 131, 34-43.	1.9	18
32232	Properties of M <sub>2</sub> O <sub>3</sub> /Au(111) Honeycomb Monolayers (M = Sc, Ti, V, Cr, Mn, Fe). <i>Tj ETQq 0 0 0 rgBT/Overlock</i>	1.5	21
32233	Symmetry Breaking at MAPb <sub>3</sub> Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain <i>ab Initio</i> Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1617-1623.	2.1	65
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32247	An insight into optical properties of Pb:CdS system (a theoretical study). <i>Materials Research Express</i> , 2019, 6, 065904.	0.8	8
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32264	Atomically Layered and Ordered Rare-Earth MAX Phases: A New Class of Magnetic Quaternary Compounds. <i>Chemistry of Materials</i> , 2019, 31, 2476-2485.	3.2	89
32265	Double-Spiral Hexagonal Boron Nitride and Shear Strained Coalescence Boundary. <i>Nano Letters</i> , 2019, 19, 4229-4236.	4.5	15
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32280	The physical properties of ThCr <sub>2</sub> Si <sub>2</sub> -type nickel-based superconductors BaNi <sub>2</sub> T <sub>2</sub> (T = P, As): An ab-initio study. <i>Chinese Journal of Physics</i> , 2019, 59, 58-69.	2.0	11
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32301	First principles calculations on CeO <sub>2</sub> doped with Tb <sup>3+</sup> ions. <i>Optical Materials</i> , 2019, 90, 76-83.	1.7	3
32302	Adsorption of Ethene-1,2-Dione on Materials Based on Graphene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6316-6325.	1.5	1
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32313	The mechanism and activity of oxygen reduction reaction on single atom doped graphene: a DFT method. <i>RSC Advances</i> , 2019, 9, 7086-7093.	1.7	31
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32365	<a href="#">xmls:mml="http://www.w3.org/1998/Math/MathML"&gt;&lt;mml:mrow&gt;&lt;mml:mi mathvariant="normal"&gt;C&lt;/mml:mi&gt;&lt;mml:msup&gt;&lt;mml:mrow&gt;&lt;mml:mi mathvariant="normal"&gt;e&lt;/mml:mi&gt;&lt;/mml:mrow&gt;&lt;mml:mrow&gt;&lt;mml:mn&gt;3&lt;/mml:mn&gt;&lt;mml:mo&gt;+&lt;/mml:mo&gt;&lt;/mml:mrow&gt;&lt;/mml:ms</a> <a href="#">-doped</a> <a href="#">&lt;mml:math</a>		

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32459	<i>In situ</i> exsolved FeNi <sub>3</sub> nanoparticles on nickel doped Sr <sub>2</sub> Fe <sub>1.5</sub> Mo <sub>0.5</sub> O <sub>6<math>\delta</math></sub> perovskite for efficient electrochemical CO <sub>2</sub> reduction reaction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11967-11975.	5.2	159
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33017	First principle study of HF molecule adsorption on TiO <sub>2</sub> (110) surface. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 655, 012043.	0.3	2
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33330	Tuning nitrogen species in three-dimensional porous carbon via phosphorus doping for ultra-fast potassium storage. <i>Nano Energy</i> , 2019, 57, 728-736.	8.2	323
33331	Assessing Correlations of Perovskite Catalytic Performance with Electronic Structure Descriptors. <i>Chemistry of Materials</i> , 2019, 31, 785-797.	3.2	106
33332	Edge-State-Enhanced CO <sub>2</sub> Electroreduction on Topological Nodal-Line Semimetal Cu <sub>2</sub> Si Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2837-2842.	1.5	26
33333	Switchable Schottky Contacts: Simultaneously Enhanced Output Current and Reduced Leakage Current. <i>Journal of the American Chemical Society</i> , 2019, 141, 1628-1635.	6.6	43
33334	Metal Hexaboride Work Functions: Surface Configurations and the Electrical Double Layer from First Principles. <i>Advanced Electronic Materials</i> , 2019, 5, 1800074.	2.6	9
33335	Reaction mechanism for NH <sub>3</sub> -SCR of NO <sub>x</sub> over CuMn <sub>2</sub> O <sub>4</sub> catalyst. <i>Chemical Engineering Journal</i> , 2019, 361, 578-587.	6.6	146
33336	Systematic analysis of the fine structure of energy levels and spin-Hamiltonian parameters of V <sup>3+</sup> ion in corundum with dynamic Jahn-Teller effect. <i>Journal of Luminescence</i> , 2019, 208, 273-278.	1.5	1
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33338	Investigation of structural models for O <sup>2-</sup> Y and O <sup>2-</sup> Y <sup>2+</sup> Ti clusters in bcc Fe: a density functional theory study. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 095701.	0.7	3
33339	Ideal half-filled intermediate band position in CuGaS <sub>2</sub> generated by Sb-related defect complex: a first-principles study. <i>Applied Physics Express</i> , 2019, 12, 021002.	1.1	3
33340	Structural and thermodynamic properties of cubic sphalerite aluminum nitride under hydrostatic compression. <i>Computational Condensed Matter</i> , 2019, 19, e00359.	0.9	13
33341	Phase Stability Analysis of Ternary Alkaline-Earth Hexaborides: Insights from DFT Calculations. <i>ACS Applied Electronic Materials</i> , 2019, 1, 105-112.	2.0	2
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33346	Band manipulation for high thermoelectric performance in SnTe through heavy CdSe-alloying. <i>Journal of Materiomics</i> , 2019, 5, 111-117.	2.8	17
33347	First-principles study of surface properties of uranium silicides. <i>Journal of Nuclear Materials</i> , 2019, 513, 192-197.	1.3	9
33348	First-principles study of thermophysical properties of interaction layer products in U-Mo/Al dispersion fuel. <i>Journal of Nuclear Materials</i> , 2019, 513, 94-101.	1.3	1
33349	Unobvious elastic anisotropy of measured single-crystal cementite. <i>Materials Research Express</i> , 2019, 6, 016531.	0.8	0
33350	Adsorption and catalytic decomposition of hydrazine on metal-free SiC <sub>3</sub> siligraphene. <i>Applied Surface Science</i> , 2019, 469, 316-324.	3.1	16
33351	Single-layer planar penta-X <sub>2</sub> N <sub>4</sub> (X = Ni, Pd and Pt) as direct-bandgap semiconductors from first principle calculations. <i>Applied Surface Science</i> , 2019, 469, 456-462.	3.1	48
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33413	Tribo-piezoelectricity in Janus transition metal dichalcogenide bilayers: A first-principles study. <i>Nano Energy</i> , 2019, 56, 33-39.	8.2	58
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33429	Basal slip of $\frac{1}{2}\langle 11\bar{2}0 \rangle$ screw dislocations in hexagonal titanium. <i>Scripta Materialia</i> , 2019, 162, 296-299.	2.6	22
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33441	2 $\sqrt{2}$ charge density wave in single-layer TiTe <sub>2</sub> . <i>2D Materials</i> , 2019, 6, 015027.	2.0	20
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34887	Boron interaction with D03 phase in Fe-(27%Ga) alloys. <i>Intermetallics</i> , 2020, 126, 106938.	1.8	0
34888	Defects and light elements (Li, Be, B, C, O and F) driven d <sub>0</sub> magnetism in InN monolayer. <i>Vacuum</i> , 2020, 181, 109720.	1.6	3
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34891	Unraveling atomic-scale lithiation mechanisms in a NiO thin film electrode. <i>Journal of Materials Chemistry A</i> , 2020, 8, 25198-25207.	5.2	7
34892	First principles calculations on theoretical band gap improvement of IIIA-VA zinc-blende semiconductor InAs. <i>International Journal of Modern Physics C</i> , 2020, 31, 2050178.	0.8	1
34893	$\text{A}_2\text{BB}_2(\text{PO}_4)_2(\text{P}_2\text{O}_7)$ (A = K, Tl) <i>ETQq1 1 0.784314 rg</i> <i>Chemistry</i> , 2020, 2020, 4007-4014.	1.0	6
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37481	Tautomerism of azo dyes in the solid state studied by <sup>15</sup> N, <sup>14</sup> N, <sup>13</sup> C and <sup>1</sup> H NMR spectroscopy, X-ray diffraction and quantum-chemical calculations. <i>Dyes and Pigments</i> , 2020, 178, 108342.	2.0	13
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37483	Surface charging activated mechanism change: A computational study of O, CO, and CO <sub>2</sub> interactions on Ag electrodes. <i>Journal of Energy Chemistry</i> , 2020, 50, 307-313.	7.1	8
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37608	First-principles study of electronic structure and optical properties of Er:Lu <sub>2</sub> O <sub>3</sub> . <i>Journal of Rare Earths</i> , 2021, 39, 453-459.	2.5	13
37609	Hydrogen storage capacities of alkali and alkaline-earth metal atoms on SiC monolayer: A first-principles study. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 20266-20279.	3.8	39
37610	Alkali and transition metal atom-functionalized germanene for hydrogen storage: A DFT investigation. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 20245-20256.	3.8	57
37611	Cu-Al spinel-oxide catalysts for selective hydrogenation of furfural to furfuryl alcohol. <i>Catalysis Today</i> , 2021, 367, 177-188.	2.2	25
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37613	Search for potential K ion battery cathodes by first principles. <i>Journal of Energy Chemistry</i> , 2021, 54, 377-385.	7.1	8
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37616	First-principles study on predicting the crystal structures, mechanical properties and electronic structures of HfC <sub>x</sub> N <sub>1-x</sub> . <i>Journal of the European Ceramic Society</i> , 2021, 41, 3037-3044.	2.8	7
37617	The effect of edge functionalization on the device performance of monolayer Si <sub>0.5</sub> Ge <sub>0.5</sub> nanoribbon transistors. <i>Journal of Computational Electronics</i> , 2021, 20, 95-106.	1.3	2
37618	Theoretical screening of the transition metal heteronuclear dimer anchored graphdiyne for electrocatalytic nitrogen reduction. <i>Journal of Energy Chemistry</i> , 2021, 54, 501-509.	7.1	116
37619	Solid phase microwave-assisted fabrication of Fe-doped ZIF-8 for single-atom Fe-N-C electrocatalysts on oxygen reduction. <i>Journal of Energy Chemistry</i> , 2021, 54, 579-586.	7.1	52
37620	Surface modification of macroporous La <sub>0.8</sub> Sr <sub>0.2</sub> CoO <sub>3</sub> perovskite oxides integrated monolithic catalysts for improved propane oxidation. <i>Catalysis Today</i> , 2021, 376, 168-176.	2.2	13
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37622	Novel green phosphorene as a superior chemical gas sensing material. <i>Journal of Hazardous Materials</i> , 2021, 401, 123340.	6.5	71
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37624	Effects of surface functionalization of mxene-based nanocatalysts on hydrogen evolution reaction performance. <i>Catalysis Today</i> , 2021, 368, 187-195.	2.2	51
37625	Combination of theoretical and <i>in situ</i> experimental investigations of the role of lithium dopant in manganese nitride: a two-stage reagent for ammonia synthesis. <i>Faraday Discussions</i> , 2021, 229, 281-296.	1.6	9
37626	The integrated DL_POLY/DL_FIELD/DL_ANALYSER software platform for molecular dynamics simulations for exploration of the synthonic interactions in saturated benzoic acid/hexane solutions. <i>Molecular Simulation</i> , 2021, 47, 257-272.	0.9	5
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37629	Clarifying the polyaniline effect on superior electrochemical performances of hydrogen storage alloys. <i>Electrochimica Acta</i> , 2021, 365, 137336.	2.6	8
37630	Theoretical study of NO <sub>2</sub> adsorption on SiCNT and P-doped SiCNT. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 127, 114519.	1.3	5
37631	Structural, mechanical, thermal, and optical properties of inverse-Heusler alloys Cr <sub>2</sub> CoZ (Z = Al, In): A first-principles investigation. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 385, 126967.	0.9	39
37632	Misfit Layer Compounds: A Platform for Heavily Doped 2D Transition Metal Dichalcogenides. <i>Advanced Functional Materials</i> , 2021, 31, 2007706.	7.8	17

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37633	Metric-driven search for structurally stable inorganic compounds. <i>Acta Materialia</i> , 2021, 202, 437-447.	3.8	6
37634	The compatibility between environmentally friendly insulation gas C <sub>4</sub> F <sub>7</sub> N and $\hat{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface: Theoretical and experimental insights. <i>Applied Surface Science</i> , 2021, 536, 147839.	3.1	6
37635	Engineering of MoS <sub>2</sub> nanoribbons as high-performance materials for biosensing applications. <i>Applied Surface Science</i> , 2021, 540, 148349.	3.1	5
37636	Crystal face-dependent methylmercury adsorption onto mackinawite (FeS) nanocrystals: A DFT-D3 study. <i>Chemical Engineering Journal</i> , 2021, 420, 127594.	6.6	16
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37638	18 and 12 $\hat{\pm}$ Member carbon rings (cyclo[n]carbons) $\hat{\pm}$ A density functional study. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 263, 114895.	1.7	6
37639	High-pressure structural, lattice dynamics, and electronic properties of beryllium aluminate studied from first-principles theory. <i>Materials Today Communications</i> , 2021, 26, 101801.	0.9	9
37640	Ab initio study of elastic properties of orthorhombic cadmium stannate as a substrate for the manufacture of MEMS devices. <i>Materials Today Communications</i> , 2021, 26, 101822.	0.9	5
37641	Tailoring the chemical bonding of GeTe-based alloys by MgB <sub>2</sub> alloying to simultaneously enhance their mechanical and thermoelectric performance. <i>Materials Today Physics</i> , 2021, 16, 100308.	2.9	29
37642	A first-principles investigation of Janus MoSSe as a catalyst for photocatalytic water-splitting. <i>Applied Surface Science</i> , 2021, 537, 147919.	3.1	36
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37647	Ultra-incompressibility and high energy density of ReN <sub>8</sub> with infinite nitrogen chains. <i>Journal of Materials Science</i> , 2021, 56, 3814-3826.	1.7	9
37648	Microstructure and electronic property of pristine and thermal barrier layers TiN/AlN/ZrB <sub>2</sub> buffered 4H-SiC/W interface from first principles study. <i>Applied Surface Science</i> , 2021, 536, 147820.	3.1	5
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37652	First-principles studies on behaviors of He impurities in d-MAX phase Zr <sub>3</sub> Al <sub>3</sub> C <sub>5</sub> . <i>Journal of Nuclear Materials</i> , 2021, 544, 152653.	1.3	1
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37656	Exploring Janus MoSSe monolayer as a workable media for SOF <sub>6</sub> decompositions sensing based on DFT calculations. <i>Computational Materials Science</i> , 2021, 186, 109976.	1.4	21
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37659	Synthesis and simulation of surfactant free chemically derived highly polycrystalline lead iodide. <i>Materials Today: Proceedings</i> , 2021, 42, 1624-1628.	0.9	0
37660	Lignin derived hierarchical porous carbon with extremely suppressed polyselenide shuttling for high-capacity and long-cycle-life lithium-selenium batteries. <i>Journal of Energy Chemistry</i> , 2021, 55, 476-483.	7.1	31
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37662	Adsorption behavior of barium ions onto ZnO surfaces: Experiments associated with DFT calculations. <i>Journal of Molecular Structure</i> , 2021, 1223, 128991.	1.8	27
37663	Towards thermoneutral hydrogen evolution reaction using noble metal free molybdenum ditelluride/graphene nanocomposites. <i>Journal of Colloid and Interface Science</i> , 2021, 581, 847-859.	5.0	16
37664	Free-standing nanoporous NiMnFeMo alloy: An efficient non-precious metal electrocatalyst for water splitting. <i>Chemical Engineering Journal</i> , 2021, 404, 126530.	6.6	88
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37668	Identifying electrocatalytic activity and mechanism of Ce <sub>1/3</sub> NbO <sub>3</sub> perovskite for nitrogen reduction to ammonia at ambient conditions. <i>Applied Catalysis B: Environmental</i> , 2021, 280, 119419.	10.8	60

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37682	Theoretical study of magneto-electronic properties of TmCo <sub>2</sub> and NdCo <sub>2</sub> intermetallic compounds through density functional theory calculations. International Journal of Quantum Chemistry, 2021, 121, e26488.	1.0	4
37683	Theoretical study of the phase transitions and electronic structure of (Zr <sub>0.5</sub> , Mg <sub>0.5</sub> )N and (Hf <sub>0.5</sub> , Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50	1.7	11
37684	Water Adsorption and Dissociation Promoted by Co <sup>*</sup> -N-C <sup>*</sup> -Biactive Sites of Metallic Co/N-Doped Carbon Hybrids for Efficient Hydrogen Evolution. Applied Catalysis B: Environmental, 2021, 282, 119463.	10.8	77
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37690	Synthesis of flower-like twin crystal ternary Ni/NiS/Zn <sub>0.2</sub> Cd <sub>0.8</sub> S catalyst for highly efficient hydrogen production. <i>Chemical Engineering Journal</i> , 2021, 406, 126878.	6.6	57
37691	Charge-regulated, electric-field and combined effect controlled switchable CO <sub>2</sub> capture and separation on penta-C <sub>2</sub> N nanosheet: A computational study. <i>Chemical Engineering Journal</i> , 2021, 407, 127194.	6.6	24
37692	Structure and electronic properties of Bi <sub>2</sub> O <sub>3</sub> tuned by vacancy and doping: A first-principles study. <i>Ceramics International</i> , 2021, 47, 205-213.	2.3	8
37693	Anisotropic elastic, thermal properties and electronic structures of M <sub>2</sub> AlB <sub>2</sub> (M=Fe, Cr, and Mn) layer structure ceramics. <i>Ceramics International</i> , 2021, 47, 1421-1428.	2.3	17
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37695	Ab-initio, Monte Carlo and experimental investigation on structural, electronic and magnetic properties of Zn <sub>1-x</sub> Ni <sub>x</sub> O nanoparticles prepared via sol-gel method. <i>Journal of Alloys and Compounds</i> , 2021, 854, 157142.	2.8	10
37696	Influence of pressure on phase transition, electronic and thermoelectric properties of SnSe. <i>Journal of Alloys and Compounds</i> , 2021, 853, 157362.	2.8	6
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37699	Germanene/2D-SiC van der Waals heterobilayer: Structural features and tunable electronic properties. <i>Materials Today Communications</i> , 2021, 26, 101718.	0.9	22
37700	An Ab Initio study of electronic, mechanical, thermoelectric and vibrational properties of Dirac Semimetals Ca <sub>3</sub> PbO and Ca <sub>3</sub> SnO. <i>Materials Today Communications</i> , 2021, 26, 101741.	0.9	2
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37702	First-Principles Simulation of Structural, Electronic and Optical Properties of Cerium Trisulfide (Ce <sub>2</sub> S <sub>3</sub> ) Compound. <i>Journal of Electronic Materials</i> , 2021, 50, 1637-1643.	1.0	9
37703	Two-dimensional carbon allotropes with tunable direct band gaps and high carrier mobility. <i>Applied Surface Science</i> , 2021, 537, 147885.	3.1	39
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37726	Noncovalent functionalization of graphene through physisorption of 1,1-diamino-2,2-dinitroethene: Impacts of and cooperativity between hydrogen bond and $\pi\text{-}\pi$ interaction. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 148, 109736.	1.9	4
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37728	Rational defect and anion chemistries in $\text{Co}_3\text{O}_4$ for enhanced oxygen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2021, 281, 119535.	10.8	90
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37860	Electronic structure, optical and vibrational properties of Ti <sub>2</sub> FeNiSb <sub>2</sub> and Ti <sub>2</sub> Ni <sub>2</sub> InSb double half heusler alloys. <i>Materials Science in Semiconductor Processing</i> , 2021, 123, 105531.	1.9	18
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37864	Interwoven scaffolded porous titanium oxide nanocubes/carbon nanotubes framework for high-performance sodium-ion battery. <i>Journal of Energy Chemistry</i> , 2021, 59, 38-46.	7.1	25
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37866	Electronic and magnetic properties of 3d transition metal atom adsorbed Zr <sub>2</sub> CO <sub>2</sub> Mxene: First-principles study. <i>Solid State Communications</i> , 2021, 325, 114140.	0.9	9



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38003	Highly efficient H <sub>2</sub> generation over Cu <sub>2</sub> Se decorated Cd <sub>0.95</sub> Se <sub>0.05</sub> nanowires by photocatalytic water reduction. <i>Chemical Engineering Journal</i> , 2021, 409, 128157.	6.6	22
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38006	Thermoelectric properties of strontium oxide under pressure: First-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 390, 127083.	0.9	9
38007	First-principles study of electronic and optical properties of ternary compounds AuBX <sub>2</sub> (X = S, Se, Te) and AuMTe <sub>2</sub> (M = Al, In, Ga). <i>Solid State Sciences</i> , 2021, 111, 106508.	1.5	27
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38009	Chiral Switchable Low-Dimensional Perovskite Ferroelectrics. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 2044-2051.	4.0	66
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38012	Suppression of isotopic polymorphism. <i>CrystEngComm</i> , 2021, 23, 769-776.	1.3	4
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38038	The potential application of VS <sub>2</sub> as an electrode material for Mg ion battery: A DFT study. <i>Applied Surface Science</i> , 2021, 544, 148775.	3.1	50
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38052	Solar Photoelectroreduction of Nitrate Ions on Pb <sub>2</sub> /Cu Nanocomposite Electrodes. <i>Solar Rrl</i> , 2021, 5, 2000418.	3.1	4
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38061	Conductance switching of a gold-covalent organic framework nanojunction via proton transfer. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 389, 127100.	0.9	2
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38087	Charge transfer driven interaction of $\text{CH}_4$ , $\text{CO}_2$ and $\text{NH}_3$ with $\text{TiS}_2$ monolayer: Influence of vacancy defect. <i>Catalysis Today</i> , 2021, 370, 189-195.	2.2	5
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38089	Insights into atomic scale structure and interfacial fracture behaviors of $\text{Ti}(0001)/\text{Ti}_3\text{Sn}(0001)$ interface. <i>Vacuum</i> , 2021, 183, 109791.	1.6	2
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38103	Electronic structure, elastic, optical and thermal properties of chalcopyrite CuBY <sub>2</sub> (B = In, Ga, In <sub>0.5</sub> ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.9	2
38104	Tailoring M <sub>7</sub> C <sub>3</sub> carbide via electron work function-guided modification. <i>Scripta Materialia</i> , 2021, 190, 168-173.	2.6	19
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38112	Interlayer coupling effect in van der Waals heterostructures of transition metal dichalcogenides. <i>Frontiers of Physics</i> , 2021, 16, 1.	2.4	15
38113	Single-Atom Cobalt-Based Electrochemical Biomimetic Uric Acid Sensor with Wide Linear Range and Ultralow Detection Limit. <i>Nano-Micro Letters</i> , 2021, 13, 7.	14.4	76
38114	Electric field-induced band modulation of predicted ternary 2D MXC <sub>3</sub> [M: X = As:Ge, Sb:Sn and Bi:Pb] with strong stability and optical properties. <i>Carbon</i> , 2021, 172, 791-803.	5.4	21
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38116	An experimental and theoretical exploration of the role of tri-element metal-nonmetal nanohybrids in photovoltaics. <i>Chemical Engineering Journal</i> , 2021, 413, 127491.	6.6	12
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38120	Structural, mechanical and phonons properties of binary intermetallic compound BaSn <sub>3</sub> under pressure. <i>Solid State Communications</i> , 2021, 323, 114110.	0.9	7
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38126	An efficient Z-scheme (Cr, B) codoped g-C <sub>3</sub> N <sub>4</sub> /BiVO <sub>4</sub> photocatalyst for water splitting: A hybrid DFT study. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 247-261.	3.8	59
38127	Bimetallic Ag-Cu nanosheets assembled flower-like structure for oxygen reduction reaction. <i>Journal of Alloys and Compounds</i> , 2021, 856, 157379.	2.8	11
38128	Isocyanic acid (HNCO) dissociation on Rh(001) surface: A DFT study with and without dispersion correction. <i>Surface Science</i> , 2021, 709, 121744.	0.8	7
38129	The Electronic Properties of Chlorine in GaN: An Ab Initio Study. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2000303.	0.7	0
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38248	Superhydrophilic Fe <sup>3+</sup> Doped TiO <sub>2</sub> Films with Long-Lasting Antifogging Performance. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 3377-3386.	4.0	40
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38266	Understanding the origin of structure sensitivity in hydrodechlorination of trichloroethylene on a palladium catalyst. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 2270-2279.	1.9	3
38267	Z-Scheme <i>versus</i> type-II junction in g-C <sub>3</sub> N <sub>4</sub> /TiO <sub>2</sub> and g-C <sub>3</sub> N <sub>4</sub> /SrTiO <sub>3</sub> /TiO <sub>2</sub> heterostructures. <i>Catalysis Science and Technology</i> , 2021, 11, 3589-3598.	2.1	25
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38270	Transition-metal single atoms embedded into defective BC <sub>3</sub> as efficient electrocatalysts for oxygen evolution and reduction reactions. <i>Nanoscale</i> , 2021, 13, 1331-1339.	2.8	27
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38279	Redox, Magnetic, and Structural Properties of $\hat{\pm}$ -NaMnO <sub>2</sub> Cathode Material Analyzed by Fitting-Free DFT+U Calculations, Parameterized by the Linear Response Approach. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1531-1543.	1.5	4
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38350	An interplay of various damage channels in polyethylene exposed to ultra-short XUV/X-ray pulses. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16193-16205.	1.3	7
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38395	An Integrated Methodology for Screening Hydrogen Evolution Reaction Catalysts: Pt/Mo <sub>2</sub> C as an Example. <i>Springer Series in Materials Science</i> , 2021, , 719-731.	0.4	0
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38403	Activated Lone-Pair Electrons Lead to Low Lattice Thermal Conductivity: A Case Study of Boron Arsenide. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
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38410	Impact of Topological Edge Defects on Spin Transport Properties of Zigzag Graphene Nanoribbons. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2000538.	0.7	2
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38427	Bandgap evolution in nanographene assemblies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11501-11506.	1.3	1
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38433	First-principle investigation of hybrid improper ferroelectricity of $A_{2n}B_{2n}R_{2n}O_{2n}$ Ruddlesden-Popper Sr <sub>3</sub> Bi <sub>2</sub> Se <sub>7</sub> ( $A = Zr, Hf$ ). <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 116302-116302.	0.2	0
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38463	Local structure and NO adsorption/desorption property of Pd <sup>2+</sup> cations at different paired Al sites in CHA zeolite. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22273-22282.	1.3	15
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38482	Crystal growth and properties characterization of Nd <sup>3+</sup> :Na <sub>5</sub> Lu(MoO <sub>4</sub> ) <sub>4</sub> for continuous multi-wavelength NIR laser emission. <i>CrystEngComm</i> , 2021, 23, 7289-7297.	1.3	2
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38934	Synthesis, Crystal Structure, Electronic Structure, and Catalytic Properties of Ni <sub>3</sub> GaSb. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 1410-1418.	1.0	3
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38961	Single-Atom High-Valent Fe(IV) for Promoted Photocatalytic Nitrogen Hydrogenation on Porous TiO <sub>2</sub> -SiO <sub>2</sub> . ACS Catalysis, 2021, 11, 4362-4371.	5.5	70
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38963	Ab-Initio Calculations of Oxygen Vacancy in Ga <sub>2</sub> O <sub>3</sub> Crystals. Latvian Journal of Physics and Technical Sciences, 2021, 58, 3-10.	0.4	12
38964	Colossal Spin Splitting in the Monolayer of the Collinear Antiferromagnet MnF <sub>2</sub> . Journal of Physical Chemistry Letters, 2021, 12, 2363-2369.	2.1	17
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38968	Influence of Se doping on recently synthesized NaInS <sub>2</sub> -xSex solid solutions for potential thermo-mechanical applications studied via first-principles method. <i>Materials Today Communications</i> , 2021, 26, 101988.	0.9	9
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38973	First-principles calculations study the mechanical and thermal properties of CrAlB ternary borides. <i>Solid State Communications</i> , 2021, 326, 114182.	0.9	16
38974	Dynamical polarizability of graphene with spatial dispersion. <i>Physical Review B</i> , 2021, 103, .	1.1	23
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38976	A Vacancy-Driven Intermetallic Phase: Rh <sub>3</sub> Cd <sub>5</sub> (̄̄̄̄ 0.56). <i>Inorganic Chemistry</i> , 2021, 60, 5488-5496.	1.9	7
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38980	Reactivity of Single Transition Metal Atoms on a Hydroxylated Amorphous Silica Surface: A Periodic Conceptual DFT Investigation. <i>Chemistry - A European Journal</i> , 2021, 27, 6050-6063.	1.7	11
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38982	Two-dimensional carbon nitride C <sub>6</sub> N nanosheet with egg-comb-like structure and electronic properties of a semimetal. <i>Nanotechnology</i> , 2021, 32, 215702.	1.3	50
38983	Theoretical Insights into Morphologies of Alkali-Promoted Cobalt Carbide Catalysts for Fischer-Tropsch Synthesis. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6061-6072.	1.5	12
38984	High-throughput first-principles search for ceramic superlattices with improved ductility and fracture resistance. <i>Acta Materialia</i> , 2021, 206, 116615.	3.8	19

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38987	Zeolitic imidazole framework-derived FeN <sub>5</sub> -doped carbon as superior CO <sub>2</sub> electrocatalysts. <i>Journal of Catalysis</i> , 2021, 395, 63-69.	3.1	27
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38995	First-Principles Calculation of the Evaporation Field and Roll-up Effect of M (M = Fe, Cu, Si, and Mn) on the Fe (001) and Fe Step Structure. <i>Microscopy and Microanalysis</i> , 2022, 28, 1181-1187.	0.2	4
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39000	Intervalence charge transfer of Ti and Fe defects in blue kyanite. <i>Journal of the Korean Physical Society</i> , 2021, 78, 671-678.	0.3	0
39001	Simulations of hydrogen outgassing and sticking coefficients at a copper electrode surface: Dependencies on temperature, incident angle and energy. <i>Physical Review Research</i> , 2021, 3, .	1.3	4
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39007	Buckling of boron nanotubes under axial compression: Insights from molecular mechanics and continuum mechanics. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114520.	1.3	3
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39019	First-principles study on the structural, elastic, piezoelectric and electronic properties of (BaTiO <sub>3</sub> ) <sub>1-x</sub> (Sr <sub>1-x</sub> TiO <sub>3</sub> ) <sub>x</sub> . Journal of Applied Physics, 2021, 129, 154101.	0.9	4
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39040	FeMoO <sub>4</sub> Revisited: Crosslike 90° Noncollinear Antiferromagnetic Structure Caused by Dzyaloshinskii-Moriya Interaction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5947-5956.	1.5	4
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39043	Impact of ordering on the reactivity of mixed crystals of topological insulators with anion substitution: Bi <sub>2</sub> SeTe <sub>2</sub> and Sb <sub>2</sub> SeTe <sub>2</sub> . <i>Applied Surface Science</i> , 2021, 541, 148490.	3.1	0
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39054	An ab initio study of structural, elastic and electronic properties of hexagonal MAuGe (M = Lu, Sc) compounds. <i>Condensed Matter Physics</i> , 2021, 24, 13706.	0.3	3
39055	Evaluation of similarities and differences of LiTaO <sub>3</sub> and LiNbO <sub>3</sub> based on high-T-conductivity, nonlinear optical fs-spectroscopy and ab initio modeling of polaronic structures. <i>New Journal of Physics</i> , 2021, 23, 033016.	1.2	19
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39061	Electric field induced topological phase transition and large enhancements of spin-orbit coupling and Curie temperature in two-dimensional ferromagnetic semiconductors. Physical Review B, 2021, 103, .	1.1	33
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39063	Effect of Ni doping on optical, structural, and morphological properties of ZnO thin films synthesized by MSILAR: Experimental and DFT study. Materialia, 2021, 15, 101015.	1.3	9
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39074	Polyelemental Nanoparticles as Catalysts for a Li-O <sub>2</sub> Battery. ACS Nano, 2021, 15, 4235-4244.	7.3	38

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39077	Impact of stoichiometry and strain on Ge <sub>1-x</sub> Sn <sub>x</sub> alloys from first principles calculations. <i>Journal Physics D: Applied Physics</i> , 2021, 54, 245103.	1.3	4
39078	Theoretical prediction of structural stability, elastic and magnetic properties for Mn <sub>2</sub> NiGa alloy. <i>Modern Physics Letters B</i> , 2021, 35, 2150231.	1.0	2
39079	Stability, electronic structure, mechanical properties and lattice thermal conductivity of FeS and FeS <sub>2</sub> polymorphs. <i>Modern Physics Letters B</i> , 2021, 35, 2150225.	1.0	1
39080	Study of the chromium doping effect in boron phosphide semiconductors. <i>International Journal of Computational Materials Science and Engineering</i> , 2021, 10, 2150006.	0.5	2
39081	Polymerization of silanes through dehydrogenative Si–Si bond formation on metal surfaces. <i>Nature Chemistry</i> , 2021, 13, 350-357.	6.6	11
39082	Effects of copper ion irradiation on supercapacitive electrodes. <i>Journal of Applied Electrochemistry</i> , 2021, 51, 829-845.		
39084	First principle study of structural, elastic, electronic and optical properties of Pb <sub>0.5</sub> Sn <sub>0.5</sub> TiO <sub>3</sub> and Pb <sub>0.5</sub> Sn <sub>0.5</sub> Ti <sub>0.5</sub> (Zr <sub>0.5</sub> )O <sub>3</sub> . <i>Condensed Matter Physics</i> , 2021, 24, 13702.	0.3	0
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39796	Kinetics-Driven One-Dimensional Growth of van der Waals Layered SnSe. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12730-12737.	1.5	8
39797	Defect Engineering in Graphene-Confined Single-Atom Iron Catalysts for Room-Temperature Methane Conversion. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12628-12635.	1.5	22
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40205	<a href="#">xmlns:mml="http://www.w3.org/1998/Math/MathML"&gt;&lt;mml:mrow&gt;&lt;mml:msub&gt;&lt;mml:mi&gt;Hf&lt;/mml:mi&gt;&lt;mml:mrow&gt;&lt;mml:mn&gt;0.5&lt;/mml:mn&gt;&lt;/mml:mrow&gt;&lt;/mml:msub&gt;&lt;/mml:mrow&gt;&lt;/mml:math&gt;&lt;math&gt;O&lt;/math&gt; grown epitaxially on &lt;math&gt;La&lt;/math&gt;.</a> <i>Physical Review Materials</i> , 2021, 5, .	0.9	15
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40611	Room-Temperature Ferroelectricity in 2D Metal-Tellurium-Oxyhalide Cd <sub>7</sub> Te <sub>7</sub> Cl <sub>8</sub> O <sub>17</sub> via Selenium-Induced Selective-Bonding Growth. <i>ACS Nano</i> , 2021, 15, 16525-16532.	7.3	12
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40620	Stability and stoichiometry of L12 Al <sub>3</sub> (Sc,Zr) dispersoids in Al-(Si)-Sc-Zr alloys. <i>Acta Materialia</i> , 2021, 216, 117117.	3.8	24
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40669	Third-generation CALPHAD description of pure GeO <sub>2</sub> at 1 atm. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021, 74, 102299.	0.7	6
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41029	Electrochemical properties of biomass-derived carbon and its composite along with Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> as potential high-performance anodes for Na-ion and Li-ion batteries. Electrochimica Acta, 2021, 392, 139026.	2.6	27
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41031	Ab initio investigation of physical properties of the graphene/As-F hetero-bilayer. Applied Surface Science, 2021, 563, 150339.	3.1	6
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41033	Impact of the charge transfer process on the Fe <sup>2+</sup> /Fe <sup>3+</sup> distribution at Fe <sub>3</sub> O <sub>4</sub> magnetic surface induced by deposited Pd clusters. Surface Science, 2021, 712, 121879.	0.8	3
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41038	Screen the thermomechanical and optical properties of the new ductile 314 MAX phase boride Zr <sub>3</sub> Cd <sub>4</sub> B <sub>4</sub> : A DFT insight. Journal of Alloys and Compounds, 2021, 877, 160248.	2.8	25
41039	Reduction of NO on chemically doped, metal-free graphene. Carbon Trends, 2021, 5, 100111.	1.4	6
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41042	From $\hat{\Gamma}$ - to $\hat{\Gamma}$ -pinning in CaKFe <sub>4</sub> As <sub>4</sub> single crystals obtained by adjusting their defect structures. Superconductor Science and Technology, 2021, 34, 115020.	1.8	12
41043	Structure, elastic, and electronic properties of the Nb <sub>2</sub> SnC <sub>1-x</sub> B <sub>x</sub> phases MAX: ab initio calculations. Materials Today Communications, 2021, , 102840.	0.9	0
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41052	Halide double perovskite Cs <sub>2</sub> AgInBr <sub>6</sub> for photovoltaic applications: Optical properties and stability. Optik, 2021, 243, 167198.	1.4	18
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41066	Computational evaluation of Mg-decorated g-CN as clean energy gas storage media. International Journal of Hydrogen Energy, 2021, 46, 35130-35136.	3.8	22
41067	Tunable Schottky Barrier and Interfacial Electronic Properties in Graphene/ZnSe Heterostructures. Frontiers in Chemistry, 2021, 9, 744977.	1.8	1
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41070	Atomic study of hydrogen behavior in different vanadium carbides. Journal of Nuclear Materials, 2021, 554, 153096.	1.3	3
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41073	The tuning on the magnetism and the electronic structures of monolayer Ti2N MXene by electric field. <i>Physica B: Condensed Matter</i> , 2021, 618, 413183.	1.3	8
41074	The effect of additional element dissolving on the solid solubility of Zn in Mg alloy: A first-principles prediction strategy. <i>Journal of Alloys and Compounds</i> , 2021, 877, 160312.	2.8	4
41075	Novel two-dimensional $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{C} \langle \text{mml:mtext} \rangle \langle \text{mml:mtext} \rangle \text{r} \langle \text{mml:mtext} \rangle \text{X} \langle \text{mml:mtext} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mtext} \rangle$ (X=Cr, Ru) metal for high NÅ©el temperature antiferromagnetic spintronics. <i>Journal of Solid State Chemistry</i> , 2021, 302, 122427.	1.4	3
41076	Influence of the Fe-doping on hydrogen behavior on the ZrCo surface. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 33877-33888.	3.8	10
41077	Reversible hydrogenation and dehydrogenation of N-ethylcarbazole over bimetallic Pd-Rh catalyst for hydrogen storage. <i>Chemical Engineering Journal</i> , 2021, 421, 127781.	6.6	40
41078	TiO2/Carbon allotrope nanohybrids for supercapacitor application with theoretical insights from density functional theory. <i>Applied Surface Science</i> , 2021, 563, 150259.	3.1	14
41079	Electron reservoir enhances methane conversion on Zn dimer supported by N doped graphene: A DFT study. <i>Applied Surface Science</i> , 2021, 563, 150328.	3.1	4
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41081	Water adsorption behaviour on (001) pyrophyllite surface from ab initio Density Functional Theory simulations. <i>Applied Clay Science</i> , 2021, 212, 106221.	2.6	6
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41083	ns2-containing vacancy-ordered double perovskites for optoelectronic applications: A first-principles investigation. <i>Solid State Communications</i> , 2021, 337, 114462.	0.9	1
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41085	Vacancy effect on the structure and diffusion of a Li adatom on the 2D Janus MoSSe monolayer. <i>Computational Materials Science</i> , 2021, 198, 110687.	1.4	2
41086	Influence of vacancy defects on the thermoelectric performance of SnSe sheet. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 134, 114814.	1.3	10
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41088	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. <i>Carbon</i> , 2021, 183, 652-659.	5.4	10
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41092	Dual-atom active sites embedded in two-dimensional C <sub>2</sub> N for efficient CO <sub>2</sub> electroreduction: A computational study. <i>Journal of Energy Chemistry</i> , 2021, 61, 507-516.	7.1	69
41093	Pt atomic clusters catalysts with local charge transfer towards selective oxidation of furfural. <i>Applied Catalysis B: Environmental</i> , 2021, 295, 120290.	10.8	52
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41095	Identifying the Critical Surface Descriptors for the Negative Slopes in the Adsorption Energy Scaling Relationships via Density Functional Theory and Compressed Sensing. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9791-9799.	2.1	5
41096	Theoretically Predicted CO Adsorption and Dissociation on Ru-doped Co(100) Surfaces. <i>Applied Surface Science</i> , 2021, 572, 151476.	3.1	1
41097	Enhanced properties of covalently coupled borophene-graphene layers through fluorination and hydrogenation. <i>Applied Surface Science</i> , 2021, 562, 150150.	3.1	17
41098	Resistive switching characteristics and theoretical simulation of a Pt/a-Ta <sub>2</sub> O <sub>5</sub> /TiN synaptic device for neuromorphic applications. <i>Journal of Alloys and Compounds</i> , 2021, 877, 160204.	2.8	20
41099	Theory prediction of band structures, densities of states, mechanical and thermodynamic properties of solid solutions Ba <sub>x</sub> K <sub>1-x</sub> BiO <sub>0.92</sub> Mg <sub>0.08</sub> O <sub>3</sub> . <i>Physica B: Condensed Matter</i> , 2021, 618, 413163.	1.3	2
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41103	Functionalization of monolayer MoS <sub>2</sub> with transition metal oxide nanoclusters. <i>Physica B: Condensed Matter</i> , 2021, 619, 413245.	1.3	2
41104	A DFT+U study about agglomeration of Au atoms on reduced surface of rutile TiO <sub>2</sub> (110). <i>Materials Chemistry and Physics</i> , 2021, 271, 124944.	2.0	8
41105	Structural, electronic, magnetic, and optical properties of new TiXY (X = F and Cl; Y = S, Se and Te) Janus monolayers: A first-principles study. <i>Optik</i> , 2021, 244, 167438.	1.4	1
41106	Semiconductor-metal transition induced by combined electric field and external strain in bilayer phosphorene. <i>Solid State Communications</i> , 2021, 337, 114434.	0.9	3
41107	Ab initio predictions of magnetism and half-metallicity of (111)-surfaces of Co <sub>2</sub> CrSi full-Heusler alloy. <i>Vacuum</i> , 2021, 192, 110455.	1.6	1

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41109	Unveiling the electronic structure nature of twisted hybrid perovskites for solar cell applications: A combined experimental and theoretical study. <i>Solar Energy</i> , 2021, 227, 151-161.	2.9	3
41110	Ni diffusion in ceria lattice: A combined experimental and theoretical study. <i>Acta Materialia</i> , 2021, 219, 117252.	3.8	9
41111	Density functional theory studies of structural, electronic and optical properties of cubic 3d-transition metal nitrides. <i>Intermetallics</i> , 2021, 137, 107272.	1.8	9
41112	Insight into the mechanism of nanoparticle induced suppression of interfacial tension. <i>Journal of Molecular Liquids</i> , 2021, 339, 117177.	2.3	3
41113	Highly selective and reversible 2D PtX <sub>2</sub> (X = Au, Ag, As) hazardous gas sensors: Ab-initio study. <i>Applied Surface Science</i> , 2021, 563, 150391.	3.1	11
41114	Elastic properties of heterodesmic composite structures: The case of calcite CaCO <sub>3</sub> (space group) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Part C: Open Access, 2021, 6, 100184.	1.5	4
41115	The precipitation competition of $\beta'$ -series precipitates and $\beta''$ precipitates in Li-containing Al-Zn-Mg-Cu alloys. <i>Computational Materials Science</i> , 2021, 198, 110707.	1.4	7
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41117	Low-Dimensional Systems and Nanostructures, 2021, 134, 114855. Structural, electronic and magnetic properties of Cr <sub>m</sub> Sn and Cr <sub>m</sub> Se <sub>n</sub> nanoflakes: An ab initio investigation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 134, 114825.	1.3	5
41118	Electrical contacts in monolayer Ga <sub>2</sub> O <sub>3</sub> field-effect transistors. <i>Applied Surface Science</i> , 2021, 564, 150386.	3.1	11
41119	A Gr $\tilde{A}$ <sup>1/4</sup> neisen tensor for rutile and its application to host-inclusion systems. <i>American Mineralogist</i> , 2021, 106, 1586-1595.	0.9	6
41120	Structural and Thermo-Physical Properties of 3C-SiC: High-Temperature and High-Pressure Effects. <i>Silicon</i> , 2022, 14, 6299-6309.	1.8	8
41121	Layer effect on thermal expansion in blue phosphorene monolayer and few-layer. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 419, 127726.	0.9	2
41122	DFT approaches unraveling the surface and morphological properties of MnMoO <sub>4</sub> . <i>Applied Surface Science</i> , 2021, 567, 150882.	3.1	13
41123	Low Ru loading RuO <sub>2</sub> /(Co,Mn) <sub>3</sub> O <sub>4</sub> nanocomposite with modulated electronic structure for efficient oxygen evolution reaction in acid. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120442.	10.8	128
41124	Layered quaternary chalcogenides KMgCuSe <sub>2</sub> and KMgCuTe <sub>2</sub> with paramagnetic semiconducting behavior. <i>Journal of Alloys and Compounds</i> , 2021, 883, 160820.	2.8	4
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41128	Doping the permanent magnet CeFe <sub>11</sub> Ti with Co and Ni using ab-initio density functional methods. Physica B: Condensed Matter, 2021, 620, 413241.	1.3	3
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41130	Synergistic effects in ordered Co oxides for boosting catalytic activity in advanced oxidation processes. Applied Catalysis B: Environmental, 2021, 297, 120463.	10.8	30
41131	First-Principles investigation of Pressure-Induced structural transformations of barium borates in the BaO-B <sub>2</sub> O <sub>3</sub> -BaF <sub>2</sub> system in the range of 0–10 GPa. Computational Materials Science, 2021, 199, 110735.	1.4	5
41132	Single-atomic Pt sites anchored on defective TiO <sub>2</sub> nanosheets as a superior photocatalyst for hydrogen evolution. Journal of Energy Chemistry, 2021, 62, 1-10.	7.1	70
41133	Influence of high pressure on structural, electronic and mechanical properties of tetragonal FeH <sub>5</sub> . Solid State Communications, 2021, 338, 114483.	0.9	1
41134	Helium migration in Zr-Nb multilayers under electric field. Journal of Nuclear Materials, 2021, 555, 153133.	1.3	3
41135	Ab initio study of local lattice distortion of hexagonal closed-packed high-entropy (Mo <sub>0.25</sub> Nb <sub>0.25</sub> Ta <sub>0.25</sub> V <sub>0.25</sub> ) (Al <sub>0.5</sub> Si <sub>0.5</sub> ) <sub>2</sub> and the influence on thermodynamic property. Journal of Solid State Chemistry, 2021, 303, 122469.	1.4	3
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41138	Differential clustering of self-interstitials during Si crystal growth. Journal of Crystal Growth, 2021, 574, 126313.	0.7	1
41139	Experimental and first-principle computational exploration on biomass cellulose/magnesium hydroxide composite: Local structure, interfacial interaction and antibacterial property. International Journal of Biological Macromolecules, 2021, 191, 584-590.	3.6	2
41140	Unraveling surface functionalization of Cr <sub>2</sub> B <sub>2</sub> T <sub>2</sub> (T = OH, O, Cl, H) MBene by first-principles calculations. Computational Materials Science, 2021, 199, 110810.	1.4	14
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41142	Strain-induced structural phase transition in GeN monolayer. Applied Surface Science, 2021, 567, 150793.	3.1	9
41143	Stabilization of unstable and metastable InP native oxide thin films by interface effects. Applied Surface Science, 2021, 567, 150848.	3.1	2

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41145	Adsorption and dissociation behavior of H <sub>2</sub> O on PuH <sub>2</sub> (1 1 0) surface: A density functional theory study. <i>Applied Surface Science</i> , 2021, 566, 150733.	3.1	6
41146	Formation of ordered B structure on W(100). <i>Surface Science</i> , 2021, 713, 121906.	0.8	7
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41148	First-principles study of the surface properties of LiAl <sub>5</sub> O <sub>8</sub> : Stability and tritiated water formation. <i>Journal of Nuclear Materials</i> , 2021, 555, 153111.	1.3	5
41149	Effect of Lu <sub>2</sub> O <sub>3</sub> addition on the oxidation behavior of SiC-ZrB <sub>2</sub> composite coating at 1500 °C: Experimental and theoretical study. <i>Corrosion Science</i> , 2021, 192, 109803.	3.0	5
41150	Positron annihilation investigation of thermal cycling induced martensitic transformation in NiTi shape memory alloy. <i>Acta Materialia</i> , 2021, 220, 117298.	3.8	6
41151	Formation of 1D coordination polymers by reaction of a tetrazine ligand and PbX <sub>2</sub> (X: Br, I) salts: Spectral, structural and theoretical studies. <i>Polyhedron</i> , 2021, 208, 115440.	1.0	3
41152	Advanced analysis of laser-driven pulsed magnetic diffusion based on quantum molecular dynamics simulation. <i>Matter and Radiation at Extremes</i> , 2021, 6, 065901.	1.5	1
41153	Spinel NiFe <sub>2</sub> O <sub>4</sub> nanoparticles decorated 2D Ti <sub>3</sub> C <sub>2</sub> MXene sheets for efficient water splitting: Experiments and theories. <i>Journal of Colloid and Interface Science</i> , 2021, 602, 232-241.	5.0	63
41154	Single tungsten atom steered band-gap engineering for graphitic carbon nitride ultrathin nanosheets boosts visible-light photocatalytic H <sub>2</sub> evolution. <i>Chemical Engineering Journal</i> , 2021, 424, 130004.	6.6	39
41155	Nb-based double transition metal silicides MAX-phase: A first-principle study. <i>Chemical Physics</i> , 2021, 551, 111321.	0.9	3
41156	Regulate chemical environment to control the formation of defects on Ta <sub>3</sub> N <sub>5</sub> (1 1 0) surface: From theoretical perspectives. <i>Chemical Physics Letters</i> , 2021, 782, 139026.	1.2	2
41157	The spintronic and optoelectronic applications of substitutional doped CoS <sub>2</sub> . <i>Materials Chemistry and Physics</i> , 2021, 272, 125052.	2.0	1
41158	Enhanced piezoresponse and surface electric potential of hybrid biodegradable polyhydroxybutyrate scaffolds functionalized with reduced graphene oxide for tissue engineering. <i>Nano Energy</i> , 2021, 89, 106473.	8.2	28
41159	Effects of external electric field on adsorption behavior of organic molecules on stanene: Highly sensitive sensor devices. <i>Solid State Communications</i> , 2021, 338, 114459.	0.9	8
41160	Dual-salt-additive electrolyte enables high-voltage lithium metal full batteries capable of fast-charging ability. <i>Nano Energy</i> , 2021, 89, 106353.	8.2	90
41161	Thermal and elastic properties of binary and ternary high borate glass networks from first-principles methods. <i>Journal of Non-Crystalline Solids</i> , 2021, 571, 121059.	1.5	5

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41163	Mechanism insight into MnO for CO activation and O removal processes on Co(0001) surface: A DFT and kMC study. Applied Surface Science, 2021, 567, 150854.	3.1	13
41164	Structural change from Pbnm to R3̄̄c phase with varying Fe/Mn content in (1-x) LaFeO <sub>3</sub> .xLaMnO <sub>3</sub> solid solution leading to modifications in octahedral tilt and valence states. Journal of Alloys and Compounds, 2021, 883, 160761.	2.8	7
41165	Adsorption and spin polarization of pyridine on Fe/W(1 1 0) interface: A DFT study. Computational Materials Science, 2021, 199, 110734.	1.4	3
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41167	First-principles analysis of desired inherent photovoltaic functionalities of tetragonal CuAlX <sub>2</sub> (X=O, S, Se, Te). Journal of Materials Research and Technology, 2021, 15, 2227-2241.	1.4	3
41168	The studies of electronic structure, mechanical properties and ideal fracture behavior of U <sub>3</sub> Si <sub>1.75</sub> Al <sub>0.25</sub> : first-principle investigations. Journal of Materials Research and Technology, 2021, 15, 1356-1369.	2.6	4
41169	One- and two-dimensional structures based on gallium nitride. Journal of Solid State Chemistry, 2021, 303, 122513.	1.4	8
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41175	Vacancy-cluster and off-lattice metal-atom diffusion mechanisms in transition metal carbides. Computational Materials Science, 2021, 199, 110713.	1.4	3
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41179	Dual-doped carbon hollow nanospheres achieve boosted pseudocapacitive energy storage for aqueous zinc ion hybrid capacitors. Energy Storage Materials, 2021, 42, 705-714.	9.5	96

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41181	Electronic and optical properties of ZnSe by theoretical simulation TB-mBJ (Tran-Blaha modified Becke) Tj ETQq1 1 0.784314 rgBT /Over Science, 2021, 566, 150690.	3.1	7
41182	DFT investigation of mechanical and vibrational properties of CuTe. <i>Physica B: Condensed Matter</i> , 2021, 620, 413214.	1.3	2
41183	Ab-initio electronic structure simulations of transition metal doped Bi <sub>2</sub> Se <sub>3</sub> topological insulator. <i>Superlattices and Microstructures</i> , 2021, 159, 107033.	1.4	4
41184	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
41185	Functional group tuning of two-dimensional carbon nanosheets for boosting oxygen reduction electrocatalysis. <i>Carbon</i> , 2021, 185, 395-403.	5.4	10
41186	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
41187	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
41188	Selectively constructing nitrogen vacancy in carbon nitrides for efficient syngas production with visible light. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120496.	10.8	31
41189	Diaphite-structured nanodiamonds with six- and twelve-fold symmetries. <i>Diamond and Related Materials</i> , 2021, 119, 108573.	1.8	16
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41191	Intrinsic point defects and charge carrier trapping in monolayer BiOX (X = I, Br, and Cl). <i>Ceramics International</i> , 2021, 47, 30523-30530.	2.3	5
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41194	In-situ exsolution of Ni nanoparticles to achieve an active and stable solid oxide fuel cell anode catalyst on A-site deficient La <sub>0.4</sub> Sr <sub>0.4</sub> Ti <sub>0.94</sub> Ni <sub>0.06</sub> O <sub>3-δ</sub> . <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 103, 264-274.	2.9	17
41195	Theoretical investigation of hydrated [Lu(OH) <sub>2</sub> ] <sup>+</sup> adsorption on kaolinite(001) surface with DFT calculations. <i>Applied Surface Science</i> , 2021, 565, 150473.	3.1	20
41196	Penta-graphene as a Metal-free catalyst for CO and NO reaction -Insights from First-principles calculations. <i>Applied Surface Science</i> , 2021, 565, 150515.	3.1	2
41197	Gas (CO and NO) adsorption and sensing based on transition metals functionalized Janus MoSSe. <i>Applied Surface Science</i> , 2021, 565, 150509.	3.1	13



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41201	Pressure-induced two magnetic collapses in the ferromagnetic L1 <sub>2</sub> -Fe <sub>3</sub> Pd alloy and related elasticity and lattice dynamics anomalies. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 538, 168322.	1.0	4
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41206	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
41207	C-doped ZnS-ZnO/Rh nanosheets as multijunctioned photocatalysts for effective H <sub>2</sub> generation from pure water under solar simulating light. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120473.	10.8	45
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41209	A lattice defect-inspired leaching strategy toward simultaneous recovery and separation of value metals from spent cathode materials. <i>Waste Management</i> , 2021, 135, 40-46.	3.7	9
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41211	Effect of a ferromagnetic STM cobalt tip on a single Co-phthalocyanine molecule adsorbed on a ferromagnetic substrate. <i>Physics Open</i> , 2021, 9, 100088.	0.7	1
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41217	A comparative study of Ag doping effects on the electronic, optical, carrier conversion, photocatalytic and electrical properties of MoS <sub>2</sub> . <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 273, 115442.	1.7	7
41218	Unraveling the relationship between bulk structure and exposed surfaces and its effect on the electronic structure and photoluminescent properties of Ba <sub>0.5</sub> Sr <sub>0.5</sub> TiO <sub>3</sub> : A joint experimental and theoretical approach. <i>Materials Research Bulletin</i> , 2021, 143, 111442.	2.7	7
41219	The enhanced near-infrared photocatalytic and photothermal effects of MXene-based heterojunction for rapid bacteria-killing. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120500.	10.8	68
41220	First principles predictions of Na and K storage in layered SnSe <sub>2</sub> . <i>Applied Surface Science</i> , 2021, 566, 150522.	3.1	29
41221	Functionalized Mo <sub>2</sub> B <sub>2</sub> MBenes: Promising anchoring and electrocatalysis materials for Lithium-Sulfur battery. <i>Applied Surface Science</i> , 2021, 566, 150634.	3.1	29
41222	Investigation on phase structure and magnetic properties of high-temperature Ni-Pt-Co-Mn-Sn magnetic shape memory alloys by first-principles calculations. <i>Computational Materials Science</i> , 2021, 199, 110748.	1.4	5
41223	Reduced interstitial mobility through multicomponent alloying in bcc W. <i>Fusion Engineering and Design</i> , 2021, 172, 112745.	1.0	0
41224	Iminodiacetonitrile induce-synthesis of two-dimensional PdNi/Ni@carbon nanosheets with uniform dispersion and strong interface bonding as an effective bifunctional electrocatalyst in air-cathode. <i>Energy Storage Materials</i> , 2021, 42, 118-128.	9.5	64
41225	Phonon thermal transport properties of GaN with symmetry-breaking and lattice deformation induced by the electric field. <i>International Journal of Heat and Mass Transfer</i> , 2021, 179, 121659.	2.5	11
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41228	Modeling the half-metallicity of the CrN/GaN (1 $\hat{1}$ 1 $\hat{1}$ ) heterostructure. <i>Applied Surface Science</i> , 2021, 566, 150637.	3.1	4
41229	Synthesize of 3D-conductive supramolecular gel and derived N-doped Fe@C as high-performance lithium-ion battery anodes. <i>Vacuum</i> , 2021, 193, 110532.	1.6	2
41230	Press dependent electronic structure and optical property of Ba <sub>2</sub> Mg(PO <sub>4</sub> ) <sub>2</sub> :Eu <sup>2+</sup> . <i>Journal of Alloys and Compounds</i> , 2021, 883, 160870.	2.8	1
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41232	A new method for calculating the thermodynamic and physical properties of compounds: Application to Laves phase Fe <sub>2</sub> Mo. <i>Physica B: Condensed Matter</i> , 2021, 621, 413307.	1.3	4
41233	Elasticity of selected icy satellite candidate materials (CO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , MgSO <sub>4</sub> ·7H <sub>2</sub> O and CaSO <sub>4</sub> ·2H <sub>2</sub> O) revisited by dispersion corrected density functional theory. <i>Icarus</i> , 2021, 368, 114611.	1.1	3

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41235	First-principles calculation of the electronic properties and external force modulation of a new tetragonal structure C <sub>3</sub> N <sub>2</sub> crystal. <i>Solid State Communications</i> , 2021, 338, 114455.	0.9	3
41236	Jadeite and related species in shocked meteorites: Limitations on inference of shock conditions. <i>American Mineralogist</i> , 2022, 107, 1868-1877.	0.9	3
41237	Impact of metal/ceramic interactions on interfacial shear strength: Study of Cr/TiN using a new modified embedded-atom potential. <i>Materials and Design</i> , 2021, 210, 110120.	3.3	4
41238	V <sub>2</sub> C MXene synergistically coupling FeNi LDH nanosheets for boosting oxygen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120474.	10.8	106
41239	The optoelectronic properties of Eu/F-codoped tin oxide, an experimental and DFT study. <i>Ceramics International</i> , 2021, 47, 31756-31764.	2.3	2
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41241	Gas sensing of fibrous red phosphorene towards inorganic air pollutants: Insights from first-principles calculations. <i>Applied Surface Science</i> , 2021, 565, 150546.	3.1	7
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41244	Ab initio thermochemistry study of polymorphism in the Si <sub>2</sub> N <sub>2</sub> (NH) analog of Si <sub>2</sub> N <sub>2</sub> O. <i>Computational Materials Science</i> , 2021, 200, 110772.	1.4	1
41245	Prediction of optoelectronic features and efficiency for CuMX <sub>2</sub> (M=Ga, In; X=S, Se) semiconductors using mbj+U approximation. <i>Current Applied Physics</i> , 2021, 32, 11-23.	1.1	1
41246	Transformations of silicon clathrate Si <sub>136</sub> under high hydrogen pressure up to 11 ÅGPa. <i>Solid State Communications</i> , 2021, 340, 114492.	0.9	1
41247	Nitrogen-doped graphdiyne for efficient electrocatalytic $N_2$ reduction: A first-principles study. <i>Applied Surface Science</i> , 2021, 570, 151109.	3.1	14
41248	Analysis of electronic structure and properties of Ga <sub>2</sub> O <sub>3</sub> /CuAlO <sub>2</sub> heterojunction. <i>Applied Surface Science</i> , 2021, 568, 150826.	3.1	16
41249	Ethane dehydrogenation over the single-atom alloy catalysts: Screening out the excellent catalyst with the dual descriptors. <i>Fuel</i> , 2021, 306, 121641.	3.4	11
41250	Electronic modulation of CoP nanoarrays by Cr-doping for efficient overall water splitting. <i>Chemical Engineering Journal</i> , 2021, 425, 130651.	6.6	72
41251	Electrochemical catalytic mechanism of single transition metal atom embedded BC <sub>3</sub> monolayer for oxygen reduction and evolution reactions. <i>Chemical Engineering Journal</i> , 2021, 425, 130631.	6.6	18

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41253	Fabrication of cellulose@Mg(OH) <sub>2</sub> composite filter via interfacial bonding and its trapping effect for heavy metal ions. <i>Chemical Engineering Journal</i> , 2021, 426, 130812.	6.6	24
41254	First-principles calculations on the adhesion strength, fracture mechanism, interfacial bonding of the semi-coherent Al(1 1 1)/Al <sub>3</sub> BC(0001) interfaces. <i>Applied Surface Science</i> , 2021, 569, 150996.	3.1	28
41255	Nd <sub>2</sub> CaB <sub>10</sub> O <sub>19</sub> : A potential self-activated and self-frequency-doubling multifunctional crystal. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122558.	1.4	4
41256	A highly efficient and durable air electrode for intermediate-temperature reversible solid oxide cells. <i>Applied Catalysis B: Environmental</i> , 2021, 299, 120631.	10.8	37
41257	Effect of heterostructure engineering on electronic structure and transport properties of two-dimensional halide perovskites. <i>Computational Materials Science</i> , 2021, 200, 110823.	1.4	10
41258	Suppressing toxic intermediates during photocatalytic degradation of glyphosate by controlling adsorption modes. <i>Applied Catalysis B: Environmental</i> , 2021, 299, 120671.	10.8	18
41259	Mechanism for enhanced oil recovery from carbonate reservoirs by adding copper ions to seawater. <i>Fuel</i> , 2021, 305, 121605.	3.4	3
41260	The formation energy and interaction energy of point defects in ZrC. <i>Journal of Nuclear Materials</i> , 2021, 557, 153235.	1.3	12
41261	Fast start-up structured CuFeMg/Al <sub>2</sub> O <sub>3</sub> catalyst applied in microreactor for efficient hydrogen production in methanol steam reforming. <i>Chemical Engineering Journal</i> , 2021, 426, 130644.	6.6	13
41262	Weak ferromagnetic $\leftrightarrow$ Antiferromagnetic transition in MnFe <sub>0.25</sub> Sb. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 539, 168380.	1.0	1
41263	Dissociation of air pollutants on the uniform surface of pentagonal BeP <sub>2</sub> . <i>Applied Surface Science</i> , 2021, 570, 151061.	3.1	3
41264	Hydrogen evolution reaction on transition metal nanoparticles from first-principles. <i>Applied Surface Science</i> , 2021, 570, 151211.	3.1	7
41265	Revealing the atomic-scale structure and the fracture mechanism of the $\hat{\Gamma}_2$ -Al <sub>2</sub> O <sub>3</sub> / $\hat{\Gamma}_3$ -Fe ceramic-metal interface. <i>Journal of Alloys and Compounds</i> , 2021, 885, 161163.	2.8	11
41266	An improved oxygen reduction reaction activity and CO <sub>2</sub> -tolerance of La <sub>0.6</sub> Sr <sub>0.4</sub> Co <sub>0.2</sub> Fe <sub>0.8</sub> O <sub>3-<math>\hat{\Gamma}</math></sub> achieved by a surface modification with barium cobaltite coatings. <i>Journal of Power Sources</i> , 2021, 514, 230573.	4.0	24
41267	Theoretical study of the pressure effects on the electronic and magnetic properties of Sc <sub>3</sub> In. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 539, 168353.	1.0	0
41268	Charge localization to optimize reactant adsorption on KCu <sub>7</sub> S <sub>4</sub> /CuO interfacial structure toward selective CO <sub>2</sub> electroreduction. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120531.	10.8	25
41269	Thermodynamic evidence of the ferroelectric Berry phase in europium-based ferrobismuthite Eu <sub>2</sub> Bi <sub>2</sub> Fe <sub>4</sub> O <sub>12</sub> . <i>Journal of Alloys and Compounds</i> , 2021, 884, 161114.	2.8	4

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41271	Mechanistic understanding of support effect on the activity and selectivity of indium oxide catalysts for CO <sub>2</sub> hydrogenation. <i>Chemical Engineering Journal</i> , 2021, 426, 131767.	6.6	19
41272	Ab initio investigations on metal ion pre-intercalation strategy of layered V <sub>2</sub> O <sub>5</sub> cathode for magnesium-ion batteries. <i>Applied Surface Science</i> , 2021, 569, 150983.	3.1	11
41273	Segregation of Ni and Si to coherent bcc Fe-Cu interfaces from density functional theory. <i>Journal of Nuclear Materials</i> , 2021, 556, 153185.	1.3	7
41274	Synthesis and characterization of new indium gallium selenides of the InSe-GaSe system. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122569.	1.4	1
41275	Single-step synthesis of oxygen-doped hollow porous graphitic carbon nitride for photocatalytic ciprofloxacin decomposition. <i>Chemical Engineering Journal</i> , 2021, 425, 130502.	6.6	41
41276	Rational design of intermetallic compound catalysts for propane dehydrogenation from a descriptor-based microkinetic analysis. <i>Journal of Catalysis</i> , 2021, 404, 32-45.	3.1	15
41277	Photocatalytic production of H <sub>2</sub> O <sub>2</sub> from water and dioxygen only under visible light using organic polymers: Systematic study of the effects of heteroatoms. <i>Applied Catalysis B: Environmental</i> , 2021, 299, 120666.	10.8	22
41278	Density functional theory calculations of the thermodynamic and kinetic properties of point defects in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"} \rangle \langle \text{mml:mi} \hat{1}^2 \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle \text{-U}$ . <i>Journal of Nuclear Materials</i> , 2021, 557, 153238.	1.3	1
41279	Supercapattery electrode materials by Design: Plasma-induced defect engineering of bimetallic oxyphosphides for energy storage. <i>Journal of Colloid and Interface Science</i> , 2021, 603, 478-490.	5.0	30
41280	Exploring reaction mechanism of CO oxidation over SrCoO <sub>3</sub> catalyst: A DFT study. <i>Applied Surface Science</i> , 2021, 570, 151234.	3.1	11
41281	Exploring the structural, elastic, lattice dynamical stability and thermoelectric properties of semiconducting novel quaternary Heusler alloy LiScPdPb. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122601.	1.4	16
41282	Sc <sub>2</sub> CO-MXene/h-BN heterostructure with synergetic effect as an anchoring and catalytic material for lithium-sulfur battery. <i>Journal of Alloys and Compounds</i> , 2021, 887, 161273.	2.8	15
41283	High-pressure study by Raman spectroscopy and DFT calculations of L-tyrosine hydrobromide crystal. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120142.	2.0	2
41284	Role of water on ozonation of cinnamaldehyde to benzaldehyde under Ca(OH) <sub>2</sub> catalysis: A combined in situ DRIFTS and DFT study. <i>Applied Surface Science</i> , 2021, 569, 151071.	3.1	11
41285	Hydrogen storage properties of hexagonal C14 Laves phase Cu <sub>2</sub> Cd: A DFT study. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122560.	1.4	7
41286	Ultrahigh thermal conductivity in hexagonal BC <sub>6</sub> N- An efficient material for nanoscale thermal management- A first principles study. <i>Computational Materials Science</i> , 2021, 200, 110773.	1.4	8
41287	Bayesian automated weighting of aggregated DFT, MD, and experimental data for candidate thermodynamic models of aluminum with uncertainty quantification. <i>Materialia</i> , 2021, 20, 101216.	1.3	4

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41290	Structure, mechanical and phonon stability of the Th-Sn system from ab initio. Journal of Nuclear Materials, 2021, 556, 153187.	1.3	1
41291	Stability and electronic properties of the graphene-supported FeO nanostructures including clusters and monolayer. Applied Surface Science, 2021, 569, 150976.	3.1	4
41292	ABX <sub>6</sub> Monolayers: A new Dirac material family containing high Fermi velocities and topological properties. Applied Surface Science, 2021, 570, 151237.	3.1	11
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41376	Existence of spin-polarized Dirac cone in Sc <sub>2</sub> CrB <sub>4</sub> monolayer PC3: A promising material for environmentally toxic nitrogen-containing multi gases. <i>Journal of Hazardous Materials</i> , 2022, 422, 126761.	1.3	4
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44087	Interfacial-confined coordination to single-atom nanotherapeutics. <i>Nature Communications</i> , 2022, 13, 91.	5.8	49
44088	Influence of Isostatic Pressure on the Elastic and Electronic Properties of K <sub>2</sub> SiF <sub>6</sub> :Mn <sup>4+</sup> . <i>Materials</i> , 2022, 15, 613.	1.3	4
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44093	<i>Ab initio</i> surface free energies of tungsten with full account of thermal excitations. <i>Physical Review B</i> , 2022, 105, .	1.1	10
44094	Stability and electronic properties of monolayer and multilayer structures of group-IV elements and compounds of complementary groups in biphenylene network. <i>Physical Review B</i> , 2022, 105, .	1.1	22
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44099	First Principles Investigation of Binary Chromium Carbides Cr <sub>7</sub> C <sub>3</sub> , Cr <sub>3</sub> C <sub>2</sub> and Cr <sub>23</sub> C <sub>6</sub> : Electronic Structures, Mechanical Properties and Thermodynamic Properties under Pressure. <i>Materials</i> , 2022, 15, 558.	1.3	18
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44113	A computational study of the interaction of oxygenates with the surface of rutile TiO <sub>2</sub> (110). Structural and electronic trends. <i>Journal of Physics Condensed Matter</i> , 2022, , .	0.7	3
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44136	Strain-Tunable Carrier Mobility of Fe-Doped GaN: A First-Principles Study. <i>SSRN Electronic Journal</i> , 0, .	0.4	0
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44177	The joint effect of spin-orbit coupling and atomistic disorder on bandgap evolution in inorganic CsSn <sub>1-x</sub> Pb <sub>x</sub> I <sub>3</sub> mixed perovskite. <i>Journal of Applied Physics</i> , 2022, 131, 055107.	1.1	1
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44186	The phase diagrams of beryllium and magnesium oxide at megabar pressures. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 144003.	0.7	3
44187	First-Principles Study of Transition Metal Ti-Based MXenes (Ti <sub>2</sub> MC <sub>2</sub> T <sub>x</sub> and T <sub>j</sub> ETQq <sub>1</sub> 1 0.784314 rgBT /Overlock 10 Tf 50 222 T <sub>d</sub> (M <sub>2</sub> /sub>2.4		
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44188	Unveiling the effect of interstitial dopants on CO <sub>2</sub> activation over CsPbBr <sub>3</sub> catalyst for efficient photothermal CO <sub>2</sub> reduction. <i>Chemical Engineering Journal</i> , 2022, 435, 135071.	6.6	35
44189	Surface half metallicity and thermodynamic stability of 001-plane Ti <sub>2</sub> XSi (X=Mn, Co) Heusler alloys (HAs): A DFT approach. <i>Surfaces and Interfaces</i> , 2022, 28, 101602.	1.5	1
44190	Okra-like hollow Cu <sub>0.15</sub> -CoP/Co <sub>3</sub> O <sub>4</sub> @CC nanotube arrays catalyst for overall water splitting. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 7168-7179.	3.8	3
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44208	Helium impurities and interactions in lithium. <i>Computational Materials Science</i> , 2022, 204, 111176.	1.4	0
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44211	NJOY+NCrystal: An open-source tool for creating thermal neutron scattering libraries with mixed elastic support. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2022, 1027, 166227.	0.7	14
44212	Effects of nanostructures on the hydrogen storage properties of MgH <sub>2</sub> - A first principles study. <i>Computational Condensed Matter</i> , 2022, 30, e00643.	0.9	8
44213	Janus RuTe <sub>2</sub> monolayer: <i>Computational Condensed Matter</i> , 2022, 30, e00644.	0.9	8
44214	Enhanced visible light photocatalytic activity of KTaO <sub>3</sub> (Se,V): DFT investigation. <i>Computational Condensed Matter</i> , 2022, 30, e00648.	0.9	1
44215	Quantum spin Hall insulating phase and van Hove singularities in Zintl single-quintuple-layer AM <sub>2</sub> X <sub>2</sub> (A = Ca, Sr, or Ba; M = Zn or Cd; X = Sb or Bi) family. <i>Applied Physics Reviews</i> , 2022, 9, .	5.5	17
44216	Boron carbide under torsional deformation: Evidence of the formation of chain vacancies in the plastic regime. <i>Acta Materialia</i> , 2022, 226, 117553.	3.8	5
44217	Rational design of microporous biochar based on ion exchange using carboxyl as an anchor for high-efficiency capture of gaseous p-xylene. <i>Separation and Purification Technology</i> , 2022, 286, 120402.	3.9	7
44218	An optimum thermoelectric figure of merit using Ge <sub>2</sub> Se <sub>2</sub> monolayer: An ab-initio approach. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 138, 115060.	1.3	5
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44221	Adsorption of metal atoms on two-dimensional BC <sub>3</sub> and AlC <sub>3</sub> nanosheets: Computational studies. <i>Chemical Physics Letters</i> , 2022, 792, 139403.	1.2	5
44222	Effect of native point defects on the photocatalytic performance of ZnIn <sub>2</sub> S <sub>4</sub> . <i>Physica B: Condensed Matter</i> , 2022, 630, 413674.	1.3	2
44223	Effects of strain and electric field on electronic and optical properties of monolayer GeX (X = Te, Se, S). <i>Physica B: Condensed Matter</i> , 2022, 630, 413674.	1.3	2
44224	Evidence of strong correlation and magnetotransport scaling in YbFe <sub>2</sub> As <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2022, 630, 413696.	1.3	0
44225	Role of Ni on the helium diffusion, stability and energetics of vacancy-type clusters in Fe <sub>6.25</sub> Cr <sub>3.13</sub> Ni (at.%) ternary alloys: From first-principles. <i>Computational Materials Science</i> , 2022, 205, 111213.	1.4	1
44226	Structure-compressibility correlation among MoB <sub>x</sub> . <i>Journal of Physics and Chemistry of Solids</i> , 2022, 163, 110599.	1.9	4
44227	Improving performance of zinc-manganese battery via efficient deposition/dissolution chemistry. <i>Energy Storage Materials</i> , 2022, 46, 165-174.	9.5	32

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44229	Ab initio molecular dynamics investigation of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"> \langle \text{mml:mi} \hat{I}^3 \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle \text{-(U,Zr)} \rangle$ structural and thermal properties as a function of temperature and composition. <i>Journal of Nuclear Materials</i> , 2022, 561, 153523.	1.3	6
44230	Narrow gap electronic structure and thermoelectric performance of p-type ErMSb (M = Ni, Pd) half Heusler compounds. <i>Physica B: Condensed Matter</i> , 2022, 631, 413709.	1.3	4
44231	Mechanism of CO <sub>2</sub> hydrogenation to methanol on the W-doped Rh(111) surface unveiled by first-principles calculation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 638, 128332.	2.3	10
44232	Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. <i>Computational Materials Science</i> , 2022, 205, 111163.	1.4	5
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44279	Chemical-Mechanical Effects in Ni-Rich Cathode Materials. Chemistry of Materials, 2022, 34, 1509-1523.	3.2	34
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44482	Prediction the Structural, Electronic, Elastic and Dynamical Properties of $\text{LiAlGe}$ and $\text{LiInGe}$ Half-Heusler Crystals by Density Functional Theory. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

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44935	Theoretical insights into the diverse and tunable charge transport behavior of stilbene-based single-molecule junctions. <i>Chemical Physics</i> , 2022, 556, 111478.	0.9	2
44936	A First-Principles Study of the Structural, Magnetic, Optical Properties and Doping Effect in Chromium Arsenide. <i>Physica Status Solidi (B): Basic Research</i> , 0, , 2200062.	0.7	0
44937	Multiscale Characterization of the Influence of the Organic-Inorganic Interface on the Dielectric Breakdown of Nanocomposites. <i>ACS Nano</i> , 2022, 16, 6744-6754.	7.3	15
44938	Oxygen Vacancy Formation and Migration within the Antiphase Boundaries in Lanthanum Scandate-Based Oxides: Computational Study. <i>Materials</i> , 2022, 15, 2695.	1.3	0
44939	Sampling lattices in semi-grand canonical ensemble with autoregressive machine learning. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	3
44940	Metal-Doped PdH(111) Catalysts for CO <sub>2</sub> Reduction. <i>ChemSusChem</i> , 2022, 15, .	3.6	7
44941	Adsorption Behavior of Pd-Doped PtS <sub>2</sub> Monolayer Upon SF <sub>6</sub> Decomposed Species and the Effect of Applied Electric Field. <i>IEEE Sensors Journal</i> , 2022, 22, 6764-6771.	2.4	22
44942	Unsupervised machine learning to classify crystal structures according to their structural distortion: A case study on Li-argyrodite solid-state electrolytes. <i>Energy and AI</i> , 2022, 9, 100159.	5.8	3
44943	Theoretical insight on dopamine, ascorbic acid and uric acid adsorption on graphene as material for biosensors. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113705.	1.1	1
44944	Bonding character of intermediates in on-surface Ullmann reactions revealed with energy decomposition analysis. <i>Journal of Computational Chemistry</i> , 2023, 44, 179-189.	1.5	2
44945	First-Principles Computational Exploration of Thermoelectric Properties of Bulk-GaN and Monolayer-GaN. <i>Journal of Electronic Materials</i> , 2022, 51, 3317-3328.	1.0	6
44946	Identification of potential metal oxides for NO <sub>2</sub> capture: A density functional theory study. <i>Journal of the American Ceramic Society</i> , 2022, 105, 5299-5308.	1.9	3
44947	First principles study of Li adsorption properties of a Borophene based hybrid 2D material B5Se. <i>Applied Surface Science Advances</i> , 2022, 8, 100218.	2.9	1
44948	First principles design of 2 dimensional Nickel dichalcogenide Janus materials NiXY (X,Y= S,Se,Te). <i>Computational Materials Science</i> , 2022, 206, 111278.	1.4	7
44949	Hydrogen adsorption behavior on AXenes Na <sub>2</sub> N and K <sub>2</sub> N: a first-principles study. <i>Materials Research Express</i> , 2022, 9, 045501.	0.8	4
44950	Ab-initio method to investigate perovskites BiXO <sub>3</sub> (X = Be, Ca, Mg, Na, K, Li) for spintronics applications. <i>Solid State Sciences</i> , 2022, 126, 106839.	1.5	9
44951	Spontaneous Magnetic Skyrmions in Single-Layer CrInX <sub>3</sub> (X = Te, Se). <i>Nano Letters</i> , 2022, 22, 3440-3446.	4.5	34
44952	Chalcogen Atom-Doped Graphene and Its Performance in N <sub>2</sub> Activation. <i>Surfaces</i> , 2022, 5, 228-237.	1.0	0

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44954	Design Principles for Metastable Standing Molecules. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6880-6891.	1.5	2
44955	First-Principles Calculations on Lateral Heterostructures of Armchair Graphene Antidot Nanoribbons for Band Alignment. <i>ACS Applied Nano Materials</i> , 2022, 5, 5699-5708.	2.4	1
44956	First-principles investigation of equilibrium phase, mechanical and thermodynamic properties of the Nowotny TM <sub>5</sub> Si <sub>3</sub> C ternary phase. <i>Ceramics International</i> , 2022, 48, 20438-20445.	2.3	49
44957	A Defect Engineered Electrocatalyst that Promotes High-Efficiency Urea Synthesis under Ambient Conditions. <i>ACS Nano</i> , 2022, 16, 8213-8222.	7.3	109
44958	Controllable repairing the single vacancies of BC <sub>3</sub> monolayer using CO and BF molecules: A first-principles study. <i>Results in Physics</i> , 2022, 35, 105365.	2.0	5
44959	Cobalt-regulation-induced dual active sites in Ni <sub>2</sub> P for hydrazine electrooxidation. <i>Chinese Journal of Catalysis</i> , 2022, 43, 1131-1138.	6.9	9
44960	Ultrahard BC <sub>5</sub> – An efficient nanoscale heat conductor through dominant contribution of optical phonons. <i>Computational Materials Science</i> , 2022, 206, 111276.	1.4	1
44961	Lead-Free Alloyed Double Perovskites: An Emerging Class of Materials for Optoelectronic Applications. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6753-6760.	1.5	5
44962	Fast and Simple Ag/Cu Ion Exchange on Cu Foil for Anode-Free Lithium-Metal Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 17454-17460.	4.0	21
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44964	Predicted superior hydrogen evolution activities of MoC via surface dopant. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 13664-13673.	3.8	7
44965	Calculation of the vibrational spectra of CdSe and CdS crystals with zinc blende structure. <i>Materials Today: Proceedings</i> , 2022, 62, 5812-5818.	0.9	2
44966	Accurate and efficient approximate quasiparticle DFT+U/2 band structure calculations of transition metal oxide perovskites. <i>Physica Status Solidi (B): Basic Research</i> , 0, , .	0.7	0
44967	Enhancement of the lattice thermal conductivity of two-dimensional functionalized MXenes by inversion symmetry breaking. <i>Physical Review B</i> , 2022, 105, .	1.1	14
44968	Novel polymerization of nitrogen in zinc nitrides at high pressures. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 235702.	0.7	3
44969	Ferroelectricity coexisted with p-orbital ferromagnetism and metallicity in two-dimensional metal oxynitrides. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	20
44970	Equilibrium phase diagrams of isostructural and heterostructural two-dimensional alloys from first principles. <i>IScience</i> , 2022, 25, 104161.	1.9	1

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44972	Effects of Mono-Vacancies of Oxygen and Manganese on the Properties of the MnO <sub>2</sub> /Graphene Heterostructure. <i>Materials</i> , 2022, 15, 2731.	1.3	2
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44975	Simulation of thermodynamic properties of magnetic transition metals from an efficient tight-binding model: The case of cobalt and beyond. <i>Physical Review B</i> , 2022, 105, .	1.1	1
44976	Nitrogen-vacancy defects in germanium. <i>AIP Advances</i> , 2022, 12, 045110.	0.6	2
44977	Theoretical study on the influence of Cr, Mo, and W alloying additions on the helium behavior in nickel. <i>Journal of Nuclear Materials</i> , 2022, 565, 153720.	1.3	5
44978	Correlation between $d$ -orbital bandwidth and local coordination environment in RE <sub>2</sub> SiO <sub>5</sub> compounds with implications in minimizing the coefficient of thermal expansion anisotropy (RE = Sc, Y, La). <i>AIP Advances</i> , 2022, 12, 045012.	0.6	1
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44981	Possibility of Chemisorption for Benzene on Stepped Surface of Coinage Metals. <i>Surface Science</i> , 2022, , 122084.	0.8	0
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44990	Superassembly of Surface-Enriched Ru Nanoclusters from Trapping—Bonding Strategy for Efficient Hydrogen Evolution. <i>ACS Nano</i> , 2022, 16, 7993-8004.	7.3	54
44991	Comprehensive Modulation of Conductance Anisotropy in Low-Symmetry $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll" \rangle \langle \text{mml:mrow} \langle \text{mml:mi} \rangle \text{Re} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \text{mathvariant="normal"} \rangle \text{S} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$	1.5	2
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44997	Structures of boundaries and corners of fully-closed hexagonal domains in HVPE-AlN film. <i>Acta Materialia</i> , 2022, 229, 117838.	3.8	0
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45004	Ohmic contact in graphene and hexagonal III-V monolayer (GaP, GaAs, InP, and InAs) van der Waals heterostructures: Role of electric field. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022, 433, 128029.	0.9	4
45005	Correlation-assisted Peierls gap in divalent metal ion (Zn <sup>2+</sup> , Cd <sup>2+</sup> , Mg <sup>2+</sup> , Ca <sup>2+</sup> , Sr <sup>2+</sup> and Ba <sup>2+</sup> ) doped M-VO <sub>2</sub> : First principle analysis. <i>Solid State Communications</i> , 2022, 347, 114710.	0.9	2
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45041	High performance Li-ion capacitor based on novel carbon-coated chalcogenide anode. Journal of Energy Storage, 2022, 50, 104251.	3.9	12
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#	Determination of thermodynamic growth conditions for a high-efficiency Cu	IF	CITATIONS
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45062	Property changes in two-dimensional electride bilayers through compression, sliding, and twisting. <i>Applied Surface Science</i> , 2022, 586, 152596.	3.1	4
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45078	First-principles study of optoelectronic and thermoelectric properties of LiCaX (X=N, P and As) half-Heusler semiconductors. <i>Journal of Solid State Chemistry</i> , 2022, 310, 123020.	1.4	17

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45738	Achieving enhanced high-temperature mechanical properties in Mg-Nd-Sm-Zn-Ca-Zr alloy by Ag addition. <i>Materials Today Communications</i> , 2022, 31, 103666.	0.9	5
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45747	Exploring original properties of GaN-BN alloys using high-throughput ab initio computation. <i>Optik</i> , 2022, 261, 169166.	1.4	0
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45754	First principles electronic structure, molecular dynamics, and optical properties of GaOF monolayer without and with defects. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2022, 281, 115736.	1.7	4
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45760	Oxidation mechanism of arsenopyrite under alkaline conditions: Experimental and theoretical analyses. <i>Journal of Cleaner Production</i> , 2022, 358, 131987.	4.6	9



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45771	Changes in electronic structure of graphene by adsorption of low melamine coverages. <i>Surface Science</i> , 2022, 723, 122120.	0.8	2
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45780	Chemically anchoring molybdenum atoms onto micropore-rich VN nanosheet for boosted nitrogen electro-fixation via hydrogen bonds. <i>Chemical Engineering Journal</i> , 2022, 446, 136915.	6.6	4
45781	First-principles screening of Pt doped Ti <sub>2</sub> CNL (Nâ€³=â€³O, S and Se, Lâ€³=â€³F, Cl, Br and I) as high-performance catalysts for ORR/OER. <i>Applied Surface Science</i> , 2022, 596, 153574.	3.1	31
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45792	Boosting the Fischer-Tropsch synthesis performances of cobalt-based catalysts via geometric and electronic engineering: Construction of hollow structures. <i>Applied Catalysis B: Environmental</i> , 2022, 313, 121469.	10.8	9
45793	Boosting the Fischer-Tropsch synthesis performances of cobalt-based catalysts via geometric and electronic engineering: Construction of hollow structures. <i>Applied Catalysis B: Environmental</i> , 2022, 313, 121469.	10.8	9
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45796	Study on the Electronic Structure and Optical Properties of Two-dimensional Monolayer MoSi <sub>2</sub> X <sub>4</sub> (X=N, P, As). <i>Acta Chimica Sinica</i> , 2022, 80, 510.	0.5	3

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46259	Screening and Design of Bipolar Magnetic-Semiconducting Monolayers and Heterostructures. <i>ACS Applied Electronic Materials</i> , 0, , .	2.0	3
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46954	First-principles study on electronic and optical properties of van der Waals heterostructures stacked by g-ZnO and Janus-WSSe monolayers. <i>Applied Surface Science</i> , 2022, 604, 154620.	3.1	10
46955	The structural, elastic, electronic, magnetic and optical properties of SrNiO <sub>3</sub> perovskite: A DFT and DFT+U study. <i>Results in Physics</i> , 2022, 41, 105920.	2.0	4
46956	Topological properties of CsCl type superconducting materials. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022, , 128385.	0.9	1
46957	Transition metal atoms anchored on nitrogen-doped $\hat{1}\pm$ -arsenene as efficient electrocatalysts for nitrogen electroreduction reaction. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 29781-29793.	3.8	7
46958	Electronic Structure-Based Modeling of Dislocation Motion and Its Application to Nanoscale Mechanics. <i>Zairyo/Journal of the Society of Materials Science, Japan</i> , 2022, 71, 660-665.	0.1	0
46959	Sticking coefficient and Si/C ratio of silicon carbide growth species on reconstructed $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 4 \langle \text{mml:mn} \rangle \langle \text{mml:mi} \text{ mathvariant="bold"} \rangle \text{H} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \text{ linebreak="goodbreak" linebreakstyle="after"} \rangle \hat{\sim} \langle \text{mml:mo} \rangle \langle \text{mml:mi} \text{ mathvariant="bold"} \rangle \text{S} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \text{ mathvariant="bold"} \rangle \text{i} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \text{ mathvariant="bold"} \rangle \text{C} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle$		

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46962	Effective Hydrogenation Strategies to Boost Efficiency over 20% for Crystalline Silicon Solar Cell with Al <sub>2</sub> O <sub>3</sub> /Cu <sub>2</sub> O Passivating Contact. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	8
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46968	Laser damage mechanism and threshold improvement of nonlinear optical La <sub>3</sub> Ga <sub>5.5</sub> Nb <sub>0.5</sub> O <sub>14</sub> crystal for a mid-infrared high-intensity laser. <i>Optical Materials Express</i> , 2022, 12, 3449.	1.6	3
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46972	DFT calculations of 2D graphene like ZnS:Mn sheet for RESOLFT microscopic applications. <i>Journal of Computational Electronics</i> , 2022, 21, 1191-1201.	1.3	1
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46974	A superhard orthorhombic carbon allotrope. <i>Chinese Journal of Physics</i> , 2022, 79, 409-419.	2.0	10
46975	Introducing Brønsted acid sites to accelerate the bridging-oxygen-assisted deprotonation in acidic water oxidation. <i>Nature Communications</i> , 2022, 13, .	5.8	42
46976	Hybrid Density Functional Investigation of Cu Doping Impact on the Electronic Structures and Optical Characteristics of TiO <sub>2</sub> for Improved Visible Light Absorption. <i>Materials</i> , 2022, 15, 5645.	1.3	7
46977	Theoretical investigation of charged vacancies and clusters in UXO <sub>2</sub> (X = La, Ce, Pu, Am). <i>Journal of Applied Physics</i> , 2022, 132, .	1.1	1
46978	Ground-State Properties of Metallic Solids from Ab Initio Coupled-Cluster Theory. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 7497-7503.	2.1	11
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48036	Switchable single-molecule electronic and thermoelectric device induced by light in a designed diarylethene molecule. <i>Physical Review B</i> , 2022, 106, .	1.1	4
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48042	Nucleation of Single-Wall Carbon Nanotubes from Faceted Pt Catalyst Particles Revealed by <i>in Situ</i> Transmission Electron Microscopy. <i>ACS Nano</i> , 2022, 16, 16574-16583.	7.3	5
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48483	Combined DFT, SCAPS-1D, and wxAMPS frameworks for design optimization of efficient Cs <sub>2</sub> BiAg <sub>6</sub> -based perovskite solar cells with different charge transport layers. <i>RSC Advances</i> , 2022, 12, 34850-34873.	1.7	92
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48508	Photocatalytic reductive carboxylation of terminal alkynes with CO <sub>2</sub> using heterostructured ZIF-7/BiOBr under visible-light illumination. <i>Journal of CO<sub>2</sub> Utilization</i> , 2023, 67, 102334.	3.3	5
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49561	Theoretical and mechanistic insights into control factor-assisted CO2 mineralization with olivine. <i>Journal of Industrial and Engineering Chemistry</i> , 2023, 122, 241-250.	2.9	0

#	Article Title	IF	CITATIONS
49562	Phonons in binary compounds $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si17.svg" display="inline" id="d1e1274"} \rangle \langle \text{mml:mi} \rangle A \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle B_i \langle \text{mml:math} \rangle T_j$ ETQq0 0 0 rgBT /Overlock 10 Tf	0.9	3
49563	Unraveling the role of Fe <sub>5</sub> C <sub>2</sub> in CH <sub>4</sub> formation during CO <sub>2</sub> hydrogenation over hydrophobic iron catalysts. Applied Catalysis B: Environmental, 2023, 327, 122449.	10.8	7
49564	Ti-decorated nitrogen-rich BeN <sub>4</sub> monolayer for reversible hydrogen storage: DFT investigations. Applied Surface Science, 2023, 622, 156806.	3.1	6
49565	New insights into the co-adsorption behavior of H <sub>2</sub> O and H <sub>2</sub> on defective PuH <sub>2</sub> (100), (110), and (111) surfaces from first-principles study. Vacuum, 2023, 212, 112044.	1.6	1
49566	Zn-doped nickel iron (oxy)hydroxide nanocubes passivated by polyanions with high catalytic activity and corrosion resistance for seawater oxidation. Journal of Energy Chemistry, 2023, 81, 82-92.	7.1	6
49567	Prediction of novel final phases in aged uranium-niobium alloys. Journal of Nuclear Materials, 2023, 579, 154394.	1.3	2
49568	Investigating the effect of Al, Mo or Mn addition to CoCrFeNi entropy alloys on the interface binding properties of WC/HEA cemented carbides. Materials Today Communications, 2023, 35, 105891.	0.9	3
49569	Theoretical study on structural transformation and mechanical properties of Ni <sub>3</sub> Ti <sub>1-x</sub> Nbx. Results in Materials, 2023, 18, 100387.	0.9	0
49570	First-principles study of Xe behavior in $\hat{\Gamma}$ -UZr <sub>2</sub> . Journal of Nuclear Materials, 2023, 579, 154387.	1.3	1
49571	First-principles study on electronic and optical properties of Cu <sub>2</sub> CoGeS <sub>4</sub> for photovoltaic conversion and photocatalytic applications. Journal of Applied Physics, 2023, 125, 155301.	2.7	4
49572	First-principles calculations to investigate structural, electronics, optical, and mechanical properties of Bi-based novel fluoroperovskites TBiF <sub>3</sub> (T = Hg, Xe) for optoelectronic applications. Materials Science in Semiconductor Processing, 2023, 160, 107399.	1.9	13
49573	Probing the structural, electronic and optical properties of Cs <sub>2</sub> Ag <sub>1-x</sub> Na <sub>x</sub> InCl <sub>6</sub> lead-free double perovskite from first principles. Journal of Solid State Chemistry, 2023, 322, 123913.	1.4	4
49574	CALPHAD aided mechanical properties screening in full composition space of NbC-TiC-VC-ZrC ultra-high temperature ceramics. International Journal of Refractory Metals and Hard Materials, 2023, 113, 106191.	1.7	3
49575	Two-dimensional van der Waals layered VSi <sub>2</sub> N <sub>4</sub> as anode materials for alkali metal (Li, Na and K) ion batteries. Journal of Physics and Chemistry of Solids, 2023, 178, 111339.	1.9	3
49576	Elucidating the dissociative and associative mechanisms on the surface-anchored Fe <sub>3</sub> cluster under the effect of external electric field. Applied Surface Science, 2023, 623, 157021.	3.1	1
49577	Atomistic mechanism of $\hat{\Gamma}$ - $\hat{\Gamma}$ transformation in Al-Zn-Mg-Cu alloys. Scripta Materialia, 2023, 231, 115474.	2.6	6
49578	Significance of different dopamine species as reducing agents of graphene oxide: Fundamental aspects. Surface Science, 2023, 732, 122285.	0.8	1
49579	Defect engineered Janus MoSiGeN <sub>4</sub> as highly efficient electrocatalyst for hydrogen evolution reaction. Applied Surface Science, 2023, 622, 156894.	3.1	9

#	ARTICLE	IF	CITATIONS
49580	Study of the brittleness mechanism of aluminum/steel laser welded joints with copper and vanadium interlayers. <i>Optics and Laser Technology</i> , 2023, 163, 109319.	2.2	3
49581	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
49582	Dual functional effect of oxygen vacancies and depolarity shield embedded NiCo <sub>2</sub> O <sub>4</sub> cathode in lithium sulfur battery. <i>Applied Surface Science</i> , 2023, 622, 156939.	3.1	3
49583	T-BN nanosheets as High-capacity anode for Li- and Na-Ion Batteries: An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114105.	1.1	1
49584	Data-driven design of Ni-based turbine disc superalloys to improve yield strength. <i>Journal of Materials Science and Technology</i> , 2023, 155, 175-191.	5.6	4
49585	Influence of Pt or Au doping on improving the detection of CO by ZnO: A first-principles calculations study. <i>Chemical Physics</i> , 2023, 570, 111908.	0.9	0
49586	Atomic-scale engineering of cation vacancies in two-dimensional unilamellar metal oxide nanosheets for electricity generation from water evaporation. <i>Nano Energy</i> , 2023, 110, 108348.	8.2	8
49587	Multi-functional lead-free Ba <sub>2</sub> X <sub>2</sub> SbO <sub>6</sub> (X=Al, Ga) double perovskites with direct bandgaps for photocatalytic and thermoelectric applications: A first principles study. <i>Materials Today Communications</i> , 2023, 35, 105617.	0.9	6
49588	Unexpectedly spontaneous water dissociation on graphene oxide supported by copper substrate. <i>Journal of Colloid and Interface Science</i> , 2023, 642, 112-119.	5.0	3
49589	A revisit to the role of Mo in an MP35N superalloy: An experimental and theoretical study. <i>Journal of Materials Science and Technology</i> , 2023, 157, 60-70.	5.6	2
49590	Length-dependent high-frequency response of aromatic and aliphatic molecules: predictions from first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 178, 111343.	1.9	3
49591	Computational investigation on CO <sub>2</sub> capturing capacity of N-doped and Na-decorated Graphdiyne. <i>Fuel</i> , 2023, 345, 128169.	3.4	3
49592	Unravelling the role of metal-metal oxide interfaces of Cu/ZnO/ZrO <sub>2</sub> /Al <sub>2</sub> O <sub>3</sub> catalyst for methanol synthesis from CO <sub>2</sub> : Insights from experiments and DFT-based microkinetic modeling. <i>Applied Catalysis B: Environmental</i> , 2023, 332, 122743.	10.8	8
49593	New Janus structure photocatalyst having widely tunable electronic and optical properties with strain engineering. <i>Journal of Materials Science and Technology</i> , 2023, 155, 142-147.	5.6	4
49594	Evaluating the potential of planar h-BSb monolayer as anode materials for sodium-ion batteries from first principles methods. <i>Journal of Energy Storage</i> , 2023, 64, 107260.	3.9	4
49595	Unusual mechanical properties of CO <sub>2</sub> @V: Auxetic potential in a high-pressure polymorph of carbon dioxide. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 178, 111349.	1.9	0
49596	Nonlinear optical crystals KPb <sub>3</sub> (3-C <sub>5</sub> H <sub>4</sub> NCOO)2Br <sub>5</sub> and KPb <sub>3</sub> (3-C <sub>5</sub> H <sub>4</sub> NCOO)2Cl <sub>3</sub> Br <sub>2</sub> with new Pb-centered nitrogen-halide polyhedrons obtained by the halide anionic substitution. <i>Journal of Alloys and Compounds</i> , 2023, 951, 169945.	2.8	0
49597	Observation of low thermal expansion behavior and weak thermal anisotropy in M3A2C phases. <i>Journal of Materials Science and Technology</i> , 2023, 154, 210-216.	5.6	2

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49598	Electronic structure and oxygen vacancy tuning of Co & Ni co-doped W18O49 nanourchins for efficient TEA gas sensing. <i>Chemical Engineering Journal</i> , 2023, 465, 142815.	6.6	16
49599	Cu4@C2N for effective electrochemical CO2 reduction and intermediates dependent adsorption behaviours: A computational study. <i>Applied Surface Science</i> , 2023, 626, 157126.	3.1	4
49600	Experimental and computational study on the C15 phase structure stability of Y Ni2-Mn system. <i>Journal of Alloys and Compounds</i> , 2023, 952, 169632.	2.8	1
49601	Design, synthesis and investigating the interaction of novel s-triazine collector with pyrite surface: A DFT-D3+U and experimental studies. <i>Surfaces and Interfaces</i> , 2023, 38, 102820.	1.5	1
49602	Introducing dual metal centers in high purity pyrrolic-N for superior oxygen reduction reaction. <i>Carbon</i> , 2023, 209, 118031.	5.4	5
49603	Low-temperature phase transitions and reorientational dynamics studied by 11B NMR in glassy crystal ortho-carborane. <i>Journal of Non-Crystalline Solids: X</i> , 2023, 18, 100180.	0.5	0
49604	Infrared and Raman vibrational modelling of $\hat{I}^2$ -C2S and C3S compounds. <i>Cement and Concrete Research</i> , 2023, 169, 107162.	4.6	7
49605	Understanding ZnO surface defects from first-principles simulation. <i>Surface Science</i> , 2023, 732, 122272.	0.8	1
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49607	Electronic excitation induced non-thermal phase transition of tungsten. <i>Journal of Alloys and Compounds</i> , 2023, 952, 170087.	2.8	1
49608	The electronic, optical, and vibrational properties of Ag <sub>3</sub> X (X = S, Se) with density functional theory. <i>Modern Physics Letters B</i> , 0, , .	1.0	0
49609	Structural and electronic properties of hexagonal MXH (M = C, Si, Ge and Sn; X = N, P, As and Sb) monolayers: A first-principles prediction. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 151, 115710.	1.3	3
49610	First-principles prediction of electronic, optical, and thermodynamic properties of c-TiAl3 with M doping (M=V, Nb, Ta). <i>Indian Journal of Physics</i> , 0, , .	0.9	0
49611	Rational design of heterogenized molecular phthalocyanine hybrid single-atom electrocatalyst towards two-electron oxygen reduction. <i>Nature Communications</i> , 2023, 14, .	5.8	36
49612	Influence of phosphorus-doped bilayer graphene configuration on the oxygen reduction reaction in acidic solution. <i>Carbon</i> , 2023, 210, 118012.	5.4	0
49613	Structural arrangement and improved thermoelectric figure of merit in hexagonal SiX(X=N,P,As,Sb,Bi) monolayers: understanding from first-principles calculations. <i>Journal Physics D: Applied Physics</i> , 0, , .	1.3	0
49614	Adsorption effects and mechanisms of phosphorus by nanosized laponite. <i>Chemosphere</i> , 2023, 331, 138684.	4.2	7
49615	Hydrogen Absorption Performance and O2 Poisoning Resistance of Pd/ZrCo Composite Film. <i>Materials</i> , 2023, 16, 3159.	1.3	0

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49616	Ab-Initio Calculation of the Electrical Conductivity, Optical Absorption, and Reflectivity of the 2D Materials SnC and NbC. Crystals, 2023, 13, 682.	1.0	1
49617	Topological semimetal phases in a family of monolayer $X_2Y_2Z_2$ ( $X = \text{Sn, Pb, Bi, Sb, As, Te, Se, S, Ge, Si, Ga, In, Al, Bi, Sb, As, Te, Se, S, Ge, Si, Ga, In, Al}$ ). Physical Review Letters, 2023, 130, 165701.	1.3	0
49618	Combining Theoretical and Experimental Methods to Probe Confinement within Microporous Solid Acid Catalysts for Alcohol Dehydration. ACS Catalysis, 2023, 13, 5955-5968.	5.5	4
49619	Removal of Pb ions using green Co <sub>3</sub> O <sub>4</sub> nanoparticles: Simulation, modeling, adsorption, and biological studies. Environmental Research, 2023, 222, 115335.	3.7	12
49620	Comparison of adsorption capacity of water and hydroxide with collector reagents on geversite (PtSb <sub>2</sub> ) mineral surface: A DFT-D insights. Computational Materials Science, 2023, 224, 112174.	1.4	3
49621	A theoretical study of the functionalized carbon dots surfaces binding with silver nanostructures. Computational and Theoretical Chemistry, 2023, 1223, 114087.	1.1	1
49622	Density Functional Theory Studies of the Direct Conversion of Methane to Methanol Using O <sub>2</sub> on Graphitic MN <sub>4</sub> G-BN (M = Fe, Co, Cu) and CuN <sub>4</sub> G-PN Single-Atom Catalysts. ACS Applied Nano Materials, 0, , .	2.4	3
49623	Synergistic double-atom catalysts of metal-boron anchored on g-C <sub>3</sub> N <sub>4</sub> for electrochemical nitrogen reduction: Mechanistic insight and catalyst screening. Journal of Energy Chemistry, 2023, 80, 350-360.	7.1	13
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49626	Understanding the hydrogen evolution reaction activity of doped single-atom catalysts on two-dimensional GaPS <sub>4</sub> by DFT and machine learning. Journal of Energy Chemistry, 2023, 81, 93-100.	7.1	17
49627	Electronic structure, phonon stability, mechanical and high-temperature thermoelectric properties of Li-based quaternary Heusler alloys. Current Applied Physics, 2023, 50, 161-167.	1.1	2
49628	Computational design of one FeCoNiCuZn high-entropy alloy for high-performance electrocatalytic nitrate reduction. Applied Surface Science, 2023, 626, 157246.	3.1	2
49629	Confined MoS <sub>2</sub> nanosheets grown on 3D interconnected N, S co-doped carbon nanofibers as a free-standing anode for sodium-ion batteries. Journal of Solid State Chemistry, 2023, 323, 124046.	1.4	0
49630	When carbon impurities trigger the synthesis of alpha boron at high pressure and high temperature. Acta Materialia, 2023, 249, 118820.	3.8	1
49631	Strain driven anomalous anisotropic enhancement in the thermoelectric performance of monolayer MoS <sub>2</sub> . Applied Surface Science, 2023, 626, 157139.	3.1	12
49632	First principles analysis on void-reduction mechanism and impact of oxygen in nitrogen-doped CZ-Si crystal. Journal of Crystal Growth, 2023, 610, 127176.	0.7	2
49633	A computational study of adsorption of H <sub>2</sub> S and SO <sub>2</sub> on the activated carbon surfaces. Journal of Molecular Graphics and Modelling, 2023, 122, 108463.	1.3	2

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49634	Chemical and interfacial design in the visible-light-absorbing ferroelectric thin films. <i>Journal of the European Ceramic Society</i> , 2023, 43, 3275-3288.	2.8	1
49635	Coordination-number-determined activity of copper catalyst in water-gas shift reaction. <i>Fuel</i> , 2023, 343, 127850.	3.4	3
49636	Investigation on the photocatalytic property of direct Z-type van der Waals g-C <sub>3</sub> N <sub>4</sub> /AlN heterojunction and its mechanism. <i>Chemical Physics</i> , 2023, 571, 111913.	0.9	5
49637	Revealing the effects of transition metal doping on CoSe cocatalyst for enhancing photocatalytic H <sub>2</sub> production. <i>Applied Catalysis B: Environmental</i> , 2023, 328, 122503.	10.8	24
49638	Preventing H <sub>2</sub> S poisoning of dense Pd membranes for H <sub>2</sub> purification using an electric-field: An Ab initio study. <i>Surface Science</i> , 2023, 733, 122303.	0.8	2
49639	Reactivity of diamanes against oxidation: A DFT study. <i>Chemical Physics</i> , 2023, 571, 111916.	0.9	1
49640	Atomistic insight into impact of solute segregation on $\hat{\pm}$ -Mg/FCC-Al <sub>2</sub> Ca interface stability. <i>Journal of Alloys and Compounds</i> , 2023, 948, 169766.	2.8	0
49641	A new carbon allotrope: Biphenylene as promising anode materials for Li-ion and Li O <sub>2</sub> batteries. <i>Solid State Ionics</i> , 2023, 395, 116214.	1.3	3
49642	Probing structural, optical and magnetic properties of Sm-doped ZnO nanomaterials via experimental and DFT approach: Enhanced photocatalytic degradation and antibacterial performance. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 668, 131470.	2.3	8
49643	Electronic structure and magnetic properties of YX $\hat{\epsilon}^2$ CrZ (X $\hat{\epsilon}^2$ $\hat{\epsilon}^{\%}$ = $\hat{\epsilon}^{\%}$ Fe, Co, Ni; Z $\hat{\epsilon}^{\%}$ = $\hat{\epsilon}^{\%}$ Al, Ga, In) quaternary Heusler alloys. <i>Indian Journal of Physics</i> , 2023, 97, 733-749.	0.9	4
49645	Fabrication and characterization of PEG-In <sub>2</sub> O <sub>3</sub> modified PbO <sub>2</sub> anode for electrochemical degradation of metronidazole. <i>Electrochimica Acta</i> , 2023, 442, 141919.	2.6	1
49646	Revealing the bifunction mechanism of LaCoO <sub>3</sub> as electrocatalyst: Oxygen vacancies effect and synergistic reaction process. <i>Journal of Alloys and Compounds</i> , 2023, 941, 168918.	2.8	3
49647	Optoelectronic properties of Portulacaxanthin III (PXIII), GQD/Os-GQD-PXIII nanocomposites, and their coupling with photoanode in dye-sensitized solar cells: Molecular and periodic DFT calculations. <i>Optik</i> , 2023, 274, 170591.	1.4	1
49648	First-principles calculations to investigate mechanical, electronic, optical, and thermodynamic properties of Zr-based ternary compounds. <i>Journal of Materials Research and Technology</i> , 2023, 23, 1417-1434.	2.6	0
49649	Unveiling the synergistic effects of Re-Mo alloying on diffusion behaviors in $\hat{1}^3$ -Ni: From a theoretical perspective. <i>Journal of Materials Research and Technology</i> , 2023, 23, 1214-1224.	2.6	3
49650	First-principles assessment of chemical lithiation of sulfide solid electrolytes and its impact on their transport, electronic and mechanical properties. <i>Journal of Power Sources</i> , 2023, 560, 232689.	4.0	4
49651	Saturation magnetisation as an indicator of the disintegration of barium hexaferrite nanoplatelets during the surface functionalisation. <i>Scientific Reports</i> , 2023, 13, .	1.6	2
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49653	Raman signature of broken symmetry states near the quantum critical point in P doped BaFe <sub>2</sub> As <sub>2</sub>	0.6	2
49654	Theoretical study on the influence of the extra N in transition metal-N <sub>4</sub> embedded graphene as efficient CO <sub>2</sub> reduction catalysts. Applied Surface Science, 2023, 616, 156494.	3.1	1
49655	Electronic properties and photon scattering of buckled and planar few-layer 2D GaN. Vacuum, 2023, 210, 111861.	1.6	10
49656	The interaction of oxygen with the $\hat{1}^3$ -U (001) and (110) surfaces: An ab initio study. Computational Materials Science, 2023, 219, 112025.	1.4	2
49657	Computational studies for boosting nitrate electroreduction activity of Fe-N <sub>4</sub> -C Single-Atom catalyst via axial fifth ligand. Applied Surface Science, 2023, 616, 156440.	3.1	6
49658	Tunable local piezopotential properties of zinc oxide nanowires grown by remote epitaxy. Materials Science in Semiconductor Processing, 2023, 157, 107345.	1.9	0
49659	Thickness-dependent oxygen chemisorption behaviors on (1 1 1) surfaces of two-dimensional FCC metals Al and Cu: First-principles study. Computational Materials Science, 2023, 219, 112022.	1.4	1
49660	First principle calculation of structural, electronic, magnetic, and elastic properties of ferromagnetic Cu <sub>2</sub> MnZ (Z = Pb, P, As, Bi, S, Se, and Te) Heusler alloys. Physica B: Condensed Matter, 2023, 653, 414673.	1.3	3
49661	Enhancement of the magnetic and mechanical properties by introducing element carbon for Ti-based alloy. Journal of Magnetism and Magnetic Materials, 2023, 568, 170438.	1.0	2
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49663	Structural features, thermal stability and catalytic implication of Fe-Ni nanoparticles. Journal of Solid State Chemistry, 2023, 320, 123863.	1.4	1
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49666	Synthesis, Crystal, and Electronic Structure of (HpipeH <sub>2</sub> ) <sub>2</sub> [Sb <sub>2</sub> 110](I <sub>2</sub> ), with I <sub>2</sub> Molecules Linking Sb <sub>2</sub> X <sub>10</sub> Dimers into a Polymeric Anion: A Strategy for Optimizing a Hybrid Compound's Band Gap. International Journal of Molecular Sciences, 2023, 24, 2201.	1.6	1
49667	Synthesis, Crystal, and Electronic Structure of (HpipeH <sub>2</sub> ) <sub>2</sub> [Sb <sub>2</sub> 110](I <sub>2</sub> ), with I <sub>2</sub> Molecules Linking Sb <sub>2</sub> X <sub>10</sub> Dimers into a Polymeric Anion: A Strategy for Optimizing a Hybrid Compound's Band Gap. International Journal of Molecular Sciences, 2023, 24, 2201.	1.8	3
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49669	As K-edge absorption at high pressures in AFeAs (A=Na/Li): First principles results. Journal of Electron Spectroscopy and Related Phenomena, 2023, 263, 147286.	0.8	1
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49672	Wave-layered dendrite-free lithium deposition with unprecedented long-term cyclability. <i>Journal of Power Sources</i> , 2023, 560, 232697.	4.0	0
49673	Pressure-dependent semiconductorâ€“metal transition and elastic, electronic, optical, and thermophysical properties of orthorhombic SnS binary chalcogenide. <i>Results in Physics</i> , 2023, 45, 106236.	2.0	2
49674	Realizing spontaneous valley polarization and topological phase transitions in monolayer ScX <sub>2</sub> (X=Al, Tl). <i>npj Computational Materials</i> , 2023, 13, 1000017.	3.8	17
49675	Red shift of lead-free halide perovskite RbCaCl <sub>3</sub> under pressure for enhancing optoelectronic performance. <i>Physica Scripta</i> , 2023, 98, 035806.	1.2	0
49676	First-Principles Microkinetic Modeling Unravelling the Performance of Edge-Decorated Nanocarbons for Hydrogen Production from Methane. <i>ACS Applied Materials &amp; Interfaces</i> , 2023, 15, 6951-6962.	4.0	9
49677	Adsorption of 3d transition-metal atoms on two-dimensional penta-graphene: A first-principles study. <i>Journal of Saudi Chemical Society</i> , 2023, 27, 101611.	2.4	3
49678	Ab-initio investigation of the structural stability, electronic and optical properties of the LiBO <sub>2</sub> compound by using the GOW0+BSE approach. <i>Computational Condensed Matter</i> , 2023, 34, e00789.	0.9	1
49679	A theoretical prediction of novel Janus NiSX (X=As, Se, Te) Monolayers: Electronic, optical, and thermoelectric properties. <i>Applied Surface Science</i> , 2023, 616, 156560.	3.1	6
49680	Strong phonon mode induced by carbon vacancy accelerating hole transfer in SiC/MoS <sub>2</sub> heterostructure. <i>Applied Surface Science</i> , 2023, 617, 156554.	3.1	5
49681	Outstanding High Field-Effect Mobility of 299 Å <sup>2</sup> V <sup>-1</sup> Å <sup>-1</sup> by Nitrogen-Doped SnO <sub>2</sub> Nanosheet Thin-Film Transistor. <i>Advanced Materials Technologies</i> , 2023, 8, .	3.0	3
49682	Electrocatalytic nitrogen fixation performance of two-dimensional Metal-Organic Frameworks Cu <sub>3</sub> (C <sub>6</sub> O <sub>6</sub> ) and TM/Cu <sub>3</sub> (C <sub>6</sub> O <sub>6</sub> ) from first-principle study. <i>Chemical Physics</i> , 2023, 568, 111837.	0.9	1
49683	First principles study on structural, vibrational, electronic and elastic properties of 2D alkaline-earth carbides as a metallic material. <i>Synthetic Metals</i> , 2023, 293, 117281.	2.1	0
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49685	Band offsets at the interfaces between Ga <sub>2</sub> O <sub>3</sub> and Al <sub>2</sub> O <sub>3</sub> . <i>Journal of Applied Physics</i> , 2023, 134, 045701.	0.9	1
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49687	Atomic structure and large magnetic anisotropy in air-sensitive layered ferromagnetic V <sub>3</sub> . <i>Nanoscale</i> , 2023, 15, 4628-4635.	2.8	1
49688	First-principles prediction of two-dimensional MnOX (X = Cl, Br) monolayers: the half-metallic multiferroics with magnetoelastic coupling. <i>Nanoscale</i> , 2023, 15, 4546-4552.	2.8	4



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