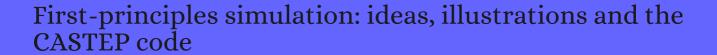
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277	Quantum optimization of complex systems with a quantum annealer. 2022, 106,	Ο
276	Constructing 1T-2H TaS2 nanosheets with architecture and defect engineering for enhance hydrogen evolution reaction. 2022 , 167877	Ο
275	Experimental and theoretical studies on the adsorption characteristics of Si/Al-based adsorbents for lead and cadmium in incineration flue gas. 2022 , 159895	Ο
274	Sn3B10O17Cl2 Achieving Birefringence Enhancement by Stereochemical Activity Lone Pair.	Ο
273	A DFT+U study of structural, electronic and optical properties of Ag- and Cu-doped ZnO.	O
272	Effects of torsional control on the optical and electronic properties of monolayer NbS2: A first-principles study. 2022 , 33, 104720	0
271	Elastic anisotropy and thermal properties of Zr-Al-N ternary nitrides using first-principles explorations. 2022 , 33, 104651	O

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269	Mechanical properties and chemical bonding transitions of Nb/NbC and ⊞e/NbC interfaces in Fe-Nb-C composites. 2022 , 33, 104791	1
268	Single Pd atom embedded Janus HfSeTe as promising sensor for dissolved gas detection in transformer oil: A density functional theory study. 2022 , 35, 102398	1
267	Atomically thin bismuthene nanosheets for sensitive electrochemical determination of heavy metal ions. 2022 , 1235, 340510	O
266	Predicting the structural, elastic, electronic, and optical properties of anti-perovskites X3SbP (XI=ICa, Sr, Ba) via first-principles. 2022 , 808, 140127	O
265	Synthesis, crystal structure, electronic structure, and intensive zero-phonon-line emission of Mn4+ in K5Nb3OF18 lattice. 2022 , 134, 113175	O
264	First-principles study on the elastic anisotropy and thermal properties of MgN compounds. 2022 , 171, 111034	О
263	Considerable improved near-infrared luminescence in ionic-free doped ZnAl2O4 by oxygen defects engineering. 2023 , 253, 119455	O
262	Elastic anisotropy and thermal properties of M-B-N (M = Al, Ga) systems using first-principles calculations. 2023 , 207, 111626	О
261	Three polar indium phosphites exhibiting diverse structural networks and SHG-activity. 2023 , 317, 123655	O
260	Effect and its mechanism of fixed-ratio and incremented 3Be-Sb complex modifier on microstructures and properties of hypereutectic Al-Si-Mg alloy. 2023 , 931, 167478	O
259	The effects of hydroxyl on selective separation of chalcopyrite from pyrite: A mechanism study. 2023 , 608, 154963	2
258	Anomalous strain-dependent charge density in honeycomb borophene. 2023 , 216, 111838	O
257	Interfacial stability analysis between Ca-doped Na3PS4 solid electrolyte and Na anode from first-principles calculations. 2023 , 216, 111848	O
256	Effects of Doped Non-Metallic Elements B, N and O on Electronic and Magnetic Properties of Monolayer PC6. 2022 , 12, 146-153	O
255	Prediction of new 2D Hf2Br2N2 monolayer as a promising candidate for photovoltaic applications. 2023 , 294, 126979	O
254	Insight of the role of F-impurity on the structural, electro-optical properties of ZnO: DFT and experiment. 2023 , 154, 107223	О
253	Coexistence of in- and out-of-plane piezoelectricity in Janus XSSiN2 (XŒCr, Mo, W) monolayers. 2023 , 610, 155586	1

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251	Facile conversion of glycerol to 1,3-dihydroxyacetone by using mesoporous CuOBnO2 composite oxide supported Au catalysts.	O
250	Filling Selenium into Sulfur Vacancies in Ultrathin Tungsten Sulfide Nanosheets for Superior Potassium Storage.	0
249	Gas-Sensitive Characteristics of Graphene Composite Tungsten Disulfide to Ammonia. 2022 , 22, 8672	O
248	Numerical Investigation of the Stimulated Growth of Single-Crystal Fibers by Point-Effect-Induced Fluid Dynamics.	0
247	The Synthesis and Characterisation of the High-Hardness Magnetic Material Mn2N0.86. 2022 , 15, 7780	O
246	First-principles calculations on the interfacial stability and bonding properties of HfN(111)/HfB2(0001) interface. 2022 , 111678	0
245	Effect of Sn addition on the mechanical properties and high-temperature oxidation resistance of intermetallic TiAl alloys by first principles study and experimental investigation. 2022 , 21, 3666-3677	O
244	Understanding the impact of Y2+ (Y Mn, Fe, and co) cations on physical properties of SrYGe2O6 clinopyroxene: A DFT insight. 2022 , 111112	O
243	Achieving Large Second Harmonic Generation Effects via Optimal Planar Alignment of Triangular Units. 2210718	3
242	Structure, electronic, optical and elastic properties of (NH4)2BeF4 crystal in paraelectric phase. 2022 ,	0
241	A type-II NGyne/GaSe heterostructure with high carrier mobility and tunable electronic properties for photovoltaic application.	О
240	Effect of halogen doping on the electronic, electrical, and optical properties of anatase TiO2. 2022 , 12, 115017	Ο
239	Experimental and DFT study of structural and optical properties of Ni-doped ZnO nanofiber thin films for optoelectronic applications. 2022 , 134, 113188	Ο
238	Two-dimensional hydrogenated/fluorinated graphyne/graphyne-like BN van der Waals heterostructures and their potential application in ultraviolet photodetection: a theoretical prediction. 2022 , 155739	O
237	DFT study of the effect of impurity defects on the inner-layer adsorption of hydrated Al(OH)2+ on the kaolinite (001) surface. 2022 , 120819	О
236	AIB3IIC3IIIQ8VI: A New Family for the Design of Infrared Nonlinear Optical Materials by Coupling Octahedra and Tetrahedra Units.	3
235	La2B3O4(OH)3(SO4)2: A new rare-earth borate-sulfate with second-harmonic generation response. 2023 , 317, 123715	O

234	Oxygen vacancy-induced spin polarization of tungsten oxide nanowires for efficient photocatalytic reduction and immobilization of uranium(VI) under simulated solar light. 2022 , 122202	О
233	First-principle study on the effect of point defects on the mechanical properties, thermal conductivity, and optical properties of wurtzite AlN. 2023 , 207, 111694	Ο
232	Integration of high-thermal-responsive color change and invisible emission intensity ratio in Gd2Mo4O15 lattice with the desired structure. 2023 , 27, 101304	O
231	Thermochemical activation of CO2 into syngas over ceria-supported niobium oxide catalyst: An integrated experimental-DFT study. 2023 , 67, 102339	Ο
230	Superior toughness and hardness in graphitelliamond hybrid induced by coherent interfaces. 2023 , 203, 357-362	O
229	Effects of long/short-range ordering on magnetic properties of Fe-23Iwt% Co alloy: A combined experimental and computational study. 2023 , 565, 170291	O
228	First-principles calculations to investigate elastic, electronic, optical and thermodynamic properties of Pt3X (X = Ti, Cu). 2023 , 44, 106141	O
227	The effect of alloying elements in Ti-5Mo-5V-8Cr-3Al alloy on growth kinetics of TiB whiskers in boride layer. 2023 , 225, 111478	O
226	Evolution of MC carbides in Ni-Mo-Cr-Ti based alloy for applications in molten salt reactors. 2023 , 196, 112588	O
225	Two-dimensional silicether: A promising anode material for sodium-ion battery. 2023 , 218, 111920	Ο
224	First-principles calculations of electronic structure, optical and thermodynamic properties of GaBN2, Ga3BN4 and GaB3N4 nitrides. 2023 , 208, 111745	0
223	Bimetallic CuCo nanocrystals to tailor absorption energy of intermediators for efficient electrochemical nitrate conversion to ammonia in neutral electrolyte. 2023 , 556, 232523	O
222	Experimental characterization and first-principles calculations to investigate structural, elastic, mechanical and optical properties of flakes-based BiOI film. 2023 , 650, 414556	O
221	Structural, electronic, and optoelectronic properties in hybrid system Cs2Sn(I1\(\mathbb{B}\)Fx)6: DFT-based study. 2023 , 218, 111961	Ο
220	Effects of VZn and Hi interstitials with different valence states and alkaline earth metal doping on carrier lifetime, activity, and oxidation reaction of ZnO. 2023 , 566, 111794	O
219	High pressure mediated physical properties of Hf2AB (A = Pb, Bi) via DFT calculations. 2023 , 34, 105147	1
218	Enhanced charge carrier density of a p-n BiOCl/BiVO4 heterostructure by Ni doping for photoelectrochemical applications. 2023 , 937, 168434	О
217	DFT approach to the stability, the structural, electronic and photocatalytic properties of the ZnV2O6(001) surface terminations. 2023 , 155, 107220	O

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214	Enhancing the reactivity of CO2 conversion to hydrocarbons by modulating the electron properties of carbon nanotube based single atom catalysts with curvature effect. 2023 , 209, 111759	Ο
213	The structural, mechanical and electronic properties of BaxNy compounds. 2023 , 156, 107268	O
212	Mechanical and thermodynamic behaviors of AlSi2Sc2 under uniaxial tensile loading: A first-principles study. 2023 , 174, 111160	O
211	Effects of Cu, Ag and Au on electronic and optical properties of ⊞a2O3 oxide according to first-principles calculations. 2023 , 174, 111152	0
210	Constructing the coherent transition interface structure for enhancing strength and ductility of hexagonal boron nitride nanosheets/Al composites. 2023 , 145, 235-248	0
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207	The Alloying Strategy to Tailor the Mechanical Properties of EAl13Fe4 Phase in Al-Mg-Fe Alloy by First-Principles Calculations. 2022 , 12, 1999	O
206	Modulation of the Phase Transition Behavior of VO2 Nanofilms by the Coupling of Zr Doping and Thickness-Dependent Band Gap.	0
205	Energy level, crystal morphology and fluorescence emission tuning in cocrystals via molecular-level engineering.	0
204	Structural stability, elasticity and minimum thermal conductivity of M-doped Mg 17 Al 12 (MIEIGa, In, Ge, Sn, Pb) compounds: A first-principles predictions.	0
203	Investigating the I-Mg17Al12 Alloy under Pressure Using First-Principles Methods: Structure, Elastic Properties, and Mechanical Properties. 2022 , 12, 1741	O
202	Core-shell LaOCl/LaFeO3 nanofibers with matched impedance for high-efficiency electromagnetic wave absorption.	O
201	Structural and optical characterization of CCBixTi1-x O (for $x = 0.04$) thin film.	O
200	Theoretical Prediction of Structural, Mechanical, and Thermophysical Properties of the Precipitates in 2xxx Series Aluminum Alloy. 2022 , 12, 2178	О
199	Reaching the Full Potential of Machine Learning in Mitigating Environmental Impacts of Functional Materials. 2022 , 260,	O

198	Modeling the structural, electronic, optoelectronic, thermodynamic, and core-level spectroscopy of XBnO3 (X = Ag, Cs, Hf) perovskites. 2022 , 114003	O
197	Analyzing the physical properties of perovskite oxides BaMO3 (M = Ru, Os) for predicting potential applications. 2022 , e00782	O
196	The Rise of 212 MAX Phase Borides: DFT Insights into the Physical Properties of Ti2PB2, Zr2PbB2, and Nb2AB2 $[A = P, S]$ for Thermomechanical Applications.	0
195	A detailed computational study to investigate the influence of metals (Bi, Sn, Tl) substitution on phase transition, electronic band structure and their implications on optical, elastic, anisotropic and mechanical properties of PbHfO3. 2023 , 55,	O
194	First principles study of the electronic and optical properties of high-valence transition metal-doped anatase titanium dioxide. 2022 , 53, 1551-1560	0
193	Fast and Durable Alkaline Hydrogen Oxidation Reaction at Electron-Deficient Ruthenium-Ruthenium Oxide Interface. 2208821	O
192	Effects of alloying elements on diamond/Cu interface properties based on first-principles calculations.	0
191	Effects of Cocrystallization on the Structure and Properties of Melt-Cast Explosive 2,4-Dinitroanisole: A Computational Study. 2022 , 27, 9010	O
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189	Detecting Common Explosive Molecules Using a Wavy Monolayer Arsenene: A Density Functional Theory Study. 2022 , 7,	O
188	Photocatalytic nitrogen fixation under an ambient atmosphere using a porous coordination polymer with bridging dinitrogen anions.	1
187	First-principles investigation of TiC(001)/TiAl(100) interface: atomic structure, stability and electronic property. 2022 , 57, 21339-21351	O
186	First-principles calculations to investigate adhesion strength, stability and electronic properties of Al(111)/TiAl3(112) interface.	0
185	Predicted High-Temperature Superconductivity in Rare Earth Hydride ErH2 at Moderate Pressure. 2022 , 39, 127403	O
184	Study on the Crystallization Behavior of Sb2Te Thin Films for Phase-Change Memory Applications.	O
183	Effect of strain on the electronic and optical properties of (non-)metal adsorbed NbS2 monolayer. 2023 , 35, 045501	O
182	The Mechanical Properties, Structural Stability and Thermal Conductivities of Y, Sc Doped AuIn2 by First P rinciples Calculations. 2022 , 12, 2121	0
181	First-Principles Calculations with Six Structures of Alkaline Earth Metal Cyanide A(CN)2 (A = Be, Mg, Ca, Sr, and Ba): Structural, Electrical, and Phonon Properties.	O

180	Deep Eutectic Solvents Synthesis of A 2 Sb(C 2 O 4)Cl 3 (AI=INH 4 , K, Rb) with Superior Optical Performance. 2202874	O
179	Coupled Evolution of Sliding and Rolling of Carbon Nanotubes: Effect of Lattice Mismatch and Size.	O
178	The effect of stress on electronic structure and optical property of cubic Ca2Ge.	0
177	The Local and Electronic Structure Study of LuxGd1᠒VO4 (0./k/和) Solid Solution Nanocrystals. 2023 , 13, 323	O
176	Heteroatom Doped Amorphous/Crystalline Ruthenium Oxide Nanocages as a Remarkable Bifunctional Electrocatalyst for Overall Water Splitting. 2207235	O
175	A first-principles study of the electronic, mechanical, vibrational, and optical properties of the zirconium carbide under high pressure.	O
174	Dual Engineering of Lattice Strain and Valence State of NiAl-LDHs for Photoreduction of CO 2 to Highly Selective CH 4. 2205770	O
173	Heterogenous Iron Oxide Assemblages for Use in Catalytic Ozonation: Reactivity, Kinetics, and Reaction Mechanism.	O
172	A comparative study of the structural, elastic, thermophysical, and optoelectronic properties of CaZn2X2 (XI=IN, P, As) semiconductors via ab-initio approach. 2023 , 44, 106214	O
171	Impacts of doping cadmium atoms on the mechanical properties of (n,0) zigzag SWCNTs: DFT approach. 2023 , 109681	O
170	Mechanisms for Radiation Resistance of InP Photovoltaic Cells: A First Principle Study. 2201042	O
169	Insights into the physical properties of newly synthesized AMn2P2 (A= Ca, Sr) via density functional theory. 2023 , 414651	O
168	First-principles calculations to investigate pressure-driven electronic phase transition of lead-free halide perovskites KMCl3 (MI=IGe, Sn) for superior optoelectronic performance. 2023 , 44, 106212	O
167	Combination of Low-Polar and Polar Binding Sites in Aliphatic MOFs for the Efficient C2H6/C2H4 Separation. 2023 , 15, 3387-3394	O
166	Investigation on the Formation Pathway of the MnSAl2O3 Inclusions at Atomic Level in High-Speed Wheel Steel.	0
165	Atomistic investigation on adhesive strength of coupling agents to aluminum. 2023, 108150	O
164	Proton-Conductive and Electrochemical-Sensitive Sensing Behavior of a New Mn(II) Chain Coordination Polymer.	О
163	Li/Na atoms' substitution effects on the structural, electronic, and mechanical properties of the CaSnO3 perovskite for battery applications. 2023 , 219, 112006	O

162	Ternary hetero-structured BiOBr/Bi2MoO6@MXene composite membrane: Construction and enhanced removal of antibiotics and dyes from water. 2023 , 669, 121329	0
161	First-principles investigation on structural and photoelectric properties of (Nb, Ta) codoped anatase TiO2. 2023 , 652, 414633	Ο
160	The influence of Cl doping on the structural, electronic properties and Li-ion migration of LiFePO4: A DFT study. 2023 , 1221, 114029	0
159	First-Principles Calculations to Investigate Effect of X+ICations Variation on Structural, Mechanical, Electronic and Optical Properties of the XCdCl3 Chloroperovskites. 2023 , 289, 116228	O
158	Effects of Sm and VZn in different valence states on the magnetic property, carrier lifetime, electric dipole moment, visible light, and redox reaction of ZnO:Hi under biaxial strain. 2023 , 297, 127362	0
157	Mechanism of Pt3Co nanocatalysts to improve the performance for oxygen reduction reactions: DFT study on oxygen adsorption and durability of different facets. 2023 , 289, 116202	Ο
156	Elastic anisotropy, thermal conductivity and tensile properties of MAX phase V2GaC, Nb2GaC and Ta2GaC: First-principles calculations. 2023 , 209, 111800	0
155	Tunable Schottky barrier of WSi2N4/graphene heterostructure via interface distance and external electric field. 2023 , 615, 156385	Ο
154	Boosting high-rate Zn-ion storage capability of EMnO2 through Tri-ion co-intercalation. 2023, 939, 168813	1
153	Comparing investigation of the anisotropic thermoelectric properties of textured KSr2Nb5O15 ceramics. 2023 , 175, 111204	Ο
152	Intensity of the Eu3+ hypersensitive transition in isostructural phosphate and vanadate compounds. 2023 , 257, 119709	Ο
151	First-Principles Calculations of Structural and Mechanical Properties of Cu N i Alloys. 2023 , 13, 43	Ο
150	A first principles study on H-atom interaction with bcc metals. 2022 ,	0
149	Effect of warpage on the electronic structure and optical properties of bilayer germanene. 2022 , 43, 122102	Ο
148	First-principles prediction of structural, electronic and optical properties of alkali metals AM4BN3H10 hydrides. 2023 ,	0
147	Structural, elastic, mechanical, electronic, damage tolerance, fracture toughness, and optical properties of Cr AlB MAB phases studied by first-principles calculations.	O
146	Internal electric field enhanced photoelectrochemical water splitting in direct Z-scheme GeC/HfS2 heterostructure: A first-principles study. 2023 , 122, 043902	0
145	Single-Layer MoS2: A Two-Dimensional Material with Negative Poisson Ratio. 2023, 13, 283	Ο

144	Investigation of the structural, electronic and mechanical properties of Ca-SiO2 compound particles in steel based on density functional theory. 2023 , 30, 744-755	O
143	First-principles calculations to investigate physical properties of orthorhombic perovskite YBO3 (B = Ti & Ti	Ο
142	Infrequent Cubane-Like Chromium Sulfide Cluster with Donor Ligands with Efficient Electrocatalytic Property Toward Hydrogen Evolution Reaction.	O
141	Reversible lewisite adsorption/desorption on the transition metal doped graphene: First-principle calculations.	O
140	Highly Nonstoichiometric YAG Ceramics with Modified Luminescence Properties. 2213418	0
139	Hydrogen-Induced Defective Crystalline Carbon Nitride with Enhanced Bidirectional Charge Migration for Persulfate Photoactivation.	O
138	Effect of Varying Stiffness and Functionalization on the Interfacial Failure Behavior of Isotactic Polypropylene on Hydroxylated □Al2O3 by MD Simulation. 2023 , 15, 6133-6141	O
137	Two Carboxylate-Cyanurates with Strong Optical Anisotropy and Large Band Gaps. 2023 , 62, 2257-2265	Ο
136	Interstitial Carbon Dopant in Palladium © old Alloy Boosting the Catalytic Performance in Vinyl Acetate Monomer Synthesis. 2023 , 145, 2985-2998	1
135	First-Principles Investigation on the High-Temperature Mechanical Properties and Thermal Properties of Pt-40Rh.	Ο
134	Revealing the interface properties of the Ti2AlC/TiAl composite from a first principles investigation. 2023 , 617, 156491	O
133	Experimental and theoretical investigation of the damage evolution of irradiated MoAlB and WAlB MAB phases. 2023 , 942, 169099	O
132	First-principles approach to the structural, physical, electronic, magnetic and optical properties of honeycomb ordered antimonates Na3Fe2SbO6. 2023 , 176, 111258	O
131	Quantum Efficiency Improvement of InGaN Near Ultraviolet LED Designs by Genetic Algorithm.	O
130	Understanding the poisoning mechanisms of Si and Zr atoms on L12 Al3Ti (111) surface: A first-principles investigation. 2023 , 210, 111891	O
129	Electron structure and exciton energy level of HgI2, CH3NH3HgI3 and (CH3NH3)2HgI4. 2023 , 137, 113598	Ο
128	The effect mechanism of HCl on chromium removal by CaO sorbent. 2023 , 397, 136559	O
127	Characterization and theoretical calculations of the T(Al20Cu2Mn3)/Al interface in 2024 alloys: TEM and DFT studies. 2023 , 210, 111884	O

126	Solution combustion synthesis of Mg-TiC@NiO nanocomposite and investigation on its metallurgical and biological properties. 2023 , 376, 121487	О
125	Vertex Strategy in Layered 2D MOFs: Simultaneous Improvement of Thermodynamics and Kinetics for Record C2H2/CO2 Separation Performance.	О
124	Phosphoric acid resistance PtCu/C oxygen reduction reaction electrocatalyst for HT-PEMFCs: A theoretical and experimental study. 2023 , 619, 156663	О
123	Ga-doped AlN monolayer nano-sheets as promising materials for environmental sensing applications. 2023 , 1223, 114086	О
122	Monolayer black phosphorus: Tunable band gap and optical properties. 2023, 657, 414780	О
121	Effects of alkali-metals (X = Li, Na, K) doping on the electronic, optoelectronic, thermodynamic, and X-ray spectroscopic properties of XBnI3 halide perovskites. 2023 , 35, e00798	О
120	Insights into the adsorption and interfacial products improving the wetting of the Ag-Ti/graphite and Cu-Ti/graphite systems: A first-principles calculation. 2023 , 38, 102840	О
119	First-principles study on p-type transformation of ZnO doped by Ag element. 2023 , 657, 414810	O
118	Tailoring the hydrogenated mechanism of Pt3Al from first-principles investigation. 2023, 212, 112033	О
117	Simultaneous S-scheme promoted Ag@AgVO3/g-C3N4/CeVO4 heterojunction with enhanced charge separation and photo redox ability towards solar photocatalysis. 2023 , 326, 138496	O
116	Electron-ion conjugation sites co-constructed by defects and heteroatoms assisted carbon electrodes for high-performance aqueous energy storage. 2023 , 640, 600-609	O
115	Comparative analysis of structure and electronic properties of doped g-GaN/Al0.5Ga0.5N heterostructure. 2023 , 292, 116423	О
114	High-throughput calculation and machine learning of two-dimensional halide perovskite materials: Formation energy and band gap. 2023 , 35, 105841	О
113	Ab-initio DFT calculations and experimental investigations into optoelectronic and structural properties of Ca9Al(PO4)7:Sm3+ orange phosphor. 2023 , 1281, 135102	О
112	A theoretical benchmark for the electronic, optical, and thermoelectrical characteristics of bulk and monolayer BiS2. 2023 , 178, 207568	О
111	Unrevealing the phase transition of high-performing high-nitrogen energetic material 1,5-diaminotetrazole-4: N-oxide via first-principles studies. 2023 , 35, 105940	О
110	First-principles study on electronic and optical properties of O-adsorbed Al0.5Ga0.5N photocathode surface. 2023 , 621, 156884	O
109	Janus monolayer SiXY (XI₽IP, as and Sb, YI₽IN, P, As) for photocatalytic water splitting. 2023 , 621, 156883	O

108	Exploring the structural, electronic, optical and mechanical properties of Mo5Si3C under pressure. 2023 , 113, 106216	O
107	First-principles calculations: Structural stability, electronic structure, optical properties and thermodynamic properties of AlBN2, Al3BN4 and AlB3N4 nitrides. 2023 , 160, 107400	O
106	Investigating the effect of Al, Mo or Mn addition to CoCrFeNi entropy alloys on the interface binding properties of WC/HEA cemented carbides. 2023 , 35, 105891	0
105	Probing the structural, electronic and optical properties of Cs2Ag1-xNaxInCl6 lead-free double perovskite from first principles. 2023 , 322, 123913	O
104	Thermodynamics of native defects in Li2O: A first-principles study. 2023 , 322, 123933	0
103	Study of the brittleness mechanism of aluminum/steel laser welded joints with copper and vanadium interlayers. 2023 , 163, 109319	Ο
102	T-BN nanosheets as High-capacity anode for Li- and Na-Ion Batteries: An ab initio study. 2023 , 1224, 114105	0
101	To explore the relationship between energy transfer rate and impact sensitivity by the first-principle calculation method. 2023 , 177, 111298	Ο
100	First-principles studies of behavior of hydrogen and mechanical properties of TiCrTaV high-entropy alloys. 2023 , 35, 105929	0
99	Photoelectrochemical and first-principles investigation on interactions between zinc ion and halide perovskite surface in the aqueous solution. 2023 , 1285, 135512	Ο
98	Comparative study of the structural, mechanical, electronic, optical and thermodynamic properties of superconducting disilicide YT2Si2 (T=Co, Ni, Ru, Rh, Pd, Ir) by DFT simulation. 2023 , 178, 111342	0
97	High hydrogen production in two-dimensional GaTe/ZnI2 type-II heterostructure for water splitting. 2023 , 178, 111317	O
96	High-entropy (Sm0.2Eu0.2Gd0.2Dy0.2Er0.2)2Hf2O7 ceramic with superb resistance to radiation-induced amorphization. 2023 , 155, 1-9	0
95	First-principles prediction of electronic, optical, and thermodynamic properties of c-TiAl3 with M doping ($M = V$, Nb, Ta).	O
94	Adhesion and mechanical properties of Zr/SiC interfaces: Insight from characteristics of structure and bonding by first-principles calculations. 2023 , 619, 156699	0
93	The lattice vibration, mechanical anisotropy, stress-strain behavior and electronic properties of HfxSiy phases: A first-principles study. 2023 , 212, 112012	О
92	Zeolitic imidazolate framework (ZIF-8)-derived acid-base bifunctional single-atom catalysts with Zn-Nx coordination for microalgal lipids conversion. 2023 , 343, 127848	0
91	Confined MoS2 nanosheets grown on 3D interconnected N, S co-doped carbon nanofibers as a free-standing anode for sodium-ion batteries. 2023 , 323, 124046	O

90	CaSiO3 (001) surface reconstruction and CO2 molecular adsorption. 2023, 323, 124027	О
89	Experimental and theoretical study on La0.5K0.5Mn1NFexO3 perovskite catalysts for mild temperature soot combustion and simultaneous removal of soot and NO. 2023 , 246, 107760	O
88	First principles study of the effect of (Mg, C) doping and Zn vacancies on the carrier activity, lifetime, visible light effect, and oxidation duction reaction of ZnO(0 0 1) monolayers. 2023 , 616, 156477	0
87	First-principles calculations to investigate mechanical, electronic, optical, and thermodynamic properties of Zr-based ternary compounds. 2023 , 23, 1417-1434	O
86	Adsorption of Pb(II) and Cd(II) hydrates via inexpensive limonitic laterite: Adsorption characteristics and mechanisms. 2023 , 310, 123234	0
85	First-principles calculations to investigate structural and mechanical properties of MoS2/MoSe2 vertical and lateral Superlattice. 2023 , 45, 106234	O
84	LnLiSiS4 (Ln = La and Ce): Promising infrared nonlinear optical materials designed by aliovalent substitution from SrCdSiS4. 2023 , 31, 100987	0
83	Defect mediated lithium adsorption on graphene-based silicon composite electrode for high capacity and high stability lithium-ion battery. 2023 , 931, 117179	O
82	Insights into thermodynamic destabilization in Mg-In-D hydrogen storage system: A combined synchrotron X-ray and neutron diffraction study. 2023 , 56, 432-442	0
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