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799	Multilayer relaxation of the Al(100) and Al(110) surfaces: an ab initio pseudopotential study. 2001 , 114-116, 501-506	7
798	Ab initio calculations on the anomalous thermal behaviour of fcc(1 1 0) surfaces. 2001 , 182, 293-296	5
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795	Reversed anisotropies and thermal contraction of fcc (110) surfaces. 2001 , 64,	15
794	Residual order within the molten Al(110) surface layer. 2002 , 65,	13
793	Thermal contraction of au nanoparticles. <i>Physical Review Letters</i> , 2002 , 89, 135504	7.4 89
792	Thermal expansion at a metal surface: A study of Mg(0001) and Be(101 $\bar{1}$ 0). 2002 , 66,	18
791	STRUCTURAL AND ELECTRONIC PROPERTIES OF AL NANOWIRES: AN AB INITIO PSEUDOPOTENTIAL STUDY. 2002 , 01, 159-169	12
790	Alkali-Aluminum surface alloys. 2002 , 225-276	1
789	FIRST PRINCIPLES MOLECULAR DYNAMICS INVOLVING EXCITED STATES AND NONADIABATIC TRANSITIONS. 2002 , 01, 319-349	125
788	First-principles study of the thermal expansion of Be(101 $\bar{1}$ 0). 2002 , 65,	47
787	Self-interstitials in V and Mo. 2002 , 66,	94
786	Melting. 2002 , 1-8	2
785	Ab initio lattice dynamics of Ag(). 2002 , 496, 331-344	13
784	Low-energy ion scattering study of Al(110) thermal disordering. 2002 , 193, 563-567	7

783	Finite temperature studies of Te adsorption on Si(001). 2002 , 519, 79-89	18
782	First-principles simulation: ideas, illustrations and the CASTEP code. 2002 , 14, 2717-2744	6910
781	Collective and single particle diffusion on surfaces. 2002 , 51, 949-1078	455
780	A low-energy ion scattering study of Al(1 1 0) surface melting. 2003 , 532-535, 13-18	10
779	Density-functional study of methanol adsorption on the Al(100) surface. 2003 , 45, 2218	3
778	Ab initio study of MoS ₂ nanotube bundles. 2003 , 68,	23
777	Quantization condition of quantum-well states in Cu/Co(001). 2003 , 68,	13
776	Multilayer thermal expansion of Be(0001) determined from surface core level shifts. 2003 , 64, 364-370	7
775	A finite temperature linear tetrahedron method for electronic structure calculations of periodic systems. 2004 , 121, 2466-70	4
774	"Hot-atom" O ₂ dissociation and oxide nucleation on Al(111). <i>Physical Review Letters</i> , 2004 , 92, 176104	7.4 67
773	Theoretical and numerical considerations on the surface energy for deformed isotropic nanocrystals. 2004 , 84, 3397-3409	4
772	Temperature dependence of atomic relaxation and vibrations for the vicinal Ni(9 7 7) surface: a molecular dynamics study. 2004 , 572, 439-448	62
771	Ab initio molecular dynamics of metal surfaces. 2004 , 16, S2575-S2596	17
770	Plane-wave pseudopotential density functional theory periodic slab calculations of CO adsorption on Cu ₂ O(111) surface. 2005 , 579, 131-140	73
769	First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives. 2005 , 71,	823
768	Negative thermal expansion. 2005 , 17, R217-R252	365
767	Theoretical study of protactinium at high pressure. 2005 , 893, 1	
766	All-electron first-principles calculations of clean surface properties of low-Miller-index Al surfaces. 2005 , 71,	51

765	Carbon monoxide reaction with UO ₂ (111) single crystal surfaces: A theoretical and experimental study. 2005 , 23, 1078-1084		17
764	THE OXIDATION OF NIAL: What Can We Learn from Ab Initio Calculations?. 2005 , 35, 167-207		112
763	Electrons and phonons in the ternary alloy CaAl ₂ Si ₆ as a function of composition. 2005 , 72,		52
762	Band structure and quantum conductance of nanostructures from maximally localized Wannier functions: the case of functionalized carbon nanotubes. <i>Physical Review Letters</i> , 2005 , 95, 076804	7.4	152
761	Oxygen Reduction on Pd _{0.75} Co _{0.25} (111) and Pt _{0.75} Co _{0.25} (111) Surfaces: An ab Initio Comparative Study. 2006 , 2, 1388-94		33
760	Adsorption and dissociation of H ₂ O ₂ on Pt and Pt-alloy clusters and surfaces. 2006 , 110, 17452-9		72
759	Cycloaddition functionalizations to preserve or control the conductance of carbon nanotubes. <i>Physical Review Letters</i> , 2006 , 97, 116801	7.4	108
758	Surface structure in simple liquid metals: An orbital-free first-principles study. 2006 , 74,		27
757	Stability of the body-centered-tetragonal phase of Fe at high pressure: Ground-state energies, phonon spectra, and molecular dynamics simulations. 2006 , 74,		20
756	First-Principles Study of Molecule/Al Interfaces. 2006 , 47, 2701-2705		1
755	Anharmonicity in Al vicinal surfaces of (1 0 0) with (1 1 1) step. 2006 , 252, 4923-4930		2
754	Thermodynamic separability of ultra-thin film surfaces and interfaces. 2006 , 600, 1012-1016		1
753	Ab initio studies of layering behavior of liquid sodium surfaces and interfaces. 2006 , 124, 174702		15
752	Momentum-resolved electron-phonon interaction in lead determined by neutron resonance spin-echo spectroscopy. <i>Physical Review Letters</i> , 2006 , 96, 225501	7.4	15
751	Ab initio calculation of the anomalous Hall conductivity by Wannier interpolation. 2006 , 74,		275
750	In-plane structure and ordering at liquid sodium surfaces and interfaces from ab initio molecular dynamics. 2007 , 127, 134703		9
749	Linear response separation of a solid into atomic constituents: Li, Al, and their evolution under pressure. 2007 , 75,		3
748	Interactions between Al atoms on Al(110) from first-principles calculations. 2007 , 75,		14

747	Fermi-surface calculation of the anomalous Hall conductivity. 2007 , 76,	96
746	Dynamical stability of Fe-H in the Earth's mantle and core regions. 2007 , 104, 9168-71	35
745	Electronic Properties of MoS ₂ Nanoparticles. 2007 , 111, 16192-16196	538
744	Spin and orbital magnetic response in metals: Susceptibility and NMR shifts. 2007 , 76,	47
743	First-Principles Prediction of High-Pressure Phase of CaC ₆ . 2007 , 24, 1668-1670	5
742	Electron-phonon interaction in graphite intercalation compounds. 2007 , 76,	55
741	Melting and superheating of crystalline solids: From bulk to nanocrystals. 2007 , 52, 1175-1262	440
740	Energetics of the adsorption and diffusion of hydrogen molecules in a (001) plate of nanocrystalline aluminum. 2008 , 81, 167-175	2
739	First-principles investigations of iridium low index surfaces. 2008 , 69, 2457-2464	6
738	Structural and dynamical properties of iridium surfaces: First principles and molecular dynamics investigations. 2008 , 403, 2748-2753	
737	Bulk aluminum at high pressure: A first-principles study. 2008 , 77,	32
736	Density-functional investigation of the rhombohedral to simple-cubic phase transition of arsenic. 2008 , 78,	18
735	First principles study of bulk CrSe and CrSe/ZnSe(001) interface. 2008 , 104, 113719	15
734	Cycloadditions to Control Bond Breaking in Naphthalenes, Fullerenes, and Carbon Nanotubes: A First-Principles Study. 2008 , 112, 4480-4485	19
733	Linear-scaling total-energy calculations with the tight-binding Korringa-Kohn-Rostoker Green function method. 2008 , 88, 2807-2815	4
732	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. 2008 , 77,	40
731	Pressure effects on the superconducting transition in nH-CaAlSi. 2008 , 77,	9
730	A Determination Method of the Work function using the Slab Model with a First-Principles Electronic Structure Calculation. 2008 , 6, 103-106	8

729	Bibliography. 419-549	
728	Electronic properties of the Pt _x Me _{1-x} /Pt(111) (Me=Au, Bi, In, Pb, Pd, Sn and Cu) surface alloys: DFT study. 2009 , 116, 94-101	29
727	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. 2009 , 30, 934-9	549
726	Ag ₂ Au alloy surfaces in an oxidizing environment: A first-principles study. 2009 , 603, 1467-1475	35
725	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. 2009 , 21, 395502	13251
724	Density functional theory study of Fe, Co, and Ni adatoms and dimers adsorbed on graphene. 2009 , 79,	174
723	Modification of electronic properties of Pt(111) surface by means of alloyed and adsorbed metals: DFT study. 2009 , 83, 1531-1536	2
722	Structures and Energetics of SrFeO _{2.875} Calculated within the GGA + U Framework. 2009 , 5, 2787-97	6
721	Spin channels in functionalized graphene nanoribbons. 2009 , 9, 3425-9	91
720	Surface energies, work functions, and surface relaxations of low-index metallic surfaces from first principles. 2009 , 80,	340
719	Ab initio study of the temperature-dependent structural properties of Al(110). 2009 , 80,	3
718	DFT study of adsorption of hydrogen and carbon monoxide on Pt _x Bi _{1-x} /Pt(111) bimetallic overlayers: correlation to surface electronic properties. 2009 , 11, 6225-33	19
717	First-principles study of neutral silicon interstitials in 3C- and 4H-SiC. 2009 , 89, 2271-2284	24
716	Structural characterization combined with the first principles simulations of barium/strontium cobaltite/ferrite as promising material for solid oxide fuel cells cathodes and high-temperature oxygen permeation membranes. 2009 , 1, 1512-9	43
715	Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. 2010 , 71, 39-57	199
714	Determining Seebeck coefficient of heavily doped La:SrTiO ₃ from density functional calculations. 2010 , 12, 1168-1172	16
713	Premelting of Al nonperfect (111) surface. 2010 , 405, 1248-1252	13
712	Halogen adsorption on crystallographic (1 1 1) planes of Pt, Pd, Cu and Au, and on Pd-monolayer catalyst surfaces: First-principles study. 2010 , 55, 1995-2003	38

711	Understanding oxygen vacancy migration and clustering in barium strontiumcobalt iron oxide. 2010 , 181, 1067-1073	23
710	Benzene adsorption on Mo2C: A theoretical and experimental study. 2010 , 379, 54-60	39
709	3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. 2010 , 39-58	7
708	Graphenelike surface boron layer: Structural phases on transition-metal diborides (0001). 2010 , 81,	29
707	Prediction of huge magnetic anisotropies of transition-metal dimer-benzene complexes from density functional theory calculations. 2010 , 82,	18
706	Predicting order-disorder phase transitions of O/Pd(111) from ab initio Wang-Landau Monte Carlo calculations. 2010 , 81,	15
705	Magnetism and clustering in Cr-doped InN. 2010 , 97, 242509	17
704	Predicting the melting temperatures of bulk materials. 2010 , 91, 46001	1
703	Many-particle effects in adsorbed magnetic atoms with easy-axis anisotropy: the case of Fe on the CuN/Cu(100) surface. 2010 , 12, 063040	41
702	Coverage-Dependent Architectures of Iron Phthalocyanine on Ag(110): a Comprehensive STM/DFT Study. 2010 , 114, 2144-2153	41
701	Weak antiferromagnetic coupling in molecular ring is predicted correctly by density functional theory plus Hubbard U. 2010 , 132, 244104	11
700	First principles study of adsorption of metals on Pt(1 1 1) surface. 2010 , 497, 38-45	16
699	Approximate quantum mechanical method for describing excitations and related properties of finite single-walled carbon nanotubes. 2010 , 81,	8
698	Effects of composition, temperature, and magnetism on phonons in bcc Fe-V alloys. 2010 , 82,	17
697	Oxygen adsorption on small PtNi nanoalloys. 2011 , 13, 7701-7	34
696	Stability of Intermediate States for Ethylene Epoxidation on AgCu Alloy Catalyst: A First-Principles Investigation. 2011 , 115, 10073-10079	14
695	Phonon-induced surface charge density oscillations in quantum wells: a first-principles study of the (2 × 2)-K overlayer on Be(0001). 2011 , 115, 7242-8	9
694	Improving the electrical conductivity of carbon nanotube networks: a first-principles study. 2011 , 5, 9726-36	53

693	Equations of state and thermodynamics of solids using empirical corrections in the quasiharmonic approximation. 2011 , 84,	54
692	Graphene-adsorbed Fe, Co, and Ni trimers and tetramers: Structure, stability, and magnetic moment. 2011 , 83,	45
691	Oxygen-vacancy formation in LaMO ₃ (M = Ti, V, Cr, Mn, Fe, Co, Ni) calculated at both GGA and GGA + U levels. 2011 , 50, 1800-1805	26
690	Ab initio lattice dynamics of CoH and NiH. 2011 , 509, S857-S859	3
689	Switchable conductance in functionalized carbon nanotubes via reversible sidewall bond cleavage. 2011 , 5, 4455-65	11
688	Hydrogenation properties of the TiB _x structures. 2011 , 36, 12268-12278	5
687	Systematic DFT-GGA study of hydrogen adsorption on transition metals. 2011 , 85, 2373-2379	21
686	Investigation of the adsorption and diffusion interaction of atomic hydrogen with low-index surfaces of crystal aluminum nanoplates. 2011 , 84, 554-566	
685	Ab initio Phonons in Magnetic Ni ₂ MnAl. 2011 , 50, 05FE07	1
684	Extremely confined quantum-well states for (2D)-K and (3B)-K on graphite: First-principles calculations. 2011 , 84,	1
683	Electronic topological transition in sliding bilayer graphene. 2011 , 84,	50
682	Structure and properties of pure and mixed transition metal dimers on graphene. 2011 , 8, 825	1
681	Magn π -like phases in epitaxial anatase TiO ₂ thin films. 2012 , 86,	22
680	Comment on Observation of anomalous peaks in the photoelectron spectra of highly oriented pyrolytic graphite: Folding of the band due to the surface charge density wave transition 2012 , 85,	
679	Oxygen vibrations and acoustic surface plasmon on Be(0001). 2012 , 86,	15
678	THERMOMAGNETIC PROPERTIES OF RARE-EARTH REPLACEMENT CRITICAL MAGNETIC MATERIALS FROM DFT CALCULATION: MnBi AND MnSb. 2012 , 01, 1250036	1
677	Orbital-free density functional theory simulations of dislocations in magnesium. 2012 , 20, 015006	41
676	First-principles calculations of lattice vibrations on LaT ₂ Zn ₂₀ (T = Ru and Ir). 2012 , 391, 012016	15

675	TiO ₂ (100)/Al ₂ O ₃ (0001) interface: A first-principles study supported by experiment. 2012 , 86,	21
674	A versatile low temperature solid-state synthesis of vanadium nitride (VN) via a "guanidinium-route": experimental and theoretical studies from the key-intermediate to the final product. 2012 , 41, 14381-90	17
673	Effect of dimensionality and spin-orbit coupling on charge-density-wave transition in 2H-TaSe ₂ . 2012 , 86,	40
672	First-Principles Characterization of Potassium Intercalation in Hexagonal 2H-MoS ₂ . 2012 , 116, 1826-1832	42
671	Electronic excitations of C ₆₀ aggregates. 2012 , 14, 13058-66	13
670	First-Principles Study of the Formamide Adsorption to the Oxygen-Covered (0001) Surface of Ruthenium. 2012 , 116, 14368-14381	5
669	Electronic and lattice instability and its relaxation mechanism in Pt-Co interfaces. 2012 , 85,	1
668	Doping of adsorbed graphene from defects and impurities in SiO ₂ substrates. 2012 , 86,	38
667	High-pressure elasticity and lattice dynamics of Mg ₂ La from first principles. 2012 , 520, 93-97	9
666	On the nature of inhibition performance of imidazole on iron surface. 2012 , 57, 254-259	51
665	First-principles determination of the absolute band-edge positions of BiOX (X=F, Cl, Br, I). 2012 , 55, 166-170	25
664	Atomic and electronic structures of Si[001] (130) symmetric tilt grain boundaries based on first-principles calculations. 2012 , 58, 38-44	12
663	Opening and tuning of band gap by the formation of diamond superlattices in twisted bilayer graphene. 2012 , 86,	46
662	Supramolecular assembly of diplatinum species through weak Pt(II)???Pt(II) intermolecular interactions: a combined experimental and computational study. 2012 , 18, 13787-99	15
661	Efficient computation of magnon dispersions within time-dependent density functional theory using maximally localized Wannier functions. 2012 , 85,	28
660	Methane and carbon dioxide adsorption on edge-functionalized graphene: a comparative DFT study. 2012 , 137, 054702	89
659	Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction. 2012 , 11, 970-7	118
658	Hydrogenation of Ferrimagnetic Graphene on a Co Surface: Significant Enhancement of Spin Moments by C-H Functionality. 2012 , 3, 2582-7	9

657	Elastic phase transitions in metals at high pressures. 2012 , 24, 195402	11
656	Raman modes and Grüneisen parameters of graphite under compressive biaxial stress. 2012 , 50, 4600-4606	24
655	First principles studies of the electronic properties and catalytic activity of single-walled carbon nanotube doped with Pt clusters and chains. 2012 , 393, 96-106	12
654	Formation dynamics of FeN thin films on Cu(100). 2012 , 523, 78-82	1
653	Trends in formation energies and elastic moduli of ternary and quaternary transition metal nitrides. 2013 , 48, 7642-7651	18
652	A computational study of the effect of alloying additions on the stability of Ni/c-ZrO ₂ interfaces. 2013 , 611, 5-9	10
651	Pressure dependence of superconductivity in simple cubic phosphorus. 2013 , 88,	18
650	Oxygen reduction reaction of PtIn alloy: Combined theoretical and experimental investigations. 2013 , 114, 706-712	16
649	Structural and hydrogen sorption properties of SmNi ₅ Ga _x system: An experimental and theoretical study. 2013 , 38, 12213-12222	4
648	Ag-Cu catalysts for ethylene epoxidation: selectivity and activity descriptors. 2013 , 138, 184707	20
647	Palladium Nanoparticles on Graphite Oxide: A Recyclable Catalyst for the Synthesis of Biaryl Cores. 2013 , 3, 2776-2789	81
646	Changes in electrodic reaction rates due to elastic stress and stress-induced surface patterns. 2013 , 111, 814-822	21
645	Evolution of the Fermi surface of arsenic through the rhombohedral to simple-cubic phase transition: A Wannier interpolation study. 2013 , 88,	3
644	Substrate-induced changes in the magnetic and electronic properties of hexagonal boron nitride. 2013 , 87,	29
643	Calculation of thermodynamic potentials with the inclusion of fractional occupation numbers and investigation of FCC-BCC structural phase transitions in alkaline-earth metals. 2013 , 55, 1991-2000	2
642	Chemical order and magnetic properties in small MxN ₂ nanoalloys. 2013 , 67, 1	13
641	DFT study of interaction of O, O ₂ , and OH with unreconstructed Pt(hkl) (h, k, l = 0, 1) surfaces: Similarities, differences, and universalities. 2013 , 87, 2214-2218	7
640	First-principles prediction of the equilibrium shape of nanoparticles under realistic electrochemical conditions. <i>Physical Review Letters</i> , 2013 , 110, 086104	7.4 50

- 639 DFT study of platinum and palladium overlayers on tungsten carbide: Structure and electrocatalytic activity toward hydrogen oxidation/evolution reaction. **2013**, 38, 5009-5018 55
- 638 Highly ordered cobalt-phthalocyanine chains on fractional atomic steps: one-dimensionality and electron hybridization. **2013**, 7, 1317-23 17
- 637 Is platinum necessary for efficient hydrogen evolution? DFT study of metal monolayers on tungsten carbide. **2013**, 38, 16071-16079 50
- 636 NH₃/O Coadsorption System on Pt(111). I. Structure of the Mixed Layer. **2013**, 117, 21186-21195 12
- 635 A Combined Experimental and Theoretical Study on the Formation of Crystalline Vanadium Nitride (VN) in Low Temperature through a Fully Solid-State Synthesis Route. **2013**, 117, 25659-25668 29
- 634 Interaction of magnetic transition metal dimers with spin-polarized hydrogenated graphene. **2013**, 138, 124709 2
- 633 Tuning patterning conditions by co-adsorption of gases: Br₂ and H₂ on Si(001). **2013**, 139, 184713 1
- 632 Extreme density-driven delocalization error for a model solvated-electron system. **2013**, 139, 184116 75
- 631 Ab initio potential for the He-Ag(110) interaction investigated using grazing-incidence fast-atom diffraction. **2013**, 87, 17
- 630 Large orbital magnetic moment in Pt_n clusters. **2014**, 26, 196006 9
- 629 Elastic properties and lattice dynamics of ruthenium at high pressures. **2014**, 490, 012059 4
- 628 Stable path to ferromagnetic hydrogenated graphene growth. **2014**, 90, 19
- 627 Rashba splitting and relativistic energy shifts in In/Si(111) nanowires. **2014**, 89, 18
- 626 Experimental assessment of the elastic properties of thin TiN/AlN superlattice and nano-multilayer coatings. **2014**, 257, 87-94 15
- 625 Structural and electronic properties of Sr₂RuO₄/Sr₃Ru₂O₇ heterostructures. **2014**, 89, 21
- 624 Inductive crystal field control in layered metal oxides with correlated electrons. **2014**, 2, 076110 11
- 623 Physical origins of weak H₂ binding on carbon nanostructures: insight from ab initio studies of chemically functionalized graphene nanoribbons. **2014**, 140, 174708 14
- 622 Investigations of the electronic and magnetic structures of Co₂YGa (Y=Cr, Mn) Heusler alloys and their (100) surfaces. **2014**, 115, 113905 15

621	Density functional study of Cr atom adsorption on hydrogen-terminated armchair boron nitride nanoribbons. 2014,	
620	Density Functional Theory Study of Metal Adatoms at or Near a Stone-wales Defect in Graphene. 2014, 93, 2-7	8
619	Elastic properties, lattice dynamics and structural transitions in molybdenum at high pressures. 2014, 81, 313-318	21
618	Elastic properties of eta carbide ($\eta\text{-Fe}_2\text{C}$) from ab initio calculations: application to cryogenically treated gear steel. 2014, 49, 2383-2390	16
617	First principles studies of Fe_mIr_n ($2 \leq m + n \leq 4$) nano clusters. 2014, 4, 593-600	4
616	DFT study of the CaNi_5H_x compounds ($0.0 \leq x \leq 1.0$). 2014, 582, 466-474	2
615	Lattice dynamics of cubic AuZn from first principles. 2014, 89,	2
614	Metallophilic interactions from dispersion-corrected density-functional theory. 2014, 140, 18A504	41
613	Investigation of hydrogen occlusion by molybdenum carbide. 2014, 469, 139-145	12
612	Improved Oxygen Reduction Performance of PtNi Nanoparticles by Adhesion on Nitrogen-Doped Graphene. 2014, 118, 2804-2811	60
611	BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. 2014, 185, 422-429	166
610	Native Defects in $\eta\text{-Mo}_2\text{C}$: Insights from First-Principles Calculations. 2014, 118, 25517-25524	13
609	Density-functional description of electrides. 2014, 16, 14584-93	59
608	Adsorbate induced vacancy formation on silver surfaces. 2014, 16, 9002-14	16
607	Adsorption and desulfurization reaction mechanism of thiophene and its hydrogenated derivatives over NbC(001) and NbN(001): an ab initio DFT study. 2014, 4, 2550-2563	15
606	Computational screening of structural and compositional factors for electrically conductive coordination polymers. 2014, 16, 14463-72	23
605	Stability of the hcp Ruthenium at high pressures from first principles. 2014, 116, 103507	11
604	Electronically driven structural transitions in $\text{A}_{10}(\text{PO}_4)_6\text{F}_2$ apatites (A = Ca, Sr, Pb, Cd and Hg). 2014, 70, 612-5	11

603	Engineering polar discontinuities in honeycomb lattices. 2014 , 5, 5157	37
602	Predictions of the Spin Configuration in Mn ₁₂ Molecular Magnets Made Accurate with the Help of Hubbard U on the Ligand Atoms. 2014 , 118, 20605-20612	5
601	Theoretical Chemistry of Graphyne: Functionalization, Symmetry Breaking, and Generation of Dirac-Fermion Mass. 2014 , 26, 3701-3708	13
600	Energy-loss contribution to grazing scattering of fast He atoms from a silver surface. 2014 , 89,	6
599	Simulating Gold's Structure-Dependent Reactivity: Nonlocal Density Functional Theory Studies of Hydrogen Activation by Gold Clusters, Nanowires, and Surfaces. 2014 , 118, 15693-15704	8
598	Thickness-dependent crossover from charge- to strain-mediated magnetoelectric coupling in ferromagnetic/piezoelectric oxide heterostructures. 2014 , 8, 894-903	54
597	Cadmium Vacancy Minority Defects as Luminescence Centers in Size and Strain Dependent Photoluminescence Shifts in CdS Nanotubes. 2014 , 118, 21604-21613	12
596	Enhanced Gas Adsorption on Graphitic Substrates via Defects and Local Curvature: A Density Functional Theory Study. 2014 , 118, 7741-7750	40
595	Refined phase coexistence line between graphite and diamond from density-functional theory and van der Waals correction. 2014 , 434, 185-193	17
594	Dimethylsulfoxide as a modifier of platinum electrocatalytic activity toward oxygen reduction reaction in aqueous solutions: Combined theoretical and experimental study. 2014 , 714-715, 11-18	4
593	Point defects in twisted bilayer graphene: A density functional theory study. 2014 , 89,	18
592	First principles explanation of the positive Seebeck coefficient of lithium. <i>Physical Review Letters</i> , 2014 , 112, 196603	7-4 52
591	Band offsets in c-Si/Si-XII heterojunctions. 2014 , 191, 6-9	
590	Density functional study of manganese atom adsorption on hydrogen-terminated armchair boron nitride nanoribbons. 2014 , 447, 65-69	4
589	Electrostatics of solvated systems in periodic boundary conditions. 2014 , 90,	60
588	Structure of Cr monolayer on Ag(001): A buried two-dimensional c(2×2) antiferromagnet. 2015 , 91,	10
587	Growth mechanism of silicene on Ag(111) determined by scanning tunneling microscopy measurements and ab initio calculations. 2015 , 92,	31
586	The influence of hydrogen on the seismic properties of solid iron. 2015 , 42, 3780-3785	28

585	Graphene oxide as an optimal candidate material for methane storage. 2015 , 143, 044704	7
584	Valence-lattice interaction on YbPd. 2015 , 592, 012061	0
583	Electronic Structure of IrO ₂ : The Role of the Metal d Orbitals. 2015 , 119, 11570-11577	54
582	Thermodynamic and spectroscopic properties of oxygen on silver under an oxygen atmosphere. 2015 , 17, 9288-312	70
581	Structural and hydrogen sorption properties of SmNi _{5-x} Al _x system [An experimental and theoretical study. 2015 , 40, 8548-8561	7
580	Calorimetric measurements on Li ₄ C ₆₀ and Na ₄ C ₆₀ . 2015 , 142, 164706	1
579	On the dynamical stability of ferromagnetic Ru and Os in the bct structure: a first-principles study. 2015 , 95, 408-415	1
578	Comprehensive Study of an Earth-Abundant Bifunctional 3D Electrode for Efficient Water Electrolysis in Alkaline Medium. 2015 , 7, 28148-55	31
577	Influence of interconfigurational electronic States On Fe, Co, Ni-silicene materials selection for spintronics. 2014 , 4, 7594	23
576	Prediction of phonon-mediated high-temperature superconductivity in LiB ₄ C ₂ . 2015 , 91,	20
575	Electronic properties and Schottky barriers at ZnO-metal interfaces from first principles. 2015 , 27, 015006	13
574	Thermoelastic properties of Iron from first-principles. 2015 , 91,	29
573	Hydrogen in palladium: Anharmonicity of lattice dynamics from first principles. 2015 , 57, 260-265	7
572	Temperature dependent lattice misfit and coherency of Al ₃ X (X = Sc, Zr, Ti and Nb) particles in an Al matrix. 2015 , 89, 109-115	49
571	Ferroelectric-Based Catalysis: Switchable Surface Chemistry. 2015 , 5, 4537-4545	90
570	Covalent and noncovalent functionalization of pristine and defective graphene by cyclohexane and dehydrogenated derivatives. 2015 , 351, 344-352	13
569	Phasego: A toolkit for automatic calculation and plot of phase diagram. 2015 , 191, 150-158	18
568	Emission properties of body-centered cubic elemental metal photocathodes. 2015 , 117, 134901	12

567	Dislocation modeling in bcc lithium: A comparison between continuum and atomistic predictions in the modified embedded atoms method. 2015 , 82, 1-9	17
566	Fracture behavior of lithium single crystal in the framework of (semi-)empirical force field derived from first-principles. 2015 , 23, 045008	9
565	Polarization screening-induced magnetic phase gradients at complex oxide interfaces. 2015 , 6, 6735	64
564	First-principles study of the interaction of hydrogen molecular on Na-adsorbed graphene. 2015 , 5, 393-402	14
563	Effect of interfacial structures on spin dependent tunneling in epitaxial L10-FePt/MgO/FePt perpendicular magnetic tunnel junctions. 2015 , 117, 083904	18
562	Landau levels in uniaxially strained graphene: A geometrical approach. 2015 , 359, 243-251	21
561	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. 2015 , 17, 31371-96	276
560	Density Functional Theory Study of Adsorption of Benzotriazole on Cu ₂ O Surfaces. 2015 , 119, 11625-11635	29
559	Vacancy formation in MoS ₂ supported on MgO: Electronic and energetic analysis. 2015 , 626, 55-62	3
558	Structure, chemisorption properties and electrocatalysis by Pd ₃ Au overlayers on tungsten carbide [A DFT study. 2015 , 40, 6085-6096	20
557	A DFT study of adsorption of imidazole, triazole, and tetrazole on oxidized copper surfaces: Cu ₂ O(111) and Cu ₂ O(111)-w/o-Cu ₂ O. 2015 , 17, 28602-15	31
556	Influence of hydrogen surface passivation on Sn segregation, aggregation, and distribution in GeSn/Ge(001) materials. 2015 , 117, 205302	10
555	Hydrogen storage on palladium adsorbed graphene: A density functional theory study. 2015 , 29, 1550143	8
554	Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures. 2015 , 15, 6229-38	64
553	First principle study of sodium decorated graphyne. 2015 , 461, 74-80	31
552	The oxidation of copper catalysts during ethylene epoxidation. 2015 , 17, 25073-89	38
551	Density functional theory analysis of hexagonal close-packed elemental metal photocathodes. 2015 , 18,	9
550	Exchange coupling and noncollinear magnetic states in Ni/Fe _n /Ni(1 0 0) multilayers. 2015 , 77, 108-123	

549	DFT study of the cohesive and structural properties of YNi ₅ H compounds. 2015 , 622, 1041-1048	5
548	Electronic and structural properties of bulk arsenopyrite and its cleavage surfaces [A DFT study]. 2015 , 5, 2013-2023	22
547	An analysis of radiation effects on NdFeB permanent magnets. 2015 , 342, 200-205	9
546	The effects of vacancies in the mechanical properties of tungsten: A first-principles study. 2015 , 342, 70-75	7
545	Bromine as a Preferred Etchant for Si Surfaces in the Supersaturation Regime: Insights from Calculations of Atomic Scale Reaction Pathways. 2016 , 120, 15230-15234	4
544	The electronic structure of iridium and its oxides. 2016 , 48, 261-273	192
543	Formation of silicene on silver: Strong interaction between Ag and Si. 2016 , 253, 206-217	8
542	Polarization-driven catalysis via ferroelectric oxide surfaces. 2016 , 18, 19676-95	55
541	Selectivity and Reactivity of Pd-Rich PdGa Surfaces toward Selective Hydrogenation of Acetylene: Interplay of Surface Roughness and Ensemble Effect. 2016 , 120, 28654-28663	15
540	Perspective: Methods for large-scale density functional calculations on metallic systems. 2016 , 145, 220901	84
539	Compton profiles of NiO and TiO ₂ obtained from first principles GWA spectral function. 2016 , 25, 067105	0
538	Noncollinear magnetic structures of FeMn ultrathin films on Cu(001). 2016 , 100, 767-779	1
537	Plane-Wave Density Functional Theory. 2016 , 135-172	
536	Erratum: Step energy and step interactions on the reconstructed GaAs(001) surface [Phys. Rev. B 90, 115314 (2014)]. 2016 , 94,	3
535	Mechanical and electronic properties of antiperovskite Ti-based compounds AXTi ₃ (X = C, N): A first-principles investigation. 2016 , 119, 044903	1
534	GW approximation study of late transition metal oxides: Spectral function clusters around Fermi energy as the mechanism behind smearing in momentum density. 2016 , 30, 1650162	
533	Photocatalytic reduction of CO ₂ with H ₂ O over modified TiO ₂ nanofibers: Understanding the reduction pathway. 2016 , 9, 1956-1968	48
532	Geometric and electric properties of graphitic carbon nitride sheet with embedded single manganese atom under bi-axial tensile strain. 2016 , 16, 809-815	17

531	Manipulating charge density waves in $1T\bar{1}TaS_2$ by charge-carrier doping: A first-principles investigation. 2016 , 94,	32
530	Non-covalently generated 3D supramolecular crystal structure in a new family of hybrid nitrates templated by piperazine: Thermal behavior and in vitro antimicrobial potential. 2016 , 119, 238-247	9
529	Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111). 2016 , 59, 1383-1393	1
528	Dirac Node Lines in Pure Alkali Earth Metals. <i>Physical Review Letters</i> , 2016 , 117, 096401	7.4 131
527	First-principles study of ferroelectricity induced by $p\bar{d}$ hybridization in ferrimagnetic $NiFe_2O_4$. 2016 , 380, 3302-3306	10
526	Oxidation of Ethylene on Oxygen Reconstructed Silver Surfaces. 2016 , 120, 28630-28638	31
525	The explicit examination of the magnetic states of electrides. 2016 , 18, 27326-27335	15
524	Magnetocrystalline anisotropy in $Gd(Co,Fe)_{12}B_6$: A first-principles study. 2016 , 688, 118-122	4
523	Cation diffusion and hybridization effects at the Mn-GaSe(0001) reacted interface: Ab initio calculations and soft x-ray electron spectroscopy studies. 2016 , 93,	3
522	Quantum stability and magic lengths of metal atom wires. 2016 , 93,	7
521	Sn/Be Sequentially co-doped Hematite Photoanodes for Enhanced Photoelectrochemical Water Oxidation: Effect of Be(2+) as co-dopant. 2016 , 6, 23183	55
520	The role of stoichiometry in superconducting NbSn: electronic and vibrational properties from ab initio calculations. 2016 , 18, 32840-32846	2
519	Determining the atomic structure of the $(4\bar{4})$ silicene layer on Ag(111) by combined grazing-incidence x-ray diffraction measurements and first-principles calculations. 2016 , 94,	20
518	Accelerated search for materials with targeted properties by adaptive design. 2016 , 7, 11241	352
517	Phonon dispersions and Fermi surfaces nesting explaining the variety of charge ordering in titanium-oxypnictides superconductors. 2016 , 6, 29661	14
516	Electronic Properties of Homo- and Heterobilayer Graphyne: The Idea of a Nanocapacitor. 2016 , 120, 26579-26587	46
515	Superconducting H $5S_2$ phase in sulfur-hydrogen system under high-pressure. 2016 , 6, 23160	49
514	Atomic-Scale Observation of Irradiation-Induced Surface Oxidation by In Situ Transmission Electron Microscopy. 2016 , 3, 1600751	10

513	Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. 2016 , 12, 3305-15	35
512	Elastic constants of beryllium: a first-principles investigation. 2016 , 28, 075401	53
511	Control of crystallite and particle size in the synthesis of layered double hydroxides: Macromolecular insights and a complementary modeling tool. 2016 , 468, 86-94	51
510	Reproducibility in density functional theory calculations of solids. 2016 , 351, aad3000	784
509	Adsorption of Acetonitrile on Platinum and its Effects on Oxygen Reduction Reaction in Acidic Aqueous Solutions Combined Theoretical and Experimental Study. 2016 , 7, 235-248	13
508	Periodic DFT Study on the Adsorption and Catalytic Desulfurization of Thiophene over VC(001) and VN(001) via Hydrogenation and Direct Pathways. 2016 , 120, 4881-4894	11
507	First principles predictions of superconductivity in doped stanene. 2016 , 118, 11-15	31
506	Ferroelectric oxide surface chemistry: water splitting via pyroelectricity. 2016 , 4, 5235-5246	78
505	Band gap engineering of carbon nanotubes via regular addition patterns of covalent functional groups. 2016 , 100, 187-195	6
504	High-pressure phase diagram of gold from first-principles calculations: Converging to an isotropic atomic stacking order. 2016 , 114, 72-78	7
503	The electronic structure of iridium oxide electrodes active in water splitting. 2016 , 18, 2292-6	215
502	A comprehensive lattice-stability limit surface for graphene. 2016 , 86, 19-41	3
501	Structure and stability of clean and adsorbate covered intermetallic PdGa surfaces: A first principles study. 2016 , 644, 69-79	5
500	AiiDA: automated interactive infrastructure and database for computational science. 2016 , 111, 218-230	275
499	Hydrides of Alkaline Earth-Tetrel (AeTt) Zintl Phases: Covalent Tt-H Bonds from Silicon to Tin. 2017 , 56, 1061-1071	20
498	First-principles investigations of electronic and magnetic properties of the FeRh/MgO (001) interface. 2017 , 700, 191-197	6
497	A New Type of Scaling Relations to Assess the Accuracy of Computational Predictions of Catalytic Activities Applied to the Oxygen Evolution Reaction. 2017 , 9, 1261-1268	61
496	Improved HER activity of Ni and stainless steel electrodes activated by NiCoMo ionic activator [A combined DFT and experimental study. 2017 , 42, 5072-5082	4

495	Suppressed superconductivity in substrate-supported $\sqrt{3} \times \sqrt{3}$ borophene by tensile strain and electron doping. 2017 , 4, 025032	63
494	Hydrogen trapping at divacancies and impurity-vacancy complexes in nickel: First principles study. 2017 , 487, 135-142	16
493	Prediction of phonon-mediated superconductivity in borophene. 2017 , 95,	138
492	Corrosion inhibition of copper in aqueous chloride solution by 1H-1,2,3-triazole and 1,2,4-triazole and their combinations: electrochemical, Raman and theoretical studies. 2017 , 19, 6113-6129	44
491	Ab initio simulations of the intercalation of iron(III) porphyrinates in Zn ₂ Al-LDH: Structural analysis and evaluation of their basic and acid sites. 2017 , 143, 220-226	6
490	The Investigation of Electronic Structure of Transition Metal Doped TiO ₂ for Diluted Magnetic Semiconductor Applications: A First Principle Study. 2017 , 170, 141-147	10
489	WITHDRAWN: Metformine-functionalized graphene oxide to immobilization of palladium nanoparticles as a heterogeneous and recyclable nanocatalyst for Suzuki coupling reactions and reduction of 4-nitrophenol. 2017 ,	
488	Unexpected coordination number and phase diagram of niobium diselenide under compression. 2017 , 19, 13219-13229	6
487	Computational Design of Ni-Zn Based Catalyst for Direct Hydrazine Fuel Cell Catalyst Using Density Functional Theory. 2017 , 170, 148-153	10
486	Thermodynamic cycles of the alkali metal-ligand complexes central to electride formation. 2017 , 19, 12816-12825	6
485	A First Principle Study of the Electronic Structures of Transition Metal Doped GaN for Diluted Magnetic Semiconductor Applications. 2017 , 170, 124-130	5
484	WITHDRAWN: Multi walled carbon nanotubes modified with mercapto-melamine groups for the stabilization of palladium nanoparticles: An efficient nanocatalyst for the Suzuki reaction in aqueous media under mild conditions. 2017 ,	
483	Two-dimensional nitrogen-rich transition metal compounds: The case of TiN ₂ . 2017 , 219, 29-34	2
482	Quantum and isotope effects in lithium metal. 2017 , 356, 1254-1259	38
481	Nitrogen and Iron-Codoped Carbon Hollow Nanotubes as High-Performance Catalysts toward Oxygen Reduction Reaction: A Combined Experimental and Theoretical Study. 2017 , 29, 5617-5628	74
480	WITHDRAWN: Multi walled carbon nanotubes modified with mercapto-melamine groups for the stabilization of palladium nanoparticles: An efficient nanocatalyst for the Suzuki reaction in aqueous media under mild conditions. 2017 ,	
479	Extra electronic outer-shell peculiarities accessible under a joint XPS and DFT study. 2017 , 19, 15842-15848	2
478	Relationships between the distribution of O atoms on partially oxidized metal (Al, Ag, Cu, Ti, Zr, Hf) surfaces and the adsorption energy: A density-functional theory study. 2017 , 121, 225303	5

477	Adsorption, dissociation and diffusion of hydrogen on the ZrCo surface and subsurface: A comprehensive study using first principles approach. 2017 , 422, 394-405	23
476	□Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations. 2017 , 121, 8653-8661	14
475	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. 2017 , 146, 114104	117
474	Non-FCC rich Au crystallites exhibiting unusual catalytic activity. 2017 , 10, 2271-2279	13
473	Electronic properties of MgZnPt ₂ at extremely high temperatures and pressures. 2017 , 55, 1011-1017	
472	First principles investigations of small bimetallic PdGa clusters as catalysts for hydrogen dissociation. 2017 , 487, 87-96	7
471	Influence of the external pressure on the quantum correlations of molecular magnets. 2017 , 117, 20004	3
470	Adsorption of graphene to nickel (111) using the exchange-hole dipole moment model. 2017 , 118, 184-191	17
469	Energetics of atomic hydrogen absorption in C15-Fe ₂ Zr Laves phases with ternary additions: A DFT study. 2017 , 42, 2157-2166	8
468	Pressure-induced superconductivity in the giant Rashba system BiTeI. 2017 , 29, 09LT02	10
467	Trends in reactivity of electrodeposited 3d transition metals on gold revealed by operando soft x-ray absorption spectroscopy during water splitting. 2017 , 50, 024002	9
466	How Density Functional Theory Surface Energies May Explain the Morphology of Particles, Nanosheets, and Conversion Films Based on Layered Double Hydroxides. 2017 , 121, 2211-2220	24
465	Tunable Broadband Nanocarbon Transparent Conductor by Electrochemical Intercalation. 2017 , 11, 788-796	27
464	The Effect of Hydrostatic Pressure on the Superconducting and Structural Properties of Nb ₃ Sn: Ab-initio Modeling and SR-XRD Investigation. 2017 , 27, 1-5	3
463	Adsorption of atoms and molecules on s-triazine sheet with embedded manganese atom: First-principles calculations. 2017 , 381, 3664-3674	14
462	The ionic versus metallic nature of 2D electrides: a density-functional description. 2017 , 19, 27343-27352	10
461	GW approximation study of the Compton profile of ZnSe. 2017 , 172, 664-677	
460	Implementation of a method for calculating temperature-dependent resistivities in the KKR formalism. 2017 , 96,	0

459	Strain-induced Weyl and Dirac states and direct-indirect gap transitions in group-V materials. 2017 , 4, 045018	16
458	Evaluation and Optimization of Interface Force Fields for Water on Gold Surfaces. 2017 , 13, 5610-5623	19
457	Modulated, three-directional, and polar structural instability in layered d1NaTiO2. 2017 , 95,	
456	Real-time atomic scale observation of void formation and anisotropic growth in II-VI semiconducting ribbons. 2017 , 9, 12479-12485	1
455	Effect of the interfacial O and Mg vacancies on electronic structure and transport properties of the FeRh/MgO/FeRh (0 0 1) magnetic tunnel junction: DFT calculations. 2017 , 444, 394-400	
454	Lithium and sodium adsorption properties of monolayer antimonene. 2017 , 5, 347-354	50
453	Adsorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model. 2017 , 124, 531-540	16
452	Theoretical investigation on the point defect formation energies in beryllium and comparison with experiments. 2017 , 12, 453-457	10
451	Ab initio study of the BaTiO3/Ge interface. 2017 , 96,	10
450	Hydrogen evolution reaction catalyzed by ruthenium ion-complexed graphitic carbon nitride nanosheets. 2017 , 5, 18261-18269	102
449	Theoretical investigation of interaction of hydrogen and intermetallic compound YCo5. 2017 , 726, 1085-1091	
448	Strain Effects on the Interaction Between NO2 and the Mo-Edge of the MoS2 Zigzag Nanoribbon. 2017 , 16, 982-990	3
447	DFT-based calculations of the adsorptions of acetic acid, triacetin, methanol and the alkoxide formation on the surfaces of zinc acetate. 2017 , 440, 43-49	7
446	Structural phase transition, electronic and superconducting properties of ScBi and YBi. 2017 , 266, 39-45	9
445	Crystallographic structure and energetics of the Rh(1 0 0)-(3 \times 1)-2O phase. 2017 , 29, 365001	
444	Understanding the cooperative atomic motion and shape change of ultrasmall Au nanoparticles below the premelting temperature. 2017 , 7, 55807-55811	1
443	Investigation into Structural Phase Transitions in Layered Titanium-Oxyphosphates by a Computational Phonon Analysis. 2017 , 56, 13732-13740	4
442	Strain-induced polar discontinuities in two-dimensional materials from combined first-principles and Schrödinger-Poisson simulations. 2017 , 96,	8

441	The Magnetic and Crystal Structure of MnGa (1.15 Å Å.8) Alloys. 2017 , 7, 646	7
440	Oxidation Mechanism of Arsenopyrite in the Presence of Water. 2017 , 121, 26887-26894	6
439	Identification of conjugate electron transitions in X-ray photoelectron spectra. 2017 , 58, 1160-1165	2
438	Possible bcc -> sc phase transitions in CaBr solid solutions under pressure. 2017 , 118, 723-730	1
437	Praseodymium Telluride: A High-Temperature, High-ZT Thermoelectric Material. 2018 , 2, 698-709	33
436	Reactive Dynamics Simulation Study on the Pyrolysis of Polymer Precursors To Generate Amorphous Silicon Oxycarbide Structures. 2018 , 122, 5767-5773	6
435	Lithium doping and vacancy effects on the structural, electronic and magnetic properties of hexagonal boron nitride sheet: A first-principles calculation. 2018 , 118, 185-195	9
434	Structural phase transition, electronic and lattice dynamical properties of half-Heusler compound CaAuBi. 2018 , 745, 240-246	8
433	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. 2018 , 13, 246-252	874
432	Quantum Capacitance Estimations of Pyrrolic-Rich Graphene for Supercapacitor Electrodes. 2018 , 17, 205-211	10
431	Ab initio calculation of spin fluctuation spectra using time-dependent density functional perturbation theory, plane waves, and pseudopotentials. 2018 , 97,	13
430	Tunable magnetotransport in Fe/hBN/graphene/hBN/Pt(Fe) epitaxial multilayers. 2018 , 51, 095302	6
429	Structural and Electronic Descriptors of Catalytic Activity of Graphene-Based Materials: First-Principles Theoretical Analysis. 2018 , 14, 1703609	37
428	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1 1 1). 2018 , 693, 28-33	11
427	The magnetic effects on the energetic landscape of Fe-Cu alloy: A model Hamiltonian approach. 2018 , 145, 163-173	4
426	Effects of atoms and molecules adsorption on electronic and magnetic properties of s-triazine with embedded Fe atom: DFT investigations. 2018 , 98, 1114-1129	8
425	Electronic structure and superconducting behaviour of LuPtBi half-Heusler compound: A first principle study. 2018 , 544, 22-26	12
424	Ab Initio Study of the Electronic Structure, Elastic Properties, Magnetic Feature and Thermodynamic Properties of the Ba ₂ NiMoO ₆ Material. 2018 , 192, 265-285	10

423	Effect of a Metal Substrate on Interlayer Interactions in Bilayer Graphene. 2018 , 122, 8910-8918	6
422	The Selective Species in Ethylene Epoxidation on Silver. 2018 , 8, 3844-3852	46
421	Surface termination analysis of stoichiometric metal hexaborides: Insights from first-principles and XPS measurements. 2018 , 144, 187-201	16
420	Droplet spreading on a surface exhibiting solid-liquid interfacial premelting. 2018 , 143, 319-328	6
419	First-principles investigation of graphitic carbon nitride monolayer with embedded Fe atom. 2018 , 667, 112-120	18
418	Effect of tetravalent dopants on hematite nanostructure for enhanced photoelectrochemical water splitting. 2018 , 427, 1203-1212	36
417	Are multiple oxygen species selective in ethylene epoxidation on silver?. 2018 , 9, 990-998	43
416	Structural and electronic properties of M-MOF-74 (M = Mg, Co or Mn). 2018 , 691, 283-290	33
415	Adhesion of electrodes on diamond (111) surface: A DFT study. 2018 , 81, 168-175	10
414	Single Atomic Layer Ferroelectric on Silicon. 2018 , 18, 241-246	16
413	Adsorption of water, sulfates and chloride on arsenopyrite surface. 2018 , 434, 389-399	12
412	Adsorption and Diffusion of Hydrogen on Low-Index (110) and (111) Surfaces of Aluminum. 2018 , 91, 1603-1616	
411	Precision and efficiency in solid-state pseudopotential calculations. 2018 , 4,	181
410	Density-functional description of alkalides: introducing the alkalide state. 2018 , 20, 26710-26718	4
409	A facile synthesis methodology for preparation of Ag-Ni-reduced graphene oxide: a magnetically separable versatile nanocatalyst for multiple organic reactions and density functional study of its electronic structures.. 2018 , 8, 37774-37788	12
408	Hidden Resources of Coordinated XPS and DFT Studies. 2018 ,	
407	Elastic anisotropy and thermal properties of extended linear chain compounds MV ₂ Ga ₄ (M = Sc, Zr, Hf) from ab-initio calculations. 2018 , 4, 529-539	6
406	Spin dynamics from time-dependent density functional perturbation theory. 2018 , 91, 1	7

405	A unique oxygen ligand environment facilitates water oxidation in hole-doped IrNiOx core-shell electrocatalysts. 2018 , 1, 841-851	253
404	DFT modeling of metallic nanoparticles. 2018 , 12, 239-293	8
403	Intercalation of alkali metals (Li, Na, and K) in molybdenum dinitride (MoN ₂) and titanium dinitride (TiN ₂) from first-principles calculations. 2018 , 17, e00335	2
402	Adsorption Energetics of Atoms and Diatomic Gases with Electrocatalysis Approach towards Hydrogen and Oxygen Evolution Reaction on Pt Surfaces. 2018 , 3, 10515-10525	6
401	Hidden order in URu ₂ Si ₂ : Symmetry-induced antitoroidal vortices. 2018 , 98,	1
400	Multigap anisotropic superconductivity in borophenes. 2018 , 98,	17
399	Microscopy of hydrogen and hydrogen-vacancy defect structures on graphene devices. 2018 , 98,	3
398	Electron-phonon interaction in a Ca ₂ N monolayer: Intrinsic mobility of electrene. 2018 , 98,	11
397	Point of Anchor: Impacts on Interfacial Charge Transfer of Metal Oxide Nanoparticles. 2018 , 140, 15290-15299	13
396	Ab-initio analysis of magnetic, structural, electronic and thermodynamic properties of the Ba ₂ TiMnO ₆ manganite. 2018 , 85, 27-36	9
395	Improving the electrochemical response of nanostructured MoO ₃ electrodes by Co doping: Synthesis and characterization. 2018 , 121, 375-385	17
394	Muon contact hyperfine field in metals: A DFT calculation. 2018 , 97,	8
393	The Crystalline Structure of Tensile Strained SrRuO ₃ : A First-Principles Investigation. 2018 , 18, 3397-3403	2
392	Pressure-Induced Isostructural Antiferromagnetic-Ferromagnetic Transition in an Organic Electride. 2018 , 122, 12742-12747	10
391	Microscopic Insights into Hydrogen Permeation Through a Model PdCu Membrane from First-Principles Investigations. 2018 , 122, 12920-12933	5
390	A molecular dynamics framework to explore the structure and dynamics of layered double hydroxides. 2018 , 163, 164-177	18
389	Seawater desalination using pillared graphene as a novel nano-membrane in reverse osmosis process: nonequilibrium MD simulation study. 2018 , 20, 22241-22248	11
388	DFT Study of Azole Corrosion Inhibitors on Cu ₂ O Model of Oxidized Copper Surfaces: I. Molecule-Surface and Cl-Surface Bonding. 2018 , 8, 310	21

- 387 DFT Study of Azole Corrosion Inhibitors on Cu₂O Model of Oxidized Copper Surfaces: II. Lateral Interactions and Thermodynamic Stability. **2018**, 8, 311 11
- 386 Charge density wave phase, Mottness, and ferromagnetism in monolayer 1T-NbSe₂. **2018**, 98, 21
- 385 Mechanisms for carbon adsorption on Au(110)-(2 × 1): A work function analysis. **2018**, 677, 232-238 4
- 384 High pressure structural, elastic and electronic properties of a new half Heusler compound: AuYPb. **2018**, 547, 83-87 8
- 383 Synthesis of multifunctional CuFeO-reduced graphene oxide nanocomposite: an efficient magnetically separable catalyst as well as high performance supercapacitor and first-principles calculations of its electronic structures.. **2018**, 8, 27725-27739 34
- 382 Electronic structure of a buried two-dimensional antiferromagnetic layer: Experimental and theoretical investigation of Ag/Cr/Ag(001). **2018**, 98, 1
- 381 Stable Red Emission from Nanosheets of Molecularly Doped Hexagonal Boron Nitride. **2018**, 122, 21076-21082
- 380 Free-atom-like d states in single-atom alloy catalysts. **2018**, 10, 1008-1015 206
- 379 Electronic and structural peculiarities of Br₂-embedded C₂F: XPS and DFT study. **2018**, 8, 085319 3
- 378 Acidic and basic sites of M₂DEBDC (M = Mg or Mn and E = O or S) acting as catalysts for cyanosilylation of aldehydes. **2018**, 154, 98-107 4
- 377 Microscopic understanding of electrocatalytic reduction of CO on Pd-polyaniline composite: an ab initio study. **2018**, 24, 248 2
- 376 Metal-support interaction in catalysis: The influence of the morphology of a nano-oxide domain on catalytic activity. **2018**, 237, 753-762 12
- 375 Structural stability of binary (hbox {Pd}_{34-n}hbox {M}_{n}) ((hbox {M}=hbox {Cu}), Ag, Au) clusters. **2018**, 137, 1 4
- 374 Graphitic Nitrogen Is Responsible for Oxygen Electroreduction on Nitrogen-Doped Carbons in Alkaline Electrolytes: Insights from Activity Attenuation Studies and Theoretical Calculations. **2018**, 8, 6827-6836 132
- 373 Enhanced Electron-Phonon Interaction in Multivalley Materials. **2019**, 9, 25
- 372 Vacuum-Level Shift at Al/LiF/Alq Interfaces: A First-Principles Study. **2019**, 4, 13426-13434 3
- 371 Interaction mechanism of CO with Pd-rich copper clusters. **2019**, 2
- 370 Electronic structure and magnetic properties of few-layer Cr₂Ge₂Te₆: the key role of nonlocal electron-electron interaction effects. **2019**, 6, 045042 18

369	Descriptor for the Efficacy of Aliovalent Doping of Oxides and Its Application for the Charging of Supported Au Clusters. 2019 , 123, 19794-19805	3
368	Diffusivity of hydrogen and properties of point defects in beryllium investigated by DFT. 2019 , 524, 323-329	4
367	Structural stability of scandium monochalcogenides ScS and ScSe under pressure and superconductivity: A first principles study. 2019 , 21, e00418	4
366	A simple descriptor for binding and charge transfer at blue phosphorene-metal interfaces. 2019 , 492, 16-22	3
365	Surface coverage dependent mechanisms for the absorption and desorption of hydrogen from the W(1 1 0) and W(1 0 0) surfaces: a density functional theory investigation. 2019 , 59, 106022	13
364	Incisive study on stability and vibrational properties of NO _x (x = 1 to 3) over Pt surfaces: A comparative analysis. 2019 , 690, 121467	1
363	Axial field induced spin response in Fe/hBN-based tunnel junctions. 2019 , 100,	3
362	Ni- and Cu-doping effects on formation and migration energies of oxygen vacancies in Ba _{0.5} Sr _{0.5} Fe _{1-x} (Cu/Ni) _x O ₃ perovskites: a DFT + U study. 2019 , 125, 1	2
361	Exfoliation of Ti ₂ C and Ti ₃ C ₂ Mxenes from bulk trigonal phases of titanium carbide: A theoretical prediction. 2019 , 299, 113657	13
360	Tuning the bandgap and introducing magnetism into monolayer BC ₃ by strain/defect engineering and adatom/molecule adsorption. 2019 , 126, 144304	44
359	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. 2019 , 5,	33
358	Structural and lattice dynamical study of half Heusler alloys RuMnX (X = P, As). 2019 ,	2
357	Surface Piezoelectricity of (0001) Sapphire. 2019 , 11,	7
356	Relative Abundance of [Formula: see text] Topological Order in Exfoliable Two-Dimensional Insulators. 2019 , 19, 8431-8440	27
355	Theoretical prediction of superconductivity in monolayer CoO. 2019 , 11, 17052-17057	4
354	Selective control of molecule charge state on graphene using tip-induced electric field and nitrogen doping. 2019 , 3,	14
353	Crystal field, ligand field, and interorbital effects in two-dimensional transition metal dichalcogenides across the periodic table. 2019 , 6, 025015	15
352	Stability and magnetism of FeN high-pressure phases. 2019 , 21, 5262-5273	8

351	A study on the formation and migration of oxygen vacancies in Ba _{0.5} Sr _{0.5} Co _{0.75} Fe _{0.25} O _{3-δ} perovskite surfaces by first-principles modelling. 2019 , 226, 371-377	3
350	Grand canonical simulations of electrochemical interfaces in implicit solvation models. 2019 , 150, 041730	80
349	Strain Engineering of Adsorbate Self-Assembly on Graphene for Band Gap Tuning. 2019 , 123, 4475-4482	11
348	Ab initio study of the LiH phase diagram at extreme pressures and temperatures. 2019 , 99,	3
347	How to control selectivity in alkane oxidation?. 2019 , 10, 2429-2443	18
346	Oxygen Reduction Reaction Catalyzed by Black-Phosphorus-Supported Metal Nanoparticles: Impacts of Interfacial Charge Transfer. 2019 , 11, 24707-24714	20
345	Anti-corrosive properties of quercetin and its derivatives on Fe(111) surface: a quantum chemical approach. 2019 , 1, 1	2
344	Spectral characterization of a Rh(110) photocathode: Band structure interpretation. 2019 , 9, 065305	4
343	Progress Report on: Sulfur in Ethylene Epoxidation on Silver (SEES2). 2019 , 167-181	
342	High pressure study of half Huesler alloy: YPdSb. 2019 ,	
341	Ferroelectric ZrO ₂ Monolayers as Buffer Layers between SrTiO ₃ and Si. 2019 , 123, 15053-15061	2
340	Equipartition of Energy Defines the Size-Thickness Relationship in Liquid-Exfoliated Nanosheets. 2019 , 13, 7050-7061	71
339	Synthesis and characterization of vacancy-doped neodymium telluride for thermoelectric applications. 2019 , 31, 4460-4468	12
338	Theory of Ferroelectric ZrO ₂ Monolayers on Si. 2019 , 123, 14350-14361	9
337	Electronic Structure, Lattice Dynamics, and Superconducting Properties of Mercury-Alkaline Earth Metal Compounds: a First-Principles Study. 2019 , 32, 3425-3430	1
336	Causes of ferroelectricity in HfO ₂ -based thin films: an ab initio perspective. 2019 , 21, 12150-12162	34
335	First principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface. 2019 , 125, 185304	1
334	Crystallographic orientation dependence of work function: carbon adsorption on Au surfaces. 2019 , 117, 2157-2161	2

333	Electron-phonon coupling and the coexistence of superconductivity and charge-density wave in monolayer NbSe ₂ . 2019 , 99,	17
332	Fluorinated MOF platform for selective removal and sensing of SO from flue gas and air. 2019 , 10, 1328	164
331	Hydrogen storage on graphitic carbon nitride and its palladium nanocomposites: A multiscale computational approach. 2019 , 44, 8325-8340	17
330	Experimental and DFT study of CoCuMo ternary ionic activator for alkaline HER on Ni cathode. 2019 , 839, 224-230	1
329	Hydrogen Effect on Electron-Phonon Interactions in L10 FePd. 2019 , 32, 3125-3133	1
328	Novel 2D materials from exfoliation of layered hydroxide salts: A theoretical study. 2019 , 483, 762-771	9
327	Ruthenium atomically dispersed in carbon outperforms platinum toward hydrogen evolution in alkaline media. 2019 , 10, 631	260
326	The Basics of Electronic Structure Theory for Periodic Systems. 2019 , 7, 106	29
325	Biogas detection on carbon nitride sheet with embedded Mn atom: dispersion-corrected density functional theory. 2019 , 6, 065603	3
324	Suzuki-Miyaura reaction by heterogeneously supported Pd nanoparticles on thio-modified multi walled carbon nanotubes as efficient nanocatalyst. 2019 , 162, 240-244	19
323	Plasmonic performance of AuAgCu alloys from many-body perturbation theory. 2019 , 31, 315901	3
322	Photorealistic modelling of metals from first principles. 2019 , 5,	10
321	An experimental and theoretical study of metallorganic coordination networks of tetrahydroquinone on Cu(111). 2019 , 43, 19186-19192	2
320	A "One-Pot" Route for the Synthesis of Snowflake-like Dendritic CoNi Alloy-Reduced Graphene Oxide-Based Multifunctional Nanocomposites: An Efficient Magnetically Separable Versatile Catalyst and Electrode Material for High-Performance Supercapacitors. 2019 , 4, 20672-20689	13
319	Unified picture of lattice instabilities in metallic transition metal dichalcogenides. 2019 , 100,	3
318	Uncovering electron-phonon scattering and phonon dynamics in type-I Weyl semimetals. 2019 , 100,	15
317	An In Situ Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO ₂ Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates. 2019 , 123, 5951-5963	78
316	Continuum models of the electrochemical diffuse layer in electronic-structure calculations. 2019 , 150, 041722	43

3 ¹⁵	Metal Hexaboride Work Functions: Surface Configurations and the Electrical Double Layer from First-Principles. 2019 , 5, 1800074	5
3 ¹⁴	Phase Stability Analysis of Ternary Alkaline-Earth Hexaborides: Insights from DFT Calculations. 2019 , 1, 105-112	2
3 ¹³	Electrochemically active Ir NPs on graphene for OER in acidic aqueous electrolyte investigated by in situ and ex situ spectroscopies. 2019 , 681, 1-8	24
3 ¹²	On the presence of antisite defect in monoclinic Li ₂ FeSiO ₄ [A combined X-Ray diffraction and DFT study. 2019 , 87, 81-86	1
3 ¹¹	Immobilization of palladium nanoparticles on Metformin-functionalized graphene oxide as a heterogeneous and recyclable nanocatalyst for Suzuki coupling reactions and reduction of 4-nitrophenol. 2019 , 158, 414-422	66
3 ¹⁰	New insights into adsorption bonding of imidazole: A viable C2H bond cleavage on copper surfaces. 2019 , 479, 463-468	11
3 ⁰⁹	Tuning the electronic and magnetic properties of Fe atom embedded heptazine sheet by atomic and molecular adsorption: First-principles calculations. 2019 , 57, 1-5	3
3 ⁰⁸	First-principles prediction of ultralow resistance-area product and high magnetoresistance ratio in magnetic tunnel junction with a rock-salt type ZnO barrier. 2019 , 58, 010910	4
3 ⁰⁷	Theoretical study of structural, electronic, phonon and thermoelectric properties of KScX (X=Sn and Pb) and KYX (X=Si and Ge) half-Heusler compounds with 8 valence electrons count. 2019 , 784, 319-329	21
3 ⁰⁶	Interaction of Hydrogen with MB (M = Ba, Ca, La, and Sr) Surfaces from First Principles. 2019 , 4, 65-72	2
3 ⁰⁵	Efficient technique for ab-initio calculation of magnetocrystalline anisotropy energy. 2019 , 238, 203-213	2
3 ⁰⁴	The Role of the Copper Oxidation State in the Electrocatalytic Reduction of CO ₂ into Valuable Hydrocarbons. 2019 , 7, 1485-1492	75
3 ⁰³	O-assisted and pristine Au-Pt(100) surfaces: A platform for adsorption and decomposition of H ₂ O. 2020 , 45, 18666-18675	4
3 ⁰²	Ab initio dielectric response function of diamond and other relevant high pressure phases of carbon. 2020 , 32, 095401	9
3 ⁰¹	Theoretical study of Mn doping effects and O or Zn vacancies on the magnetic properties in wurtzite ZnO. 2020 , 63, 63-69	8
3 ⁰⁰	High-throughput computational screening for solid-state Li-ion conductors. 2020 , 13, 928-948	42
299	Investigating hydrogen evolution reaction properties of a new honeycomb 2D ALC. 2020 , 45, 18602-18611	2
298	Site preference of V and its influence on the elastic properties in the boride series V _x Mo _{5-x} SiB ₂ as studied by first principles density functional theory. 2020 , 819, 153041	2

297	Intrinsic point defects in half-Heusler AuMnSn. 2020 , 139, 109328	6
296	Comparison of computational methods for the electrochemical stability window of solid-state electrolyte materials. 2020 , 8, 1347-1359	27
295	Uncovering the structural, electronic and vibrational properties of atomically precise PdCu clusters and their interaction with CO molecule. 2020 , 229, 117912	4
294	Green synthesis and characterization of nontoxic L-methionine capped silver and gold nanoparticles. 2020 , 204, 110958	14
293	Raman spectrum of layered jacutingaite (Pt ₂ HgSe ₃) crystals Experimental and theoretical study. 2020 , 51, 357-365	5
292	Ripples in isotropically compressed graphene. 2020 , 173, 109422	3
291	Spectroscopic and first-principles investigations of iodine species incorporation into ettringite: Implications for iodine migration in cement waste forms. 2020 , 389, 121880	27
290	First Principles Density Functional Theory Prediction of the Crystal Structure and the Elastic Properties of Mo ₂ ZrB ₂ and Mo ₂ HfB ₂ . 2020 , 10, 865	0
289	Role of OH Intermediates during the Au Oxide Electro-Reduction at Low pH Elucidated by Electrochemical Surface-Enhanced Raman Spectroscopy and Implicit Solvent Density Functional Theory. 2020 , 10, 12716-12726	6
288	Electronic, vibrational, and electron-phonon coupling properties in SnSe ₂ and SnS ₂ under pressure. 2020 , 8, 16404-16417	3
287	Finite-temperature-based time-dependent density-functional theory method for static electron correlation systems. 2020 , 152, 244111	0
286	Theoretical study of structural, electronic and lattice dynamical properties of novel AlNiP half-Heusler alloy. 2020 , 100, 2785-2801	9
285	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of Mn _x Gey compounds. 2020 , 127, 244901	12
284	Enhanced Thermopower in the Antiferromagnetic Phase of Mn _{2-x} Cr _x Sb. 2020 , 89, 124601	1
283	Tuning Structural, Electronic, and Magnetic Properties of C Sites Vacancy Defects in Graphene/MoS ₂ van der Waals Heterostructure Materials: A First-Principles Study. 2020 , 2020, 1-11	4
282	Dynamical stability of two-dimensional metals in the periodic table. 2020 , 102,	12
281	Experimental and DFT Study of Metal-Free Catalyst for Selective Oxidation of Biomass-Derived Molecule (HMF). 2020 , 59, 13335-13342	3
280	Ultrafast photoluminescence in metals: Theory and its application to silver. 2020 , 102,	5

279	Tetragonal and uniaxial strains in pristine and doped half-Heusler AuMnSn alloy. 2020 , 848, 156186	3
278	Hydrogen Adsorption on Ordered and Disordered Pt-Ni Alloys. 2020 , 63, 714-727	3
277	Tuning Structural and Electronic Properties of Phosphorene with Vacancies. 2020 , 6, 7-15	0
276	First-principles study of electronic and magnetic properties of nickel doped hexagonal boron nitride (h-BN). 2020 , 93, 1	3
275	Lithium Polysulfide Interaction with Group III Atoms-Doped Graphene: A Computational Insight. 2020 , 6, 46	3
274	Electrosorption at metal surfaces from first principles. 2020 , 6,	25
273	Features of Extended XPS Spectra of C2FBr0.15 Intercalate and Silver Foil. 2020 , 61, 523-532	0
272	Spin-polarized electrical transport in transition metal encapsulated C20 fullerenes: A theoretical account. 2020 , 1, 100002	1
271	Enhanced hydrogen evolution reactivity on $(\text{Mo})_2\text{C}/(\text{Mo})_2\text{N}$ composites. 2020 , 43, 1	3
270	Stationary interatomic force constant matrix method with ultrasoft pseudopotentials. 2020 , 102,	0
269	First principles density functional theory calculations on the elastic properties of Mo-Si based solid solutions. 2020 , 882, 012024	1
268	Thermoelectric response of anti-fluoride Sr2Ge semiconducting material: A first-principles study. 2020 ,	
267	Degrading CO poisoning over foreign atom seized Ag12M icosahedral bimetallic clusters. 2020 ,	1
266	Lattice dynamics of novel Heusler alloys MnYZ_2 (Z=Al and Si). 2020 , 590, 412222	14
265	AFeSe_2 (A=Tl, K, Rb, or Cs): Iron-based superconducting analog of the cuprates. 2020 , 101,	1
264	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. 2020 , 101,	8
263	Low-temperature electron-phonon relaxation in Cu and Ag thin films. 2020 , 101,	1
262	Preferential out-of-plane conduction and quasi-one-dimensional electronic states in layered 1T-TaS2. 2020 , 4,	19

261	Modeling Morphology and Catalytic Activity of Nanoparticle Ensembles Under Reaction Conditions. 2020 , 10, 6149-6158		16
260	Hydrogen trapping at surface and subsurface vacancies of low-index surfaces of Pd. 2020 , 698, 121610		2
259	Strain-induced room-temperature ferroelectricity in SrTiO membranes. 2020 , 11, 3141		51
258	Why are MoS ₂ monolayers not a good catalyst for the oxygen evolution reaction?. 2020 , 528, 146591		10
257	CO capture, activation and dissociation on the TiC surface and TiC MXene: the role of surface structure. 2020 , 22, 14599-14612		10
256	Suppression of nano-hydride growth on Nb(100) due to nitrogen doping. 2020 , 152, 214703		6
255	Atomically thin half-van der Waals metals enabled by confinement heteroepitaxy. 2020 , 19, 637-643		53
254	Data-driven design of B20 alloys with targeted magnetic properties guided by machine learning and density functional theory. 2020 , 35, 890-897		4
253	Frustration and Atomic Ordering in a Monolayer Semiconductor Alloy. <i>Physical Review Letters</i> , 2020 , 124, 096101	7-4	10
252	Achieving Minimal Heat Conductivity by Ballistic Confinement in Phononic Metalattices. 2020 , 14, 4235-4243		12
251	Bulk and Surface Electronic Structure of the Dual-Topology Semimetal Pt ₂ HgSe ₃ . <i>Physical Review Letters</i> , 2020 , 124, 106402	7-4	20
250	ELSI [An open infrastructure for electronic structure solvers. 2020 , 256, 107459		14
249	Blocking of the martensitic transition at the nanoscale in a Ti ₂ NiCu wedge. 2020 , 101,		3
248	Structure, electronic and magnetic properties of 2D Graphene-Molybdenum diSulphide (G-MoS ₂) Heterostructure (HS) with vacancy defects at Mo sites. 2020 , 24, e00489		7
247	First-Principles Study of Molecular Adsorption of Hydrogen/s on Co-Adatom Graphene. 2020 , 25, 15-23		1
246	Multicomponent gas separation and purification using advanced 2D carbonaceous nanomaterials.. 2020 , 10, 24255-24264		9
245	Motif based high-throughput structure prediction of superconducting monolayer titanium boride. 2020 , 22, 16236-16243		3
244	Metal-free ferromagnetic semiconductor: Mechanical, electronic and magnetic properties of boron doped graphitic carbon nitride (gC ₆ N ₆) sheet. 2020 , 254, 123470		8

243	Structural stability, electronic and thermoelectric properties of ruthenium silicide. 2020 , 826, 154164	2
242	Effects of surface charge and cluster size on the electrochemical dissolution of platinum nanoparticles using COMB3 and continuum electrolyte models. 2020 , 152, 064102	1
241	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. 2020 , 101,	14
240	Doping induced charge density wave in monolayer TiS ₂ and phonon-mediated superconductivity. 2020 , 127, 044301	5
239	Numerical quadrature in the Brillouin zone for periodic Schrödinger operators. 2020 , 144, 479-526	3
238	Structural Phases of Alkanethiolate Self-Assembled Monolayers (C112) on Cu[100] by Density Functional Theory. 2020 , 124, 3802-3811	2
237	On-surface synthesis of extended linear graphyne molecular wires by protecting the alkynyl group. 2020 , 22, 12180-12186	7
236	Tuning electronic and magnetic properties of the graphone/Ni(111) interface by oxygen intercalation: A first-principles prediction. 2020 , 101,	1
235	Nanocatalysts Unravel the Selective State of Ag. 2020 , 12, 2977-2988	4
234	Ab initio thermodynamic properties of certain compounds in Nd-Fe-B system. 2020 , 180, 109696	2
233	The role of oxophilic Mo species in Pt/MgO catalysts as extremely active sites for enhanced hydrodeoxygenation of dibenzofuran. 2020 , 10, 2948-2960	9
232	Support work function as a descriptor and predictor for the charge and morphology of deposited Au nanoparticles. 2020 , 152, 144704	2
231	First-principles investigation on the electronic, mechanical and lattice dynamical properties of novel AlNiX (X = As and Sb) half-Heusler alloys. 2021 , 26, 101885	7
230	Artificial neural network potential for pure zinc. 2021 , 188, 110207	6
229	A first principle study of structural, elastic, electronic and thermodynamic properties of Half-Heusler compounds; YNiPn (Pn=As, sb, and bi). 2021 , 112, 106507	2
228	Synergistic effect of 2-mercaptobenzimidazole and octylphosphonic acid as corrosion inhibitors for copper and aluminium [An electrochemical, XPS, FTIR and DFT study. 2021 , 182, 109082	30
227	Role of geometry, charge and fluxionality of clusters in CO ₂ activation on supported sub-nanometer metal clusters: The case of Cu tetramers on pristine and O-terminated MXene. 2021 , 370, 93-103	3
226	Molecular Analysis of the Unusual Stability of an IrNbO Catalyst for the Electrochemical Water Oxidation to Molecular Oxygen (OER). 2021 , 13, 3748-3761	5

225	First-principles prediction of structural stability and thermoelectric properties of SrGaSnH.. 2021 , 11, 3304-3314	2
224	First-principles study of nickel reactivity under two-dimensional cover: Ni ₂ C formation at rotated graphene/Ni(111) interface. 2021 , 5,	
223	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. 2021 , 15, 148-155	257
222	Organically Capped Iridium Nanoparticles as High-Performance Bifunctional Electrocatalysts for Full Water Splitting in Both Acidic and Alkaline Media: Impacts of MetalLigand Interfacial Interactions. 2021 , 11, 1179-1188	21
221	Theoretical investigation of superconductivity in diamond: Effects of doping and pressure. 2021 , 129, 043903	4
220	Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations. 2021 , 103,	14
219	Outstanding Thermoelectric Performance of MCu ₃ X ₄ (M = V, Nb, Ta; X = S, Se, Te) with Unaffected Band Degeneracy under Pressure. 2021 , 4, 1942-1953	4
218	Emergence of intrinsic superconductivity in monolayer W ₂ N ₃ . 2021 , 103,	4
217	Coexistence of topological Weyl and nodal-ring states in ferromagnetic and ferrimagnetic double perovskites. 2021 , 103,	1
216	First-principles study of structure, electronic, and magnetic properties of C sites vacancy defects in water adsorbed graphene/MoS van der Waals heterostructures. 2021 , 27, 82	5
215	Thermodynamic Cyclic Voltammograms Based on Calculations: Ag(111) in Halide-Containing Solutions. 2021 , 17, 1782-1794	8
214	Electron-phonon contribution in aluminene: Superconductive and transport properties. 2021 , 151, 106822	2
213	Extensive Benchmarking of DFT+U Calculations for Predicting Band Gaps. 2021 , 11, 2395	14
212	Predicting the Pseudocapacitive Windows for MXene Electrodes with Voltage-Dependent Cluster Expansion Models. 2021 , 4, 3151-3159	6
211	Dependence of characteristics of Hf(M)SiBCN (M = Y, Ho, Ta, Mo) thin films on the M choice: Ab-initio and experimental study. 2021 , 206, 116628	3
210	Effect of the density of states at the Fermi level on defect free energies and superconductivity: A case study of Nb ₃ Sn. 2021 , 103,	2
209	Lattice stability of ordered Au-Cu alloys in the warm dense matter regime. 2021 , 103,	2
208	High-throughput computational search for two-dimensional binary compounds: Energetic stability versus synthesizability of three-dimensional counterparts. 2021 , 103,	5

- 207 Ab Initio Study of the Electron-Phonon Coupling in Ultrathin Al Layers. **2021**, 203, 180-193
- 206 Effects of copper ion irradiation on Cu_2S and Cu_2O based supercapacitive electrodes. **2021**, 51, 829-845
- 205 Interplay between London Dispersion, Hubbard U , and Metastable States for Uranium Compounds. **2021**, 125, 2791-2799 1
- 204 A promising Zn-Ti layered double hydroxide/Fe-bearing montmorillonite composite as an efficient photocatalyst for Cr(VI) reduction: Insight into the role of Fe impurity in montmorillonite. **2021**, 546, 148835 13
- 203 Ab initio modeling and experimental investigation of Fe₂P by DFT and spin spectroscopies. **2021**, 5,
- 202 Gate-tunable imbalanced Kane-Mele model in encapsulated bilayer jacutingaite. **2021**, 5, 3
- 201 Coverage dependent CO₂ activation on Ti₂C(111) surface: Effect of intrinsic subsurface Carbon vacancies. **2021**, 706, 121798 1
- 200 Structure, Energetics, and Thermal Behavior of Bimetallic Re-Pt Clusters. **2021**, 125, 4294-4305 2
- 199 First principles study on the lattice dynamics and electron-phonon interaction of HfOs and HfRu compounds. **2021**, 584, 1353862
- 198 Development and Applications of ReaxFF Reactive Force Fields for Group-III Gas-Phase Precursors and Surface Reactions with Graphene in Metal-Organic Chemical Vapor Deposition Synthesis. **2021**, 125, 10747-10758 3
- 197 A computational study of physical, electronic, thermal and transport properties of one-dimensional boron and boron nitride systems. **2021**, 297, 122037 3
- 196 Evolutionary search for cobalt-rich compounds in the yttrium-cobalt-boron system. **2021**, 5, 0
- 195 Dynamical Stability and Superconductivity in Two-dimensional Nodal Line Semimetal CuSe and Cu₂Si. **2021**, 34, 2229-2237 0
- 194 Study Of Mercaptobenzimidazoles As Inhibitors For Copper Corrosion: Down to the Molecular Scale. **2021**, 168, 051504 9
- 193 Chemical control of the Rashba spin splitting size of Bi₂Te₃(111) surface states by adjusting the potential at the topmost atomic layer. **2021**, 103, 0
- 192 Switching of the electron-phonon interaction in 1T'₂Se₂ assisted by hot carriers. **2021**, 103, 2
- 191 Requirements for an accurate dispersion-corrected density functional. **2021**, 154, 230902 13
- 190 Structural, electronic and magnetic properties of S sites vacancy defects graphene/MoS₂ van der Waals heterostructures: First-principles study. **2021**, 10, 2150009 3

189	Compressibility and Phase Stability of Iron-Rich Ankerite. 2021 , 11, 607	3
188	Leveraging Polar Discontinuities to Tune the Binding of Methanol on BCN and GrapheneBN Lateral Heterostructures. 2021 , 125, 15012-15024	1
187	Theoretical study of thermo-dynamical and thermoelectric properties of novel half-Heusler alloys AlNiAs and AlNiSb. 2021 , 27, 102195	6
186	Dynamic recrystallization of Silver nanocubes during high-velocity impacts. 2021 , 212, 116892	4
185	Investigations of mechanical and thermoelectric properties of AlNiP novel half-Heusler alloy. 2021 , 265, 124518	9
184	Pressure evolution of the electronic structure of non-centrosymmetric EuRhGe3. 2021 , 3, 034002	0
183	Dichotomy of saddle points in energy bands of monolayer NbSe2. 2021 , 104,	0
182	Superconductivity in highly doped diamond: Role of group III and V impurities. 2021 , 130, 043903	
181	Mechanical properties of layered tilkerodeite (Pd2HgSe3) and jacutingaite (Pt2HgSe3) crystals: Insights on the interlayer, intralayer interactions, and phonons. 2021 , 130, 015105	1
180	Emergence of Nontrivial Spin Textures in Frustrated Van Der Waals Ferromagnets. 2021 , 11,	2
179	Metastability relationship between two- and three-dimensional crystal structures: a case study of the Cu-based compounds. 2021 , 11, 14588	2
178	Benzylic Csp3-Bond Oxidation on the (111) Facets of Octahedral Cu2O Nanocrystals. 2021 , 4, 7840-7855	1
177	Electronic, optical, mechanical, and thermal properties of diphenylacetylene-based graphyne nanosheet using density functional theory. 2021 , 32,	1
176	Quantifying multipoint ordering in alloys. 2021 , 104,	
175	Size effect on phonon hydrodynamics in graphite microstructures and nanostructures. 2021 , 104,	2
174	Theoretical prediction on the immiscible Pb-Sn alloy stabilized on metal surfaces. 2021 , 776, 138696	1
173	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. 2021 , 21, 7631-7636	1
172	Effect of vacancy defects in 2D vdW graphene/h-BN heterostructure: First-principles study. 2021 , 11, 085218	4

171	Electrolyte-Guided Design of Electroreductive CO Coupling on Copper Surfaces. 2021 , 4, 8201-8210	3
170	Surface Electron-Hole Rich Species Active in the Electrocatalytic Water Oxidation. 2021 , 143, 12524-12534	22
169	A Density-Functional Theory Structural Database for Discovery of Novel Actinide Waste Forms. 2021 , 21, 5100-5107	0
168	Electrochemical and quantum mechanical investigation of various small molecule organic compounds as corrosion inhibitors in mild steel. 2021 , 7, e07952	3
167	Adsorbate Partition Functions via Phase Space Integration: Quantifying the Effect of Translational Anharmonicity on Thermodynamic Properties. 2021 , 125, 20249-20260	2
166	Evaluating the stability and activity of dilute Cu-based alloys for electrochemical CO reduction. 2021 , 155, 114702	3
165	Electron-phonon superconductivity in C-doped topological nodal-line semimetal ZrPt: a muon spin rotation and relaxation (μ SR) study. 2021 , 34,	1
164	Coherent energy exchange between carriers and phonons in Peierls-distorted bismuth unveiled by broadband XUV pulses. 2021 , 3,	1
163	Synthesis, crystal and electronic structure of CaNi_2Al_8 . 2021 ,	1
162	Anisotropic phonon-mediated electronic transport in chiral Weyl semimetals. 2021 , 5,	1
161	Study of lattice dynamic, electronic and mechanical properties of Half-Heusler RuCrP alloy. 2021 , 29, 102799	1
160	Exploring the structural, elastic, lattice dynamical stability and thermoelectric properties of semiconducting novel quaternary Heusler alloy LiScPdPb . 2021 , 304, 122601	2
159	Effect of spin-polarization on structural, electronic, and lattice dynamical properties of MnY_2Ga Full Heusler alloy. 2022 , 624, 413425	1
158	CH_4 activation and $\text{C}\equiv\text{C}$ coupling on the $\text{Ti}_2\text{C}(100)$ surface in the presence of intrinsic C-vacancies: is excess good?.	
157	Vacuum ultraviolet enhanced atomic layer etching of ruthenium films. 2021 , 39, 012601	1
156	The effect of elastic strains on the adsorption energy of H, O, and OH in transition metals. 2021 , 23, 21295-21306	
155	Data-driven analysis of the electronic-structure factors controlling the work functions of perovskite oxides. 2021 , 23, 6880-6887	3
154	Effect of 3d transition metal substitutional dopants and adatoms on mono layer TcS_2 ab initio insights. 2020 , 123, 114165	3

153	Operando XANES from first-principles and its application to iridium oxide. 2020 , 22, 10807-10818	10
152	Adsorption of methane on single metal atoms supported on graphene: Role of electron back-donation in binding and activation. 2020 , 153, 244701	2
151	Raman spectrum of layered tilkerodeite (PdHgSe) topological insulator: the palladium analogue of jacutingaite (PtHgSe). 2021 , 33, 065401	2
150	Ab initio theory of the impact of grain boundaries and substitutional defects on superconducting Nb ₃ Sn. 2021 , 34, 015015	5
149	Mott-to-Goodenough insulator-insulator transition in LiVO ₂ . 2017 , 95,	2
148	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. 2018 , 2,	115
147	Influence of surface restructuring on the activity of SrTiO ₃ photoelectrodes for photocatalytic hydrogen reduction. 2019 , 3,	2
146	Probing the pseudocapacitance and energy-storage performance of RuO ₂ facets from first principles. 2019 , 3,	4
145	Electron-phonon coupling and hot electron thermalization in titanium nitride. 2019 , 3,	11
144	Theoretical investigation of charge density wave instability in CuS ₂ . 2020 , 4,	4
143	Optoelectronic response of the type-I Weyl semimetals TaAs and NbAs from first principles. 2020 , 2,	9
142	Nanowrinkled Carbon Aerogels Embedded with FeN Sites as Effective Oxygen Electrodes for Rechargeable Zinc-Air Battery. 2019 , 2019, 6813585	18
141	Importance of intersite Hubbard interactions in MnO ₂ : A first-principles DFT+U+V study. 2021 , 5,	1
140	Lattice dynamics of photoexcited insulators from constrained density-functional perturbation theory. 2021 , 104,	1
139	Large Magnetoresistance in Scandium Nitride Magnetic Tunnel Junctions Using First Principles. 2021 , 4, 2100309	
138	Graphene composites with Ru-RuO ₂ heterostructures: Highly efficient Mott-Schottky-type electrocatalysts for pH-universal water splitting and flexible zinc-air batteries. 2022 , 302, 120838	23
137	Strong Electron-Phonon Coupling in 3D WN and Coexistence of Intrinsic Superconductivity and Topological Nodal Line in Its 2D Limit. 2100477	
136	Structure of Liquid Metal Surfaces. 2011 ,	

135	Ab initio Phonons in Magnetic Ni ₂ MnAl. 2011 , 50, 05FE07	
134	Introduction. 2015 , 1-7	
133	Modelling of Phase Transitions in Calcium Strontium Superstructures at Low Pressures.. 2017 , 39, 113-125	
132	Chapter 7: First-Principles Computational Approaches to Superconducting Transition Temperatures: Phonon-Mediated Mechanism and Beyond. 2018 , 198-239	
131	Prediction of the fundamental properties of novel Be-B-Ta-based ternary compounds from first-principles calculations. 2019 , 3,	1
130	Comprehensive search for buckled honeycomb binary compounds based on noble metals (Cu, Ag, and Au). 2021 , 5,	1
129	Machine-learning interatomic potential for radiation damage effects in bcc-iron. 2022 , 202, 110960	1
128	Ground State Structural, Elastic, Electronic Properties and Pressure-Induced Structural Phase Transition of XCoSb (X = Sc, Ti, V, Cr and Mn). 2020 , 33, 1821-1829	0
127	Analysis of Ionicity-Magnetism Competition in 2D-MX ₃ Halides towards a Low-Dimensional Materials Study Based on GPU-Enabled Computational Systems. 2021 , 11,	0
126	Stability and molecular pathways to the formation of spin defects in silicon carbide. 2021 , 12, 6325	1
125	Oxygen Reduction Reaction Catalyzed by Carbon-Supported Platinum Few-Atom Clusters: Significant Enhancement by Doping of Atomic Cobalt. 2020 , 2020, 9167829	8
124	Identifying resonant dopants in BaCu ₂ S ₂ for thermoelectric applications: A density functional theory based study. 2022 , 342, 114592	
123	Topological nodal line and superconductivity of highly thermally stable two-dimensional TiB ₄ . 2021 , 104,	2
122	Maximal superconductivity in proximity to the charge density wave quantum critical point in Cu _x TiSe ₂ . 2021 , 104,	0
121	Vacancies and substitutional defects in multicomponent diboride TiZrHfTaB: first-principle study. 2021 , 34,	0
120	X-ray Absorption Spectroscopy of Trivalent Eu, Gd, Tb, and Dy Chlorides and Oxichlorides. 2021 , 897, 162629	0
119	Investigation of mechanical, thermodynamical, dynamical and electronic properties of RuAs (Cr and Fe) alloys. 2021 , 34,	1
118	Electronic and magnetic properties of RuO ₂ monolayer: DFT+U investigation. 2021 , 29, e00614	0

117	Blue and black phosphorene on metal substrates: a density functional theory study. 2021 , 34,		0
116	Intrinsic Nature of Spontaneous Magnetic Fields in Superconductors with Time-Reversal Symmetry Breaking.. <i>Physical Review Letters</i> , 2021 , 127, 237002	7.4	1
115	Palladium Nanoparticles-Decorated β -Cyclodextrin-Cyanoguanidine Modified Graphene Oxide: A Heterogeneous Nanocatalyst for Suzuki-Miyaura Coupling and Reduction of 4-Nitrophenol Reactions in Aqueous Media. 2022 , 32, 791		1
114	A periodic DFT study of CO adsorption over PdCu alloy (111) surfaces. 2022 , 48, 853		
113	Investigation of Metastable Low Dimensional Halometallates.. 2022 , 27,		0
112	Structural, electronic, elastic, phonon and thermoelectric properties of Heusler-structured intermetallic HfCu ₂ In: Using density functional theory. 2022 , 629, 413633		0
111	Adsorption and decomposition of H ₂ S on C ₂ N sheet with embedded manganese atom: First-principles calculations. 2022 , 555, 111443		0
110	Electronegativity Difference as a Descriptor for the Oxidation-Inhibiting Effect of the Alloying Element during the Early Stages of Titanium Oxidation.. 2022 ,		1
109	Computational Studies of MoS ₂ Nanotubes for Hydrodesulfurization.		0
108	Exploring the Compositional Space of High-Entropy Alloys for Cost-Effective High-Temperature Applications. 2022 , 8,		1
107	First-principles investigation of a symmetry incompatible adsorbate-substrate system: PF ₃ on Cu(001). 2022 , 719, 122045		
106	Ab initio theory of magnetism in two-dimensional 1T-TaS ₂ . 2022 , 105,		0
105	High-T _c Superconducting Hydrides Formed by LaH ₂₄ and YH ₂₄ Cage Structures as Basic Blocks. 2021 , 33, 9501-9507		1
104	First Principles Study of the Electronic Structure, Charge Density Contours and Fermi Surfaces of Zirconium-Based Weyl Semi-Metals ZrX (X = S, Se, and Te). 2022 , 487-496		
103	Computational design of a new layered superconductor LaOTf.. 2022 ,		
102	Interaction of water with nitrogen-doped graphene. 2022 , 105,		0
101	Multiple strong topological gaps and hexagonal warping in Bi ₄ Te ₃ . 2022 , 105,		2
100	Borophene and Pristine Graphene 2D Sheets as Potential Surfaces for the Adsorption of Electron-Rich and Electron-Deficient π -Systems: A Comparative DFT Study.. 2022 , 12,		0

- 99 Al₂O₃/Au Thin Films for Thermally Stable and Highly Sensitive Plasmonic Sensors. **2022**, 126, 5628-5639 0
- 98 SrAl₅Pt₃ and Sr₂Al₁₆Pt₉ Two new strontium aluminum platinides. **2022**, 11, 111539 1
- 97 Adsorption of water on C sites vacancy defected graphene/h-BN: First-principles study.. **2022**, 28, 107 0
- 96 Metastable hexagonal close-packed palladium hydride in liquid cell TEM.. **2022**, 603, 631-636 4
- 95 The effects of Pt doping on the optical properties of Au₂₀.
- 94 Investigation of Rare Earth-Containing Double Phosphates of the Type A₃Ln(PO₄)₂ (Ln = Y, La, Pr, Nd, and Sm) as Potential Nuclear Waste Forms. 0
- 93 Probing the elastic, mechanical and thermodynamic properties of Weyl semimetals ZrX (X=S and Te). **2022**, 96, 1
- 92 First principles study of Li adsorption properties of a Borophene based hybrid 2D material B₅Se. **2022**, 8, 100218 1
- 91 Role of intercalated cobalt in the electronic structure of Co_{1/3}NbS₂. **2022**, 105, 105105 0
- 90 DFT study of hydrogen bonding between metal hydroxides and organic molecules containing N, O, S, and P heteroatoms: clusters vs. surfaces. **2022**, 111539 0
- 89 Hydrogen evolution reaction activity of III-V heterostructure nanowires. **2022**, 111539 0
- 88 Structural and electronic properties of Sn sheets grown on Cd(0001). **2022**, 32, 1 1
- 87 Prediction of some physical properties in new half Heusler alloy NbAgSi. **2022**, 310, 122999 2
- 86 Evidence for multiband superconductivity and charge density waves in Ni-doped ZrTe₂. **2022**, 907, 164477 1
- 85 Unraveling Mg <c + a> slip using neural network potential. **2022**, 102, 651-673 2
- 84 Light-Tunable Charge Density Wave Orders in MoTe₂ and WTe₂ Single Layers.. *Physical Review Letters*, **2021**, 127, 257401 7.4 0
- 83 Frustrated network of indirect exchange paths between tetrahedrally coordinated Co in Ba₂CoO₄. **2021**, 5, 051101 0
- 82 Direct driving of electronic and phononic degrees of freedom in a honeycomb bilayer with infrared light. **2021**, 104, 104104 0

81	Unexpected Electron Transport Suppression in a Heterostructured Graphene-MoS Multiple Field-Effect Transistor Architecture.. 2021 ,	0
80	ReaxFF Force Field Development and Application for Toluene Adsorption on MnMO (M = Cu, Fe, Ni) Catalysts. 2021 ,	
79	Spin-dependent vibronic response of a carbon radical ion in two-dimensional WS.. 2021 , 12, 7287	2
78	First-principles study of the electronic structure of CaKRu4P4. 2021 , 104,	
77	Adsorption of Water Molecule in Graphene/MoS2 Heterostructure with Vacancy Defects in Mo Sites. 2022 , 2022, 1-18	
76	The binding of atomic hydrogen on graphene from density functional theory and diffusion Monte Carlo calculations.. 2022 , 156, 144702	0
75	Operando Structure-Activity-Stability Relationship of Iridium Oxides during the Oxygen Evolution Reaction. 5174-5184	3
74	Rapid preparation of carbon-supported ruthenium nanoparticles by magnetic induction heating for efficient hydrogen evolution reaction in both acidic and alkaline media.	1
73	Revealing the Origin of Low-Temperature Activity of Ni-Rh Nanostructures during CO Oxidation Reaction with Operando TEM.. 2022 , e2105599	0
72	Role of the M point phonons for the dynamical stability of B2 compounds.. 2022 , 12, 7258	
71	Structural and electronic properties of double perovskite ruthenates; A2GdRuO6 (where A = Ba, Sr). 2022 , 913, 165177	2
70	Distinctive Features of Semiconducting and Brittle Half-Heusler Alloys; LiXP (X=Zn, Cd). 2022 , 181-197	
69	Anisotropic Phononic and Electronic Thermal Transport in BeN.. 2022 , 4501-4505	1
68	Modeling Metallic Halide Local Structures in Salt Melts Using a Genetic Algorithm.	
67	Quantum Phase Transition in the Spin Transport Properties of Ferromagnetic Metal-Insulator-Metal Hybrid Materials. 2022 , 12, 1836	0
66	Electronic and Band Structure calculation of Wurtzite CdS Using GGA and GGA+U functionals. 2022 , 2267, 012155	1
65	Microstructure Formation of Cast and Directionally Solidified Mo-Ti-B Alloys. 2022 , 12, 916	
64	Enhancing thermoelectric properties in TiNiSi structure-type semimetal ZrNiSi by doping. 2022 , 6,	

63	Emergence of superconductivity in an InSe monolayer: Roles of deposited metal and biaxial strain. 2022 , 110823	0
62	A transferable prediction model of molecular adsorption on metals based on adsorbate and substrate properties.	1
61	HP Γ A code for the calculation of Hubbard parameters using density-functional perturbation theory. 2022 , 108455	1
60	Comparative density functional theory study for predicting oxygen reduction activity of single-atom catalyst. 2022 , 122144	0
59	Nodal-line driven anomalous susceptibility in ZrSiS. 2022 , 105,	
58	Gaussian approximation potential for amorphous Si:H. 2022 , 6,	2
57	Evidence for Jahn-Teller-driven metal-insulator transition in strained SrCrO ₃ from first-principles calculations. 2022 , 6,	0
56	DFT Study of Small Re-Pt Clusters Supported on γ -Al ₂ O ₃ . 2022 , 122157	
55	First principle study of the electronic and structural properties of NaFeAs superconductor. 2022 ,	
54	A charge transfer framework that describes supramolecular interactions governing structure and properties of 2D perovskites. 2022 , 13,	3
53	Differentiating the {100} surfaces of Cu ₂ O nanocrystals from {111} and {110} for benzylic Csp ³ -H bond oxidation: Oxidations of diphenyl methane to benzophenone and cumene to cumene hydroperoxide under mild conditions. 2022 , 528, 112490	
52	Exploring unusual temperature-dependent optical properties of graphite single crystal by spectroscopic ellipsometry. 2022 , 197, 485-493	0
51	Evolution of geometric and electronic structures of oxygen-induced superstructures on Mo(110) surface: A LEED, ARPES, and DFT study. 2022 , 106,	
50	Learning Grain-Boundary Segregation: From First Principles to Polycrystals. 2022 , 129,	1
49	Two-dimensional anisotropic Dirac materials PtN ₄ C ₂ and Pt ₂ N ₈ . 2022 , 6,	0
48	Multitemperature Modeling of Thermal Transport across a Au/GaN Interface from Ab Initio Calculations.	0
47	Optimization of configurations of atomic species on two-dimensional hexagonal lattices for copper-based systems. 2022 , 12, 085313	
46	Rational design of graphyne-based dual-atom site catalysts for CO oxidation.	0

- 45 Pivotal Role of Intersite Hubbard Interactions in Fe-Doped MnO_2 . **2022**, 126, 14353-14365 1
- 44 Effect of oxygen vacancy defects on electronic and optical properties of MgO monolayers: First principles study. **2022**, 286, 115974 0
- 43 $\text{V}_8\text{Si}_4\text{B}_4$ A new ternary phase in the VB_2B system. **2022**, 151, 107691 0
- 42 A two-dimensional topological nodal-line material MgN_4 with extremely large magnetoresistance. **2022**, 14, 14191-14198 0
- 41 A low cost bimetallic AuCu_3 tetramer on Ti_2CO_2 MXene as an efficient catalyst for CO oxidation: a theoretical prediction. **2022**, 24, 19512-19520 0
- 40 Modeling Short-Range Ordering in Binary BCC Ti-X (X = Nb, V, Zr) Alloys using CE-CVM. **2022**, 43, 511-526 0
- 39 Predicting hot-electron free energies from ground-state data. **2022**, 106, 0
- 38 Adsorption Behavior of Toxic Carbon Dichalcogenides (CX_2 ; X = O, S, or Se) on h^2 Borophene and Pristine Graphene Sheets: A DFT Study. **2022**, 12, 3411 0
- 37 Enhancing the Electrochemical Performance of Olivine LiMnPO_4 as Cathode Materials for Li-Ion Batteries by Ni^{II}e Codoping. **2022**, 5, 10591-10603 0
- 36 Heisenberg's uncertainty principle in the PTOLEMY project: A theory update. **2022**, 106, 0
- 35 First-Principles Study of Induced Magnetism in Tungsten Vanadium Selenide Alloys for Spintronic Applications. 0
- 34 Intrinsic glassy-metallic transport in an amorphous coordination polymer. 1
- 33 An introduction to the theory of inorganic solid surfaces. **2022**, 0
- 32 Impact of Anionic Substitution in $\text{Yb}_{14}\text{MgSb}_{11}\text{As}_x$ Compounds on the Electronic and Thermoelectric Properties. **2022**, 126, 18490-18504 0
- 31 Tuning transport properties of B and C sites vacancy defects Graphene/h-BN heterostructures: first-principles study. **2022**, 95, 0
- 30 Accurate Electronic Properties and Intercalation Voltages of Olivine-Type Li-Ion Cathode Materials from Extended Hubbard Functionals. **2022**, 1, 1
- 29 Heat-conserving three-temperature model for ultrafast demagnetization in nickel. **2022**, 106, 0
- 28 Tailoring the Properties of $\text{Ni}(111)$ /Graphene Interfaces by Intercalation of Al and Na: A DFT Study. **2022**, 8, 62 0

- 27 High-pressure synthesis of seven lanthanum hydrides with a significant variability of hydrogen content. **2022**, 13, ○
- 26 Growing borophene on metal substrates: A theoretical study of the role of oxygen on Al(111). **2022**, 6, ○
- 25 Density Functional Studies on the Atomistic Structure and Properties of Iron Oxides: A Parametric Study. **2022**, 15, 8316 ○
- 24 Structural and electronic properties of the Te-Si(111) surface from first principles. **2022**, 106, ○
- 23 Configuration Space Integration for Adsorbate Partition Functions: The Effect of Anharmonicity on the Thermophysical Properties of CO/Pt(111) and CH₃OH/Cu(111). 19-32 ○
- 22 Polarization-dependent electronic structure of Ag quantum well states on the MoS₂ (0001) surface using ARPES and DFT studies. **2022**, 106, ○
- 21 Facile Low-Energy and Open-Air Synthesis of Mixed-Cation Perovskite Quantum Dots for High-Performance Solar Cells. **2022**, 141107 ○
- 20 Synergism between B and Nb Improves Fire Resistance in Microalloyed Steels. **2023**, 13, 84 ○
- 19 Exploring the Dirac nature of RbBi₂. **2023**, 107, ○
- 18 Structural, mechanical, electronic, vibrational and thermoelectric properties of novel double perovskites Ba₂MgPdO₆ and Ba₂MgPtO₆ within DFT framework. **2023**, 158, 107381 ○
- 17 Stabilization of Ti₅Al₁₁ at room temperature in ternary Ti-Al-Me (Me = Au, Pd, Mn, Pt) systems. **2023**, 944, 169244 ○
- 16 Adjusting the Chemical Reactivity of Oxygen for Propylene Epoxidation on Silver by Rational Design: The Use of an Oxyanion and Cl. 5906-5913 ○
- 15 First-principles calculations of hematite (Fe₂O₃) by self-consistent DFT+U+V. **2023**, 26, 106033 ○
- 14 First-principles study of the strain effect with half-metallic ferromagnetism in Cd_{1-x}V_xTe alloys: supercell approaches. **2023**, 98, 035828 ○
- 13 Unraveling the effects of inter-site Hubbard interactions in spinel Li-ion cathode materials. **2023**, 25, 9061-9072 ○
- 12 Innate dynamics and identity crisis of a metal surface unveiled by machine learning of atomic environments. **2023**, 158, 124701 ○
- 11 Role of spin-orbit coupling effects in rare-earth metallic tetra-borides: a first principle study. **2023**, 96, ○
- 10 Eu₄Al₁₃Pt₉ is a coloring variant of the Ho₄Ir₁₃Ge₉ type structure. **2023**, 78, 147-156 ○

- 9 Accelerating self-consistent field iterations in Kohn-Sham density functional theory using a low-rank approximation of the dielectric matrix. **2023**, 107, 1
- 8 Direct Laser Writing of Multimetal Bifunctional Catalysts for Overall Water Splitting. **2023**, 6, 3756-3768 0
- 7 Magnetic frustration and fractionalization in oligo(indenoindenes). **2023**, 107, 0
- 6 Magnetic properties and muon localization in Cr₂S₃. **2023**, 2462, 012006 0
- 5 Hybrid interatomic potential for Sn. **2023**, 7, 0
- 4 Exploring the Charge Density Wave Phase of 1T $\bar{1}$ WSe₂ : Mott or Charge-Transfer Gap?. **2023**, 130, 0
- 3 Long-range electrostatic contribution to electron-phonon couplings and mobilities of two-dimensional and bulk materials. **2023**, 107, 0
- 2 Site selective behaviour of B, C and N doping in MgO monolayers towards spintronic and optoelectronic applications. **2023**, 162, 107514 0
- 1 Semimetallic, Half-Metallic, Semiconducting, and Metallic States in Gd-Sb Compounds. **2023**, 24, 8778 0