Hoat Do Minh

List of Publications by Year in Descending Order

99 papers	929 citations	16 h-index	25 g-index
109 ext. papers	1,345 ext. citations	2.8 avg, IF	5.56 L-index

#	Paper	IF	Citations
99	Controlling magnetic-semiconductor properties of the Si- and Al-doped blue phosphorene monolayer. *Journal Physics D: Applied Physics*, **2022**, 55, 165302	3	0
98	Prediction of a Beryllium Phosphide Iodide Monolayer as a Photocatalyst for Water Splitting by Density Functional Theory. *Journal of Electronic Materials*, **2022**, 51, 2077	1.9	
97	Exploring a silicene monolayer as a promising sensor platform to detect and capture NO and CO gas.. *RSC Advances*, **2022**, 12, 9828-9835	3.7	1
96	First-principles calculations to investigate Structural, electronic, and optical properties of MgF2 monolayer in 1T-phase and 2H-phase using hybrid functional. *Chemical Physics*, **2022**, 557, 111473	2.3	
95	Study of vacancy, voids, atom adsorption and domain substitution in hexagonal gallium nitride monolayer. *Surfaces and Interfaces*, **2022**, 30, 101898	4.1	
94	First principles prediction of the stable MgFCl Janus monolayer with tunable properties. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 137, 115023	3	0
93	Effect of adsorption and substitutional B doping at different concentrations on the electronic and magnetic properties of a BeO monolayer: a first-principles study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24922-24931	3.6	2
92	Effects of the Gas Molecules (H2, CO, NO) and Transition Metal Atoms (Cr, Au) Adsorbed on Hexagonal Boron Nitride Layers. *Journal of the Physical Society of Japan*, **2021**, 90, 114601	1.5	0
91	Developing feature-rich electronic and magnetic properties in the □As monolayer for spintronic and optoelectronic applications by C and Si doping: A first-principles study. *Surfaces and Interfaces*, **2021**, 27, 101534	4.1	0
90	Electronic, optical and thermoelectric properties of a novel two-dimensional SbXY (X = Se, Te; Y = Br, I) family: perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 25866-25876	3.6	3
89	Tuning MoSO monolayer properties for optoelectronic and spintronic applications: effect of external strain, vacancies and doping.. *RSC Advances*, **2021**, 11, 35614-35623	3.7	1
88	Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. *Indian Journal of Physics*, **2021**, 95, 2365	1.4	11
87	Feature-rich structural, electronic, magnetic and optical properties of the fluorine- and nitrogen-incorporated CaF2 compound. *International Journal of Quantum Chemistry*, **2021**, 121, e26672	2.1	
86	Structural, electronic, magnetic and optical properties of CaO induced by oxygen incorporation effects: A first-principles study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2021**, 397, 127241	2.3	0
85	Nitrogen doping and oxygen vacancy effects on the fundamental properties of BeO monolayer: a DFT study. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	3
84	Opening the germanene monolayer band gap using halogen atoms: An efficient approach studied by first-principles calculations. *Applied Surface Science*, **2021**, 551, 149318	6.7	4
83	Theoretical prediction of the PtOX (X = S and Se) monolayers as promising optoelectronic and thermoelectric 2D materials. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 131, 114732	3	3

82	Theoretical analysis of the HfS2 monolayer electronic structure and optical properties under vertical strain effects. *Optik*, **2021**, 225, 165718	2.5	6
81	Prediction of a new 2D B2CO monolayer from density functional theory. *Computational Materials Science*, **2021**, 186, 109975	3.2	1
80	First principles analysis of the half-metallic ferromagnetism, elastic and thermodynamic properties of equiatomic quaternary Heusler compound CoCrRhSi. *Materials Chemistry and Physics*, **2021**, 257, 123695	4.4	4
79	Investigations of thermoelectric properties of ZnO monolayers from the first-principles approach. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 126, 114444	3	17
78	Strain-tunable electronic, optical and thermoelectric properties of BP monolayer investigated by FP-LAPW calculations. *Physica B: Condensed Matter*, **2021**, 603, 412757	2.8	3
77	Pressure effects on the electronic, magnetic, thermoelectric, and thermodynamic properties of Mn2CoSi half-metallic compound. *International Journal of Quantum Chemistry*, **2021**, 121, e26445	2.1	1
76	Novel two-dimensional ZnO2, CdO2 and HgO2 monolayers: a first-principles-based prediction. *New Journal of Chemistry*, **2021**, 45, 9368-9374	3.6	2
75	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties an electric field and mechanical strain. *Physical Chemistry Chemical Physics*, **2021**, 23, 15216-15223	3.6	17
74	MoSi2N4 single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. *Journal Physics D: Applied Physics*, **2021**, 54, 155303	3	68
73	Strain-driven modulation of the electronic, optical and thermoelectric properties of □antimonene monolayer: A hybrid functional study. *Materials Science in Semiconductor Processing*, **2021**, 131, 105878	4.3	1
72	Structural, electronic, magnetic, and optical properties of new TiXY (X = F and Cl; Y = S, Se and Te) Janus monolayers: A first-principles study. *Optik*, **2021**, 244, 167438	2.5	0
71	Engineering the electronic and magnetic properties of nitrogene monolayer and bilayer by doping: A first-principles study. *Applied Surface Science*, **2021**, 566, 150711	6.7	2
70	Two-dimensional buckled tetragonal cadmium chalcogenides including CdS, CdSe, and CdTe monolayers as photo-catalysts for water splitting. *Physical Chemistry Chemical Physics*, **2021**, 23, 12226-12232	3.6	11
69	Strain tunable electronic and optical properties of 2D orthorhombic lithium sulfur monolayer. *Chemical Physics*, **2020**, 535, 110762	2.3	
68	Electronic structure, optical and thermoelectric properties of cadmium chalcogenides monolayers. *Optik*, **2020**, 210, 164567	2.5	10
67	P-substitution effects on the electronic structure and thermal properties of the half-metallic half-Heusler NaCrBi compound. *Chemical Physics*, **2020**, 537, 110848	2.3	4
66	Mn2CoX (X = P and As) full-Heusler compounds for spintronic applications: Half-metallicity and elastic properties. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126589	2.3	14
65	LiCl monolayer for UV detection: First principles prediction. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 123, 114168	3	3

64	First-principles investigation of nonmetal doped single-layer BiOBr as a potential photocatalyst with a low recombination rate. *Physical Chemistry Chemical Physics*, **2020**, 22, 15354-15364	3.6	45
63	Half-metal effect on the MnAs/InP (0□0□1)-(2□□4) interface. *Computational Materials Science*, **2020**, 175, 109603	3.2	4
62	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties.. *RSC Advances*, **2020**, 10, 10731-10739	3.7	10
61	Computational prediction of the spin-polarized semiconductor equiatomic quaternary Heusler compound MnVZrP as a spin-filter.. *RSC Advances*, **2020**, 10, 25609-25617	3.7	2
60	Structural, electronic and optical properties of CdO monolayer and bilayers: Stacking effect investigations. *Superlattices and Microstructures*, **2020**, 145, 106644	2.8	8
59	New equiatomic quaternary Heusler compounds without transition metals KCaBX (X□= S and Se): Robust half-metallicity and optical properties. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107642	2.8	6
58	DFT prediction of structural, electronic and magnetic properties of Sr0.75TM0.25S (TM is 3d transition metals). *Philosophical Magazine Letters*, **2020**, 100, 95-104	1	3
57	The characteristics of defective ZrS2 monolayers adsorbed various gases on S-vacancies: A first-principles study. *Superlattices and Microstructures*, **2020**, 140, 106454	2.8	12
56	First principles insight into the structural, electronic, optical and thermodynamic properties of CsPb2Br5 compound. *Chemical Physics*, **2020**, 533, 110704	2.3	5
55	An assessment of the structural, electronic, optical and thermoelectric properties of the BaAg2GeS4 compound. *Journal of Solid State Chemistry*, **2020**, 285, 121260	3.3	4
54	2D Hexagonal SnTe monolayer: a quasi direct band gap semiconductor with strain sensitive electronic and optical properties. *European Physical Journal B*, **2020**, 93, 1	1.2	4
53	Half-metallicity and magnetism in BAs monolayer induced by anchoring 3d transition metals (TM = V, Cr and Mn). *Superlattices and Microstructures*, **2020**, 139, 106399	2.8	10
52	Functionalizing AlN monolayer with hydroxyl group: Effect on the structural and electronic properties. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126444	2.3	10
51	A comprehensive investigation on electronic structure, optical and thermoelectric properties of the HfSSe Janus monolayer. *Journal of Physics and Chemistry of Solids*, **2020**, 144, 109490	3.9	14
50	Fluorinating the graphene-like BeO monolayer: A spin-polarized first principles study of the electronic, magnetic and optical properties. *Physica Scripta*, **2020**, 95, 105806	2.6	7
49	Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study. *Superlattices and Microstructures*, **2020**, 137, 106320	2.8	11
48	Tuning the electronic, photocatalytic and optical properties of hydrogenated InN monolayer by biaxial strain and electric field. *Chemical Physics*, **2020**, 532, 110677	2.3	8
47	Reducing the electronic band gap of BN monolayer by coexistence of P(As)-doping and external electric field. *Superlattices and Microstructures*, **2020**, 137, 106357	2.8	9

46	Examining the uniform strain effect on elastic, electronic and optical properties of CsPbCl3 through FP-LAPW calculations. *Chemical Physics*, **2020**, 531, 110654	2.3	5
45	Electronic and optical properties of wide band gap Tl3TaS4: A promising surface acoustic wave material. *Optical Materials*, **2020**, 99, 109601	3.3	5
44	Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties. *Superlattices and Microstructures*, **2020**, 137, 106359	2.8	10
43	Theoretical prediction of 2D XI (X=Si, Ge, Sn, Pb) monolayers by density functional theory. *Journal of Molecular Graphics and Modelling*, **2020**, 95, 107501	2.8	9
42	On the structural, electronic, optical and thermoelectric properties of CdIn2Se4 ordered-vacancy compound. *Journal of Solid State Chemistry*, **2020**, 282, 121078	3.3	1
41	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. *Materials Research Express*, **2020**, 7, 015013	1.7	8
40	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 117, 113857	3	6
39	Examining the half-metallicity and thermoelectric properties of new equiatomic quaternary Heusler compound CoVRhGe under pressure. *Physica B: Condensed Matter*, **2020**, 583, 412058	2.8	15
38	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study.. *RSC Advances*, **2020**, 10, 40411-40420	3.7	3
37	Electronic, optical and thermoelectric properties of CaO mono- and bi-layers: Theoretical comparative investigation. *Optik*, **2020**, 218, 165115	2.5	1
36	The mechanical, electronic, optical and thermoelectric properties of two-dimensional honeycomb-like of XSb (X = Si, Ge, Sn) monolayers: a first-principles calculations.. *RSC Advances*, **2020**, 10, 30398-30405	3.7	20
35	Theoretical investigation of the AlN (0 0 0 1)-(2□2) surface doped with nickel: Structural, electronic and magnetic properties. *Journal of Crystal Growth*, **2020**, 551, 125907	1.6	2
34	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. *Chemical Physics*, **2020**, 529, 110543	2.3	41
33	Ternary sulfides BaLa2S4 and CaLa2S4 as promising photocatalytic water splitting and thermoelectric materials: First-principles DFT calculations. *International Journal of Hydrogen Energy*, **2020**, 45, 22600-22612	6.7	8
32	Electronic and thermoelectric properties of RbYSn half-Heusler compound with 8 valence electrons: Spin-orbit coupling effect. *Chemical Physics*, **2020**, 528, 110510	2.3	11
31	Theoretical prediction of electronic and optical properties of haft-hydrogenated InN monolayers. *Superlattices and Microstructures*, **2020**, 142, 106519	2.8	4
30	Tuning the electronic structure of 2D materials by strain and external electric field: Case of GeI2 monolayer. *Chemical Physics*, **2019**, 527, 110499	2.3	40
29	First principles investigation on elastic, optoelectronic and thermoelectric properties of KYX (X□= Ge, Sn and Pb) half-heusler compounds. *Journal of Molecular Graphics and Modelling*, **2019**, 92, 249-255	2.8	9

28	Electronic and magnetic properties of single-layer boron phosphide associated with materials processing defects. *Computational Materials Science*, **2019**, 170, 109201	3.2	44
27	Prediction of 2D Li2X (X=Se, Te) monolayer semiconductors by first principles calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 125992	2.3	6
26	Theoretical study of electronic structure, thermoelectric and thermodynamic properties of 2H-AgAlO2. *Physica B: Condensed Matter*, **2019**, 558, 109-115	2.8	4
25	Electronic structure, chemical bonding, optical, elastic and dynamical properties of MeB2 compounds: Effect of transition metal Me = Sc, Ti and Zr. *Computational Condensed Matter*, **2019**, 21, e00406	1.7	3
24	Structural, electronic, optical and thermodynamic properties of AeBiO (Ae= Sr and Ba): Insights from first principles study. *Journal of Molecular Graphics and Modelling*, **2019**, 90, 153-160	2.8	7
23	Investigation on new equiatomic quaternary Heusler compound CoCrIrSi via FP-LAPW calculations. *Chemical Physics*, **2019**, 523, 130-137	2.3	21
22	Assessing optoelectronic properties of PbI2 monolayer under uniaxial strain from first principles calculations. *Superlattices and Microstructures*, **2019**, 130, 354-360	2.8	25
21	Structural, optoelectronic and thermoelectric properties of antiperovskite compounds Ae3PbS (Ae = Ca, Sr and Ba): A first principles study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 1648-1654	2.3	16
20	Improving the Calculations of Electronic and Magnetic Properties of Sr2CrMoO6 Double-Perovskite with LDA+U and mBJ Potential. *Journal of Electronic Materials*, **2019**, 48, 6406-6413	1.9	4
19	Effect of DFT methods on electronic structure and K-absorption spectra of InPS4: detailed studies of the optical, thermoelectric and elastic properties. *Materials Research Express*, **2019**, 6, 106320	1.7	3
18	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. *Superlattices and Microstructures*, **2019**, 136, 106270	2.8	9
17	Computational investigation of the structural, electronic, optical and thermoelectric properties of T2-Al2MgC2 compound. *Journal of Solid State Chemistry*, **2019**, 280, 120999	3.3	5
16	Investigation on structural, electronic, magnetic and thermodynamic properties of antiperovskites Mn3XC (X=Al, Zn and Ga). *International Journal of Modern Physics B*, **2019**, 33, 1950337	1.1	2
15	Electronic and optical properties of Janus ZrSSe by density functional theory.. *RSC Advances*, **2019**, 9, 41058-41065	3.7	45
14	Comparative study of structural, electronic, optical and thermoelectric properties of GaS bulk and monolayer. *Philosophical Magazine*, **2019**, 99, 736-751	1.6	7
13	Electronic structure and thermoelectric properties of Ta-based half-Heusler compounds with 18 valence electrons. *Computational Materials Science*, **2019**, 159, 470-477	3.2	24
12	Investigation on electronic structure and luminescence mechanism of CaF2:Eu3+ from first principles calculations. *Optik*, **2019**, 181, 1023-1027	2.5	4
11	Theoretical investigations on physical properties of SrFCuCh (Ch=S and Se). *Journal of Solid State Chemistry*, **2019**, 271, 191-198	3.3	1

10	Systematic study of structural, electronic, optical and thermodynamic properties of SrFCuTe compound. *Journal of Solid State Chemistry*, **2019**, 270, 85-91	3.3	6
9	Theoretical study of electronic and optical properties of antiferromagnetic MnS using the modified Becke Johnson (mBJ) potential. *Journal of Physics and Chemistry of Solids*, **2019**, 128, 310-315	3.9	4
8	FP-LAPW investigation on structural, electronic and optical properties of Eu2+-doped MF2 (M = Ca and Ba). *Optik*, **2018**, 161, 335-341	2.5	4
7	First principles study of structural, electronic and optical properties of perovskites CaZrO 3 and CaHfO 3 in cubic phase. *Solid State Communications*, **2018**, 275, 29-34	1.6	20
6	First principles study of structural, electronic, elastic and thermodynamic properties of cubic HfO2 under pressure. *Physica B: Condensed Matter*, **2018**, 545, 55-61	2.8	9
5	Investigation on the structural, elastic, electronic, and magnetic properties of half-metallic (hbox {Co}_{2}hbox {MnSi}) and CoMnIrSi via first-principles calculations. *Journal of Computational Electronics*, **2018**, 17, 1470-1477	1.8	18
4	Search for new d0 half-metallic materials: theoretical investigation on KCaC1Six (x = 0; 0.25; 0.5; 0.75 and 1) compounds. *Chinese Journal of Physics*, **2018**, 56, 3078-3084	3.5	6
3	First principles study on structural, electronic and optical properties of Ga 1 B x P ternary alloys (x = 0, 0.25, 0.5, 0.75 and 1). *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2018**, 382, 1942-1949	2.3	4
2	Insight into the structural, elastic, electronic and thermal properties of YMgX4 (X = Co, Ni and Cu) from ab initio calculations. *Materials Research Express*, **2018**, 5, 066549	1.7	5
1	Effect of pressure on structural, electronic and optical properties of SrF2: a first principles study. *Revista Mexicana De Fsica*, **2017**, 64, 94-100	3.5	6