

# Hoat Do Minh

## List of Publications by Citations

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papers

929  
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109  
ext. papers

1,345  
ext. citations

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#	Paper	IF	Citations
99	MoSi <sub>2</sub> N <sub>4</sub> single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. <i>Journal Physics D: Applied Physics</i> , <b>2021</b> , 54, 155303	3	68
98	First-principles investigation of nonmetal doped single-layer BiOBr as a potential photocatalyst with a low recombination rate. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 15354-15364	3.6	45
97	Electronic and optical properties of Janus ZrSSe by density functional theory.. <i>RSC Advances</i> , <b>2019</b> , 9, 41058-41065	3.7	45
96	Electronic and magnetic properties of single-layer boron phosphide associated with materials processing defects. <i>Computational Materials Science</i> , <b>2019</b> , 170, 109201	3.2	44
95	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. <i>Chemical Physics</i> , <b>2020</b> , 529, 110543	2.3	41
94	Tuning the electronic structure of 2D materials by strain and external electric field: Case of GeI <sub>2</sub> monolayer. <i>Chemical Physics</i> , <b>2019</b> , 527, 110499	2.3	40
93	Assessing optoelectronic properties of PbI <sub>2</sub> monolayer under uniaxial strain from first principles calculations. <i>Superlattices and Microstructures</i> , <b>2019</b> , 130, 354-360	2.8	25
92	Electronic structure and thermoelectric properties of Ta-based half-Heusler compounds with 18 valence electrons. <i>Computational Materials Science</i> , <b>2019</b> , 159, 470-477	3.2	24
91	Investigation on new equiatomic quaternary Heusler compound CoCrIrSi via FP-LAPW calculations. <i>Chemical Physics</i> , <b>2019</b> , 523, 130-137	2.3	21
90	First principles study of structural, electronic and optical properties of perovskites CaZrO <sub>3</sub> and CaHfO <sub>3</sub> in cubic phase. <i>Solid State Communications</i> , <b>2018</b> , 275, 29-34	1.6	20
89	The mechanical, electronic, optical and thermoelectric properties of two-dimensional honeycomb-like of XSb (X = Si, Ge, Sn) monolayers: a first-principles calculations.. <i>RSC Advances</i> , <b>2020</b> , 10, 30398-30405	3.7	20
88	Investigation on the structural, elastic, electronic, and magnetic properties of half-metallic (hbox {Co}_{2}hbox {MnSi}) and CoMnIrSi via first-principles calculations. <i>Journal of Computational Electronics</i> , <b>2018</b> , 17, 1470-1477	1.8	18
87	Investigations of thermoelectric properties of ZnO monolayers from the first-principles approach. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 126, 114444	3	17
86	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties an electric field and mechanical strain. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 15216-15223	3.6	17
85	Structural, optoelectronic and thermoelectric properties of antiperovskite compounds Ae <sub>3</sub> PbS (Ae = Ca, Sr and Ba): A first principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2019</b> , 383, 1648-1654	2.3	16
84	Examining the half-metallicity and thermoelectric properties of new equiatomic quaternary Heusler compound CoVRhGe under pressure. <i>Physica B: Condensed Matter</i> , <b>2020</b> , 583, 412058	2.8	15
83	Mn <sub>2</sub> CoX (X = P and As) full-Heusler compounds for spintronic applications: Half-metallicity and elastic properties. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2020</b> , 384, 126589	2.3	14

82	A comprehensive investigation on electronic structure, optical and thermoelectric properties of the HfSSe Janus monolayer. <i>Journal of Physics and Chemistry of Solids</i> , <b>2020</b> , 144, 109490	3.9	14
81	The characteristics of defective ZrS <sub>2</sub> monolayers adsorbed various gases on S-vacancies: A first-principles study. <i>Superlattices and Microstructures</i> , <b>2020</b> , 140, 106454	2.8	12
80	Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study. <i>Superlattices and Microstructures</i> , <b>2020</b> , 137, 106320	2.8	11
79	Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. <i>Indian Journal of Physics</i> , <b>2021</b> , 95, 2365	1.4	11
78	Electronic and thermoelectric properties of RbYSn half-Heusler compound with 8 valence electrons: Spin-orbit coupling effect. <i>Chemical Physics</i> , <b>2020</b> , 528, 110510	2.3	11
77	Two-dimensional buckled tetragonal cadmium chalcogenides including CdS, CdSe, and CdTe monolayers as photo-catalysts for water splitting. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 12226-12232	3.6	11
76	Electronic structure, optical and thermoelectric properties of cadmium chalcogenides monolayers. <i>Optik</i> , <b>2020</b> , 210, 164567	2.5	10
75	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties.. <i>RSC Advances</i> , <b>2020</b> , 10, 10731-10739	3.7	10
74	Half-metallicity and magnetism in BAs monolayer induced by anchoring 3d transition metals (TM = V, Cr and Mn). <i>Superlattices and Microstructures</i> , <b>2020</b> , 139, 106399	2.8	10
73	Functionalizing AlN monolayer with hydroxyl group: Effect on the structural and electronic properties. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2020</b> , 384, 126444	2.3	10
72	Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties. <i>Superlattices and Microstructures</i> , <b>2020</b> , 137, 106359	2.8	10
71	First principles investigation on elastic, optoelectronic and thermoelectric properties of KYX (X=Ge, Sn and Pb) half-heusler compounds. <i>Journal of Molecular Graphics and Modelling</i> , <b>2019</b> , 92, 249-255	2.8	9
70	First principles study of structural, electronic, elastic and thermodynamic properties of cubic HfO <sub>2</sub> under pressure. <i>Physica B: Condensed Matter</i> , <b>2018</b> , 545, 55-61	2.8	9
69	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. <i>Superlattices and Microstructures</i> , <b>2019</b> , 136, 106270	2.8	9
68	Reducing the electronic band gap of BN monolayer by coexistence of P(As)-doping and external electric field. <i>Superlattices and Microstructures</i> , <b>2020</b> , 137, 106357	2.8	9
67	Theoretical prediction of 2D XI (X=Si, Ge, Sn, Pb) monolayers by density functional theory. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 95, 107501	2.8	9
66	Structural, electronic and optical properties of CdO monolayer and bilayers: Stacking effect investigations. <i>Superlattices and Microstructures</i> , <b>2020</b> , 145, 106644	2.8	8
65	Tuning the electronic, photocatalytic and optical properties of hydrogenated InN monolayer by biaxial strain and electric field. <i>Chemical Physics</i> , <b>2020</b> , 532, 110677	2.3	8

64	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. <i>Materials Research Express</i> , <b>2020</b> , 7, 015013	1.7	8
63	Ternary sulfides BaLa <sub>2</sub> S <sub>4</sub> and CaLa <sub>2</sub> S <sub>4</sub> as promising photocatalytic water splitting and thermoelectric materials: First-principles DFT calculations. <i>International Journal of Hydrogen Energy</i> , <b>2020</b> , 45, 22600-22612	6.7	8
62	Structural, electronic, optical and thermodynamic properties of AeBiO (Ae = Sr and Ba): Insights from first principles study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2019</b> , 90, 153-160	2.8	7
61	Fluorinating the graphene-like BeO monolayer: A spin-polarized first principles study of the electronic, magnetic and optical properties. <i>Physica Scripta</i> , <b>2020</b> , 95, 105806	2.6	7
60	Comparative study of structural, electronic, optical and thermoelectric properties of GaS bulk and monolayer. <i>Philosophical Magazine</i> , <b>2019</b> , 99, 736-751	1.6	7
59	Prediction of 2D Li <sub>2</sub> X (X=Se, Te) monolayer semiconductors by first principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2019</b> , 383, 125992	2.3	6
58	New equiatomic quaternary Heusler compounds without transition metals KCaBX (X = S and Se): Robust half-metallicity and optical properties. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 100, 107642	2.8	6
57	Effect of pressure on structural, electronic and optical properties of SrF <sub>2</sub> : a first principles study. <i>Revista Mexicana De Física</i> , <b>2017</b> , 64, 94-100	3.5	6
56	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2020</b> , 117, 113857	3	6
55	Systematic study of structural, electronic, optical and thermodynamic properties of SrFCuTe compound. <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 270, 85-91	3.3	6
54	Theoretical analysis of the HfS <sub>2</sub> monolayer electronic structure and optical properties under vertical strain effects. <i>Optik</i> , <b>2021</b> , 225, 165718	2.5	6
53	Search for new d0 half-metallic materials: theoretical investigation on KCaC <sub>1-x</sub> Si <sub>x</sub> (x = 0; 0.25; 0.5; 0.75 and 1) compounds. <i>Chinese Journal of Physics</i> , <b>2018</b> , 56, 3078-3084	3.5	6
52	First principles insight into the structural, electronic, optical and thermodynamic properties of CsPb <sub>2</sub> Br <sub>5</sub> compound. <i>Chemical Physics</i> , <b>2020</b> , 533, 110704	2.3	5
51	Computational investigation of the structural, electronic, optical and thermoelectric properties of T <sub>2</sub> -Al <sub>2</sub> MgC <sub>2</sub> compound. <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 280, 120999	3.3	5
50	Examining the uniform strain effect on elastic, electronic and optical properties of CsPbCl <sub>3</sub> through FP-LAPW calculations. <i>Chemical Physics</i> , <b>2020</b> , 531, 110654	2.3	5
49	Electronic and optical properties of wide band gap Tl <sub>3</sub> Ta <sub>4</sub> S <sub>4</sub> : A promising surface acoustic wave material. <i>Optical Materials</i> , <b>2020</b> , 99, 109601	3.3	5
48	Insight into the structural, elastic, electronic and thermal properties of YMgX <sub>4</sub> (X = Co, Ni and Cu) from ab initio calculations. <i>Materials Research Express</i> , <b>2018</b> , 5, 066549	1.7	5
47	Theoretical study of electronic structure, thermoelectric and thermodynamic properties of 2H-AgAlO <sub>2</sub> . <i>Physica B: Condensed Matter</i> , <b>2019</b> , 558, 109-115	2.8	4

46	P-substitution effects on the electronic structure and thermal properties of the half-metallic half-Heusler NaCrBi compound. <i>Chemical Physics</i> , <b>2020</b> , 537, 110848	2.3	4
45	Half-metal effect on the MnAs/InP (0001)-(2004) interface. <i>Computational Materials Science</i> , <b>2020</b> , 175, 109603	3.2	4
44	An assessment of the structural, electronic, optical and thermoelectric properties of the BaAg <sub>2</sub> GeS <sub>4</sub> compound. <i>Journal of Solid State Chemistry</i> , <b>2020</b> , 285, 121260	3.3	4
43	2D Hexagonal SnTe monolayer: a quasi direct band gap semiconductor with strain sensitive electronic and optical properties. <i>European Physical Journal B</i> , <b>2020</b> , 93, 1	1.2	4
42	FP-LAPW investigation on structural, electronic and optical properties of Eu <sup>2+</sup> -doped MF <sub>2</sub> (M = Ca and Ba). <i>Optik</i> , <b>2018</b> , 161, 335-341	2.5	4
41	Improving the Calculations of Electronic and Magnetic Properties of Sr <sub>2</sub> CrMoO <sub>6</sub> Double-Perovskite with LDA+U and mBJ Potential. <i>Journal of Electronic Materials</i> , <b>2019</b> , 48, 6406-6413	1.9	4
40	Opening the germanene monolayer band gap using halogen atoms: An efficient approach studied by first-principles calculations. <i>Applied Surface Science</i> , <b>2021</b> , 551, 149318	6.7	4
39	Investigation on electronic structure and luminescence mechanism of CaF <sub>2</sub> :Eu <sup>3+</sup> from first principles calculations. <i>Optik</i> , <b>2019</b> , 181, 1023-1027	2.5	4
38	Theoretical study of electronic and optical properties of antiferromagnetic EMnS using the modified Becke Johnson (mBJ) potential. <i>Journal of Physics and Chemistry of Solids</i> , <b>2019</b> , 128, 310-315	3.9	4
37	Theoretical prediction of electronic and optical properties of haft-hydrogenated InN monolayers. <i>Superlattices and Microstructures</i> , <b>2020</b> , 142, 106519	2.8	4
36	First principles analysis of the half-metallic ferromagnetism, elastic and thermodynamic properties of equiatomic quaternary Heusler compound CoCrRhSi. <i>Materials Chemistry and Physics</i> , <b>2021</b> , 257, 123695	4.4	4
35	First principles study on structural, electronic and optical properties of Ga <sub>1-x</sub> B <sub>x</sub> P ternary alloys (x = 0, 0.25, 0.5, 0.75 and 1). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2018</b> , 382, 1942-1949	2.3	4
34	Electronic structure, chemical bonding, optical, elastic and dynamical properties of MeB <sub>2</sub> compounds: Effect of transition metal Me = Sc, Ti and Zr. <i>Computational Condensed Matter</i> , <b>2019</b> , 21, e00406	1.7	3
33	LiCl monolayer for UV detection: First principles prediction. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2020</b> , 123, 114168	3	3
32	DFT prediction of structural, electronic and magnetic properties of Sr <sub>0.75</sub> TM <sub>0.25</sub> S (TM is 3d transition metals). <i>Philosophical Magazine Letters</i> , <b>2020</b> , 100, 95-104	1	3
31	Effect of DFT methods on electronic structure and K-absorption spectra of InPS <sub>4</sub> : detailed studies of the optical, thermoelectric and elastic properties. <i>Materials Research Express</i> , <b>2019</b> , 6, 106320	1.7	3
30	Electronic, optical and thermoelectric properties of a novel two-dimensional SbXY (X = Se, Te; Y = Br, I) family: perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 25866-25876	3.6	3
29	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study.. <i>RSC Advances</i> , <b>2020</b> , 10, 40411-40420	3.7	3

28	Nitrogen doping and oxygen vacancy effects on the fundamental properties of BeO monolayer: a DFT study. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 33,	1.8	3
27	Theoretical prediction of the PtOX (X = S and Se) monolayers as promising optoelectronic and thermoelectric 2D materials. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 131, 114732 <sup>3</sup>		3
26	Strain-tunable electronic, optical and thermoelectric properties of BP monolayer investigated by FP-LAPW calculations. <i>Physica B: Condensed Matter</i> , <b>2021</b> , 603, 412757	2.8	3
25	Computational prediction of the spin-polarized semiconductor equiatomic quaternary Heusler compound MnVZrP as a spin-filter.. <i>RSC Advances</i> , <b>2020</b> , 10, 25609-25617	3.7	2
24	Effect of adsorption and substitutional B doping at different concentrations on the electronic and magnetic properties of a BeO monolayer: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24922-24931	3.6	2
23	Theoretical investigation of the AlN (0 0 0 1)-(2 $\times$ 2) surface doped with nickel: Structural, electronic and magnetic properties. <i>Journal of Crystal Growth</i> , <b>2020</b> , 551, 125907	1.6	2
22	Investigation on structural, electronic, magnetic and thermodynamic properties of antiperovskites Mn <sub>3</sub> XC (X=Al, Zn and Ga). <i>International Journal of Modern Physics B</i> , <b>2019</b> , 33, 1950337	1.1	2
21	Novel two-dimensional ZnO <sub>2</sub> , CdO <sub>2</sub> and HgO <sub>2</sub> monolayers: a first-principles-based prediction. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 9368-9374	3.6	2
20	Engineering the electronic and magnetic properties of nitrogene monolayer and bilayer by doping: A first-principles study. <i>Applied Surface Science</i> , <b>2021</b> , 566, 150711	6.7	2
19	Tuning MoSO monolayer properties for optoelectronic and spintronic applications: effect of external strain, vacancies and doping.. <i>RSC Advances</i> , <b>2021</b> , 11, 35614-35623	3.7	1
18	On the structural, electronic, optical and thermoelectric properties of CdIn <sub>2</sub> Se <sub>4</sub> ordered-vacancy compound. <i>Journal of Solid State Chemistry</i> , <b>2020</b> , 282, 121078	3.3	1
17	Electronic, optical and thermoelectric properties of CaO mono- and bi-layers: Theoretical comparative investigation. <i>Optik</i> , <b>2020</b> , 218, 165115	2.5	1
16	Theoretical investigations on physical properties of SrFCuCh (Ch=S and Se). <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 271, 191-198	3.3	1
15	Prediction of a new 2D B <sub>2</sub> CO monolayer from density functional theory. <i>Computational Materials Science</i> , <b>2021</b> , 186, 109975	3.2	1
14	Pressure effects on the electronic, magnetic, thermoelectric, and thermodynamic properties of Mn <sub>2</sub> CoSi half-metallic compound. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26445	2.1	1
13	Strain-driven modulation of the electronic, optical and thermoelectric properties of Antimonene monolayer: A hybrid functional study. <i>Materials Science in Semiconductor Processing</i> , <b>2021</b> , 131, 105878	4.3	1
12	Exploring a silicene monolayer as a promising sensor platform to detect and capture NO and CO gas.. <i>RSC Advances</i> , <b>2022</b> , 12, 9828-9835	3.7	1
11	Controlling magnetic-semiconductor properties of the Si- and Al-doped blue phosphorene monolayer. <i>Journal Physics D: Applied Physics</i> , <b>2022</b> , 55, 165302	3	0

10	First principles prediction of the stable MgFCl Janus monolayer with tunable properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 137, 115023	3	○
9	Effects of the Gas Molecules (H <sub>2</sub> , CO, NO) and Transition Metal Atoms (Cr, Au) Adsorbed on Hexagonal Boron Nitride Layers. <i>Journal of the Physical Society of Japan</i> , <b>2021</b> , 90, 114601	1.5	○
8	Developing feature-rich electronic and magnetic properties in the EAs monolayer for spintronic and optoelectronic applications by C and Si doping: A first-principles study. <i>Surfaces and Interfaces</i> , <b>2021</b> , 27, 101534	4.1	○
7	Structural, electronic, magnetic and optical properties of CaO induced by oxygen incorporation effects: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2021</b> , 397, 127241	2.3	○
6	Structural, electronic, magnetic, and optical properties of new TiXY (X = F and Cl; Y = S, Se and Te) Janus monolayers: A first-principles study. <i>Optik</i> , <b>2021</b> , 244, 167438	2.5	○
5	Strain tunable electronic and optical properties of 2D orthorhombic lithium sulfur monolayer. <i>Chemical Physics</i> , <b>2020</b> , 535, 110762	2.3	
4	Prediction of a Beryllium Phosphide Iodide Monolayer as a Photocatalyst for Water Splitting by Density Functional Theory. <i>Journal of Electronic Materials</i> , <b>2022</b> , 51, 2077	1.9	
3	Feature-rich structural, electronic, magnetic and optical properties of the fluorine- and nitrogen-incorporated CaF <sub>2</sub> compound. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26672	2.1	
2	First-principles calculations to investigate Structural, electronic, and optical properties of MgF <sub>2</sub> monolayer in 1T-phase and 2H-phase using hybrid functional. <i>Chemical Physics</i> , <b>2022</b> , 557, 111473	2.3	
1	Study of vacancy, voids, atom adsorption and domain substitution in hexagonal gallium nitride monolayer. <i>Surfaces and Interfaces</i> , <b>2022</b> , 30, 101898	4.1	