Hoat Do Minh

List of Publications by Year
in descending order

107 papers	1,788 citations	331259 21 h-index	360668 35 g-index
109 all docs	109 docs citations	109 times ranked	1075 citing authors

#	Article	IF	Citations
1	MoSi₂N₄ single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. Journal Physics D: Applied Physics, 2021, 54, 155303.	1.3	160
2	Electronic and optical properties of Janus ZrSSe by density functional theory. RSC Advances, 2019, 9, 41058-41065.	1.7	81
3	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.	1.3	74
4	Electronic and magnetic properties of single-layer boron phosphide associated with materials processing defects. Computational Materials Science, 2019, 170, 109201.	1.4	63
5	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. Chemical Physics, 2020, 529, 110543.	0.9	60
6	Tuning the electronic structure of 2D materials by strain and external electric field: Case of GeI2 monolayer. Chemical Physics, 2019, 527, 110499.	0.9	53
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.	0.9	41
8	Assessing optoelectronic properties of PbI2 monolayer under uniaxial strain from first principles calculations. Superlattices and Microstructures, 2019, 130, 354-360.	1.4	41
9	Electronic structure and thermoelectric properties of Ta-based half-Heusler compounds with 18 valence electrons. Computational Materials Science, 2019, 159, 470-477.	1.4	41
10	Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. Indian Journal of Physics, 2021, 95, 2365-2373.	0.9	39
11	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.	1.9	36
12	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.	1.3	35
13	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties via an electric field and mechanical strain. Physical Chemistry Chemical Physics, 2021, 23, 15216-15223.	1.3	32
14	Opening the germanene monolayer band gap using halogen atoms: An efficient approach studied by first-principles calculations. Applied Surface Science, 2021, 551, 149318.	3.1	30
15	Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study. Superlattices and Microstructures, 2020, 137, 106320.	1.4	28
16	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.	0.9	28
17	Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties. Superlattices and Microstructures, 2020, 137, 106359.	1.4	26
18	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.	1.7	26

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19	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.	1.3	26
20	Investigation on new equiatomic quaternary Heusler compound CoCrIrSi via FP-LAPW calculations. Chemical Physics, 2019, 523, 130-137.	0.9	25
21	Investigations of thermoelectric properties of ZnO monolayers from the first-principles approach. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 126, 114444.	1.3	25
22	Examining the half-metallicity and thermoelectric properties of new equiatomic quaternary Heusler compound CoVRhGe under pressure. Physica B: Condensed Matter, 2020, 583, 412058.	1.3	23
23	Structural, optoelectronic and thermoelectric properties of antiperovskite compounds Ae3PbS (Ae =) Tj ETQq1 1 0.784314 rgBT /Ove Physics, 2019, 383, 1648-1654.	0.9	22
24	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study. RSC Advances, 2020, 10, 40411-40420.	1.7	22
25	Electronic and thermoelectric properties of RbYSn half-Heusler compound with 8 valence electrons: Spin-orbit coupling effect. Chemical Physics, 2020, 528, 110510.	0.9	20
26	Reducing the electronic band gap of BN monolayer by coexistence of P(As)-doping and external electric field. Superlattices and Microstructures, 2020, 137, 106357.	1.4	20
27	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.	3.8	19
28	Theoretical prediction of 2D XI2 (X=Si, Ge, Sn, Pb) monolayers by density functional theory. Journal of Molecular Graphics and Modelling, 2020, 95, 107501.	1.3	19
29	The characteristics of defective ZrS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1160" altimg="si64.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> monolayers adsorbed various gases on S-vacancies: A first-principles study. Superlattices and Microstructures, 2020, 140, 106454.	1.4	19
30	Investigation on the structural, elastic, electronic, and magnetic properties of half-metallic $$hbox {Co}_{2}hbox {MnSi}$$ Co 2 MnSi and CoMnIrSi via first-principles calculations. Journal of Computational Electronics, 2018, 17, 1470-1477.	1.3	18
31	First principles investigation on elastic, optoelectronic and thermoelectric properties of KYX (XÂ= Ge,) Tj ETQq1 1 0.784314 rgBT /Over	1.3	18
32	Half-metallicity and magnetism in BAs monolayer induced by anchoring 3d transition metals (TM = V,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.4	17
33	Electronic, optical and thermoelectric properties of a novel two-dimensional SbXY (X = Se, Te; Y = Br, I) family: ab initio perspective. Physical Chemistry Chemical Physics, 2021, 23, 25866-25876.	1.3	17
34	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.	0.9	16
35	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. Materials Research Express, 2020, 7, 015013.	0.8	16
36	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113857.	1.3	16

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37	Theoretical analysis of the HfS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math> monolayer electronic structure and optical properties under vertical strain effects. Optik, 2021, 225, 165718.	1.4	16
38	First principles study of structural, electronic, elastic and thermodynamic properties of cubic HfO2 under pressure. Physica B: Condensed Matter, 2018, 545, 55-61.	1.3	15
39	Electronic structure, optical and thermoelectric properties of cadmium chalcogenides monolayers. Optik, 2020, 210, 164567.	1.4	15
40	Comparative study of structural, electronic, optical and thermoelectric properties of GaS bulk and monolayer. Philosophical Magazine, 2019, 99, 736-751.	0.7	14
41	Structural, electronic and optical properties of CdO monolayer and bilayers: Stacking effect investigations. Superlattices and Microstructures, 2020, 145, 106644.	1.4	14
42	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. Superlattices and Microstructures, 2019, 136, 106270.	1.4	13
43	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties. RSC Advances, 2020, 10, 10731-10739.	1.7	13
44	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.	0.9	13
45	Electronic structure, chemical bonding, optical, elastic and dynamical properties of MeB2 compounds: Effect of transition metal Meâ€¯=â€¯Sc, Ti and Zr. Computational Condensed Matter, 2019, 21, e00406.	0.9	12
46	2D Hexagonal SnTe monolayer: a quasi direct band gap semiconductor with strain sensitive electronic and optical properties. European Physical Journal B, 2020, 93, 1.	0.6	12
47	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.	0.9	12
48	Exploring a silicene monolayer as a promising sensor platform to detect and capture NO and CO gas. RSC Advances, 2022, 12, 9828-9835.	1.7	12
49	First principles study on structural, electronic and optical properties of Ga 1â^'x B x P ternary alloys () Tj ETQq1 1 0.784314 rgBT /Over 1942-1949.	0.9	10
50	Systematic study of structural, electronic, optical and thermodynamic properties of SrFCuTe compound. Journal of Solid State Chemistry, 2019, 270, 85-91.	1.4	10
51	Tuning the electronic, photocatalytic and optical properties of hydrogenated InN monolayer by biaxial strain and electric field. Chemical Physics, 2020, 532, 110677.	0.9	10
52	Engineering the electronic and magnetic properties of nitrogene monolayer and bilayer by doping: A first-principles study. Applied Surface Science, 2021, 566, 150711.	3.1	10
53	Fluorinating the graphene-like BeO monolayer: A spin-polarized first principles study of the electronic, magnetic and optical properties. Physica Scripta, 2020, 95, 105806.	1.2	10
54	Defective and doped MgO monolayer as promising 2D materials for optoelectronic and spintronic applications. Materials Science in Semiconductor Processing, 2022, 149, 106876.	1.9	10

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55	Insight into the structural, elastic, electronic and thermal properties of YMgX₄ (X = Co,) Tj ETQq1 1 0.784314 rgBT /Ove	0.8	9
56	New equiatomic quaternary Heusler compounds without transition metals KCaBX (XÂ= S and Se): Robust half-metallicity and optical properties. Journal of Molecular Graphics and Modelling, 2020, 100, 107642.	1.3	9
57	Strain-tunable electronic, optical and thermoelectric properties of BP monolayer investigated by FP-LAPW calculations. Physica B: Condensed Matter, 2021, 603, 412757.	1.3	9
58	Nitrogen doping and oxygen vacancy effects on the fundamental properties of BeO monolayer: a DFT study. Journal of Physics Condensed Matter, 2021, 33, 325305.	0.7	9
59	Exploring the electronic band gap of Janus MoSeO and WSeO monolayers and their heterostructures. New Journal of Chemistry, 0, , .	1.4	9
60	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.	1.0	8
61	Structural, electronic, optical and thermodynamic properties of AeBi2O6 (AeÂ= Sr and Ba): Insights from first principles study. Journal of Molecular Graphics and Modelling, 2019, 90, 153-160.	1.3	8
62	Examining the uniform strain effect on elastic, electronic and optical properties of CsPbCl3 through FP-LAPW calculations. Chemical Physics, 2020, 531, 110654.	0.9	8
63	P-substitution effects on the electronic structure and thermal properties of the half-metallic half-Heusler NaCrBi compound. Chemical Physics, 2020, 537, 110848.	0.9	8
64	An assessment of the structural, electronic, optical and thermoelectric properties of the BaAg2GeS4 compound. Journal of Solid State Chemistry, 2020, 285, 121260.	1.4	8
65	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.	2.0	8
66	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.	1.3	8
67	Effect of pressure on structural, electronic and optical properties of SrF2: a first principles study. Revista Mexicana De FÃsica, 2017, 64, 94-100.	0.2	8
68	Search for new d0 half-metallic materials: theoretical investigation on KCaC1â^'xSi (x = 0; 0.25; 0.5; 0.75) Tj ETQq0 0 0 rgBT /Overlock 1	2.0	7
69	Electronic and optical properties of wide band gap Tl3TaS4: A promising surface acoustic wave material. Optical Materials, 2020, 99, 109601.	1.7	7
70	LiCl monolayer for UV detection: First principles prediction. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 123, 114168.	1.3	7
71	First principles insight into the structural, electronic, optical and thermodynamic properties of CsPb2Br5 compound. Chemical Physics, 2020, 533, 110704.	0.9	7
72	Computational investigation of the structural, electronic, optical and thermoelectric properties of T2-Al2MgC2 compound. Journal of Solid State Chemistry, 2019, 280, 120999.	1.4	6

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73	Theoretical study of electronic structure, thermoelectric and thermodynamic properties of 2H-AgAlO2. Physica B: Condensed Matter, 2019, 558, 109-115.	1.3	6
74	Novel two-dimensional ZnO₂, CdO₂ and HgO₂ monolayers: a first-principles-based prediction. New Journal of Chemistry, 2021, 45, 9368-9374.	1.4	6
75	Tuning MoSO monolayer properties for optoelectronic and spintronic applications: effect of external strain, vacancies and doping. RSC Advances, 2021, 11, 35614-35623.	1.7	6
76	Theoretical study of electronic and optical properties of antiferromagnetic Î²-MnS using the modified Becke Johnson (mBJ) potential. Journal of Physics and Chemistry of Solids, 2019, 128, 310-315.	1.9	5
77	Half-metal effect on the MnAs/InP (0ÂÔÂ1)-(2ÂÃ—Â4) interface. Computational Materials Science, 2020, 175, 109603.	1.4	5
78	Theoretical prediction of electronic and optical properties of haft-hydrogenated InN monolayers. Superlattices and Microstructures, 2020, 142, 106519.	1.4	5
79	Strain-driven modulation of the electronic, optical and thermoelectric properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e158" altimg="si13.svg"><mml:mi>Î²</mml:mi></mml:math>-antimonene monolayer: A hybrid functional study. Materials Science in Semiconductor Processing, 2021, 131, 105878.	1.9	5
80	First principles prediction of the stable MgFCl Janus monolayer with tunable properties. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 137, 115023.	1.3	5
81	FP-LAPW investigation on structural, electronic and optical properties of Eu2+-doped MF2 (Mâ€¯=â€¯Ca and) Tj ETQq1 1 0.784314 rgBT	1.4	4
82	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.	0.8	4
83	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.	1.0	4
84	Investigation on electronic structure and luminescence mechanism of CaF2:Eu3+ from first principles calculations. Optik, 2019, 181, 1023-1027.	1.4	4
85	Computational prediction of the spin-polarized semiconductor equiatomic quaternary Heusler compound MnVZrP as a spin-filter. RSC Advances, 2020, 10, 25609-25617.	1.7	4
86	DFT prediction of structural, electronic and magnetic properties of Sr_{0.75}TM_{0.25}S (TM is 3d transition metals). Philosophical Magazine Letters, 2020, 100, 95-104.	0.5	4
87	Prediction of a new 2D B2CO monolayer from density functional theory. Computational Materials Science, 2021, 186, 109975.	1.4	4
88	Electronic, optical and thermoelectric properties of CaO mono- and bi-layers: Theoretical comparative investigation. Optik, 2020, 218, 165115.	1.4	3
89	Theoretical investigation of the AlN (0 0 0 1)-(2ÂÃ—Â2) surface doped with nickel: Structural, electronic and magnetic properties. Journal of Crystal Growth, 2020, 551, 125907.	0.7	3
90	Ferromagnetic half-metallicity of the cubic NaMgO₃ perovskite: from bulk to (001) surfaces. Physical Chemistry Chemical Physics, 2022, 24, 2209-2218.	1.3	3

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91	Controlling magnetic-semiconductor properties of the Si- and Al-doped blue phosphorene monolayer. Journal Physics D: Applied Physics, 2022, 55, 165302.	1.3	3
92	Theoretical investigations on physical properties of SrFCuCh (Ch=S and Se). Journal of Solid State Chemistry, 2019, 271, 191-198.	1.4	2
93	On the structural, electronic, optical and thermoelectric properties of CdIn2Se4 ordered-vacancy compound. Journal of Solid State Chemistry, 2020, 282, 121078.	1.4	2
94	Pressure effects on the electronic, magnetic, thermoelectric, and thermodynamic properties of Mn 2 CoSi halfâ€metallic compound. International Journal of Quantum Chemistry, 2021, 121, e26445.	1.0	2
95	Firstâ€principles investigation of the (HfSe ₂) _{4â^' n} â€"(HfSSe) _n (n Â=Â0, 1, 2, 3, 4) lateral heterostructures. International Journal of Quantum Chemistry, 2022, 122, .	1.0	2
96	Exploring the sensing ability of <scp>B</scp> â€•and <scp>Si</scp> â€•doped <scp> WS ₂ </scp> monolayer toward <scp>CO</scp> and <scp>NO</scp> gas. International Journal of Quantum Chemistry, 0, , .	1.0	2
97	Antiferromagnetic ordering in the TM-adsorbed AlN monolayer (TM = V and Cr). RSC Advances, 2022, 12, 16677-16683.	1.7	2
98	Designing doping strategy in arsenene monolayer for spintronic and optoelectronic applications: a case study of germanium and nitrogen as dopants. Journal of Physics Condensed Matter, 2022, 34, 355301.	0.7	2
99	Electronic and magnetic properties of the WSO Janus monolayer engineered by intrinsic defects. Surfaces and Interfaces, 2022, 32, 102114.	1.5	2
100	Strain tunable electronic and optical properties of 2D orthorhombic lithium sulfur monolayer. Chemical Physics, 2020, 535, 110762.	0.9	1
101	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.	1.4	1
102	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.	0.7	1
103	Developing feature-rich electronic and magnetic properties in the Î²-As monolayer for spintronic and optoelectronic applications by C and Si doping: A first-principles study. Surfaces and Interfaces, 2021, 27, 101534.	1.5	1
104	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.	0.9	1
105	Study of vacancy, voids, atom adsorption and domain substitution in hexagonal gallium nitride monolayer. Surfaces and Interfaces, 2022, 30, 101898.	1.5	1
106	Featureâ€rich structural, electronic, magnetic and optical properties of the fluorineâ€•and nitrogenâ€•incorporated CaF 2 compound. International Journal of Quantum Chemistry, 2021, 121, e26672.	1.0	0
107	Prediction of a Beryllium Phosphide Iodide Monolayer as a Photocatalyst for Water Splitting by Density Functional Theory. Journal of Electronic Materials, 2022, 51, 2077-2082.	1.0	0