Tuan V Vu

List of Publications by Year
in descending order

		76196	143772
188	5,055	40	57
papers	citations	h-index	g-index

189	189	189	2357
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Layered graphene/GaS van der Waals heterostructure: Controlling the electronic properties and Schottky barrier by vertical strain. Applied Physics Letters, 2018, 113, .	1.5	171
2	Rashba spin splitting and photocatalytic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>GeC</mml:mi><mml:mo>â^'</mml:mo><mml:mi>M</mml:mi><mml:m (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 697 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:r	1.1	144
3	Graphene/WSeTe van der Waals heterostructure: Controllable electronic properties and Schottky barrier via interlayer coupling and electric field. Applied Surface Science, 2020, 507, 145036.	3.1	133
4	Interfacial characteristics, Schottky contact, and optical performance of a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>graphene</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mrow><mathvariant="normal">S</mml:mi><mml:mi>Se</mml:mi></mml:math> van der Waals heterostructure: Strain engineering and electric field tunability. Physical Review B, 2020, 102, .	1.1	100
5	Interlayer coupling and electric field tunable electronic properties and Schottky barrier in a graphene/bilayer-GaSe van der Waals heterostructure. Physical Chemistry Chemical Physics, 2018, 20, 17899-17908.	1.3	99
6	A type-II GaSe/HfS2 van der Waals heterostructure as promising photocatalyst with high carrier mobility. Applied Surface Science, 2020, 534, 147607.	3.1	97
7	Theoretical prediction of electronic, transport, optical, and thermoelectric properties of Janus monolayers <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:mm		

#	Article	IF	Citations
19	A van der Waals heterostructure of MoS₂/MoSi₂N₄: a first-principles study. New Journal of Chemistry, 2021, 45, 8291-8296.	1.4	59
20	First-principles study of the structural and electronic properties of graphene/MoS2 interfaces. Journal of Applied Physics, 2017, 122, .	1.1	57
21	Electronic structure and optical properties of Ag2HgSnSe4: First-principles DFT calculations and X-ray spectroscopy studies. Journal of Alloys and Compounds, 2018, 732, 372-384.	2.8	57
22	Graphene hetero-multilayer on layered platinum mineral jacutingaite (Pt₂HgSe₃): van der Waals heterostructures with novel optoelectronic and thermoelectric performances. Journal of Materials Chemistry A, 2020, 8, 13248-13260.	5.2	57
23	First principles study of the electronic properties and Schottky barrier in vertically stacked graphene on the Janus MoSeS under electric field. Computational Materials Science, 2018, 153, 438-444.	1.4	56
24	Tunable type-II band alignment and electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:msub><mml:mi>MoSi</mml:mi><mml:mi mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> heterostructure: Interlayer coupling and electric. Physical Review B, 2022, 105, .	1.1	56
25	Enhancement of monolayer SnSe light absorption by strain engineering: A DFT calculation. Chemical Physics, 2019, 521, 5-13.	0.9	54
26	Two-Dimensional Boron Phosphide/MoGe₂N₄ van der Waals Heterostructure: A Promising Tunable Optoelectronic Material. Journal of Physical Chemistry Letters, 2021, 12, 5076-5084.	2.1	54
27	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
28	First-principles investigation of structural, elastic, thermodynamic, electronic and optical properties of lead-free double perovskites halides: Cs2LiYX6 (X = Br, I). Materials Chemistry and Physics, 2021, 258, 123945.	2.0	52
29	Interfacial Electronic Properties and Tunable Contact Types in Graphene/Janus MoGeSiN₄ Heterostructures. Journal of Physical Chemistry Letters, 2021, 12, 3934-3940.	2.1	52
30	Van der Waals graphene/g-GaSe heterostructure: Tuning the electronic properties and Schottky barrier by interlayer coupling, biaxial strain, and electric gating. Journal of Alloys and Compounds, 2018, 750, 765-773.	2.8	51
31	Effect of biaxial strain and external electric field on electronic properties of MoS 2 monolayer: A first-principle study. Chemical Physics, 2016, 468, 9-14.	0.9	49
32	Tailoring the structural and electronic properties of an SnSe₂/MoS₂ van der Waals heterostructure with an electric field and the insertion of a graphene sheet. Physical Chemistry Chemical Physics, 2019, 21, 22140-22148.	1.3	48
33	Linear and nonlinear magneto-optical properties of monolayer phosphorene. Journal of Applied Physics, 2017, 121, .	1.1	47
34	First-principles investigations of Na2CuMCl6 (M = Bi, Sb) double perovskite semiconductors: Materials for green technology. Materials Science in Semiconductor Processing, 2022, 150, 106947.	1.9	45
35	First principles study of single-layer SnSe2 under biaxial strain and electric field: Modulation of electronic properties. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 201-205.	1.3	44
36	Electric gating and interlayer coupling controllable electronic structure and Schottky contact of graphene/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>BiI</mml:mi></mml:mrow><mml:mn>3</mml:mn> van der Waals heterostructure. Physical Review B, 2021, 103, .	1.1	43

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37	First-principles investigations of Ba2NaIO6 double Perovskite semiconductor: Material for low-cost energy technologies. Materials Chemistry and Physics, 2022, 275, 125237.	2.0	42
38	Tuning the electronic properties and Schottky barrier height of the vertical graphene/MoS 2 heterostructure by an electric gating. Superlattices and Microstructures, 2018, 116, 79-87.	1.4	41
39	A theoretical and experimental study of the valence-band electronic structure and optical constants of quaternary copper mercury tin sulfide, Cu2HgSnS4, a potential material for optoelectronics and solar cells. Optical Materials, 2019, 96, 109296.	1.7	41
40	Assessing optoelectronic properties of PbI2 monolayer under uniaxial strain from first principles calculations. Superlattices and Microstructures, 2019, 130, 354-360.	1.4	41
41	Band alignment and optical features in Janus-MoSeTe/X(OH)₂ (X = Ca, Mg) van der Waals heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 25849-25858.	1.3	40
42	Structural, electronic, and transport properties of quintuple atomic Janus monolayers <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m mathvariant="normal">S</mml:mi><mml:msub><mml:mi>X</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 532 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:m	1.1	40
43	First principle study on the electronic properties and Schottky contact of graphene adsorbed on MoS 2 monolayer under applied out-plane strain. Surface Science, 2018, 668, 23-28.	0.8	39
44	Computational prediction of electronic and optical properties of Janus Ga₂SeTe monolayer. Journal Physics D: Applied Physics, 2020, 53, 455302.	1.3	39
45	Vertical strain and electric field tunable electronic properties of type-II band alignment C2N/InSe van der Waals heterostructure. Chemical Physics Letters, 2019, 716, 155-161.	1.2	38
46	van der Waals heterostructures based on MSSe (M = Mo, W) and graphene-like GaN: enhanced optoelectronic and photocatalytic properties for water splitting. Physical Chemistry Chemical Physics, 2020, 22, 20704-20711.	1.3	37
47	Oxygenation of janus group III monochalcogenides: First principles insights into <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>GaIn</mml:mi><mml:mi>X</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 342 Td (2021, 104. .	1.1	37
48	Electric-field tunable electronic properties and Schottky contact of graphene/phosphorene heterostructure. Vacuum, 2018, 149, 231-237.	1.6	36
49	Theoretical investigation of electronic structure and thermoelectric properties of MX2 (M=Zr, Hf;) Tj ETQq1 1 0.784314 rgBT /Overlock	1.9	36
50	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
51	Particular features of the electronic structure and optical properties of Ag2PbGeS4 as evidenced from first-principles DFT calculations and XPS studies. Materials Chemistry and Physics, 2018, 208, 268-280.	2.0	35
52	First principles study of optical properties of molybdenum disulfide: From bulk to monolayer. Superlattices and Microstructures, 2018, 115, 10-18.	1.4	35
53	Investigation of strain and doping on the electronic properties of single layers of C₆N₆ and C₆N₈: a first principles study. RSC Advances, 2020, 10, 27743-27751.	1.7	35
54	Electronic and optical properties of bulk and surface of CsPbBr3 inorganic halide perovskite a first principles DFT 1/2 approach. Scientific Reports, 2021, 11, 20622.	1.6	35

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55	Electronic structure and optical properties of RbPb2Br5. Journal of Physics and Chemistry of Solids, 2016, 91, 25-33.	1.9	33
56	Spinâ€“orbit coupling effect on electronic, optical, and thermoelectric properties of Janus Ga₂SSe. RSC Advances, 2020, 10, 44785-44792.	1.7	32
57	Electronic properties and optical behaviors of bulk and monolayer ZrS2: A theoretical investigation. Superlattices and Microstructures, 2019, 125, 205-213.	1.4	31
58	Gas adsorption properties (N₂, H₂, O₂, NO, NO₂, CO,) Tj ETQq0 0 0 rgBT /Overlock first-principles study. New Journal of Chemistry, 2020, 44, 18763-18769.	1.4	30
59	Electric field and substrateâ€“induced modulation of spin-polarized transport in graphene nanoribbons on A3B5 semiconductors. Journal of Applied Physics, 2015, 117, .	1.1	29
60	Linear and nonlinear magneto-optical properties of monolayer MoS2. Journal of Applied Physics, 2018, 123, .	1.1	29
61	Effects of different surface functionalization on the electronic properties and contact types of graphene/functionalized-GeC van der Waals heterostructures. Physical Chemistry Chemical Physics, 2020, 22, 7952-7961.	1.3	29
62	Electronic structure and optical properties of noncentrosymmetric LiGaSe 2 : Experimental measurements and DFT band structure calculations. Optical Materials, 2017, 66, 149-159.	1.7	28
63	Out-of-plane strain and electric field tunable electronic properties and Schottky contact of graphene/antimonene heterostructure. Superlattices and Microstructures, 2017, 112, 554-560.	1.4	27
64	Electric field tunable electronic properties of P-ZnO and SiC-ZnO van der Waals heterostructures. Computational Materials Science, 2019, 164, 166-170.	1.4	27
65	Electronic structure and optical properties of Cs2HgI4: Experimental study and band-structure DFT calculations. Optical Materials, 2015, 42, 351-360.	1.7	26
66	Linear and nonlinear magneto-optical absorption coefficients and refractive index changes in graphene. Optical Materials, 2017, 69, 328-332.	1.7	26
67	Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties. Superlattices and Microstructures, 2020, 137, 106359.	1.4	26
68	Electronic properties and low lattice thermal conductivity (Îº_l) of mono-layer (ML) MoS₂: FP-LAPW incorporated with spinâ€“orbit coupling (SOC). RSC Advances, 2020, 10, 18830-18840.	1.7	26
69	Effect of electric field on the electronic and magnetic properties of a graphene nanoribbon/aluminium nitride bilayer system. RSC Advances, 2015, 5, 49308-49316.	1.7	25
70	Electronic structure and optical properties of noncentrosymmetric LiGaGe 2 Se 6 , a promising nonlinear optical material. Physica B: Condensed Matter, 2016, 501, 74-83.	1.3	25
71	Specific features of the electronic structure and optical properties of KPb2Br5: DFT calculations and X-ray spectroscopy measurements. Optical Materials, 2016, 53, 64-72.	1.7	25
72	Ab-initio study of electronic and optical properties of biaxially deformed single-layer GeS. Superlattices and Microstructures, 2018, 120, 501-507.	1.4	25

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73	Magneto-optical absorption in silicene and germanene induced by electric and Zeeman fields. Physical Review B, 2020, 101, .	1.1	25
74	Electronic structure and optical properties of Cu2CdGeS4: DFT calculations and X-ray spectroscopy measurements. Optical Materials, 2015, 47, 435-444.	1.7	24
75	Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides. Journal of Physics Condensed Matter, 2021, 33, 225503.	0.7	24
76	Electronic and optical properties of 2D monolayer (ML) MoS2 with vacancy defect at S sites. Nano Structures Nano Objects, 2020, 21, 100404.	1.9	23
77	Dispersion-Corrected Density Functional Theory Investigations of Structural and Electronic Properties of Bulk MoS2: Effect of Uniaxial Strain. Nanoscale Research Letters, 2015, 10, 433.	3.1	22
78	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study. RSC Advances, 2020, 10, 40411-40420.	1.7	22
79	Effect of strains on electronic and optical properties of monolayer SnS: Ab-initio study. Physica B: Condensed Matter, 2018, 545, 255-261.	1.3	21
80	Strain and electric field tunable electronic properties of type-II band alignment in van der Waals GaSe/MoSe2 heterostructure. Chemical Physics, 2019, 521, 92-99.	0.9	21
81	Modulation of electronic properties of monolayer InSe through strain and external electric field. Chemical Physics, 2019, 516, 213-217.	0.9	21
82	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
83	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
84	Efficient Broadband Truncated-Pyramid-Based Metamaterial Absorber in the Visible and Near-Infrared Regions. Crystals, 2020, 10, 784.	1.0	19
85	Electronic and optoelectronic properties of van der Waals heterostructure based on graphene-like GaN, blue phosphorene, SiC, and ZnO: A first principles study. Journal of Applied Physics, 2020, 127, .	1.1	19
86	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
87	Janus Ga2STe monolayer under strain and electric field: Theoretical prediction of electronic and optical properties. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114358.	1.3	18
88	Structural, elastic, and electronic properties of chemically functionalized boron phosphide monolayer. RSC Advances, 2021, 11, 8552-8558.	1.7	18
89	Rashba-type spin splitting and transport properties of novel Janus XWGeN₂ (X = O, S, Se,) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	18
90	Manifestation of Anomalous Weak Space-Charge-Density Acentricity for a Tl₄HgBr₆Single Crystal. Inorganic Chemistry, 2016, 55, 10547-10557.	1.9	17

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91	Electronic, magnetic and optical properties of monolayer (ML) hexagonal ZnSe on vacancy defects at Zn sites from DFT-1/2 approach. Vacuum, 2020, 182, 109597.	1.6	17
92	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
93	Induced ferromagnetism in bilayer hexagonal Boron Nitride (h-BN) on vacancy defects at B and N sites. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 126, 114436.	1.3	17
94	First-principles DFT calculations of the electronic structure and optical properties of TlInGe2Se6, a prospective NLO material. Materials Chemistry and Physics, 2018, 219, 162-174.	2.0	16
95	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. Materials Research Express, 2020, 7, 015013.	0.8	16
96	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113857.	1.3	16
97	Modulation of electronic and optical properties of GaTe monolayer by biaxial strain and electric field. Superlattices and Microstructures, 2020, 140, 106435.	1.4	16
98	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
99	Crystal growth, electronic and optical properties of Tl2CdSnSe4, a recently discovered prospective semiconductor for application in thin film solar cells and optoelectronics. Optical Materials, 2021, 111, 110656.	1.7	16
100	Band Gap Modulation of Bilayer MoS2 Under Strain Engineering and Electric Field: A Density Functional Theory. Journal of Electronic Materials, 2016, 45, 4038-4043.	1.0	15
101	Tuning the Electronic and Optical Properties of Two-Dimensional Graphene-like $$hbox {C}_2hbox {N}$$ C 2 N Nanosheet by Strain Engineering. Journal of Electronic Materials, 2018, 47, 4594-4603.	1.0	15
102	Electronic, Optical and Elastic Properties of Cu2CdGeSe4: A First-Principles Study. Journal of Electronic Materials, 2019, 48, 705-715.	1.0	15
103	Effects of electric field and strain engineering on the electronic properties, band alignment and enhanced optical properties of ZnO/Janus ZrSSe heterostructures. RSC Advances, 2020, 10, 9824-9832.	1.7	15
104	Stacking and electric field effects on the band alignment and electronic properties of the GeC/GaSe heterostructure. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 120, 114050.	1.3	15
105	Electronic structure and optical constants of CsPbCl3: The effect of approaches within ab initio calculations in relation to X-ray spectroscopy experiments. Materials Chemistry and Physics, 2021, 261, 124216.	2.0	15
106	Effects of electric field and biaxial strain on the (NO2, NO, O2, and SO2) gas adsorption properties of Sc2CO2 monolayer. Superlattices and Microstructures, 2022, 163, 107135.	1.4	15
107	Single crystal growth, electronic structure and optical properties of Cs2HgBr4. Journal of Physics and Chemistry of Solids, 2015, 85, 254-263.	1.9	14
108	Strain-Tunable Electronic and Optical Properties of Monolayer Germanium Monosulfide: Ab-Initio Study. Journal of Electronic Materials, 2019, 48, 2902-2909.	1.0	14

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109	Quaternary Cu2HgGeSe4 selenide: Its electronic and optical properties as elucidated from TB-mBJ band-structure calculations and XPS and XES measurements. Chemical Physics, 2020, 536, 110821.	0.9	14
110	Structural, electronic and optical properties of CdO monolayer and bilayers: Stacking effect investigations. Superlattices and Microstructures, 2020, 145, 106644.	1.4	14
111	TlInGe2S6, A Prospective Nonlinear Optical Material: First-Principles DFT Calculations of the Electronic Structure and Optical Properties. Journal of Electronic Materials, 2018, 47, 5525-5536.	1.0	13
112	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. Superlattices and Microstructures, 2019, 136, 106270.	1.4	13
113	Tri-layered van der Waals heterostructures based on graphene, gallium selenide and molybdenum selenide. Journal of Applied Physics, 2019, 125, .	1.1	13
114	Electronic and optical properties of quaternary sulfide Tl2HgSnS4, a promising optoelectronic semiconductor: A combined experimental and theoretical study. Optical Materials, 2019, 92, 294-302.	1.7	13
115	Electronic and optical properties of layered van der Waals heterostructure based on MS₂ (M = Mo, W) monolayers. Materials Research Express, 2019, 6, 065060.	0.8	13
116	Theoretical and experimental study on the electronic and optical properties of K_{0.5}Rb_{0.5}Pb₂Br₅: a promising laser host material. RSC Advances, 2020, 10, 11156-11164.	1.7	13
117	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties. RSC Advances, 2020, 10, 10731-10739.	1.7	13
118	Promising optoelectronic response of 2D monolayer MoS2: A first principles study. Chemical Physics, 2020, 538, 110824.	0.9	13
119	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
120	First-principles DFT computation and X-ray spectroscopy study of the electronic band structure and optical constants of Cu2HgGeS4. Solid State Sciences, 2020, 104, 106287.	1.5	13
121	Effect of oxygen adsorption on structural and electronic properties of defective surfaces (0 0 1), (1 1) Tj ETQq1 1 0.784314 rgBT /Ove	1.4	12
122	DFT study and XPS measurements elucidating the electronic and optical properties of KPb2Cl5. Optical Materials, 2020, 102, 109793.	1.7	12
123	Computational insights into structural, electronic and optical characteristics of GeC/C₂N van der Waals heterostructures: effects of strain engineering and electric field. RSC Advances, 2020, 10, 2967-2974.	1.7	12
124	Understanding the electronic properties, contact types and optical performances in graphene/InN heterostructure: Role of electric gating. Diamond and Related Materials, 2020, 106, 107851.	1.8	12
125	Electronic structure and optical properties of LiGa0.5In0.5Se2 single crystal, a nonlinear optical mid-IR material. Optical Materials, 2018, 80, 12-21.	1.7	11
126	Electronic band structure and basic optical constants of TlGaSn2Se6, a promising NLO semiconductor: First-principles calculations under DFT framework. Optik, 2019, 181, 673-685.	1.4	11

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127	TlSbP2Se6 - a new layered single crystal: growth, structure and electronic properties. Journal of Alloys and Compounds, 2020, 848, 156485.	2.8	11
128	Outstanding elastic, electronic, transport and optical properties of a novel layered material C₄F₂: first-principles study. RSC Advances, 2021, 11, 23280-23287.	1.7	11
129	Electronic structure and optical properties of Cs 2 HgCl 4 : DFT calculations and X-ray photoelectron spectroscopy measurements. Optical Materials, 2016, 60, 169-180.	1.7	10
130	Structural, electronic, optical and elastic properties of XLa2S4 (Xâ€¯=â€¯Ba; Ca): Ab initio study. Physica B: Condensed Matter, 2019, 558, 91-99.	1.3	10
131	Tuning the electronic properties of GaS monolayer by strain engineering and electric field. Chemical Physics, 2019, 524, 101-105.	0.9	10
132	Schottky anomaly and NÃ©el temperature treatment of possible perturbed hydrogenated AA-stacked graphene, SiC, and h-BN bilayers. RSC Advances, 2019, 9, 41569-41580.	1.7	10
133	Simulation within a DFT framework and experimental study of the valence-band electronic structure and optical properties of quaternary selenide Cu2HgSnSe4. Optik, 2020, 202, 163709.	1.4	10
134	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
135	Low-energy bands, optical properties, and spin/valley-Hall conductivity of silicene and germanene. Journal of Materials Science, 2020, 55, 14848-14857.	1.7	10
136	Theoretical insights into tunable electronic and optical properties of Janus Al2SSe monolayer through strain and electric field. Optik, 2021, 238, 166761.	1.4	10
137	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
138	Novel Janus GaInX₃ (X = S, Se, Te) single-layers: first-principles prediction on structural, electronic, and transport properties. RSC Advances, 2022, 12, 7973-7979.	1.7	10
139	Ni-doped WO3 flakes-based sensor for fast and selective detection of H2S. Journal of Materials Science: Materials in Electronics, 2020, 31, 12783-12795.	1.1	9
140	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
141	First-principles calculations to investigate electronic properties of ZnO/PtSSe van der Waals heterostructure: Effects of vertical strain and electric field. Chemical Physics, 2021, 551, 111333.	0.9	9
142	Calculations within DFT framework of the electronic and optical properties of quaternary sulfide Tl2PbSiS4, a prospective optoelectronic semiconductor. Computational Condensed Matter, 2019, 21, e00392.	0.9	8
143	Optical and electronic properties of lithium thiogallate (LiGaS₂): experiment and theory. RSC Advances, 2020, 10, 26843-26852.	1.7	8
144	First-principles study of structure, electronic properties and stability of tungsten adsorption on TiC(111) surface with disordered vacancies. Physica B: Condensed Matter, 2017, 526, 28-36.	1.3	7

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145	Structural properties and variable-range hopping conductivity of Cu₂SnS₃. Materials Research Express, 2019, 6, 055915.	0.8	7
146	Electronic and optical properties of wide band gap Tl3TaS4: A promising surface acoustic wave material. Optical Materials, 2020, 99, 109601.	1.7	7
147	LiCl monolayer for UV detection: First principles prediction. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 123, 114168.	1.3	7
148	Electronic structure and optical performance of PbI2/SnSe2 heterostructure. Chemical Physics, 2020, 533, 110736.	0.9	7
149	Valence-band electronic structure and main optical properties of Cu2HgGeTe4: Theoretical simulation within a DFT framework and experimental XPS study. Materials Today Communications, 2020, 23, 100828.	0.9	7
150	Stacking effects in van der Waals heterostructures of blueP and Janus XYO (X = Ti, Zr, Hf: Y = S, Se) monolayers. RSC Advances, 2021, 11, 12189-12199.	1.7	7
151	A theoretical study on elastic, electronic, transport, optical and thermoelectric properties of Janus SnSO monolayer. Journal Physics D: Applied Physics, 2021, 54, 475306.	1.3	7
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