Tuan V Vu

List of Publications by Year in Descending Order

180 papers	2,934 citations	31 h-index	43 g-index
189 ext. papers	3,966 ext. citations	3.2 avg, IF	6.09 L-index

#	Paper	IF	Citations
180	Tunable type-II band alignment and electronic structure of C3N4/MoSi2N4 heterostructure: Interlayer coupling and electric field. *Physical Review B*, **2022**, 105,	3.3	9
179	Janus monolayer HfSO with improved optical properties as a novel material for photovoltaic and photocatalyst applications. *New Journal of Chemistry*, **2022**, 46, 1557-1568	3.6	1
178	Growth of a novel K0.4Rb0.6Pb2Cl5 crystal and theoretical and experimental studies of its electronic and optical properties. *Optical Materials*, **2022**, 124, 112050	3.3	0
177	Structural, electronic, and transport properties of quintuple atomic Janus monolayers Ga2SX2 (X= O, S, Se, Te): First-principles predictions. *Physical Review B*, **2022**, 105,	3.3	6
176	Highly anisotropic layered crystal AgBiP2Se6: Growth, electronic band-structure and optical properties. *Materials Chemistry and Physics*, **2022**, 277, 125556	4.4	0
175	First-principles investigations of Ba2NaIO6 double Perovskite semiconductor: Material for low-cost energy technologies. *Materials Chemistry and Physics*, **2022**, 275, 125237	4.4	2
174	Novel Janus GaInX (X = S, Se, Te) single-layers: first-principles prediction on structural, electronic, and transport properties.. *RSC Advances*, **2022**, 12, 7973-7979	3.7	0
173	Layered post-transition-metal dichalcogenide SnGeN as a promising photoelectric material: a DFT study.. *RSC Advances*, **2022**, 12, 10249-10257	3.7	1
172	Monoelemental two-dimensional iodinene nanosheets: a first-principles study of the electronic and optical properties. *Journal Physics D: Applied Physics*, **2022**, 55, 135104	3	
171	Intriguing interfacial characteristics of the CS contact with MX (M = Mo, W; X = S, Se, Te) and MXY ((X Y) = S, Se, Te) monolayers.. *RSC Advances*, **2022**, 12, 12292-12302	3.7	0
170	Theoretical prediction of Janus PdXO (X = S, Se, Te) monolayers: structural, electronic, and transport properties.. *RSC Advances*, **2022**, 12, 12971-12977	3.7	0
169	Electronic and optical properties of bulk and surface of CsPbBr inorganic halide perovskite a first principles DFT 1/2 approach. *Scientific Reports*, **2021**, 11, 20622	4.9	9
168	Electric gating and interlayer coupling controllable electronic structure and Schottky contact of graphene/BiI3 van der Waals heterostructure. *Physical Review B*, **2021**, 103,	3.3	13
167	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	4.4	4
166	DFT calculations and experimental studies of the electronic structure and optical properties of Tl4PbI6. *Optical Materials*, **2021**, 114, 110982	3.3	4
165	Interfacial Electronic Properties and Tunable Contact Types in Graphene/Janus MoGeSiN Heterostructures. *Journal of Physical Chemistry Letters*, **2021**, 12, 3934-3940	6.4	17
164	Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	9

163	Two-Dimensional Boron Phosphide/MoGeN van der Waals Heterostructure: A Promising Tunable Optoelectronic Material. *Journal of Physical Chemistry Letters*, **2021**, 12, 5076-5084	6.4	21
162	A DFT Study of Structural, Elastic, Thermodynamic, Magneto-optical, and Electrical Properties of Double-Perovskite Bi2CrMO6 (M = Zn, Ni) Using GGA and TB-mBj Functionals. *Journal of Superconductivity and Novel Magnetism*, **2021**, 34, 2105-2119	1.5	2
161	Theoretical analysis of the HfS2 monolayer electronic structure and optical properties under vertical strain effects. *Optik*, **2021**, 225, 165718	2.5	6
160	Ab initio study of the structural, electronic, optical and elastic properties of promising optoelectronic and thermoelectric compounds MgSc2X4 (X = S; Se). *Journal of Solid State Chemistry*, **2021**, 293, 121763	3.3	2
159	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	3.3	8
158	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	3	9
157	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
156	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	4.4	11
155	Electronic and optical properties of gyrotropic □Hg3S2Cl2: insights from an ab initio study. *Indian Journal of Physics*, **2021**, 95, 73-82	1.4	0
154	Structural, elastic, and electronic properties of chemically functionalized boron phosphide monolayer.. *RSC Advances*, **2021**, 11, 8552-8558	3.7	3
153	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	3.7	4
152	Outstanding elastic, electronic, transport and optical properties of a novel layered material CF: first-principles study.. *RSC Advances*, **2021**, 11, 23280-23287	3.7	3
151	A van der Waals heterostructure of MoS2/MoSi2N4: a first-principles study. *New Journal of Chemistry*, **2021**, 45, 8291-8296	3.6	20
150	Theoretical prediction of electronic, transport, optical, and thermoelectric properties of Janus monolayers In2XO (X=S,Se,Te). *Physical Review B*, **2021**, 103,	3.3	39
149	Theoretical insights into tunable electronic and optical properties of Janus Al2SSe monolayer through strain and electric field. *Optik*, **2021**, 238, 166761	2.5	2
148	Quantum magnetotransport properties of silicene: Influence of the acoustic phonon correction. *Physical Review B*, **2021**, 104,	3.3	1
147	Oxygenation of Janus group III monochalcogenides: First-principles insights into GaInXO (X=S, Se, Te) monolayers. *Physical Review B*, **2021**, 104,	3.3	12
146	A theoretical study on elastic, electronic, transport, optical and thermoelectric properties of Janus SnSO monolayer. *Journal Physics D: Applied Physics*, **2021**, 54, 475306	3	3

145	Quaternary Tl2CdGeSe4 selenide: Electronic structure and optical properties of a novel semiconductor for potential application in optoelectronics. *Journal of Solid State Chemistry*, **2021**, 302, 122453	3.3	1
144	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	2.3	1
143	Effects of electric field and biaxial strain on the (NO2, NO, O2, and SO2) gas adsorption properties of Sc2CO2 monolayer. *Superlattices and Microstructures*, **2021**, 107135	2.8	1
142	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	2.3	5
141	Electronic and optical properties of a Janus SnSSe monolayer: effects of strain and electric field. *Physical Chemistry Chemical Physics*, **2020**, 22, 11637-11643	3.6	33
140	Magneto-optical absorption in silicene and germanene induced by electric and Zeeman fields. *Physical Review B*, **2020**, 101,	3.3	17
139	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	13	44
138	LiCl monolayer for UV detection: First principles prediction. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 123, 114168	3	3
137	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
136	Interlayer coupling and electric field controllable Schottky barriers and contact types in graphene/PbI2 heterostructures. *Physical Review B*, **2020**, 101,	3.3	45
135	Theoretical and experimental study on the electronic and optical properties of KRbPbBr: a promising laser host material.. *RSC Advances*, **2020**, 10, 11156-11164	3.7	4
134	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties.. *RSC Advances*, **2020**, 10, 10731-10739	3.7	10
133	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	3.7	9
132	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	3.6	15
131	DFT study and XPS measurements elucidating the electronic and optical properties of KPb2Cl5. *Optical Materials*, **2020**, 102, 109793	3.3	7
130	Structural, electronic and optical properties of CdO monolayer and bilayers: Stacking effect investigations. *Superlattices and Microstructures*, **2020**, 145, 106644	2.8	8
129	Ni-doped WO3 flakes-based sensor for fast and selective detection of H2S. *Journal of Materials Science: Materials in Electronics*, **2020**, 31, 12783-12795	2.1	3
128	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, 245302	2.5	7

127	Computational prediction of electronic and optical properties of Janus Ga2SeTe monolayer. *Journal Physics D: Applied Physics*, **2020**, 53, 455302	3	13
126	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	3	7
125	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
124	On the in-plane electronic thermal conductivity of biased nanosheet borophene. *Physical Chemistry Chemical Physics*, **2020**, 22, 6318-6325	3.6	0
123	Electronic structure and optical performance of PbI2/SnSe2 heterostructure. *Chemical Physics*, **2020**, 533, 110736	2.3	2
122	Modulation of electronic and optical properties of GaTe monolayer by biaxial strain and electric field. *Superlattices and Microstructures*, **2020**, 140, 106435	2.8	4
121	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
120	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	2.5	4
119	Computational insights into structural, electronic and optical characteristics of GeC/CN van der Waals heterostructures: effects of strain engineering and electric field.. *RSC Advances*, **2020**, 10, 2967-2974	3.7	7
118	Magneto-optical transport properties of monolayer transition metal dichalcogenides. *Physical Review B*, **2020**, 101,	3.3	44
117	Promising optoelectronic response of 2D monolayer MoS2: A first principles study. *Chemical Physics* , **2020**, 538, 110824	2.3	6
116	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
115	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
114	Highly anisotropic layered selenophosphate AgSbP2Se6: The electronic structure and optical properties by experimental measurements and first-principles calculations. *Chemical Physics*, **2020**, 536, 110813	2.3	2
113	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	3.4	7
112	Electronic properties and low lattice thermal conductivity ( ) of mono-layer (ML) MoS: FP-LAPW incorporated with spin-orbit coupling (SOC).. *RSC Advances*, **2020**, 10, 18830-18840	3.7	13
111	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
110	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	2.5	6

109	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
108	Graphene/WSeTe van der Waals heterostructure: Controllable electronic properties and Schottky barrier via interlayer coupling and electric field. *Applied Surface Science*, **2020**, 507, 145036	6.7	92
107	DFT-investigation on anisotropy degree of electronic, optical, and mechanical properties of olivine ZnRE2S4 (RE = Er, Tm) compounds. *Materials Research Express*, **2020**, 7, 016305	1.7	2
106	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
105	Electronic and optical properties of wide band gap Tl3TaS4: A promising surface acoustic wave material. *Optical Materials*, **2020**, 99, 109601	3.3	5
104	Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties. *Superlattices and Microstructures*, **2020**, 137, 106359	2.8	10
103	Electronic and optical properties of 2D monolayer (ML) MoS2 with vacancy defect at S sites. *Nano Structures Nano Objects*, **2020**, 21, 100404	5.6	12
102	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. *Materials Research Express*, **2020**, 7, 015013	1.7	8
101	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 117, 113857	3	6
100	A type-II GaSe/HfS2 van der Waals heterostructure as promising photocatalyst with high carrier mobility. *Applied Surface Science*, **2020**, 534, 147607	6.7	40
99	Janus monolayer PtSSe under external electric field and strain: A first principles study on electronic structure and optical properties. *Superlattices and Microstructures*, **2020**, 147, 106683	2.8	39
98	Electronic structure and band alignment of Blue Phosphorene/Janus ZrSSe heterostructure: A first principles study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 124, 114369	3	1
97	Optical and electronic properties of lithium thiogallate (LiGaS): experiment and theory.. *RSC Advances*, **2020**, 10, 26843-26852	3.7	4
96	Proposal of new spinel oxides semiconductors ZnGaO, [ZnGaO]:Mn and Rh: ab-initio calculations and prospects for thermophysical and optoelectronic applications. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107750	2.8	
95	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study.. *RSC Advances*, **2020**, 10, 40411-40420	3.7	3
94	Interfacial characteristics, Schottky contact, and optical performance of a graphene/Ga2SSe van der Waals heterostructure: Strain engineering and electric field tunability. *Physical Review B*, **2020**, 102,	3.3	55
93	Low-energy bands, optical properties, and spin/valley-Hall conductivity of silicene and germanene. *Journal of Materials Science*, **2020**, 55, 14848-14857	4.3	4
92	TlSbP2Se6 - a new layered single crystal: growth, structure and electronic properties. *Journal of Alloys and Compounds*, **2020**, 848, 156485	5.7	6

91	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	3	9
90	Investigation of strain and doping on the electronic properties of single layers of CN and CN: a first principles study.. *RSC Advances*, **2020**, 10, 27743-27751	3.7	23
89	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	3.7	8
88	Efficient Broadband Truncated-Pyramid-Based Metamaterial Absorber in the Visible and Near-Infrared Regions. *Crystals*, **2020**, 10, 784	2.3	8
87	Gas adsorption properties (N2, H2, O2, NO, NO2, CO, CO2, and SO2) on a Sc2CO2 monolayer: a first-principles study. *New Journal of Chemistry*, **2020**, 44, 18763-18769	3.6	8
86	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	3.6	11
85	Spin-orbit coupling effect on electronic, optical, and thermoelectric properties of Janus GaSSe.. *RSC Advances*, **2020**, 10, 44785-44792	3.7	12
84	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. *Chemical Physics*, **2020**, 529, 110543	2.3	41
83	Computational understanding of the band alignment engineering in PbI2/PtS2 heterostructure: Effects of electric field and vertical strain. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 115, 113706	3	4
82	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
81	Understanding the electronic properties, contact types and optical performances in graphene/InN heterostructure: Role of electric gating. *Diamond and Related Materials*, **2020**, 106, 107851	3.5	7
80	Theoretical prediction of electronic and optical properties of haft-hydrogenated InN monolayers. *Superlattices and Microstructures*, **2020**, 142, 106519	2.8	4
79	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
78	Electronic and magnetic properties of single-layer boron phosphide associated with materials processing defects. *Computational Materials Science*, **2019**, 170, 109201	3.2	44
77	Structural, electronic, optical and elastic properties of XLa2S4 (X = Ba; Ca): Ab initio study. *Physica B: Condensed Matter*, **2019**, 558, 91-99	2.8	5
76	Tri-layered van der Waals heterostructures based on graphene, gallium selenide and molybdenum selenide. *Journal of Applied Physics*, **2019**, 125, 225304	2.5	10
75	Tuning the electronic properties of GaS monolayer by strain engineering and electric field. *Chemical Physics*, **2019**, 524, 101-105	2.3	6
74	Calculations within DFT framework of the electronic and optical properties of quaternary sulfide Tl2PbSiS4, a prospective optoelectronic semiconductor. *Computational Condensed Matter*, **2019**, 21, e00392	1.7	7

73	Electronic and optical properties of quaternary sulfide Tl2HgSnS4, a promising optoelectronic semiconductor: A combined experimental and theoretical study. *Optical Materials*, **2019**, 92, 294-302	3.3	6
72	Assessing optoelectronic properties of PbI2 monolayer under uniaxial strain from first principles calculations. *Superlattices and Microstructures*, **2019**, 130, 354-360	2.8	25
71	Electronic and optical properties of layered van der Waals heterostructure based on MS2 (M = Mo, W) monolayers. *Materials Research Express*, **2019**, 6, 065060	1.7	7
70	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	3	31
69	Electric field tunable electronic properties of P-ZnO and SiC-ZnO van der Waals heterostructures. *Computational Materials Science*, **2019**, 164, 166-170	3.2	20
68	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	3.3	23
67	Strain and electric field engineering of band alignment in InSe/Ca(OH)2 heterostructure. *Chemical Physics Letters*, **2019**, 732, 136649	2.5	5
66	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
65	Tunable electronic properties of InSe by biaxial strain: from bulk to single-layer. *Materials Research Express*, **2019**, 6, 115002	1.7	2
64	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. *Superlattices and Microstructures*, **2019**, 136, 106270	2.8	9
63	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
62	Rashba spin splitting and photocatalytic properties of GeCTMSSe (M=Mo, W) van der Waals heterostructures. *Physical Review B*, **2019**, 100,	3.3	92
61	Strain-Tunable Electronic and Optical Properties of Monolayer Germanium Monosulfide: Ab-Initio Study. *Journal of Electronic Materials*, **2019**, 48, 2902-2909	1.9	8
60	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	2.3	15
59	Structural properties and variable-range hopping conductivity of Cu2SnS3. *Materials Research Express*, **2019**, 6, 055915	1.7	4
58	Band alignment and optical features in Janus-MoSeTe/X(OH) (X = Ca, Mg) van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2019**, 21, 25849-25858	3.6	36
57	Tailoring the structural and electronic properties of an SnSe/MoS van der Waals heterostructure with an electric field and the insertion of a graphene sheet. *Physical Chemistry Chemical Physics*, **2019**, 21, 22140-22148	3.6	32
56	Schottky anomaly and Nl temperature treatment of possible perturbed hydrogenated AA-stacked graphene, SiC, and h-BN bilayers.. *RSC Advances*, **2019**, 9, 41569-41580	3.7	5

55	Electronic and optical properties of Janus ZrSSe by density functional theory.. *RSC Advances*, **2019**, 9, 41058-41065	3.7	45
54	Modulation of electronic properties of monolayer InSe through strain and external electric field. *Chemical Physics*, **2019**, 516, 213-217	2.3	14
53	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	2.5	30
52	Electronic band structure and basic optical constants of TlGaSn2Se6, a promising NLO semiconductor: First-principles calculations under DFT framework. *Optik*, **2019**, 181, 673-685	2.5	9
51	Electronic, Optical and Elastic Properties of Cu2CdGeSe4: A First-Principles Study. *Journal of Electronic Materials*, **2019**, 48, 705-715	1.9	10
50	Electronic properties and optical behaviors of bulk and monolayer ZrS2: A theoretical investigation. *Superlattices and Microstructures*, **2019**, 125, 205-213	2.8	15
49	Enhancement of monolayer SnSe light absorption by strain engineering: A DFT calculation. *Chemical Physics*, **2019**, 521, 5-13	2.3	34
48	Theoretical investigation of electronic structure and thermoelectric properties of MX2 (M=Zr, Hf; X=S, Se) van der Waals heterostructures. *Journal of Physics and Chemistry of Solids*, **2019**, 126, 304-309	3.9	19
47	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	5.7	45
46	Tuning the electronic properties and Schottky barrier height of the vertical graphene/MoS2 heterostructure by an electric gating. *Superlattices and Microstructures*, **2018**, 116, 79-87	2.8	32
45	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	4.4	23
44	Linear and nonlinear magneto-optical properties of monolayer MoS2. *Journal of Applied Physics*, **2018**, 123, 034301	2.5	16
43	First principles study of optical properties of molybdenum disulfide: From bulk to monolayer. *Superlattices and Microstructures*, **2018**, 115, 10-18	2.8	23
42	Electric-field tunable electronic properties and Schottky contact of graphene/phosphorene heterostructure. *Vacuum*, **2018**, 149, 231-237	3.7	31
41	Tuning the Electronic and Optical Properties of Two-Dimensional Graphene-like (hbox {C}_2hbox {N}) Nanosheet by Strain Engineering. *Journal of Electronic Materials*, **2018**, 47, 4594-4603	1.9	11
40	Electronic structure and optical properties of LiGa0.5In0.5Se2 single crystal, a nonlinear optical mid-IR material. *Optical Materials*, **2018**, 80, 12-21	3.3	8
39	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	5.7	40
38	First principle study on the electronic properties and Schottky contact of graphene adsorbed on MoS2 monolayer under applied out-plane strain. *Surface Science*, **2018**, 668, 23-28	1.8	31

37	Tuning the Electronic Properties, Effective Mass and Carrier Mobility of MoS2 Monolayer by Strain Engineering: First-Principle Calculations. *Journal of Electronic Materials*, **2018**, 47, 730-736	1.9	42
36	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	3.2	45
35	Electronic band-structure and optical constants of Pb2GeS4: Ab initio calculations and X-ray spectroscopy experiments. *Journal of Materials Science: Materials in Electronics*, **2018**, 29, 16088-16100	2.1	4
34	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	4.4	11
33	Ab-initio study of electronic and optical properties of biaxially deformed single-layer GeS. *Superlattices and Microstructures*, **2018**, 120, 501-507	2.8	17
32	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	3.6	76
31	Electronic structure and optical properties of defect chalcopyrite HgGa2Se4. *Optical Materials*, **2018**, 75, 538-546	3.3	6
30	Structural and electronic properties of a van der Waals heterostructure based on silicene and gallium selenide: effect of strain and electric field. *Physical Chemistry Chemical Physics*, **2018**, 20, 27856-27864	3.6	54
29	Layered graphene/GaS van der Waals heterostructure: Controlling the electronic properties and Schottky barrier by vertical strain. *Applied Physics Letters*, **2018**, 113, 171605	3.4	141
28	Electronic structure and basic optical constants of TlHgBr3: Density functional theory calculations. *Optical Materials*, **2018**, 86, 191-197	3.3	5
27	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	1.9	11
26	Effect of strains on electronic and optical properties of monolayer SnS: Ab-initio study. *Physica B: Condensed Matter*, **2018**, 545, 255-261	2.8	16
25	Linear and nonlinear magneto-optical properties of monolayer phosphorene. *Journal of Applied Physics*, **2017**, 121, 045107	2.5	33
24	Electronic structure and optical properties of noncentrosymmetric LiGaSe2: Experimental measurements and DFT band structure calculations. *Optical Materials*, **2017**, 66, 149-159	3.3	21
23	Linear and nonlinear magneto-optical absorption coefficients and refractive index changes in graphene. *Optical Materials*, **2017**, 69, 328-332	3.3	17
22	Out-of-plane strain and electric field tunable electronic properties and Schottky contact of graphene/antimonene heterostructure. *Superlattices and Microstructures*, **2017**, 112, 554-560	2.8	22
21	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	2.8	6
20	First-principles study of the structural and electronic properties of graphene/MoS2 interfaces. *Journal of Applied Physics*, **2017**, 122, 104301	2.5	43

19	Magneto-optical transport properties of monolayer MoS2 on polar substrates. *Physical Review B*, **2017**, 96,	3.3	61
18	Experimental and theoretical study of the electronic energy structure of phosphorus containing sulfides InPS4, Tl3PS4 and Sn2P2S6. *Journal of Structural Chemistry*, **2017**, 58, 1220-1225	0.9	3
17	Electronic structure and optical properties of noncentrosymmetric LiGaGe 2 Se 6 , a promising nonlinear optical material. *Physica B: Condensed Matter*, **2016**, 501, 74-83	2.8	21
16	Effect of oxygen adsorption on structural and electronic properties of defective surfaces (0 0 1), (1 1 1), and (1 1 0) TiC: Ab initio study. *Computational Materials Science*, **2016**, 124, 344-352	3.2	10
15	Specific features of the electronic structure and optical properties of KPb2Br5: DFT calculations and X-ray spectroscopy measurements. *Optical Materials*, **2016**, 53, 64-72	3.3	19
14	Electronic structure and optical properties of RbPb2Br5. *Journal of Physics and Chemistry of Solids*, **2016**, 91, 25-33	3.9	25
13	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	2.3	33
12	Band Gap Modulation of Bilayer MoS2 Under Strain Engineering and Electric Field: A Density Functional Theory. *Journal of Electronic Materials*, **2016**, 45, 4038-4043	1.9	13
11	Manifestation of Anomalous Weak Space-Charge-Density Acentricity for a TlHgBr Single Crystal. *Inorganic Chemistry*, **2016**, 55, 10547-10557	5.1	16
10	Electronic structure and optical properties of Cs2HgCl4: DFT calculations and X-ray photoelectron spectroscopy measurements. *Optical Materials*, **2016**, 60, 169-180	3.3	7
9	Quantum-mechanical calculations for the electron structure of phosphorus-containing sulfides Sn2P2S6 and Tl3PS4. *Bulletin of the Russian Academy of Sciences: Physics*, **2015**, 79, 802-806	0.4	1
8	Electronic structure and optical properties of Cu2CdGeS4: DFT calculations and X-ray spectroscopy measurements. *Optical Materials*, **2015**, 47, 435-444	3.3	22
7	Effect of electric field on the electronic and magnetic properties of a graphene nanoribbon/aluminium nitride bilayer system. *RSC Advances*, **2015**, 5, 49308-49316	3.7	25
6	Dispersion-Corrected Density Functional Theory Investigations of Structural and Electronic Properties of Bulk MoS2: Effect of Uniaxial Strain. *Nanoscale Research Letters*, **2015**, 10, 433	5	18
5	Electric field and substrate-induced modulation of spin-polarized transport in graphene nanoribbons on A3B5 semiconductors. *Journal of Applied Physics*, **2015**, 117, 174309	2.5	28
4	Single crystal growth, electronic structure and optical properties of Cs2HgBr4. *Journal of Physics and Chemistry of Solids*, **2015**, 85, 254-263	3.9	12
3	Electronic structure and optical properties of Cs2HgI4: Experimental study and band-structure DFT calculations. *Optical Materials*, **2015**, 42, 351-360	3.3	23
2	Ab initio calculations of Electronic, Magneto-Optical, and Transport Properties of the Ga1-2xSmxEuxN alloy (x = 0.0625) by GGA, GGA + U, and TB-mBj approximations. *Indian Journal of Physics*,1	1.4	

1 Ab initio Insight of the Electronic, Structural, Mechanical and Optical Properties of X(_3)P(_2) (X= Mg, Ca) from GGA and Hybrid Functional (HSE06). *Journal of Superconductivity and Novel Magnetism*,1 1.5