Nguyen N Hieu

List of Publications by Citations

213 papers	3,270 citations	32 h-index	44 g-index
226 ext. papers	4,390 ext. citations	3 avg, IF	6.19 L-index

#	Paper	IF	Citations
213	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
212	Rashba spin splitting and photocatalytic properties of GeCl2MSSe (M=Mo, W) van der Waals heterostructures. *Physical Review B*, **2019**, 100,	3.3	92
211	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
210	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
209	Magneto-optical transport properties of monolayer MoS2 on polar substrates. *Physical Review B*, **2017**, 96,	3.3	61
208	Electronic structure, optical and photocatalytic performance of SiC-MX (M = Mo, W and X = S, Se) van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2018**, 20, 24168-24175	3.6	60
207	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
206	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
205	Electronic and photocatalytic performance of boron phosphide-blue phosphorene vdW heterostructures. *Applied Surface Science*, **2020**, 523, 146483	6.7	47
204	Van der Waals heterostructures of P, BSe, and SiC monolayers. *Journal of Applied Physics*, **2019**, 125, 094301	2.5	45
203	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
202	Interlayer coupling and electric field controllable Schottky barriers and contact types in graphene/PbI2 heterostructures. *Physical Review B*, **2020**, 101,	3.3	45
201	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
200	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
199	Electronic and optical properties of Janus ZrSSe by density functional theory.. *RSC Advances*, **2019**, 9, 41058-41065	3.7	45
198	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
197	Magneto-optical transport properties of monolayer transition metal dichalcogenides. *Physical Review B*, **2020**, 101,	3.3	44

196	First-principles study of the structural and electronic properties of graphene/MoS2 interfaces. *Journal of Applied Physics*, **2017**, 122, 104301	2.5	43
195	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
194	Tunable optical and electronic properties of Janus monolayers Ga2SSe, Ga2STe, and Ga2SeTe as promising candidates for ultraviolet photodetectors applications. *Superlattices and Microstructures*, **2019**, 125, 1-7	2.8	41
193	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. *Chemical Physics*, **2020**, 529, 110543	2.3	41
192	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
191	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
190	Effective Photocatalytic Activity of Mixed Ni/Fe-Base Metal-Organic Framework under a Compact Fluorescent Daylight Lamp. *Catalysts*, **2018**, 8, 487	4	39
189	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
188	Enhancement of monolayer SnSe light absorption by strain engineering: A DFT calculation. *Chemical Physics*, **2019**, 521, 5-13	2.3	34
187	Linear and nonlinear magneto-optical properties of monolayer phosphorene. *Journal of Applied Physics*, **2017**, 121, 045107	2.5	33
186	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
185	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
184	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
183	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
182	Synergy of physical properties of low-dimensional carbon-based systems for nanoscale device design. *Materials Research Express*, **2019**, 6, 042002	1.7	32
181	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
180	Electric-field tunable electronic properties and Schottky contact of graphene/phosphorene heterostructure. *Vacuum*, **2018**, 149, 231-237	3.7	31
179	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

178	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
177	Electronic properties of WS2 and WSe2 monolayers with biaxial strain: A first-principles study. *Chemical Physics*, **2019**, 519, 69-73	2.3	30
176	Nonlinear optical absorption in parabolic quantum well via two-photon absorption process. *Optics Communications*, **2015**, 335, 37-41	2	28
175	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
174	Magneto-optical effect in GaAs/GaAlAs semi-parabolic quantum well. *Thin Solid Films*, **2019**, 682, 10-17	2.2	26
173	Magneto-optical properties of semi-parabolic plus semi-inverse squared quantum wells. *Physica B: Condensed Matter*, **2018**, 539, 117-122	2.8	26
172	Nonlinear optical absorption in graphene via two-photon absorption process. *Optics Communications*, **2015**, 344, 12-16	2	26
171	Electronic properties and enhanced photocatalytic performance of van der Waals heterostructures of ZnO and Janus transition metal dichalcogenides. *Physical Chemistry Chemical Physics*, **2020**, 22, 10351-10359	3.6	26
170	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
169	First principles study of optical properties of molybdenum disulfide: From bulk to monolayer. *Superlattices and Microstructures*, **2018**, 115, 10-18	2.8	23
168	Uniaxially deformed (5,5) carbon nanotube: Structural transitions. *Chemical Physics Letters*, **2008**, 464, 187-191	2.5	23
167	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
166	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
165	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
164	First principles study on the electronic properties and Schottky barrier of Graphene/InSe heterostructure. *Superlattices and Microstructures*, **2018**, 122, 570-576	2.8	21
163	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
162	LO-phonon-assisted cyclotron resonance in a special asymmetric hyperbolic-type quantum well. *Superlattices and Microstructures*, **2018**, 120, 738-746	2.8	20
161	A van der Waals heterostructure of MoS2/MoSi2N4: a first-principles study. *New Journal of Chemistry*, **2021**, 45, 8291-8296	3.6	20

160	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
159	Controlling electronic properties of PtS2/InSe van der Waals heterostructure via external electric field and vertical strain. *Chemical Physics Letters*, **2019**, 724, 1-7	2.5	18
158	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
157	Linear and nonlinear magneto-optical absorption coefficients and refractive index changes in graphene. *Optical Materials*, **2017**, 69, 328-332	3.3	17
156	Magneto-optical absorption in silicene and germanene induced by electric and Zeeman fields. *Physical Review B*, **2020**, 101,	3.3	17
155	Ab-initio study of electronic and optical properties of biaxially deformed single-layer GeS. *Superlattices and Microstructures*, **2018**, 120, 501-507	2.8	17
154	Interfacial Electronic Properties and Tunable Contact Types in Graphene/Janus MoGeSiN Heterostructures. *Journal of Physical Chemistry Letters*, **2021**, 12, 3934-3940	6.4	17
153	Linear and nonlinear magneto-optical properties of monolayer MoS2. *Journal of Applied Physics*, **2018**, 123, 034301	2.5	16
152	Structural phase transition and band gap of uniaxially deformed (6, 0) carbon nanotube. *Chemical Physics Letters*, **2012**, 545, 71-77	2.5	16
151	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
150	Prediction of two-dimensional bismuth-based chalcogenides Bi2X3(X = S, Se, Te) monolayers with orthorhombic structure: a first-principles study. *Journal Physics D: Applied Physics*, **2021**, 54, 395103	3	16
149	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
148	First principles study of the electronic properties and band gap modulation of two-dimensional phosphorene monolayer: Effect of strain engineering. *Superlattices and Microstructures*, **2018**, 118, 289-297	2.8	15
147	Point Defects in a Two-Dimensional ZnSnN2 Nanosheet: A First-Principles Study on the Electronic and Magnetic Properties. *Journal of Physical Chemistry C*, **2021**, 125, 13067-13075	3.8	15
146	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
145	Electronic properties and optical behaviors of bulk and monolayer ZrS2: A theoretical investigation. *Superlattices and Microstructures*, **2019**, 125, 205-213	2.8	15
144	Pyramidal core-shell quantum dot under applied electric and magnetic fields. *Scientific Reports*, **2020**, 10, 8961	4.9	14
143	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

142	Modulation of electronic properties of monolayer InSe through strain and external electric field. *Chemical Physics*, **2019**, 516, 213-217	2.3	14
141	Investigation of cyclotron-phonon resonance in monolayer molybdenum disulfide. *Journal of Physics and Chemistry of Solids*, **2019**, 125, 74-79	3.9	14
140	Strain effects on the electronic and optical properties of Van der Waals heterostructure MoS2/WS2: A first-principles study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 116, 113799	3	14
139	Surface modification of titanium carbide MXene monolayers (TiC and TiC) chalcogenide and halogenide atoms. *Physical Chemistry Chemical Physics*, **2021**, 23, 15319-15328	3.6	14
138	Tailoring electronic properties and Schottky barrier in sandwich heterostructure based on graphene and tungsten diselenide. *Diamond and Related Materials*, **2019**, 94, 129-136	3.5	13
137	Computational prediction of electronic and optical properties of Janus Ga2SeTe monolayer. *Journal Physics D: Applied Physics*, **2020**, 53, 455302	3	13
136	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
135	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
134	Phonon-assisted cyclotron resonance in P□chl-Teller quantum well. *Journal of Applied Physics*, **2019**, 126, 124301	2.5	12
133	Strain-induced electronic phase transition in phosphorene: A Green□ function study. *Chemical Physics*, **2019**, 522, 249-255	2.3	12
132	Modulation of the band structure in bilayer zigzag graphene nanoribbons on hexagonal boron nitride using the force and electric fields. *Materials Chemistry and Physics*, **2015**, 154, 78-83	4.4	12
131	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
130	First principles calculations of the geometric structures and electronic properties of van der Waals heterostructure based on graphene, hexagonal boron nitride and molybdenum diselenide. *Diamond and Related Materials*, **2018**, 88, 151-157	3.5	12
129	Magnetically operated nanorelay based on two single-walled carbon nanotubes filled with endofullerenes Fe@C20. *Journal of Nanophotonics*, **2010**, 4, 041675	1.1	12
128	Oxygenation of Janus group III monochalcogenides: First-principles insights into GaInXO (X=S, Se, Te) monolayers. *Physical Review B*, **2021**, 104,	3.3	12
127	One- and two-photon-induced cyclotron□phonon resonance in modified-P□chl□eller quantum well. *Applied Physics A: Materials Science and Processing*, **2019**, 125, 1	2.6	11
126	Electronic structure, optoelectronic properties and enhanced photocatalytic response of GaN-GeC van der Waals heterostructures: a first principles study.. *RSC Advances*, **2020**, 10, 24127-24133	3.7	11
125	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

124	First principles investigations of the influence of O-adsorption on the structural and electronic properties of TiC(111) surfaces with vacancies. *Surface Science*, **2016**, 649, 20-26	1.8	11
123	Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study. *Superlattices and Microstructures*, **2020**, 137, 106320	2.8	11
122	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
121	Hexagonal boron nitride (h-BN) nanosheet as a potential hydrogen adsorption material: A density functional theory (DFT) study. *Surfaces and Interfaces*, **2021**, 24, 101043	4.1	11
120	Refractive index changes and optical absorption involving 1s1p excitonic transitions in quantum dot under pressure and temperature effects. *Applied Physics A: Materials Science and Processing*, **2019**, 125, 1	2.6	11
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117	Tuning the electronic properties of armchair graphene nanoribbons by strain engineering. *Physica Scripta*, **2015**, 90, 015802	2.6	10
116	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties.. *RSC Advances*, **2020**, 10, 10731-10739	3.7	10
115	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
114	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
113	Linear and nonlinear magneto-optical absorption in parabolic quantum well. *Optik*, **2016**, 127, 10519-10526	2.5	10
112	Electronic properties of GaSe/MoS2 and GaS/MoSe2 heterojunctions from first principles calculations. *AIP Advances*, **2018**, 8, 075207	1.5	10
111	Band gap and electronic properties of molybdenum disulphide under strain engineering: density functional theory calculations. *Molecular Simulation*, **2017**, 43, 86-91	2	10
110	Electronic, Optical and Elastic Properties of Cu2CdGeSe4: A First-Principles Study. *Journal of Electronic Materials*, **2019**, 48, 705-715	1.9	10
109	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
108	First-principles study of the structural and electronic properties of graphene absorbed on MnO(111) surfaces. *Computational and Theoretical Chemistry*, **2016**, 1098, 22-30	2	9
107	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. *Superlattices and Microstructures*, **2019**, 136, 106270	2.8	9

106	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
105	First principles study of structural, optoelectronic and photocatalytic properties of SnS, SnSe monolayers and their van der Waals heterostructure. *Chemical Physics*, **2020**, 539, 110939	2.3	9
104	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
103	Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	9
102	Phonon-assisted cyclotron resonance in special symmetric quantum wells. *Applied Physics A: Materials Science and Processing*, **2018**, 124, 1	2.6	9
101	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
100	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. *Materials Research Express*, **2020**, 7, 015013	1.7	8
99	Induced magnetic states upon electron–hole injection at B and N sites of hexagonal boron nitride bilayer: A density functional theory study. *International Journal of Quantum Chemistry*, **2021**, 121, e26680	2.1	8
98	Strain-Tunable Electronic and Optical Properties of Monolayer Germanium Monosulfide: Ab-Initio Study. *Journal of Electronic Materials*, **2019**, 48, 2902-2909	1.9	8
97	Fundamental exciton transitions in SiO2/Si/SiO2 cylindrical core/shell quantum dot. *Journal of Applied Physics*, **2018**, 124, 144303	2.5	8
96	Excitonic nonlinear optical properties in AlN/GaN spherical core/shell quantum dots under pressure. *MRS Communications*, **2019**, 9, 663-669	2.7	7
95	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
94	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
93	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
92	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
91	Band structure of deformed armchair nanoribbon with bond alternation. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 60, 91-94	3	7
90	Effect of Peierls transition in armchair carbon nanotube on dynamical behaviour of encapsulated fullerene. *Nanoscale Research Letters*, **2011**, 6, 216	5	7
89	Electronic energy band structure of uniaxially deformed (5,5) armchair carbon nanotube. *Molecular Simulation*, **2009**, 35, 681-684	2	7

88	Band-gap engineering, magnetic behavior and Dirac-semimetal character in the MoSi2N4 nanoribbon with armchair and zigzag edges. *Journal Physics D: Applied Physics*, **2022**, 55, 035301	3	7
87	Electronic and photocatalytic properties of two-dimensional boron phosphide/SiC van der Waals heterostructure with direct type-II band alignment: a first principles study.. *RSC Advances*, **2020**, 10, 32027-32033	3.7	7
86	Type-I band alignment of BX-ZnO (X = As, P) van der Waals heterostructures as high-efficiency water splitting photocatalysts: a first-principles study.. *RSC Advances*, **2020**, 10, 44545-44550	3.7	7
85	Linear magneto-electron-light interaction in ultranarrow armchair graphene and boronitrene nanoribbons. *Diamond and Related Materials*, **2019**, 92, 86-91	3.5	7
84	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
83	Tuning the electronic properties of GaS monolayer by strain engineering and electric field. *Chemical Physics*, **2019**, 524, 101-105	2.3	6
82	Linear and nonlinear magneto-optical absorption in a triangular quantum well. *International Journal of Modern Physics B*, **2018**, 32, 1850162	1.1	6
81	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
80	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
79	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 117, 113857	3	6
78	Defect-Induced Gas-Sensing Properties of a Flexible SnS Sensor under UV Illumination at Room Temperature. *Sensors*, **2020**, 20,	3.8	6
77	Exciton states in conical quantum dots under applied electric and magnetic fields. *Optics and Laser Technology*, **2021**, 139, 106953	4.2	6
76	First-principles study of W, N, and O adsorption on TiB2(0001) surface with disordered vacancies. *Superlattices and Microstructures*, **2018**, 123, 414-426	2.8	6
75	Strain and electric field engineering of band alignment in InSe/Ca(OH)2 heterostructure. *Chemical Physics Letters*, **2019**, 732, 136649	2.5	5
74	Modified tailoring the electronic phase and emergence of midstates in impurity-imbrued armchair graphene nanoribbons. *Scientific Reports*, **2019**, 9, 10651	4.9	5
73	Interwall conductance in double-walled armchair carbon nanotubes. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 5706-5711	2.3	5
72	Electronic structures, and optical and photocatalytic properties of the BP**B**Se van der Waals heterostructures. *New Journal of Chemistry*, **2020**, 44, 14964-14969	3.6	5
71	Nonlinear magneto-optical absorption in a finite semi-parabolic quantum well. *Optical and Quantum Electronics*, **2021**, 53, 1	2.4	5

70	Oscillations of the electron energy loss rate in two-dimensional transition-metal dichalcogenides in the presence of a quantizing magnetic field. *Physical Review B*, **2021**, 103,	3.3	5
69	Schottky anomaly and Nēl temperature treatment of possible perturbed hydrogenated AA-stacked graphene, SiC, and h-BN bilayers.. *RSC Advances*, **2019**, 9, 41569-41580	3.7	5
68	Two-Dimensional Metal/Semiconductor Contact in a Janus MoSH/MoSiN van der Waals Heterostructure.. *Journal of Physical Chemistry Letters*, **2022**, 2576-2582	6.4	5
67	Strain engineering and electric field tunable electronic properties of Ti2CO2 MXene monolayer. *Materials Research Express*, **2019**, 6, 065910	1.7	4
66	Quantum Chemical Calculation of Reactions Involving C20, C60, Graphene and H2O. *International Journal of Nanoscience*, **2019**, 18, 1940008	0.6	4
65	Substrate-induced band structure and electronic properties in graphene/Al2O3(0001) interface. *Surface Science*, **2015**, 632, 111-117	1.8	4
64	Modulation of electronic and optical properties of GaTe monolayer by biaxial strain and electric field. *Superlattices and Microstructures*, **2020**, 140, 106435	2.8	4
63	First-principles study of electronic properties of AB-stacked bilayer armchair graphene nanoribbons under out-plane strain. *Indian Journal of Physics*, **2018**, 92, 447-452	1.4	4
62	Enhanced anisotropic electrical conductivity of perturbed monolayer Ēborophene. *Physical Chemistry Chemical Physics*, **2019**, 22, 286-294	3.6	4
61	Strain engineering of the electro-optical and photocatalytic properties of single-layered Janus MoSSe: First principles calculations. *Optik*, **2020**, 224, 165503	2.5	4
60	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
59	Opening a band gap in graphene by C□C bond alternation: a tight binding approach. *Materials Research Express*, **2019**, 6, 045605	1.7	4
58	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
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56	Study of the Elastic Properties of the Energetic Molecular Crystals Using Density Functionals with van der Waals Corrections. *ACS Omega*, **2021**, 6, 642-648	3.9	4
55	Computational insights into structural, electronic, and optical properties of Janus GeSO monolayer.. *RSC Advances*, **2021**, 11, 28381-28387	3.7	4
54	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
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