

Nguyen N Hieu

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Tunable type-II band alignment and electronic structure of C ₃ N ₄ /MoSi ₂ N ₄ heterostructure: Interlayer coupling and electric field. <i>Physical Review B</i> , 2022 , 105,	3.3	9
212	Structural, electronic, and transport properties of quintuple atomic Janus monolayers Ga ₂ SX ₂ (X= O, S, Se, Te): First-principles predictions. <i>Physical Review B</i> , 2022 , 105,	3.3	6
211	Band-gap engineering, magnetic behavior and Dirac-semimetal character in the MoSi ₂ N ₄ nanoribbon with armchair and zigzag edges. <i>Journal Physics D: Applied Physics</i> , 2022 , 55, 035301	3	7
210	Novel Janus GaInX (X = S, Se, Te) single-layers: first-principles prediction on structural, electronic, and transport properties.. <i>RSC Advances</i> , 2022 , 12, 7973-7979	3.7	0
209	Thermoelectric properties of doped graphene nanoribbons: density functional theory calculations and electrical transport.. <i>RSC Advances</i> , 2022 , 12, 6174-6180	3.7	0
208	Two-Dimensional Metal/Semiconductor Contact in a Janus MoSH/MoSiN van der Waals Heterostructure.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 2576-2582	6.4	5
207	Study of electronic and mechanical properties of single walled Carbon nanotube (SWCNT) via substitutional Boron doping in zigzag and armchair pattern. <i>Surfaces and Interfaces</i> , 2022 , 29, 101815	4.1	3
206	Two-dimensional XY monolayers (X = Al, Ga, In; Y = N, P, As) with a double layer hexagonal structure: A first-principles perspective. <i>Applied Surface Science</i> , 2022 , 590, 152998	6.7	3
205	Intriguing interfacial characteristics of the CS contact with MX (M = Mo, W; X = S, Se, Te) and MXY ((X Y) = S, Se, Te) monolayers.. <i>RSC Advances</i> , 2022 , 12, 12292-12302	3.7	0
204	Theoretical prediction of Janus PdXO (X = S, Se, Te) monolayers: structural, electronic, and transport properties.. <i>RSC Advances</i> , 2022 , 12, 12971-12977	3.7	0
203	First-principles insights onto structural, electronic and optical properties of Janus monolayers CrXO (X = S, Se, Te).. <i>RSC Advances</i> , 2021 , 11, 39672-39679	3.7	0
202	Two-dimensional Dirac half-metal in porous carbon nitride CNmonolayer via atomic doping. <i>Nanotechnology</i> , 2021 , 33,	3.4	3
201	Electric gating and interlayer coupling controllable electronic structure and Schottky contact of graphene/Bil ₃ van der Waals heterostructure. <i>Physical Review B</i> , 2021 , 103,	3.3	13
200	Effects of La and Ce doping on electronic structure and optical properties of janus MoSSe monolayer. <i>Superlattices and Microstructures</i> , 2021 , 151, 106841	2.8	1
199	Computational study on strain and electric field tunable electronic and optical properties of InTe monolayer. <i>Superlattices and Microstructures</i> , 2021 , 151, 106816	2.8	0
198	Nonlinear magneto-optical absorption in a finite semi-parabolic quantum well. <i>Optical and Quantum Electronics</i> , 2021 , 53, 1	2.4	5
197	Interfacial Electronic Properties and Tunable Contact Types in Graphene/Janus MoGeSiN Heterostructures. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 3934-3940	6.4	17

196	Induced magnetic states upon electron-hole injection at B and N sites of hexagonal boron nitride bilayer: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26680	2.1	8
195	Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	9
194	Two-Dimensional Boron Phosphide/MoGeN van der Waals Heterostructure: A Promising Tunable Optoelectronic Material. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 5076-5084	6.4	21
193	Oscillations of the electron energy loss rate in two-dimensional transition-metal dichalcogenides in the presence of a quantizing magnetic field. <i>Physical Review B</i> , 2021 , 103,	3.3	5
192	Hexagonal boron nitride (h-BN) nanosheet as a potential hydrogen adsorption material: A density functional theory (DFT) study. <i>Surfaces and Interfaces</i> , 2021 , 24, 101043	4.1	11
191	Point Defects in a Two-Dimensional ZnSnN ₂ Nanosheet: A First-Principles Study on the Electronic and Magnetic Properties. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13067-13075	3.8	15
190	Exciton states in conical quantum dots under applied electric and magnetic fields. <i>Optics and Laser Technology</i> , 2021 , 139, 106953	4.2	6
189	Ab initio study of the structural, electronic, optical and elastic properties of promising optoelectronic and thermoelectric compounds MgSc ₂ X ₄ (X = S; Se). <i>Journal of Solid State Chemistry</i> , 2021 , 293, 121763	3.3	2
188	Exchange field effects on the electronic properties of heterostructured ferromagnetic/topological crystalline insulator. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 126, 114441	3	1
187	Study of the Elastic Properties of the Energetic Molecular Crystals Using Density Functionals with van der Waals Corrections. <i>ACS Omega</i> , 2021 , 6, 642-648	3.9	4
186	Computational insights into structural, electronic, and optical properties of Janus GeSO monolayer.. <i>RSC Advances</i> , 2021 , 11, 28381-28387	3.7	4
185	Structural, elastic, and electronic properties of chemically functionalized boron phosphide monolayer.. <i>RSC Advances</i> , 2021 , 11, 8552-8558	3.7	3
184	Stacking effects in van der Waals heterostructures of blueP and Janus XYO (X = Ti, Zr, Hf; Y = S, Se) monolayers.. <i>RSC Advances</i> , 2021 , 11, 12189-12199	3.7	4
183	Outstanding elastic, electronic, transport and optical properties of a novel layered material CF: first-principles study.. <i>RSC Advances</i> , 2021 , 11, 23280-23287	3.7	3
182	A van der Waals heterostructure of MoS ₂ /MoSi ₂ N ₄ : a first-principles study. <i>New Journal of Chemistry</i> , 2021 , 45, 8291-8296	3.6	20
181	Surface modification of titanium carbide MXene monolayers (TiC and TiC) chalcogenide and halogenide atoms. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 15319-15328	3.6	14
180	Relativistic electric potential near a resting straight carbon nanotube of a finite-length with stationary current. <i>Journal of the Belarusian State University Physics</i> , 2021 , 20-25	0.3	1
179	Theoretical prediction of electronic, transport, optical, and thermoelectric properties of Janus monolayers In ₂ XO (X=S,Se,Te). <i>Physical Review B</i> , 2021 , 103,	3.3	39

178	Electronic structure of vertically coupled quantum dot-ring heterostructures under applied electromagnetic probes. A finite-element approach. <i>Scientific Reports</i> , 2021 , 11, 4015	4.9	3
177	Prediction of two-dimensional bismuth-based chalcogenides Bi ₂ X ₃ (X = S, Se, Te) monolayers with orthorhombic structure: a first-principles study. <i>Journal Physics D: Applied Physics</i> , 2021 , 54, 395103	3	16
176	Theoretical insights into tunable electronic and optical properties of Janus Al ₂ SSe monolayer through strain and electric field. <i>Optik</i> , 2021 , 238, 166761	2.5	2
175	Quantum magnetotransport properties of silicene: Influence of the acoustic phonon correction. <i>Physical Review B</i> , 2021 , 104,	3.3	1
174	Oxygenation of Janus group III monochalcogenides: First-principles insights into GaInXO (X=S, Se, Te) monolayers. <i>Physical Review B</i> , 2021 , 104,	3.3	12
173	A theoretical study on elastic, electronic, transport, optical and thermoelectric properties of Janus SnSO monolayer. <i>Journal Physics D: Applied Physics</i> , 2021 , 54, 475306	3	3
172	Anisotropy of effective masses induced by strain in Janus MoSSe and WSSe monolayers. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 134, 114826	3	2
171	First-principles calculations to investigate electronic properties of ZnO/PtSSe van der Waals heterostructure: Effects of vertical strain and electric field. <i>Chemical Physics</i> , 2021 , 551, 111333	2.3	1
170	Electronic and optical properties of a Janus SnSSe monolayer: effects of strain and electric field. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 11637-11643	3.6	33
169	Magneto-optical absorption in silicene and germanene induced by electric and Zeeman fields. <i>Physical Review B</i> , 2020 , 101,	3.3	17
168	Graphene hetero-multilayer on layered platinum mineral jacutingaitite (Pt ₂ HgSe ₃): van der Waals heterostructures with novel optoelectronic and thermoelectric performances. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 13248-13260	13	44
167	First-principles investigation of nonmetal doped single-layer BiOBr as a potential photocatalyst with a low recombination rate. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15354-15364	3.6	45
166	Intra- and inter-band magneto-optical absorption in monolayer WS ₂ . <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 124, 114315	3	0
165	Pyramidal core-shell quantum dot under applied electric and magnetic fields. <i>Scientific Reports</i> , 2020 , 10, 8961	4.9	14
164	Interlayer coupling and electric field controllable Schottky barriers and contact types in graphene/PbI ₂ heterostructures. <i>Physical Review B</i> , 2020 , 101,	3.3	45
163	Low-energy bands and optical properties of monolayer WS ₂ . <i>Optik</i> , 2020 , 209, 164581	2.5	2
162	First-principles prediction of chemically functionalized InN monolayers: electronic and optical properties.. <i>RSC Advances</i> , 2020 , 10, 10731-10739	3.7	10
161	Effects of electric field and strain engineering on the electronic properties, band alignment and enhanced optical properties of ZnO/Janus ZrSSe heterostructures.. <i>RSC Advances</i> , 2020 , 10, 9824-9832	3.7	9

160	Effects of different surface functionalization on the electronic properties and contact types of graphene/functionalized-GeC van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 7952-7961	3.6	15
159	Electronic structure, optoelectronic properties and enhanced photocatalytic response of GaN-GeC van der Waals heterostructures: a first principles study.. <i>RSC Advances</i> , 2020 , 10, 24127-24133	3.7	11
158	Electronic and optoelectronic properties of van der Waals heterostructure based on graphene-like GaN, blue phosphorene, SiC, and ZnO: A first principles study. <i>Journal of Applied Physics</i> , 2020 , 127, 245302	3.5	7
157	Computational prediction of electronic and optical properties of Janus Ga ₂ SeTe monolayer. <i>Journal Physics D: Applied Physics</i> , 2020 , 53, 455302	3	13
156	Stacking and electric field effects on the band alignment and electronic properties of the GeC/GaSe heterostructure. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 120, 114050	3	7
155	The characteristics of defective ZrS ₂ monolayers adsorbed various gases on S-vacancies: A first-principles study. <i>Superlattices and Microstructures</i> , 2020 , 140, 106454	2.8	12
154	Electronic structure and optical performance of PbI ₂ /SnSe ₂ heterostructure. <i>Chemical Physics</i> , 2020 , 533, 110736	2.3	2
153	Modulation of electronic and optical properties of GaTe monolayer by biaxial strain and electric field. <i>Superlattices and Microstructures</i> , 2020 , 140, 106435	2.8	4
152	Half-metallicity and magnetism in BAs monolayer induced by anchoring 3d transition metals (TM = V, Cr and Mn). <i>Superlattices and Microstructures</i> , 2020 , 139, 106399	2.8	10
151	Computational insights into structural, electronic and optical characteristics of GeC/CN van der Waals heterostructures: effects of strain engineering and electric field.. <i>RSC Advances</i> , 2020 , 10, 2967-2974	3.7	7
150	Magneto-optical transport properties of monolayer transition metal dichalcogenides. <i>Physical Review B</i> , 2020 , 101,	3.3	44
149	Stark and Zeeman effects on the topological phase and transport properties of topological crystalline insulator thin films. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 12129-12139	3.6	
148	Electronic and photocatalytic performance of boron phosphide-blue phosphorene vdW heterostructures. <i>Applied Surface Science</i> , 2020 , 523, 146483	6.7	47
147	A comprehensive investigation on electronic structure, optical and thermoelectric properties of the HfSSe Janus monolayer. <i>Journal of Physics and Chemistry of Solids</i> , 2020 , 144, 109490	3.9	14
146	Effects of charged impurity scattering and substrate on the magneto-optical absorption properties in gapped monolayer graphene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 121, 114149	3	19
145	The geometry of a bilayer nanoscroll rolled from zigzag nanoribbons of graphene and boron nitride. <i>Proceedings of the National Academy of Sciences of Belarus Physics and Mathematics Series</i> , 2020 , 56, 411-418	0.2	1
144	Magneto-optical absorption in Pöschl-Teller-like quantum well. <i>Physica B: Condensed Matter</i> , 2020 , 592, 412279	2.8	3
143	Power loss of hot Dirac fermions in silicene and its near equivalence with graphene. <i>Semiconductor Science and Technology</i> , 2020 , 36, 025005	1.8	3

142	Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study. <i>Superlattices and Microstructures</i> , 2020 , 137, 106320	2.8	11
141	Tuning the electronic, photocatalytic and optical properties of hydrogenated InN monolayer by biaxial strain and electric field. <i>Chemical Physics</i> , 2020 , 532, 110677	2.3	8
140	Graphene/WSeTe van der Waals heterostructure: Controllable electronic properties and Schottky barrier via interlayer coupling and electric field. <i>Applied Surface Science</i> , 2020 , 507, 145036	6.7	92
139	Structural and electronic properties of chemically functionalized SnC monolayer: a first principles study. <i>Materials Research Express</i> , 2020 , 7, 015013	1.7	8
138	Electronic, optical and photocatalytic properties of fully hydrogenated GeC monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 117, 113857	3	6
137	Defect-Induced Gas-Sensing Properties of a Flexible SnS Sensor under UV Illumination at Room Temperature. <i>Sensors</i> , 2020 , 20,	3.8	6
136	Janus monolayer PtSSe under external electric field and strain: A first principles study on electronic structure and optical properties. <i>Superlattices and Microstructures</i> , 2020 , 147, 106683	2.8	39
135	Strain engineering of the electro-optical and photocatalytic properties of single-layered Janus MoSSe: First principles calculations. <i>Optik</i> , 2020 , 224, 165503	2.5	4
134	Electronic structure and band alignment of Blue Phosphorene/Janus ZrSSe heterostructure: A first principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 124, 114369	3	1
133	Quantum Chemical Calculations of Carbon Nanoscroll Energy Rolled from Zigzag Graphene Nanoribbon. <i>Semiconductors</i> , 2020 , 54, 1678-1681	0.7	2
132	Structural, electronic and optical properties of pristine and functionalized MgO monolayers: a first principles study.. <i>RSC Advances</i> , 2020 , 10, 40411-40420	3.7	3
131	Interfacial characteristics, Schottky contact, and optical performance of a graphene/Ga2SSe van der Waals heterostructure: Strain engineering and electric field tunability. <i>Physical Review B</i> , 2020 , 102,	3.3	55
130	Electronic structures, and optical and photocatalytic properties of the BPBSe van der Waals heterostructures. <i>New Journal of Chemistry</i> , 2020 , 44, 14964-14969	3.6	5
129	Low-energy bands, optical properties, and spin/valley-Hall conductivity of silicene and germanene. <i>Journal of Materials Science</i> , 2020 , 55, 14848-14857	4.3	4
128	First principles study of structural, optoelectronic and photocatalytic properties of SnS, SnSe monolayers and their van der Waals heterostructure. <i>Chemical Physics</i> , 2020 , 539, 110939	2.3	9
127	Janus Ga2STe monolayer under strain and electric field: Theoretical prediction of electronic and optical properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 124, 114358	3	9
126	Investigation of strain and doping on the electronic properties of single layers of CN and CN: a first principles study.. <i>RSC Advances</i> , 2020 , 10, 27743-27751	3.7	23
125	Electronic and photocatalytic properties of two-dimensional boron phosphide/SiC van der Waals heterostructure with direct type-II band alignment: a first principles study.. <i>RSC Advances</i> , 2020 , 10, 32027-32033	3.7	23

124	van der Waals heterostructures based on MS ₂ Se (M = Mo, W) and graphene-like GaN: enhanced optoelectronic and photocatalytic properties for water splitting. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 20704-20711	3.6	11
123	Type-I band alignment of BX-ZnO (X = As, P) van der Waals heterostructures as high-efficiency water splitting photocatalysts: a first-principles study.. <i>RSC Advances</i> , 2020 , 10, 44545-44550	3.7	7
122	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. <i>Chemical Physics</i> , 2020 , 529, 110543	2.3	41
121	Computational understanding of the band alignment engineering in PbI ₂ /PtS ₂ heterostructure: Effects of electric field and vertical strain. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 115, 113706	3	4
120	Strain effects on the electronic and optical properties of Van der Waals heterostructure MoS ₂ /WS ₂ : A first-principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 116, 113799	3	14
119	Electronic properties and enhanced photocatalytic performance of van der Waals heterostructures of ZnO and Janus transition metal dichalcogenides. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10351-10359 ²⁶	3.6	26
118	Understanding the electronic properties, contact types and optical performances in graphene/InN heterostructure: Role of electric gating. <i>Diamond and Related Materials</i> , 2020 , 106, 107851	3.5	7
117	Theoretical prediction of electronic and optical properties of haft-hydrogenated InN monolayers. <i>Superlattices and Microstructures</i> , 2020 , 142, 106519	2.8	4
116	Phonon-assisted cyclotron resonance in Pöschl-Teller quantum well. <i>Journal of Applied Physics</i> , 2019 , 126, 124301	2.5	12
115	One- and two-photon-induced cyclotron-phonon resonance in modified-Pöschl-Teller quantum well. <i>Applied Physics A: Materials Science and Processing</i> , 2019 , 125, 1	2.6	11
114	Tri-layered van der Waals heterostructures based on graphene, gallium selenide and molybdenum selenide. <i>Journal of Applied Physics</i> , 2019 , 125, 225304	2.5	10
113	Cyclotron-phonon resonance line-width in monolayer silicene. <i>Superlattices and Microstructures</i> , 2019 , 131, 117-123	2.8	2
112	Coulomb Green's functions in the problem of photodetachment of the negatively charged hydrogen ion. <i>European Physical Journal D</i> , 2019 , 73, 1	1.3	
111	Two-photon induced magneto-optical absorption in finite semi-parabolic quantum wells. <i>Superlattices and Microstructures</i> , 2019 , 130, 446-453	2.8	
110	Tuning the electronic properties of GaS monolayer by strain engineering and electric field. <i>Chemical Physics</i> , 2019 , 524, 101-105	2.3	6
109	Excitonic nonlinear optical properties in AlN/GaN spherical core/shell quantum dots under pressure. <i>MRS Communications</i> , 2019 , 9, 663-669	2.7	7
108	Magneto-optical effect in GaAs/GaAlAs semi-parabolic quantum well. <i>Thin Solid Films</i> , 2019 , 682, 10-17	2.2	26
107	Tailoring electronic properties and Schottky barrier in sandwich heterostructure based on graphene and tungsten diselenide. <i>Diamond and Related Materials</i> , 2019 , 94, 129-136	3.5	13

106	Strain engineering and electric field tunable electronic properties of Ti ₂ CO ₂ MXene monolayer. <i>Materials Research Express</i> , 2019 , 6, 065910	1.7	4
105	Van der Waals heterostructures of P, BSe, and SiC monolayers. <i>Journal of Applied Physics</i> , 2019 , 125, 094301	2.5	45
104	Strain-induced electronic phase transition in phosphorene: A Green's function study. <i>Chemical Physics</i> , 2019 , 522, 249-255	2.3	12
103	Electronic and optical properties of layered van der Waals heterostructure based on MS ₂ (M = Mo, W) monolayers. <i>Materials Research Express</i> , 2019 , 6, 065060	1.7	7
102	First principles study of single-layer SnSe ₂ under biaxial strain and electric field: Modulation of electronic properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019 , 111, 201-205	3	31
101	Electric field tunable electronic properties of P-ZnO and SiC-ZnO van der Waals heterostructures. <i>Computational Materials Science</i> , 2019 , 164, 166-170	3.2	20
100	Controlling electronic properties of PtS ₂ /InSe van der Waals heterostructure via external electric field and vertical strain. <i>Chemical Physics Letters</i> , 2019 , 724, 1-7	2.5	18
99	Quantum Chemical Calculation of Reactions Involving C ₂₀ , C ₆₀ , Graphene and H ₂ O. <i>International Journal of Nanoscience</i> , 2019 , 18, 1940008	0.6	4
98	Strain and electric field engineering of band alignment in InSe/Ca(OH) ₂ heterostructure. <i>Chemical Physics Letters</i> , 2019 , 732, 136649	2.5	5
97	Strain and electric field engineering of electronic structures and Schottky contact of layered graphene/Ca(OH) ₂ heterostructure. <i>Superlattices and Microstructures</i> , 2019 , 133, 106185	2.8	3
96	Electric field tuning of dynamical dielectric function in phosphorene. <i>Chemical Physics Letters</i> , 2019 , 731, 136606	2.5	1
95	Computational understanding of electronic properties of graphene/PtS ₂ heterostructure under electric field. <i>Applied Physics A: Materials Science and Processing</i> , 2019 , 125, 1	2.6	3
94	Modified tailoring the electronic phase and emergence of midstates in impurity-imbrued armchair graphene nanoribbons. <i>Scientific Reports</i> , 2019 , 9, 10651	4.9	5
93	Tunable electronic properties of InSe by biaxial strain: from bulk to single-layer. <i>Materials Research Express</i> , 2019 , 6, 115002	1.7	2
92	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. <i>Superlattices and Microstructures</i> , 2019 , 136, 106270	2.8	9
91	Rashba spin splitting and photocatalytic properties of GeMSSe (M=Mo, W) van der Waals heterostructures. <i>Physical Review B</i> , 2019 , 100,	3.3	92
90	Enhanced anisotropic electrical conductivity of perturbed monolayer Eborophene. <i>Physical Chemistry Chemical Physics</i> , 2019 , 22, 286-294	3.6	4
89	Strain-Tunable Electronic and Optical Properties of Monolayer Germanium Monosulfide: Ab-Initio Study. <i>Journal of Electronic Materials</i> , 2019 , 48, 2902-2909	1.9	8

88	Strain and electric field tunable electronic properties of type-II band alignment in van der Waals GaSe/MoSe ₂ heterostructure. <i>Chemical Physics</i> , 2019 , 521, 92-99	2.3	15
87	Band alignment and optical features in Janus-MoSeTe/X(OH) (X = Ca, Mg) van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 25849-25858	3.6	36
86	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. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22140-22148	3.6	32
85	Schottky anomaly and NBE temperature treatment of possible perturbed hydrogenated AA-stacked graphene, SiC, and h-BN bilayers.. <i>RSC Advances</i> , 2019 , 9, 41569-41580	3.7	5
84	Electronic and optical properties of Janus ZrSSe by density functional theory.. <i>RSC Advances</i> , 2019 , 9, 41058-41065	3.7	45
83	Modulation of electronic properties of monolayer InSe through strain and external electric field. <i>Chemical Physics</i> , 2019 , 516, 213-217	2.3	14
82	Nonlinear optical absorption and cyclotron impurity resonance in monolayer silicene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019 , 105, 168-173	3	
81	Vertical strain and electric field tunable electronic properties of type-II band alignment C ₂ N/InSe van der Waals heterostructure. <i>Chemical Physics Letters</i> , 2019 , 716, 155-161	2.5	30
80	Opening a band gap in graphene by C-C bond alternation: a tight binding approach. <i>Materials Research Express</i> , 2019 , 6, 045605	1.7	4
79	Electronic properties of WS ₂ and WSe ₂ monolayers with biaxial strain: A first-principles study. <i>Chemical Physics</i> , 2019 , 519, 69-73	2.3	30
78	Linear magneto-electron-light interaction in ultranarrow armchair graphene and boronitrene nanoribbons. <i>Diamond and Related Materials</i> , 2019 , 92, 86-91	3.5	7
77	Synergy of physical properties of low-dimensional carbon-based systems for nanoscale device design. <i>Materials Research Express</i> , 2019 , 6, 042002	1.7	32
76	Electronic, Optical and Elastic Properties of Cu ₂ CdGeSe ₄ : A First-Principles Study. <i>Journal of Electronic Materials</i> , 2019 , 48, 705-715	1.9	10
75	Modulation of electronic properties and Schottky barrier in the graphene/GaS heterostructure by electric gating. <i>Physica B: Condensed Matter</i> , 2019 , 555, 69-73	2.8	0
74	Electronic properties and optical behaviors of bulk and monolayer ZrS ₂ : A theoretical investigation. <i>Superlattices and Microstructures</i> , 2019 , 125, 205-213	2.8	15
73	Enhancement of monolayer SnSe light absorption by strain engineering: A DFT calculation. <i>Chemical Physics</i> , 2019 , 521, 5-13	2.3	34
72	Tunable optical and electronic properties of Janus monolayers Ga ₂ SSe, Ga ₂ STe, and Ga ₂ SeTe as promising candidates for ultraviolet photodetectors applications. <i>Superlattices and Microstructures</i> , 2019 , 125, 1-7	2.8	41
71	Refractive index changes and optical absorption involving 1s _{np} excitonic transitions in quantum dot under pressure and temperature effects. <i>Applied Physics A: Materials Science and Processing</i> , 2019 , 125, 1	2.6	11

70	Theoretical investigation of electronic structure and thermoelectric properties of MX ₂ (M=Zr, Hf; X=S, Se) van der Waals heterostructures. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 126, 304-309	3.9	19
69	Investigation of cyclotron-phonon resonance in monolayer molybdenum disulfide. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 125, 74-79	3.9	14
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62	Linear and nonlinear magneto-optical properties of monolayer MoS ₂ . <i>Journal of Applied Physics</i> , 2018 , 123, 034301	2.5	16
61	First principles study of optical properties of molybdenum disulfide: From bulk to monolayer. <i>Superlattices and Microstructures</i> , 2018 , 115, 10-18	2.8	23
60	Electric-field tunable electronic properties and Schottky contact of graphene/phosphorene heterostructure. <i>Vacuum</i> , 2018 , 149, 231-237	3.7	31
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55	First principles study of the electronic properties and Schottky barrier in vertically stacked graphene on the Janus MoSeS under electric field. <i>Computational Materials Science</i> , 2018 , 153, 438-444	3.2	45
54	Electronic properties of GaSe/MoS ₂ and GaS/MoSe ₂ heterojunctions from first principles calculations. <i>AIP Advances</i> , 2018 , 8, 075207	1.5	10
53	First principles calculations of the geometric structures and electronic properties of van der Waals heterostructure based on graphene, hexagonal boron nitride and molybdenum diselenide. <i>Diamond and Related Materials</i> , 2018 , 88, 151-157	3.5	12

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51	Magneto-optical absorption in quantum dot via two-photon absorption process. <i>Optik</i> , 2018 , 173, 263-270	2.5	3
50	Ab-initio study of electronic and optical properties of biaxially deformed single-layer GeS. <i>Superlattices and Microstructures</i> , 2018 , 120, 501-507	2.8	17
49	Interlayer coupling and electric field tunable electronic properties and Schottky barrier in a graphene/bilayer-GaSe van der Waals heterostructure. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 17899-17908	3.6	76
48	Structural and electronic properties of a van der Waals heterostructure based on silicene and gallium selenide: effect of strain and electric field. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 27856-27864	3.6	54
47	First-principles study of W, N, and O adsorption on TiB ₂ (0001) surface with disordered vacancies. <i>Superlattices and Microstructures</i> , 2018 , 123, 414-426	2.8	6
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45	Effective Photocatalytic Activity of Mixed Ni/Fe-Base Metal-Organic Framework under a Compact Fluorescent Daylight Lamp. <i>Catalysts</i> , 2018 , 8, 487	4	39
44	Layered graphene/GaS van der Waals heterostructure: Controlling the electronic properties and Schottky barrier by vertical strain. <i>Applied Physics Letters</i> , 2018 , 113, 171605	3.4	141
43	Electronic structure, optical and photocatalytic performance of SiC-MX (M = Mo, W and X = S, Se) van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 24168-24175	3.6	60
42	Phonon-assisted cyclotron resonance in special symmetric quantum wells. <i>Applied Physics A: Materials Science and Processing</i> , 2018 , 124, 1	2.6	9
41	First principles study on the electronic properties and Schottky barrier of Graphene/InSe heterostructure. <i>Superlattices and Microstructures</i> , 2018 , 122, 570-576	2.8	21
40	Effect of strains on electronic and optical properties of monolayer SnS: Ab-initio study. <i>Physica B: Condensed Matter</i> , 2018 , 545, 255-261	2.8	16
39	Linear and nonlinear magneto-optical properties of monolayer phosphorene. <i>Journal of Applied Physics</i> , 2017 , 121, 045107	2.5	33
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37	First principles study of structural, electronic and magnetic properties of graphene adsorbed on the O-terminated MnO(111) surface. <i>Diamond and Related Materials</i> , 2017 , 74, 31-40	3.5	10
36	Linear and nonlinear magneto-optical absorption coefficients and refractive index changes in graphene. <i>Optical Materials</i> , 2017 , 69, 328-332	3.3	17
35	Out-of-plane strain and electric field tunable electronic properties and Schottky contact of graphene/antimonene heterostructure. <i>Superlattices and Microstructures</i> , 2017 , 112, 554-560	2.8	22

34	First-principles study of structure, electronic properties and stability of tungsten adsorption on TiC(111) surface with disordered vacancies. <i>Physica B: Condensed Matter</i> , 2017 , 526, 28-36	2.8	6
33	First-principles study of the structural and electronic properties of graphene/MoS2 interfaces. <i>Journal of Applied Physics</i> , 2017 , 122, 104301	2.5	43
32	Magneto-optical transport properties of monolayer MoS2 on polar substrates. <i>Physical Review B</i> , 2017 , 96,	3.3	61
31	Band gap and electronic properties of molybdenum disulphide under strain engineering: density functional theory calculations. <i>Molecular Simulation</i> , 2017 , 43, 86-91	2	10
30	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. <i>Computational Materials Science</i> , 2016 , 124, 344-352	3.2	10
29	Linear and nonlinear magneto-optical absorption in parabolic quantum well. <i>Optik</i> , 2016 , 127, 10519-10526	2.6	10
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21	Effect of electric field on the electronic and magnetic properties of a graphene nanoribbon/aluminium nitride bilayer system. <i>RSC Advances</i> , 2015 , 5, 49308-49316	3.7	25
20	Tuning the electronic properties of armchair graphene nanoribbons by strain engineering. <i>Physica Scripta</i> , 2015 , 90, 015802	2.6	10
19	Nonlinear optical absorption in parabolic quantum well via two-photon absorption process. <i>Optics Communications</i> , 2015 , 335, 37-41	2	28
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15	Nonlinear optical absorption in graphene via two-photon absorption process. <i>Optics Communications</i> , 2015 , 344, 12-16	2	26
14	Band structure of deformed armchair nanoribbon with bond alternation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014 , 60, 91-94	3	7
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