Asadollah Bafekry

List of Publications by Citations

74 papers	1,709 citations	26 h-index	37 g-index
80 ext. papers	2,341 ext. citations	4 avg, IF	6.34 L-index

#	Paper	IF	Citations
74	A first-principles study of the effects of atom impurities, defects, strain, electric field and layer thickness on the electronic and magnetic properties of the C2N nanosheet. *Carbon*, **2020**, 157, 371-384	10.4	81
73	MoSi2N4 single-layer: a novel two-dimensional material with outstanding mechanical, thermal, electronic and optical properties. *Journal Physics D: Applied Physics*, **2021**, 54, 155303	3	68
72	C3N Monolayer: Exploring the Emerging of Novel Electronic and Magnetic Properties with Adatom Adsorption, Functionalizations, Electric Field, Charging, and Strain. *Journal of Physical Chemistry C*, **2019**, 123, 12485-12499	3.8	57
71	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
70	Introducing novel electronic and magnetic properties in CN nanosheets by defect engineering and atom substitution. *Physical Chemistry Chemical Physics*, **2019**, 21, 21070-21083	3.6	52
69	Van der Waals heterostructures of MoS2 and Janus MoSSe monolayers on graphitic boron-carbon-nitride (BC 3, C 3 N, C3N4 and C4N3) nanosheets: a first-principles study. *Journal Physics D: Applied Physics*, **2020**, 53, 355106	3	50
68	Electro-optical properties of monolayer and bilayer boron-doped C3N: Tunable electronic structure via strain engineering and electric field. *Carbon*, **2020**, 168, 220-229	10.4	49
67	Two-dimensional carbon nitride (2DCN) nanosheets: Tuning of novel electronic and magnetic properties by hydrogenation, atom substitution and defect engineering. *Journal of Applied Physics*, **2019**, 126, 215104	2.5	49
66	Tunable electronic and magnetic properties of graphene/carbon-nitride van der Waals heterostructures. *Applied Surface Science*, **2020**, 505, 144450	6.7	47
65	Graphene-like BC6N single-layer: Tunable electronic and magnetic properties via thickness, gating, topological defects, and adatom/molecule. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 118, 113850	3	47
64	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
63	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
62	Tuning the bandgap and introducing magnetism into monolayer BC3 by strain/defect engineering and adatom/molecule adsorption. *Journal of Applied Physics*, **2019**, 126, 144304	2.5	44
61	Adsorption of molecules on C3N nanosheet: A first-principles calculations. *Chemical Physics*, **2019**, 526, 110442	2.3	40
60	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
59	Tuning the electronic and magnetic properties of antimonene nanosheets via point defects and external fields: first-principles calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 10552-10566	3.6	37
58	Tuning the electronic properties of graphene□graphitic carbon nitride heterostructures and heterojunctions by using an electric field. *Physical Review B*, **2020**, 101,	3.3	36

57	Strain, electric-field and functionalization induced widely tunable electronic properties in MoS/BC , /C N and /[Formula: see text] van der Waals heterostructures. *Nanotechnology*, **2020**, 31, 295202	3.4	34
56	Tunable electronic and magnetic properties of MoSi2N4 monolayer via vacancy defects, atomic adsorption and atomic doping. *Applied Surface Science*, **2021**, 559, 149862	6.7	34
55	Exploiting the Novel Electronic and Magnetic Structure of C3N via Functionalization and Conformation. *Advanced Electronic Materials*, **2019**, 5, 1900459	6.4	33
54	Control of CN and CN carbon nitride nanosheetsTelectronic and magnetic properties through embedded atoms. *Physical Chemistry Chemical Physics*, **2020**, 22, 2249-2261	3.6	32
53	A Dirac-semimetal two-dimensional BeN4: Thickness-dependent electronic and optical properties. *Applied Physics Letters*, **2021**, 118, 203103	3.4	32
52	Two-dimensional graphitic carbon nitrides: Strain-tunable ferromagnetic ordering. *Physical Review B*, **2020**, 101,	3.3	30
51	A First-Principles Study of C N Nanostructures: Control and Engineering of the Electronic and Magnetic Properties of Nanosheets, Tubes and Ribbons. *ChemPhysChem*, **2020**, 21, 164-174	3.2	30
50	The Electronic, Optical, and Thermoelectric Properties of Monolayer PbTe and the Tunability of the Electronic Structure by External Fields and Defects. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 2000182	1.3	28
49	Embedding of atoms into the nanopore sites of the CN and CN porous carbon nitride monolayers with tunable electronic properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 6418-6433	3.6	27
48	Band-gap control of graphenelike borocarbonitride gBC6N bilayers by electrical gating. *Physical Review B*, **2020**, 102,	3.3	26
47	Dirac half-metallicity of Thin PdCl Nanosheets: Investigation of the Effects of External Fields, Surface Adsorption and Defect Engineering on the Electronic and Magnetic Properties. *Scientific Reports*, **2020**, 10, 213	4.9	26
46	Band gap and magnetism engineering in Dirac half-metallic Na2C nanosheet via layer thickness, strain and point defects. *Journal of Magnetism and Magnetic Materials*, **2019**, 491, 165565	2.8	26
45	Two-dimensional carbon nitride C6N nanosheet with egg-comb-like structure and electronic properties of a semimetal. *Nanotechnology*, **2020**,	3.4	25
44	Modulating the electro-optical properties of doped C3N monolayers and graphene bilayers via mechanical strain and pressure. *New Journal of Chemistry*, **2020**, 44, 15785-15792	3.6	24
43	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
42	Effect of electric field and vertical strain on the electro-optical properties of the MoSi2N4 bilayer: A first-principles calculation. *Journal of Applied Physics*, **2021**, 129, 155103	2.5	23
41	Strain and electric field tuning of semi-metallic character WCrCO MXenes with dual narrow band gap. *Journal of Physics Condensed Matter*, **2020**, 32, 355504	1.8	21
40	Two-dimensional silicon bismotide (SiBi) monolayer with a honeycomb-like lattice: first-principles study of tuning the electronic properties.. *RSC Advances*, **2020**, 10, 31894-31900	3.7	21

39	Electronic and magnetic properties of two-dimensional of FeX (X = S, Se, Te) monolayers crystallize in the orthorhombic structures. *Applied Physics Letters*, **2021**, 118, 143102	3.4	21
38	The mechanical, electronic, optical and thermoelectric properties of two-dimensional honeycomb-like of XSb (X = Si, Ge, Sn) monolayers: a first-principles calculations.. *RSC Advances*, **2020**, 10, 30398-30405	3.7	20
37	Ab initio prediction of semiconductivity in a novel two-dimensional SbX (X= S, Se, Te) monolayers with orthorhombic structure. *Scientific Reports*, **2021**, 11, 10366	4.9	20
36	A van der Waals heterostructure of MoS2/MoSi2N4: a first-principles study. *New Journal of Chemistry*, **2021**, 45, 8291-8296	3.6	20
35	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties an electric field and mechanical strain. *Physical Chemistry Chemical Physics*, **2021**, 23, 15216-15223	3.6	17
34	ZnN and ZnP as novel graphene-like materials with high Li-ion storage capacities. *Materials Today Energy*, **2020**, 16, 100392	7	16
33	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
32	Adsorption of habitat and industry-relevant molecules on the MoSi2N4 monolayer. *Applied Surface Science*, **2021**, 564, 150326	6.7	16
31	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
30	Tunable electronic properties of the dynamically stable layered mineral PtHgSe (Jacutingaite). *Physical Chemistry Chemical Physics*, **2020**, 22, 24471-24479	3.6	14
29	Vertical two-dimensional layered conjugated porous organic network structures of poly-benzimidazobenzophenanthroline (BBL): A first-principles study. *Applied Physics Letters*, **2020**, 117, 233101	3.4	14
28	Oxygen Vacancies in the Single Layer of Ti2CO2 MXene: Effects of Gating Voltage, Mechanical Strain, and Atomic Impurities. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 2000343	1.3	14
27	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
26	Two-dimensional porous graphitic carbon nitride C6N7 monolayer: First-principles calculations. *Applied Physics Letters*, **2021**, 119, 142102	3.4	12
25	Surface functionalization of the honeycomb structure of zinc antimonide (ZnSb) monolayer: A first-Principles study. *Surface Science*, **2021**, 707, 121796	1.8	12
24	Biphenylene monolayer as a two-dimensional nonbenzenoid carbon allotrope: a first-principles study. *Journal of Physics Condensed Matter*, **2021**, 34,	1.8	11
23	Two-dimensional buckled tetragonal cadmium chalcogenides including CdS, CdSe, and CdTe monolayers as photo-catalysts for water splitting. *Physical Chemistry Chemical Physics*, **2021**, 23, 12226-12232	3.6	11
22	Ab-initio-driven prediction of puckered penta-like PdPSeX (X= O, S, Te) Janus monolayers: Study on the electronic, optical, mechanical and photocatalytic properties. *Applied Surface Science*, **2022**, 582, 152356	6.7	9

21	Semiconducting Chalcogenide Alloys Based on the (Ge, Sn, Pb) (S, Se, Te) Formula with Outstanding Properties: A First-Principles Calculation Study. *ACS Omega*, **2021**, 6, 9433-9441	3.9	9
20	Electronic and optical properties of two-dimensional heterostructures and heterojunctions between doped-graphene and C- and N-containing materials. *Physical Chemistry Chemical Physics*, **2021**, 23, 4865-4873	3.6	9
19	Electro-optical and mechanical properties of Zinc antimonide (ZnSb) monolayer and bilayer: A first-principles study. *Applied Surface Science*, **2021**, 540, 148289	6.7	8
18	Novel two-dimensional AlSb and InSb monolayers with a double-layer honeycomb structure: a first-principles study. *Physical Chemistry Chemical Physics*, **2021**, 23, 18752-18759	3.6	8
17	Van der Waals heterostructure of graphene and germanane: tuning the ohmic contact by electrostatic gating and mechanical strain. *Physical Chemistry Chemical Physics*, **2021**, 23, 21196-21206	3.6	8
16	First-principles investigation of electronic, mechanical and thermoelectric properties of graphene-like XBi (X = Si, Ge, Sn) monolayers. *Physical Chemistry Chemical Physics*, **2021**, 23, 12471-12478	3.6	8
15	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
14	Two-dimensional FeTe and predicted Janus FeXS (X: Te and Se) monolayers with intrinsic half-metallic character: tunable electronic and magnetic properties strain and electric field. *Physical Chemistry Chemical Physics*, **2021**, 23, 24336-24343	3.6	5
13	A novel two-dimensional boron□carbon□nitride (BCN) monolayer: A first-principles insight. *Journal of Applied Physics*, **2021**, 130, 114301	2.5	5
12	Tunable electronic properties of porous graphitic carbon nitride (C6N7) monolayer by atomic doping and embedding: A first-principle study. *Applied Surface Science*, **2022**, 583, 152270	6.7	3
11	Two-dimensional Dirac half-metal in porous carbon nitride CNmonolayer via atomic doping. *Nanotechnology*, **2021**, 33,	3.4	3
10	Electronic, optical and thermoelectric properties of a novel two-dimensional SbXY (X = Se, Te; Y = Br, I) family: perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 25866-25876	3.6	3
9	Theoretical prediction of the PtOX (X = S and Se) monolayers as promising optoelectronic and thermoelectric 2D materials. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 131, 114732	3	3
8	Two-dimensional XY monolayers (X = Al, Ga, In; Y = N, P, As) with a double layer hexagonal structure: A first-principles perspective. *Applied Surface Science*, **2022**, 590, 152998	6.7	3
7	Effect of adsorption and substitutional B doping at different concentrations on the electronic and magnetic properties of a BeO monolayer: a first-principles study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24922-24931	3.6	2
6	Novel two-dimensional ZnO2, CdO2 and HgO2 monolayers: a first-principles-based prediction. *New Journal of Chemistry*, **2021**, 45, 9368-9374	3.6	2
5	Point defects in two-dimensional BeO monolayer: a first-principles study on electronic and magnetic properties. *Physical Chemistry Chemical Physics*, **2021**, 23, 24301-24312	3.6	2
4	Investigation of vacancy defects and substitutional doping in AlSb monolayer with double layer honeycomb structure: a first-principles calculation. *Journal of Physics Condensed Matter*, **2021**, 34,	1.8	1

3	Developing feature-rich electronic and magnetic properties in the As monolayer for spintronic and optoelectronic applications by C and Si doping: A first-principles study. *Surfaces and Interfaces*, **2021**, 27, 101534	4.1	0
2	Thermoelectric properties of doped graphene nanoribbons: density functional theory calculations and electrical transport.. *RSC Advances*, **2022**, 12, 6174-6180	3.7	0
1	Monoelemental two-dimensional iodinene nanosheets: a first-principles study of the electronic and optical properties. *Journal Physics D: Applied Physics*, **2022**, 55, 135104	3	