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List of Publications by Year
in descending order

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51 papers	2,209 citations	117453 34 h-index	223531 46 g-index
62 all docs	62 docs citations	62 times ranked	1115 citing authors

#	Article	IF	Citations
1	Unraveling the effect of Gd doping on the structural, optical, and magnetic properties of ZnO based diluted magnetic semiconductor nanorods. RSC Advances, 2019, 9, 33207-33221.	1.7	123
2	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.	1.4	77
3	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.	1.3	74
4	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.	1.4	69
5	A Dirac-semimetal two-dimensional BeN4: Thickness-dependent electronic and optical properties. Applied Physics Letters, 2021, 118, .	1.5	64
6	Electronic and magnetic properties of single-layer boron phosphide associated with materials processing defects. Computational Materials Science, 2019, 170, 109201.	1.4	63
7	Tunable electronic and optical properties of new two-dimensional GaN/BAs van der Waals heterostructures with the potential for photovoltaic applications. Chemical Physics Letters, 2019, 728, 124-131.	1.2	63
8	Stacking impact on the optical and electronic properties of two-dimensional MoSe2/PtS2 heterostructures formed by PtS2 and MoSe2 monolayers. Chemical Physics, 2020, 532, 110679.	0.9	63
9	Strain-tunable electronic and optical properties of monolayer GeSe: Promising for photocatalytic water splitting applications. Chemical Physics, 2020, 529, 110543.	0.9	60
10	Two-dimensional porous graphitic carbon nitride C6N7 monolayer: First-principles calculations. Applied Physics Letters, 2021, 119, .	1.5	57
11	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.	3.1	55
12	Tuning the electronic structure of 2D materials by strain and external electric field: Case of GeI2 monolayer. Chemical Physics, 2019, 527, 110499.	0.9	53
13	Two-dimensional penta-like PdPSe with a puckered pentagonal structure: a first-principles study. Physical Chemistry Chemical Physics, 2022, 24, 9990-9997.	1.3	53
14	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.	3.1	53
15	Tunable optical and electronic properties of gallium telluride monolayer for photovoltaic absorbers and ultraviolet detectors. Chemical Physics Letters, 2018, 713, 46-51.	1.2	52
16	Tunable electronic and optical properties of GaS/GaSe van der Waals heterostructure. Current Applied Physics, 2018, 18, 673-680.	1.1	51
17	Two-dimensional carbon nitride C₆N nanosheet with egg-comb-like structure and electronic properties of a semimetal. Nanotechnology, 2021, 32, 215702.	1.3	50
18	Adsorption of molecules on C3N nanosheet: A first-principles calculations. Chemical Physics, 2019, 526, 110442.	0.9	49

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19	Biphenylene monolayer as a two-dimensional nonbenzenoid carbon allotrope: a first-principles study. Journal of Physics Condensed Matter, 2022, 34, 015001.	0.7	45
20	First principles study of single-layer SnSe2 under biaxial strain and electric field: Modulation of electronic properties. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 201-205.	1.3	44
21	Two-dimensional ZnI2 monolayer as a photocatalyst for water splitting and improvement its electronic and optical properties by strains. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 126, 114487.	1.3	44
22	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.	1.3	44
23	Ab initio prediction of semiconductivity in a novel two-dimensional Sb2X3 (X= S, Se, Te) monolayers with orthorhombic structure. Scientific Reports, 2021, 11, 10366.	1.6	44
24	Tuning optical and electronic properties of 2D ZnI2/CdS heterostructure by biaxial strains for optical nanodevices: A first-principles study. Journal of Applied Physics, 2021, 129, .	1.1	44
25	Two-dimensional FeTe₂ and predicted Janus FeXS (X: Te and Se) monolayers with intrinsic half-metallic character: tunable electronic and magnetic properties via strain and electric field. Physical Chemistry Chemical Physics, 2021, 23, 24336-24343.	1.3	44
26	The electronic, half-metallic, and magnetic properties of Ca1-Cr S ternary alloys: Insights from the first-principle calculations. Journal of Molecular Graphics and Modelling, 2019, 89, 22-32.	1.3	43
27	Prediction of two-dimensional bismuth-based chalcogenides Bi₂X₃(X = S, Se,) Tj ETQq1 1 0.784314 rgBT /O Physics, 2021, 54, 395103.	1.3	42
28	Assessing optoelectronic properties of PbI2 monolayer under uniaxial strain from first principles calculations. Superlattices and Microstructures, 2019, 130, 354-360.	1.4	41
29	Electronic band structure, thermodynamics and optical characteristics of BeO1â^'A (Aâ€¯=â€¯S, Se, Te) alloys: Insights from ab initio study. Chemical Physics, 2019, 526, 110414.	0.9	39
30	Electronic and magnetic properties of two-dimensional of FeX (X = S, Se, Te) monolayers crystallize in the orthorhombic structures. Applied Physics Letters, 2021, 118, .	1.5	39
31	Electronic Properties of Adsorption of CO, CO₂, NH₃, NO, NO₂ and SO₂ on Nitrogen Doped Graphene for Gas Sensor Applications. Sensor Letters, 2017, 15, 432-439.	0.4	35
32	Electronic Properties of CO and CO₂ Adsorbed Silicene/Graphene Nanoribbons as a Promising Candidate for a Metal-Free Catalyst and a Gas Sensor. Sensor Letters, 2016, 14, 989-995.	0.4	34
33	Electronic and Structural Properties of Gas Adsorbed Graphene-Silicene Hybrid as a Gas Sensor. Journal of Nanoelectronics and Optoelectronics, 2017, 12, 742-747.	0.1	33
34	Simulation of Electronic Structure of Aluminum Phosphide Nanocrystals Using Ab Initio Large Unit Cell Method. Advances in Materials Science and Engineering, 2012, 2012, 1-6.	1.0	29
35	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.	1.6	20
36	Puckered Penta-like PdPX (X = O, S, Te) Semiconducting Nanosheets: First-Principles Study of the Mechanical, Electro-Optical, and Photocatalytic Properties. ACS Applied Materials & Interfaces, 2022, 14, 21577-21584.	4.0	19

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37	Investigation of vacancy defects and substitutional doping in AlSb monolayer with double layer honeycomb structure: a first-principles calculation. Journal of Physics Condensed Matter, 2022, 34, 065701.	0.7	18
38	Prediction of two-dimensional AlBrSe monolayer as a highly efficient photocatalytic for water splitting. Surfaces and Interfaces, 2022, 31, 102020.	1.5	18
39	Electronic, optical and thermoelectric properties of a novel two-dimensional SbXY (X = Se, Te; Y = Br, I) family: ab initio perspective. Physical Chemistry Chemical Physics, 2021, 23, 25866-25876.	1.3	17
40	Structural, electronic and optical properties of ABTe2 (A = Li, Na, K, Rb, Cs and B = Sc, Y, La): Insights from first-principles computations. Journal of Solid State Chemistry, 2019, 279, 120954.	1.4	13
41	Electronic Structure of AlP Under Pressure Using Semiempirical Method. The Open Condensed Matter Physics Journal, 2010, 3, 1-7.	0.2	12
42	Theoretical study of thermal conductivity, mechanical, vibrational and thermodynamical properties of Ln2Zr2O7 (LnÂ=ÂLa, Nd, Sm, and Eu) pyrochlore. Inorganic Chemistry Communication, 2021, 127, 108495.	1.8	9
43	Tilted electric field effects on the electronic states in a GaAs quantum disk. Superlattices and Microstructures, 2012, 52, 1078-1082.	1.4	7
44	Electronic band structure, elastic, optical and thermodynamic characteristic of cubic YF3: An ab initio study. Optik, 2021, 239, 166680.	1.4	7
45	Al-Doped Graphene as a Sensor for Harmful Gases (CO, CO₂, NH₃, NO,) Tj ETQq1 1 0.784314 rgBT /Overlock	0.4	7
46	Tunable electronic properties of InSe by biaxial strain: from bulk to single-layer. Materials Research Express, 2019, 6, 115002.	0.8	6
47	Insight view of mechanical, electronic and thermodynamic properties of the novel intermetallic $$hbox {REPt}_{{4}}$$ $$hbox {In}_{{4}}$$ (RE $$=$$ Eu, Gd, Tb, Dy, Ho) compounds via ab initio calculations. Bulletin of Materials Science, 2020, 43, 1.	0.8	3
48	Electronic Structure Properties of Twisted Armchair (3, 3) and Zigzag (5, 0) Carbon Nanotube: A Density Functional Study. Materials Focus, 2016, 5, 158-164.	0.4	2
49	Structural, Electronic and Optical Properties of Transition Metal Dichalcogenides Layer PtS₂(Se₂) for Nano Devices Applications. Key Engineering Materials, 0, 886, 48-56.	0.4	1
50	Hydrogenation of Zigzag (5, 0) and (6, 0) Single-Walled Carbon Nanotubes Using Density Functional Theory. Journal of Advanced Physics, 2016, 5, 140-144.	0.4	1
51	Electronic and Optical Properties of Indium Selenide Nanosheet Using First-Principle Calculations. Advanced Science, Engineering and Medicine, 2019, 11, 1148-1154.	0.3	0