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List of Publications by Year in Descending Order

79 papers	7,163 citations	26 h-index	84 g-index
85 ext. papers	8,043 ext. citations	3.8 avg, IF	6.11 L-index

#	Paper	IF	Citations
79	First-principles and Monte Carlo investigation of magnetic properties of two-dimensional transition metal alloyed boron-carbide CrFeBC sheet. *Computational Materials Science*, **2022**, 202, 110964	3.2	1
78	Doping-Driven Antiferromagnetic to Ferromagnetic Phase Transition in Tetragonal Cr 2 B 2 Monolayer. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000396	1.3	3
77	Theoretical Screening of Metal Borocarbide Sheets for High-Capacity and High-Rate Li- and Na-Ion Batteries. *Physical Review Applied*, **2021**, 16,	4.3	4
76	High uptake and fixation ability of BC monolayer for CO and NO toxic gases: a computational analysis. *Journal of Materials Science*, **2021**, 56, 18566	4.3	
75	Novel two-dimensional CrXB2 (X=Cr, Ru) metal for high Nēl temperature antiferromagnetic spintronics. *Journal of Solid State Chemistry*, **2021**, 302, 122427	3.3	0
74	Functionalization of monolayer MoS2 with transition metal oxide nanoclusters. *Physica B: Condensed Matter*, **2021**, 619, 413245	2.8	0
73	Ferromagnetic TMBC (TM = Cr, Mn) monolayers for spintronic devices with high Curie temperature. *Physical Chemistry Chemical Physics*, **2021**, 23, 6107-6115	3.6	9
72	Above Room Temperature Ferromagnetism in Gd2B2 Monolayer with High Magnetic Anisotropy. *Journal of Physical Chemistry C*, **2020**, 124, 12816-12823	3.8	12
71	Two dimensional ruthenium carbide: structural and electronic features. *Physical Chemistry Chemical Physics*, **2020**, 22, 15488-15495	3.6	1
70	Tuning the electronic structure of RhX (X = Cl, Br, I) nonmagnetic monolayers: effects of charge-injection and external strain. *Physical Chemistry Chemical Physics*, **2020**, 22, 4561-4573	3.6	3
69	Adsorption of small molecules on a Pmma CO monolayer. *Journal of Physics and Chemistry of Solids*, **2020**, 139, 109300	3.9	
68	Free-standing and supported phosphorene nanoflakes: Shape- and size-dependent properties. *Applied Surface Science*, **2020**, 506, 144756	6.7	5
67	Electronic structure, cohesive and magnetic properties of iridium oxide clusters adsorbed on graphene. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107726	2.8	0
66	Interactions of selected organic molecules with a blue phosphorene monolayer: self-assembly, solvent effect, enhanced binding and fixation through coadsorbed gold clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 26552-26561	3.6	5
65	Exploring the potential of MnX (S, Sb) monolayers for antiferromagnetic spintronics: A theoretical investigation. *Journal of Applied Physics*, **2020**, 128, 113903	2.5	6
64	A tetragonal phase MnB sheet: a stable room temperature ferromagnet with sizable magnetic anisotropy. *Physical Chemistry Chemical Physics*, **2020**, 22, 10893-10899	3.6	11
63	Enhanced Interactions of Amino Acids and Nucleic Acid Bases with Bare Black Phosphorene Monolayer Mediated by Coadsorbed Species. *Journal of Physical Chemistry C*, **2019**, 123, 23691-23704	3.8	7

62	Deformed octagon-hexagon-square structure of group-IV and group-V elements and III-V compounds. *Physical Review B*, **2019**, 100,	3.3	3
61	Stable, one-dimensional suspended and supported monatomic chains of pnictogens: a metal-insulator framework. *Physical Chemistry Chemical Physics*, **2019**, 21, 14832-14845	3.6	4
60	Novel Metallic Clathrates of Group-IV Elements and Their Compounds in a Dense Hexagonal Lattice. *Journal of Physical Chemistry C*, **2019**, 123, 15330-15338	3.8	3
59	Effect of point defects on electronic and magnetic properties of single-layer SiO. *Philosophical Magazine*, **2019**, 99, 2340-2353	1.6	2
58	Two-dimensional pnictogens: A review of recent progresses and future research directions. *Applied Physics Reviews*, **2019**, 6, 021308	17.3	97
57	Functionalization of monolayer AsP phases by adatoms: a first-principles study. *Materials Research Express*, **2019**, 6, 065032	1.7	1
56	Strain effects on electronic and magnetic properties of the monolayer □ RuCl 3: A first-principles and Monte Carlo study. *Journal of Applied Physics*, **2019**, 125, 083903	2.5	20
55	A new single-layer structure of MBene family: TiB. *Journal of Physics Condensed Matter*, **2019**, 31, 505401	1.8	11
54	Mechanical and Electrical Monitoring in the Dynamics of Twisted Phosphorene Nanoflakes on 2D Monolayers. *Journal of Physical Chemistry C*, **2019**, 123, 30704-30713	3.8	2
53	Exploring the electronic and magnetic properties of new metal halides from bulk to two-dimensional monolayer: RuX3 (X = Br, I). *Journal of Magnetism and Magnetic Materials*, **2019**, 476, 111-119	2.8	32
52	Glycine self-assembled on graphene enhances the solar absorbance performance. *Carbon*, **2019**, 143, 329-334	10.4	14
51	Tuning electronic and magnetic properties of single-layer PN phases by point defects. *Journal of Physics and Chemistry of Solids*, **2019**, 125, 80-89	3.9	1
50	Fundamentals, progress, and future directions of nitride-based semiconductors and their composites in two-dimensional limit: A first-principles perspective to recent synthesis. *Applied Physics Reviews*, **2018**, 5, 011105	17.3	50
49	Influence of chalcogen composition on the structural transition and on the electronic and optical properties of the monolayer titanium trichalcogenide ordered alloys. *Physical Chemistry Chemical Physics*, **2018**, 20, 1431-1439	3.6	8
48	Metal□nsulator Transition and Heterostructure Formation by Glycines Self-Assembled on Defect-Patterned Graphene. *Journal of Physical Chemistry C*, **2018**, 122, 14598-14605	3.8	18
47	Diffusion quantum Monte Carlo and density functional calculations of the structural stability of bilayer arsenene. *Journal of Chemical Physics*, **2018**, 148, 214706	3.9	19
46	Electronic and magnetic properties of monolayer □RuCl: a first-principles and Monte Carlo study. *Physical Chemistry Chemical Physics*, **2018**, 20, 997-1004	3.6	42
45	Chemical and substitutional doping, and anti-site and vacancy formation in monolayer AlN and GaN. *Physical Chemistry Chemical Physics*, **2018**, 20, 16077-16091	3.6	24

44	Functionalization of Single-Layer Nitrogene by Vacancy, Adatoms, and Molecules. *Journal of Physical Chemistry C*, **2017**, 121, 6329-6338	3.8	11
43	Tunable dynamics of a flake on graphene: Libration frequency. *Physical Review B*, **2017**, 95,	3.3	6
42	Point defects in buckled and asymmetric washboard phases of arsenic phosphorus: A first principles study. *Computational Materials Science*, **2017**, 140, 290-298	3.2	15
41	The effect of vacancies and the substitution of p-block atoms on single-layer buckled germanium selenide. *RSC Advances*, **2017**, 7, 37815-37822	3.7	15
40	Half metallicity and pressure-induced electronic structure of monolayer FeX2 (X = S, Se). *Materials Research Express*, **2017**, 4, 116305	1.7	4
39	Theoretical investigation of lithium adsorption, diffusion and coverage on MX 2 (M = Mo, W; X = O, S, Se, Te) monolayers. *Applied Surface Science*, **2017**, 425, 301-306	6.7	38
38	Modification of electronic structure, magnetic structure, and topological phase of bismuthene by point defects. *Physical Review B*, **2017**, 96,	3.3	44
37	Investigation of adatom adsorption on single layer buckled germanium selenide. *Applied Surface Science*, **2016**, 390, 185-189	6.7	4
36	Single and bilayer bismuthene: Stability at high temperature and mechanical and electronic properties. *Physical Review B*, **2016**, 94,	3.3	224
35	Point defects in hexagonal germanium carbide monolayer: A first-principles calculation. *Applied Surface Science*, **2016**, 389, 1-6	6.7	44
34	Adsorption of alkali and alkaline-earth metal atoms on stanene: A first-principles study. *Materials Chemistry and Physics*, **2016**, 180, 326-331	4.4	29
33	Interaction of Adatoms and Molecules with Single-Layer Arsenene Phases. *Journal of Physical Chemistry C*, **2016**, 120, 14345-14355	3.8	88
32	Effects of adatoms and physisorbed molecules on the physical properties of antimonene. *Physical Review B*, **2016**, 93,	3.3	76
31	Stable single-layer structure of group-V elements. *Physical Review B*, **2016**, 94,	3.3	88
30	T-ZrS nanoribbons: structure and electronic properties. *Philosophical Magazine*, **2016**, 96, 2074-2087	1.6	5
29	Effect of adatoms and molecules on the physical properties of platinum-doped and -substituted silicene: A first-principles investigation. *Applied Surface Science*, **2016**, 371, 314-321	6.7	17
28	Stable monolayer honeycomb-like structures of RuX2 (X=S,Se). *Physical Review B*, **2016**, 94,	3.3	28
27	Interactions of h-AlN monolayer with platinum, oxygen, and their clusters. *Chemical Physics*, **2015**, 455, 73-80	2.3	8

26	Adsorption and Diffusion of Lithium on Monolayer Transition Metal Dichalcogenides (MoS2(1⊠)Se2x) Alloys. *Journal of Physical Chemistry C*, **2015**, 119, 28648-28653	3.8	63
25	A first-principles study of n-type and p-type doping of germanium carbide sheet. *Applied Surface Science*, **2015**, 332, 147-151	6.7	37
24	Effects of silver adatoms on the electronic structure of silicene. *Applied Surface Science*, **2014**, 311, 9-13	6.7	22
23	Electronic structure of BSb defective monolayers and nanoribbons. *Journal of Physics Condensed Matter*, **2014**, 26, 325303	1.8	9
22	Bimetallic two-dimensional PtAg coverage on h-BN substrate: First-principles calculations. *Applied Surface Science*, **2014**, 303, 306-311	6.7	18
21	Silicon-based counterpart of alpha-graphyne. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 1313-1315	2.3	2
20	Oxygen adsorption on honeycomb BC2N monolayers. *Materials Letters*, **2013**, 106, 168-170	3.3	5
19	Adsorption of carbon adatoms to graphene and its nanoribbons. *Journal of Applied Physics*, **2011**, 109, 013704	2.5	53
18	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS2. *Journal of Physical Chemistry C*, **2011**, 115, 16354-16361	3.8	250
17	Mechanical and Electronic Properties of MoS2 Nanoribbons and Their Defects. *Journal of Physical Chemistry C*, **2011**, 115, 3934-3941	3.8	391
16	DIPEPTIDE ADSORPTION ON Si(100)-2 □ ASYMMETRIC SURFACE BY FIRST PRINCIPLES. *International Journal of Modern Physics C*, **2010**, 21, 97-106	1.1	1
15	Effects of silicon and germanium adsorbed on graphene. *Applied Physics Letters*, **2010**, 96, 123112	3.4	55
14	First-principles study of the iron pnictide superconductor BaFe2As2. *Physical Review B*, **2009**, 79,	3.3	38
13	JOINT ENTROPY OF THE HARMONIC OSCILLATOR WITH TIME-DEPENDENT MASS AND/OR FREQUENCY. *International Journal of Modern Physics B*, **2009**, 23, 2449-2461	1.1	4
12	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. *Physical Review B*, **2009**, 79,	3.3	277
11	Monolayer honeycomb structures of group-IV elements and III-V binary compounds: First-principles calculations. *Physical Review B*, **2009**, 80,	3.3	1401
10	First-principles study of two- and one-dimensional honeycomb structures of boron nitride. *Physical Review B*, **2009**, 79,	3.3	503
9	Two- and one-dimensional honeycomb structures of silicon and germanium. *Physical Review Letters*, **2009**, 102, 236804	7.4	2380

8	First-principles approach to monitoring the band gap and magnetic state of a graphene nanoribbon via its vacancies. *Physical Review B*, **2008**, 78,	3.3	108
7	High-capacity hydrogen storage by metallized graphene. *Applied Physics Letters*, **2008**, 93, 043123	3.4	356
6	Time Dependence of Joint Entropy of Oscillating Quantum Systems. *International Journal of Theoretical Physics*, **2008**, 47, 3207-3218	1.1	4
5	Can Sobolev Inequality Be Written for Sharma-Mittal Entropy?. *International Journal of Theoretical Physics*, **2008**, 47, 3310-3320	1.1	9
4	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. *Journal of Molecular Structure*, **2008**, 886, 144-147	3.4	
3	Nonextensive Statistical Mechanics Application to Vibrational Dynamics of Protein Folding. *International Journal of Theoretical Physics*, **2007**, 46, 2945-2949	1.1	2
2	THE STRUCTURE OF THE FREE ENERGY SURFACE OF COARSE-GRAINED OFF-LATTICE PROTEIN MODELS. *International Journal of Modern Physics C*, **2007**, 18, 99-106	1.1	2
1	SOLVATION EFFECTS ON FREE ENERGY SURFACE OF POLYALANINE. *International Journal of Modern Physics C*, **2005**, 16, 1489-1496	1.1	5