

List of Publications by Citations

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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.

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	Two- and one-dimensional honeycomb structures of silicon and germanium. <i>Physical Review Letters</i> , 2009 , 102, 236804	7.4	2380
78	Monolayer honeycomb structures of group-IV elements and III-V binary compounds: First-principles calculations. <i>Physical Review B</i> , 2009 , 80,	3.3	1401
77	First-principles study of two- and one-dimensional honeycomb structures of boron nitride. <i>Physical Review B</i> , 2009 , 79,	3.3	503
76	Mechanical and Electronic Properties of MoS ₂ Nanoribbons and Their Defects. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 3934-3941	3.8	391
75	High-capacity hydrogen storage by metallized graphene. <i>Applied Physics Letters</i> , 2008 , 93, 043123	3.4	356
74	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. <i>Physical Review B</i> , 2009 , 79,	3.3	277
73	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS ₂ . <i>Journal of Physical Chemistry C</i> , 2011 , 115, 16354-16361	3.8	250
72	Single and bilayer bismuthene: Stability at high temperature and mechanical and electronic properties. <i>Physical Review B</i> , 2016 , 94,	3.3	224
71	First-principles approach to monitoring the band gap and magnetic state of a graphene nanoribbon via its vacancies. <i>Physical Review B</i> , 2008 , 78,	3.3	108
70	Two-dimensional pnictogens: A review of recent progresses and future research directions. <i>Applied Physics Reviews</i> , 2019 , 6, 021308	17.3	97
69	Interaction of Adatoms and Molecules with Single-Layer Arsenene Phases. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 14345-14355	3.8	88
68	Stable single-layer structure of group-V elements. <i>Physical Review B</i> , 2016 , 94,	3.3	88
67	Effects of adatoms and physisorbed molecules on the physical properties of antimonene. <i>Physical Review B</i> , 2016 , 93,	3.3	76
66	Adsorption and Diffusion of Lithium on Monolayer Transition Metal Dichalcogenides (MoS ₂ (1-x)Se _{2x}) Alloys. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 28648-28653	3.8	63
65	Effects of silicon and germanium adsorbed on graphene. <i>Applied Physics Letters</i> , 2010 , 96, 123112	3.4	55
64	Adsorption of carbon adatoms to graphene and its nanoribbons. <i>Journal of Applied Physics</i> , 2011 , 109, 013704	2.5	53
63	Fundamentals, progress, and future directions of nitride-based semiconductors and their composites in two-dimensional limit: A first-principles perspective to recent synthesis. <i>Applied Physics Reviews</i> , 2018 , 5, 011105	17.3	50

62	Point defects in hexagonal germanium carbide monolayer: A first-principles calculation. <i>Applied Surface Science</i> , 2016 , 389, 1-6	6.7	44
61	Modification of electronic structure, magnetic structure, and topological phase of bismuthene by point defects. <i>Physical Review B</i> , 2017 , 96,	3.3	44
60	Electronic and magnetic properties of monolayer β -RuCl ₃ : a first-principles and Monte Carlo study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 997-1004	3.6	42
59	Theoretical investigation of lithium adsorption, diffusion and coverage on MX ₂ (M = Mo, W; X = O, S, Se, Te) monolayers. <i>Applied Surface Science</i> , 2017 , 425, 301-306	6.7	38
58	First-principles study of the iron pnictide superconductor BaFe ₂ As ₂ . <i>Physical Review B</i> , 2009 , 79,	3.3	38
57	A first-principles study of n-type and p-type doping of germanium carbide sheet. <i>Applied Surface Science</i> , 2015 , 332, 147-151	6.7	37
56	Exploring the electronic and magnetic properties of new metal halides from bulk to two-dimensional monolayer: RuX ₃ (X = Br, I). <i>Journal of Magnetism and Magnetic Materials</i> , 2019 , 476, 111-119	2.8	32
55	Adsorption of alkali and alkaline-earth metal atoms on stanene: A first-principles study. <i>Materials Chemistry and Physics</i> , 2016 , 180, 326-331	4.4	29
54	Stable monolayer honeycomb-like structures of RuX ₂ (X=S,Se). <i>Physical Review B</i> , 2016 , 94,	3.3	28
53	Chemical and substitutional doping, and anti-site and vacancy formation in monolayer AlN and GaN. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16077-16091	3.6	24
52	Effects of silver adatoms on the electronic structure of silicene. <i>Applied Surface Science</i> , 2014 , 311, 9-13	6.7	22
51	Strain effects on electronic and magnetic properties of the monolayer β -RuCl ₃ : A first-principles and Monte Carlo study. <i>Journal of Applied Physics</i> , 2019 , 125, 083903	2.5	20
50	Diffusion quantum Monte Carlo and density functional calculations of the structural stability of bilayer arsenene. <i>Journal of Chemical Physics</i> , 2018 , 148, 214706	3.9	19
49	Metallinsulator Transition and Heterostructure Formation by Glycines Self-Assembled on Defect-Patterned Graphene. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 14598-14605	3.8	18
48	Bimetallic two-dimensional PtAg coverage on h-BN substrate: First-principles calculations. <i>Applied Surface Science</i> , 2014 , 303, 306-311	6.7	18
47	Effect of adatoms and molecules on the physical properties of platinum-doped and -substituted silicene: A first-principles investigation. <i>Applied Surface Science</i> , 2016 , 371, 314-321	6.7	17
46	Point defects in buckled and asymmetric washboard phases of arsenic phosphorus: A first principles study. <i>Computational Materials Science</i> , 2017 , 140, 290-298	3.2	15
45	The effect of vacancies and the substitution of p-block atoms on single-layer buckled germanium selenide. <i>RSC Advances</i> , 2017 , 7, 37815-37822	3.7	15

44	Glycine self-assembled on graphene enhances the solar absorbance performance. <i>Carbon</i> , 2019 , 143, 329-334	10.4	14
43	Above Room Temperature Ferromagnetism in Gd ₂ B ₂ Monolayer with High Magnetic Anisotropy. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 12816-12823	3.8	12
42	Functionalization of Single-Layer Nitrogen by Vacancy, Adatoms, and Molecules. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6329-6338	3.8	11
41	A new single-layer structure of MBene family: TiB. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 505401	1.8	11
40	A tetragonal phase MnB sheet: a stable room temperature ferromagnet with sizable magnetic anisotropy. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10893-10899	3.6	11
39	Electronic structure of BSb defective monolayers and nanoribbons. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 325303	1.8	9
38	Can Sobolev Inequality Be Written for Sharma-Mittal Entropy?. <i>International Journal of Theoretical Physics</i> , 2008 , 47, 3310-3320	1.1	9
37	Ferromagnetic TMBC (TM = Cr, Mn) monolayers for spintronic devices with high Curie temperature. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 6107-6115	3.6	9
36	Influence of chalcogen composition on the structural transition and on the electronic and optical properties of the monolayer titanium trichalcogenide ordered alloys. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 1431-1439	3.6	8
35	Interactions of h-AlN monolayer with platinum, oxygen, and their clusters. <i>Chemical Physics</i> , 2015 , 455, 73-80	2.3	8
34	Enhanced Interactions of Amino Acids and Nucleic Acid Bases with Bare Black Phosphorene Monolayer Mediated by Coadsorbed Species. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 23691-23704	3.8	7
33	Tunable dynamics of a flake on graphene: Libration frequency. <i>Physical Review B</i> , 2017 , 95,	3.3	6
32	Exploring the potential of MnX (S, Sb) monolayers for antiferromagnetic spintronics: A theoretical investigation. <i>Journal of Applied Physics</i> , 2020 , 128, 113903	2.5	6
31	Oxygen adsorption on honeycomb BC ₂ N monolayers. <i>Materials Letters</i> , 2013 , 106, 168-170	3.3	5
30	SOLVATION EFFECTS ON FREE ENERGY SURFACE OF POLYALANINE. <i>International Journal of Modern Physics C</i> , 2005 , 16, 1489-1496	1.1	5
29	Free-standing and supported phosphorene nanoflakes: Shape- and size-dependent properties. <i>Applied Surface Science</i> , 2020 , 506, 144756	6.7	5
28	Interactions of selected organic molecules with a blue phosphorene monolayer: self-assembly, solvent effect, enhanced binding and fixation through coadsorbed gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 26552-26561	3.6	5
27	T-ZrS nanoribbons: structure and electronic properties. <i>Philosophical Magazine</i> , 2016 , 96, 2074-2087	1.6	5

26	Stable, one-dimensional suspended and supported monatomic chains of pnictogens: a metal-insulator framework. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 14832-14845	3.6	4
25	Investigation of adatom adsorption on single layer buckled germanium selenide. <i>Applied Surface Science</i> , 2016 , 390, 185-189	6.7	4
24	Half metallicity and pressure-induced electronic structure of monolayer FeX ₂ (X = S, Se). <i>Materials Research Express</i> , 2017 , 4, 116305	1.7	4
23	JOINT ENTROPY OF THE HARMONIC OSCILLATOR WITH TIME-DEPENDENT MASS AND/OR FREQUENCY. <i>International Journal of Modern Physics B</i> , 2009 , 23, 2449-2461	1.1	4
22	Time Dependence of Joint Entropy of Oscillating Quantum Systems. <i>International Journal of Theoretical Physics</i> , 2008 , 47, 3207-3218	1.1	4
21	Theoretical Screening of Metal Borocarbide Sheets for High-Capacity and High-Rate Li- and Na-Ion Batteries. <i>Physical Review Applied</i> , 2021 , 16,	4.3	4
20	Deformed octagon-hexagon-square structure of group-IV and group-V elements and III-V compounds. <i>Physical Review B</i> , 2019 , 100,	3.3	3
19	Novel Metallic Clathrates of Group-IV Elements and Their Compounds in a Dense Hexagonal Lattice. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15330-15338	3.8	3
18	Tuning the electronic structure of RhX (X = Cl, Br, I) nonmagnetic monolayers: effects of charge-injection and external strain. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4561-4573	3.6	3
17	Doping-Driven Antiferromagnetic to Ferromagnetic Phase Transition in Tetragonal Cr ₂ B ₂ Monolayer. <i>Physica Status Solidi (B): Basic Research</i> , 2021 , 258, 2000396	1.3	3
16	Effect of point defects on electronic and magnetic properties of single-layer SiO. <i>Philosophical Magazine</i> , 2019 , 99, 2340-2353	1.6	2
15	Silicon-based counterpart of alpha-graphyne. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 1313-1315	2.3	2
14	Nonextensive Statistical Mechanics Application to Vibrational Dynamics of Protein Folding. <i>International Journal of Theoretical Physics</i> , 2007 , 46, 2945-2949	1.1	2
13	THE STRUCTURE OF THE FREE ENERGY SURFACE OF COARSE-GRAINED OFF-LATTICE PROTEIN MODELS. <i>International Journal of Modern Physics C</i> , 2007 , 18, 99-106	1.1	2
12	Mechanical and Electrical Monitoring in the Dynamics of Twisted Phosphorene Nanoflakes on 2D Monolayers. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 30704-30713	3.8	2
11	Functionalization of monolayer AsP phases by adatoms: a first-principles study. <i>Materials Research Express</i> , 2019 , 6, 065032	1.7	1
10	Two dimensional ruthenium carbide: structural and electronic features. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15488-15495	3.6	1
9	DIPEPTIDE ADSORPTION ON Si(100)-2 × 1 ASYMMETRIC SURFACE BY FIRST PRINCIPLES. <i>International Journal of Modern Physics C</i> , 2010 , 21, 97-106	1.1	1

8	First-principles and Monte Carlo investigation of magnetic properties of two-dimensional transition metal alloyed boron-carbide CrFeBC sheet. <i>Computational Materials Science</i> , 2022 , 202, 110964	3.2	1
7	Tuning electronic and magnetic properties of single-layer PN phases by point defects. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 125, 80-89	3.9	1
6	Electronic structure, cohesive and magnetic properties of iridium oxide clusters adsorbed on graphene. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107726	2.8	0
5	Novel two-dimensional CrXB ₂ (X=Cr, Ru) metal for high Néel temperature antiferromagnetic spintronics. <i>Journal of Solid State Chemistry</i> , 2021 , 302, 122427	3.3	0
4	Functionalization of monolayer MoS ₂ with transition metal oxide nanoclusters. <i>Physica B: Condensed Matter</i> , 2021 , 619, 413245	2.8	0
3	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. <i>Journal of Molecular Structure</i> , 2008 , 886, 144-147	3.4	
2	Adsorption of small molecules on a Pmma CO monolayer. <i>Journal of Physics and Chemistry of Solids</i> , 2020 , 139, 109300	3.9	
1	High uptake and fixation ability of BC monolayer for CO and NO toxic gases: a computational analysis. <i>Journal of Materials Science</i> , 2021 , 56, 18566	4.3	