E AktÃ¼rk

List of Publications by Year
in descending order

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84 papers	8,807 citations	185998 28 h-index	60497 81 g-index
85 all docs	85 docs citations	85 times ranked	7547 citing authors

#	Article	IF	Citations
1	Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium. Physical Review Letters, 2009, 102, 236804.	2.9	2,837
2	Monolayer honeycomb structures of group-IV elements and III-V binary compounds: First-principles calculations. Physical Review B, 2009, 80, .	1.1	1,769
3	First-principles study of two- and one-dimensional honeycomb structures of boron nitride. Physical Review B, 2009, 79, .	1.1	580
4	Mechanical and Electronic Properties of MoS₂ Nanoribbons and Their Defects. Journal of Physical Chemistry C, 2011, 115, 3934-3941.	1.5	427
5	High-capacity hydrogen storage by metallized graphene. Applied Physics Letters, 2008, 93, .	1.5	397
6	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. Physical Review B, 2009, 79, .	1.1	314
7	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS₂. Journal of Physical Chemistry C, 2011, 115, 16354-16361.	1.5	298
8	Single and bilayer bismuthene: Stability at high temperature and mechanical and electronic properties. Physical Review B, 2016, 94, .	1.1	295
9	Two-dimensional pnictogens: A review of recent progresses and future research directions. Applied Physics Reviews, 2019, 6, .	5.5	143
10	First-principles approach to monitoring the band gap and magnetic state of a graphene nanoribbon via its vacancies. Physical Review B, 2008, 78, .	1.1	120
11	Stable single-layer structure of group-V elements. Physical Review B, 2016, 94, .	1.1	108
12	Interaction of Adatoms and Molecules with Single-Layer Arsenene Phases. Journal of Physical Chemistry C, 2016, 120, 14345-14355.	1.5	98
13	Effects of adatoms and physisorbed molecules on the physical properties of antimonene. Physical Review B, 2016, 93, .	1.1	84
14	Adsorption and Diffusion of Lithium on Monolayer Transition Metal Dichalcogenides (MoS_{2(1â€“x)}Se_{2x}) Alloys. Journal of Physical Chemistry C, 2015, 119, 28648-28653.	1.5	76
15	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, .	5.5	71
16	Effects of silicon and germanium adsorbed on graphene. Applied Physics Letters, 2010, 96, .	1.5	63
17	Point defects in hexagonal germanium carbide monolayer: A first-principles calculation. Applied Surface Science, 2016, 389, 1-6.	3.1	62
18	Adsorption of carbon adatoms to graphene and its nanoribbons. Journal of Applied Physics, 2011, 109, 013704.	1.1	59

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19	Electronic and magnetic properties of monolayer Î±-RuCl₃: a first-principles and Monte Carlo study. Physical Chemistry Chemical Physics, 2018, 20, 997-1004.	1.3	57
20	Theoretical investigation of lithium adsorption, diffusion and coverage on MX 2 (M = Mo, W; X = O, S,) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.1	55
21	Modification of electronic structure, magnetic structure, and topological phase of bismuthene by point defects. Physical Review B, 2017, 96, .	1.1	54
22	Exploring the electronic and magnetic properties of new metal halides from bulk to two-dimensional monolayer: RuX3 (Xâ€¯=â€¯Br, I). Journal of Magnetism and Magnetic Materials, 2019, 476, 111-119.	1.0	48
23	Chemical and substitutional doping, and anti-site and vacancy formation in monolayer AlN and GaN. Physical Chemistry Chemical Physics, 2018, 20, 16077-16091.	1.3	45
24	First-principles study of the iron pnictide superconductorBaFe2As2. Physical Review B, 2009, 79, .	1.1	43
25	A first-principles study of n-type and p-type doping of germanium carbide sheet. Applied Surface Science, 2015, 332, 147-151.	3.1	41
26	Adsorption of alkali and alkaline-earth metal atoms on stanene: A first-principles study. Materials Chemistry and Physics, 2016, 180, 326-331.	2.0	33
27	Strain effects on electronic and magnetic properties of the monolayer Î±-RuCl3: A first-principles and Monte Carlo study. Journal of Applied Physics, 2019, 125, .	1.1	32
28	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.	3.1	30
29	Stable monolayer honeycomb-like structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mtext>Ru</mml:mtext><mml:msub><mml:mi>X</mml:mi><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mrow><mml:mi>X</mml:mi><mml:mo>=</mml:mo> Physical Review B, 2016, 94, .	11	30
30	Ferromagnetic TM₂BC (TM = Cr, Mn) monolayers for spintronic devices with high Curie temperature. Physical Chemistry Chemical Physics, 2021, 23, 6107-6115.	1.3	29
31	Metalâ€“Insulator Transition and Heterostructure Formation by Glycines Self-Assembled on Defect-Patterned Graphene. Journal of Physical Chemistry C, 2018, 122, 14598-14605.	1.5	28
32	A tetragonal phase Mn₂B₂ sheet: a stable room temperature ferromagnet with sizable magnetic anisotropy. Physical Chemistry Chemical Physics, 2020, 22, 10893-10899.	1.3	28
33	A new single-layer structure of MBene family: Ti₂B. Journal of Physics Condensed Matter, 2019, 31, 505401.	0.7	27
34	Effects of silver adatoms on the electronic structure of silicene. Applied Surface Science, 2014, 311, 9-13.	3.1	25
35	Above Room Temperature Ferromagnetism in Gd₂B₂ Monolayer with High Magnetic Anisotropy. Journal of Physical Chemistry C, 2020, 124, 12816-12823.	1.5	25
36	Diffusion quantum Monte Carlo and density functional calculations of the structural stability of bilayer arsenene. Journal of Chemical Physics, 2018, 148, 214706.	1.2	23

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37	Stability and electronic properties of monolayer and multilayer structures of group-IV elements and compounds of complementary groups in biphenylene network. Physical Review B, 2022, 105, .	1.1	22
38	Glycine self-assembled on graphene enhances the solar absorbance performance. Carbon, 2019, 143, 329-334.	5.4	21
39	Bimetallic two-dimensional PtAg coverage on h-BN substrate: First-principles calculations. Applied Surface Science, 2014, 303, 306-311.	3.1	20
40	The effect of vacancies and the substitution of p-block atoms on single-layer buckled germanium selenide. RSC Advances, 2017, 7, 37815-37822.	1.7	20
41	Point defects in buckled and asymmetric washboard phases of arsenic phosphorus: A first principles study. Computational Materials Science, 2017, 140, 290-298.	1.4	19
42	Functionalization of Single-Layer Nitrogene by Vacancy, Adatoms, and Molecules. Journal of Physical Chemistry C, 2017, 121, 6329-6338.	1.5	16
43	Exploring the potential of MnX (S, Sb) monolayers for antiferromagnetic spintronics: A theoretical investigation. Journal of Applied Physics, 2020, 128, .	1.1	15
44	Theoretical Screening of Metal Borocarbide Sheets for High-Capacity and High-Rate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Li</mml:mi></mml:math> - and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Na</mml:mi></mml:math> -Ion Batteries. Physical Review Applied, 2021, 16, .	1.5	15
45	Interactions of h-AlN monolayer with platinum, oxygen, and their clusters. Chemical Physics, 2015, 455, 73-80.	0.9	13
46	Can Sobolev Inequality Be Written for Sharma-Mittal Entropy?. International Journal of Theoretical Physics, 2008, 47, 3310-3320.	0.5	12
47	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.	1.5	10
48	Columnar antiferromagnetic order of a MBene monolayer. Physical Review B, 2021, 103, .	1.1	10
49	Electronic structure of BSb defective monolayers and nanoribbons. Journal of Physics Condensed Matter, 2014, 26, 325303.	0.7	9
50	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.	1.3	9
51	Stable, one-dimensional suspended and supported monatomic chains of pnictogens: a metalâ€“insulator framework. Physical Chemistry Chemical Physics, 2019, 21, 14832-14845.	1.3	9
52	Dopingâ€Driven Antiferromagnetic to Ferromagnetic Phase Transition in Tetragonal Cr2B2 Monolayer. Physica Status Solidi (B): Basic Research, 2021, 258, 2000396.	0.7	9
53	Functional Carbon and Silicon Monolayers in Biphenylene Network. ACS Applied Electronic Materials, 2022, 4, 3056-3070.	2.0	9
54	T-ZrS nanoribbons: structure and electronic properties. Philosophical Magazine, 2016, 96, 2074-2087.	0.7	8

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55	Free-standing and supported phosphorene nanoflakes: Shape- and size-dependent properties. Applied Surface Science, 2020, 506, 144756.	3.1	8
56	Tunable dynamics of a flake on graphene: Libration frequency. Physical Review B, 2017, 95, .	1.1	7
57	Deformed octagon-hexagon-square structure of group-IV and group-V elements and III-V compounds. Physical Review B, 2019, 100, .	1.1	7
58	Half metallicity and pressure-induced electronic structure of monolayer FeX2 (X = S, Se). Materials Research Express, 2017, 4, 116305.	0.8	6
59	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.	1.3	6
60	SOLVATION EFFECTS ON FREE ENERGY SURFACE OF POLYALANINE. International Journal of Modern Physics C, 2005, 16, 1489-1496.	0.8	5
61	Oxygen adsorption on honeycomb <mml:math altimg="si0001.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.co. Ma	1.3	5
62	Novel Metallic Clathrates of Group-IV Elements and Their Compounds in a Dense Hexagonal Lattice. Journal of Physical Chemistry C, 2019, 123, 15330-15338.	1.5	5
63	Functionalization of monolayer AsP phases by adatoms: a first-principles study. Materials Research Express, 2019, 6, 065032.	0.8	5
64	Tuning the electronic structure of RhX₃ (X = Cl, Br, I) nonmagnetic monolayers: effects of charge-injection and external strain. Physical Chemistry Chemical Physics, 2020, 22, 4561-4573.	1.3	5
65	Influence of Doping with Selected Organic Molecules on Magnetic and Electronic Properties of Bare, Surface Terminated and Defect Patterned Ti2C MXene Monolayer. Physical Chemistry Chemical Physics, 2022, , .	1.3	5
66	Magnetization of silicene via coverage with gadolinium: Effects of thickness, symmetry, strain, and coverage. Physical Review B, 2021, 104, .	1.1	5
67	Time Dependence of Joint Entropy of Oscillating Quantum Systems. International Journal of Theoretical Physics, 2008, 47, 3207-3218.	0.5	4
68	JOINT ENTROPY OF THE HARMONIC OSCILLATOR WITH TIME-DEPENDENT MASS AND/OR FREQUENCY. International Journal of Modern Physics B, 2009, 23, 2449-2461.	1.0	4
69	Investigation of adatom adsorption on single layer buckled germanium selenide. Applied Surface Science, 2016, 390, 185-189.	3.1	4
70	Silicon-based counterpart of alpha-graphyne. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1313-1315.	0.9	3
71	Effect of point defects on electronic and magnetic properties of single-layer SiO. Philosophical Magazine, 2019, 99, 2340-2353.	0.7	3
72	Tuning electronic and magnetic properties of single-layer PN phases by point defects. Journal of Physics and Chemistry of Solids, 2019, 125, 80-89.	1.9	3

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73	Novel two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mtext>C</mml:mtext><mml:mtext>r</mml:mtext><mml:mtext>X</mml:mtext><mml:msub><mml:mi	1.4	3
	(X=Cr, Ru) metal for high NÃ©el temperature antiferromagnetic spintronics. Journal of Solid State Chemistry, 2021, 302, 122427.		
74	THE STRUCTURE OF THE FREE ENERGY SURFACE OF COARSE-GRAINED OFF-LATTICE PROTEIN MODELS. International Journal of Modern Physics C, 2007, 18, 99-106.	0.8	2
75	Nonextensive Statistical Mechanics Application to Vibrational Dynamics of Protein Folding. International Journal of Theoretical Physics, 2007, 46, 2945-2949.	0.5	2
76	Mechanical and Electrical Monitoring in the Dynamics of Twisted Phosphorene Nanoflakes on 2D Monolayers. Journal of Physical Chemistry C, 2019, 123, 30704-30713.	1.5	2
77	Two dimensional ruthenium carbide: structural and electronic features. Physical Chemistry Chemical Physics, 2020, 22, 15488-15495.	1.3	2
78	Functionalization of monolayer MoS2 with transition metal oxide nanoclusters. Physica B: Condensed Matter, 2021, 619, 413245.	1.3	2
79	First-principles and Monte Carlo investigation of magnetic properties of two-dimensional transition metal alloyed boron-carbide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mi mathvariant="normal">r</mml:mi><mml:mi mathvariant="normal">F</mml:mi><mml:mi mathvariant="normal">e</mml:mi><mml:mi mathvariant="normal">B</mml:mi><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math>sheet. Computational Materials Science,	1.4	2
80	DIPEPTIDE ADSORPTION ON Si(100)-2 Ã— 1 ASYMMETRIC SURFACE BY FIRST PRINCIPLES. International Journal of Modern Physics C, 2010, 21, 97-106.	0.8	1
81	Electronic structure, cohesive and magnetic properties of iridium oxide clusters adsorbed on graphene. Journal of Molecular Graphics and Modelling, 2020, 101, 107726.	1.3	1
82	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. Journal of Molecular Structure, 2008, 886, 144-147.	1.8	0
83	Adsorption of small molecules on a Pmma CO monolayer. Journal of Physics and Chemistry of Solids, 2020, 139, 109300.	1.9	0
84	High uptake and fixation ability of BC monolayer for CO and NO toxic gases: a computational analysis. Journal of Materials Science, 2021, 56, 18566-18580.	1.7	0