E AktÃ¼rk

List of Publications by Year
in descending order

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	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	1.4	2
2	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
3	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
4	Functional Carbon and Silicon Monolayers in Biphenylene Network. ACS Applied Electronic Materials, 2022, 4, 3056-3070.	2.0	9
5	Dopingâ€Driven Antiferromagnetic to Ferromagnetic Phase Transition in Tetragonal Cr2B2 Monolayer. Physica Status Solidi (B): Basic Research, 2021, 258, 2000396.	0.7	9
6	Columnar antiferromagnetic order of a MBene monolayer. Physical Review B, 2021, 103, .	1.1	10
7	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
8	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
9	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:m (X=Cr, Ru) metal for high NÃ©el temperature antiferromagnetic spintronics. Journal of Solid State Chemistry, 2021, 302, 122427.	1.4	3
10	Functionalization of monolayer MoS2 with transition metal oxide nanoclusters. Physica B: Condensed Matter, 2021, 619, 413245.	1.3	2
11	Ferromagnetic TM₂BC (TM = Cr, Mn) monolayers for spintronic devices with high Curie temperature. Physical Chemistry Chemical Physics, 2021, 23, 6107-6115.	1.3	29
12	Magnetization of silicene via coverage with gadolinium: Effects of thickness, symmetry, strain, and coverage. Physical Review B, 2021, 104, .	1.1	5
13	Adsorption of small molecules on a Pmma CO monolayer. Journal of Physics and Chemistry of Solids, 2020, 139, 109300.	1.9	0
14	Free-standing and supported phosphorene nanoflakes: Shape- and size-dependent properties. Applied Surface Science, 2020, 506, 144756.	3.1	8
15	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
16	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
17	Exploring the potential of MnX (S, Sb) monolayers for antiferromagnetic spintronics: A theoretical investigation. Journal of Applied Physics, 2020, 128, .	1.1	15
18	Above Room Temperature Ferromagnetism in Gd₂B₂ Monolayer with High Magnetic Anisotropy. Journal of Physical Chemistry C, 2020, 124, 12816-12823.	1.5	25

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19	Two dimensional ruthenium carbide: structural and electronic features. Physical Chemistry Chemical Physics, 2020, 22, 15488-15495.	1.3	2
20	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
21	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
22	A new single-layer structure of MBene family: Ti₂B. Journal of Physics Condensed Matter, 2019, 31, 505401.	0.7	27
23	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
24	Deformed octagon-hexagon-square structure of group-IV and group-V elements and III-V compounds. Physical Review B, 2019, 100, .	1.1	7
25	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
26	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
27	Effect of point defects on electronic and magnetic properties of single-layer SiO. Philosophical Magazine, 2019, 99, 2340-2353.	0.7	3
28	Two-dimensional pnictogens: A review of recent progresses and future research directions. Applied Physics Reviews, 2019, 6, .	5.5	143
29	Functionalization of monolayer AsP phases by adatoms: a first-principles study. Materials Research Express, 2019, 6, 065032.	0.8	5
30	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
31	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
32	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
33	Glycine self-assembled on graphene enhances the solar absorbance performance. Carbon, 2019, 143, 329-334.	5.4	21
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	Functionalization of Single-Layer Nitrogene by Vacancy, Adatoms, and Molecules. Journal of Physical Chemistry C, 2017, 121, 6329-6338.	1.5	16
42	Tunable dynamics of a flake on graphene: Libration frequency. Physical Review B, 2017, 95, .	1.1	7
43	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
44	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
45	Half metallicity and pressure-induced electronic structure of monolayer FeX2 (X = S, Se). Materials Research Express, 2017, 4, 116305.	0.8	6
46	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
47	Modification of electronic structure, magnetic structure, and topological phase of bismuthene by point defects. Physical Review B, 2017, 96, .	1.1	54
48	Stable single-layer structure of group-V elements. Physical Review B, 2016, 94, .	1.1	108
49	T-ZrS nanoribbons: structure and electronic properties. Philosophical Magazine, 2016, 96, 2074-2087.	0.7	8
50	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
51	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:mo>(</mml:mo><mml:mrow><mml:mi>X</mml:mi><mml:mo>=</mml:mo> Physical Review B, 2016, 94, .	1.1	30
52	Investigation of adatom adsorption on single layer buckled germanium selenide. Applied Surface Science, 2016, 390, 185-189.	3.1	4
53	Single and bilayer bismuthene: Stability at high temperature and mechanical and electronic properties. Physical Review B, 2016, 94, .	1.1	295
54	Point defects in hexagonal germanium carbide monolayer: A first-principles calculation. Applied Surface Science, 2016, 389, 1-6.	3.1	62

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55	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
56	Interaction of Adatoms and Molecules with Single-Layer Arsenene Phases. Journal of Physical Chemistry C, 2016, 120, 14345-14355.	1.5	98
57	Effects of adatoms and physisorbed molecules on the physical properties of antimonene. Physical Review B, 2016, 93, .	1.1	84
58	Interactions of h-AlN monolayer with platinum, oxygen, and their clusters. Chemical Physics, 2015, 455, 73-80.	0.9	13
59	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
60	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
61	Silicon-based counterpart of alpha-graphyne. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1313-1315.	0.9	3
62	Effects of silver adatoms on the electronic structure of silicene. Applied Surface Science, 2014, 311, 9-13.	3.1	25
63	Electronic structure of BSb defective monolayers and nanoribbons. Journal of Physics Condensed Matter, 2014, 26, 325303.	0.7	9
64	Bimetallic two-dimensional PtAg coverage on h-BN substrate: First-principles calculations. Applied Surface Science, 2014, 303, 306-311.	3.1	20
65	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... M...	1.3	5
66	Adsorption of carbon adatoms to graphene and its nanoribbons. Journal of Applied Physics, 2011, 109, 013704.	1.1	59
67	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS₂. Journal of Physical Chemistry C, 2011, 115, 16354-16361.	1.5	298
68	Mechanical and Electronic Properties of MoS₂ Nanoribbons and Their Defects. Journal of Physical Chemistry C, 2011, 115, 3934-3941.	1.5	427
69	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
70	Effects of silicon and germanium adsorbed on graphene. Applied Physics Letters, 2010, 96, .	1.5	63
71	First-principles study of the iron pnictide superconductorBaFe2As2. Physical Review B, 2009, 79, .	1.1	43
72	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

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73	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. Physical Review B, 2009, 79, .	1.1	314
74	Monolayer honeycomb structures of group-IV elements and III-V binary compounds: First-principles calculations. Physical Review B, 2009, 80, .	1.1	1,769
75	First-principles study of two- and one-dimensional honeycomb structures of boron nitride. Physical Review B, 2009, 79, .	1.1	580
76	Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium. Physical Review Letters, 2009, 102, 236804.	2.9	2,837
77	Time Dependence of Joint Entropy of Oscillating Quantum Systems. International Journal of Theoretical Physics, 2008, 47, 3207-3218.	0.5	4
78	Can Sobolev Inequality Be Written for Sharma-Mittal Entropy?. International Journal of Theoretical Physics, 2008, 47, 3310-3320.	0.5	12
79	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. Journal of Molecular Structure, 2008, 886, 144-147.	1.8	0
80	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
81	High-capacity hydrogen storage by metallized graphene. Applied Physics Letters, 2008, 93, .	1.5	397
82	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
83	Nonextensive Statistical Mechanics Application to Vibrational Dynamics of Protein Folding. International Journal of Theoretical Physics, 2007, 46, 2945-2949.	0.5	2
84	SOLVATION EFFECTS ON FREE ENERGY SURFACE OF POLYALANINE. International Journal of Modern Physics C, 2005, 16, 1489-1496.	0.8	5