Yi Ding

List of Publications by Year in descending order

68 papers	3,844 citations	159585 30 h-index	123424 61 g-index
68 all docs	68 docs citations	68 times ranked	4520 citing authors

#	Article	IF	Citations
1	First principles study of structural, vibrational and electronic properties of graphene-like MX2 (M=Mo, Nb, W, Ta; X=S, Se, Te) monolayers. Physica B: Condensed Matter, 2011, 406, 2254-2260.	2.7	613
2	Ab initioprediction of stable boron sheets and boron nanotubes: Structure, stability, and electronic properties. Physical Review B, 2008, 77, .	3.2	315
3	Electronic structures of silicon nanoribbons. Applied Physics Letters, 2009, 95, .	3.3	276
4	Density Functional Theory Study of the Silicene-like SiX and XSi₃ (X = B, C, N, Al, P) Honeycomb Lattices: The Various Buckled Structures and Versatile Electronic Properties. Journal of Physical Chemistry C, 2013, 117, 18266-18278.	3.1	271
5	Structural, Electronic, and Magnetic Properties of Adatom Adsorptions on Black and Blue Phosphorene: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 10610-10622.	3.1	196
6	Electronic structures of silicene fluoride and hydride. Applied Physics Letters, 2012, 100, .	3.3	165
7	Electronic Structure and Carrier Mobilities of Arsenene and Antimonene Nanoribbons: A First-Principle Study. Nanoscale Research Letters, 2015, 10, 955.	5.7	137
8	Strain-induced self-doping in silicene and germanene from first-principles. Solid State Communications, 2013, 155, 6-11.	1.9	131
9	Electronic properties of graphene nanoribbons embedded in boron nitride sheets. Applied Physics Letters, 2009, 95, .	3.3	123
10	Electronic structures of silicene/GaS heterosheets. Applied Physics Letters, 2013, 103, .	3.3	105
11	Hydrogen-induced stabilization and tunable electronic structures of penta-silicene: a computational study. Journal of Materials Chemistry C, 2015, 3, 11341-11348.	5.5	85
12	Electronic structures of zigzag silicene nanoribbons with asymmetric sp2âˆ’sp3 edges. Applied Physics Letters, 2013, 102, .	3.3	74
13	Geometric and Electronic Structures of Two-Dimensional SiC₃ Compound. Journal of Physical Chemistry C, 2014, 118, 4509-4515.	3.1	74
14	The stabilities of boron nitride nanoribbons with different hydrogen-terminated edges. Applied Physics Letters, 2009, 94, .	3.3	73
15	Fluorination-induced half-metallicity in zigzag boron nitride nanoribbons: First-principles calculations. Physical Review B, 2010, 81, .	3.2	66
16	Highly active, stable and self-antimicrobial enzyme catalysts prepared by biomimetic mineralization of copper hydroxysulfate. Nanoscale, 2016, 8, 17440-17445.	5.6	60
17	Electronic structures of BC3 nanoribbons. Applied Physics Letters, 2009, 94, .	3.3	58
18	The electronic structures of group-Vâ€“group-IV hetero-bilayer structures: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 27769-27776.	2.8	54

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19	Electronic Structures of Porous Graphene, BN, and BC₂N Sheets with One- and Two-Hydrogen Passivations from First Principles. Journal of Physical Chemistry C, 2011, 115, 5334-5343.	3.1	48
20	Electronic structures of reconstructed zigzag silicene nanoribbons. Applied Physics Letters, 2014, 104, .	3.3	46
21	Electronic structures of zigzag SiC nanoribbons with asymmetric hydrogen-terminations. Applied Physics Letters, 2012, 101, 013102.	3.3	42
22	Electronic structures of boron nanoribbons. Applied Physics Letters, 2008, 93, .	3.3	40
23	Tuning Electronic Properties of Hydro-Boronâ^'Carbon Compounds by Hydrogen and Boron Contents: A First Principles Study. Journal of Physical Chemistry C, 2009, 113, 18468-18472.	3.1	39
24	Mechanical and electronic properties of stoichiometric silicene and germanene oxides from firstâ€principles. Physica Status Solidi - Rapid Research Letters, 2013, 7, 410-413.	2.4	38
25	Structural, Electronic, and Magnetic Properties of Defects in the BC₃ Sheet from First Principles. Journal of Physical Chemistry C, 2010, 114, 12416-12421.	3.1	37
26	An enzymeâ€“copper nanoparticle hybrid catalyst prepared from disassembly of an enzymeâ€“inorganic nanocrystal three-dimensional nanostructure. RSC Advances, 2016, 6, 20772-20776.	3.6	36
27	The hydrogen-induced structural stability and promising electronic properties of molybdenum and tungsten dinitride nanosheets: a first-principles study. Journal of Materials Chemistry C, 2016, 4, 7485-7493.	5.5	35
28	Electronic structures of graphane sheets with foreign atom substitutions. Applied Physics Letters, 2011, 98, .	3.3	34
29	Unexpected buckled structures and tunable electronic properties in arsenic nanosheets: insights from first-principles calculations. Journal of Physics Condensed Matter, 2015, 27, 225304.	1.8	33
30	Uncovering a Stable Phase in Group V Transition-metal Dinitride (MN₂, M = Ta, Nb, V) Nanosheets and Their Electronic Properties via First-principles Investigations. Journal of Physical Chemistry C, 2018, 122, 26748-26755.	3.1	32
31	Anisotropic elastic behaviour and one-dimensional metal in phosphorene. Physica Status Solidi - Rapid Research Letters, 2014, 8, 939-942.	2.4	29
32	Unusual structural and electronic properties of porous silicene and germanene: insights from first-principles calculations. Nanoscale Research Letters, 2015, 10, 13.	5.7	29
33	Electronic structures of fully fluorinated and semifluorinated zinc oxide sheets. Applied Physics Letters, 2010, 96, .	3.3	26
34	Electronic structures of Fe-terminated armchair boron nitride nanoribbons. Applied Physics Letters, 2011, 99, .	3.3	25
35	Computational Exploration of Stable 4d/5d Transition-Metal MSi₂N₄ (M =) Tj ETQq1 1 0.784314 rgBT /Ove Physical Chemistry C, 2021, 125, 19580-19591.	3.1	25
36	Quasi-Free-Standing Features of Stanene/Stanane on InSe and GaTe Nanosheets: A Computational Study. Journal of Physical Chemistry C, 2015, 119, 27848-27854.	3.1	24

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37	A first-principles study of a real energetically stable MoN₂ nanosheet and its tunable electronic structure. Journal of Materials Chemistry C, 2018, 6, 2245-2251.	5.5	23
38	Electronic and magnetic properties of 3d transition-metal selenides from first principles. Solid State Communications, 2009, 149, 505-509.	1.9	22
39	Switchable valley polarization and quantum anomalous Hall state in the VN2X2Y2 nanosheets (Xâ€‰=â€‰group-III and Yâ€‰=â€‰group-VI elements). Applied Physics Letters, 2021, 119, .	3.3	22
40	First-principles study of half-metallicity in semi-hydrogenated BC3, BC5, BC7, and B-doped graphone sheets. Nanoscale Research Letters, 2011, 6, 190.	5.7	20
41	Enhanced piezoelectricity and half-metallicity of fluorinated AlN nanosheets and nanoribbons: a first-principles study. Journal of Materials Chemistry C, 2016, 4, 1517-1526.	5.5	19
42	Firstâ€principles study of the electronic and magnetic properties of 4â€8 lineâ€defectâ€embedded BN sheets decorated with transition metals. Annalen Der Physik, 2014, 526, 415-422.	2.4	18
43	Tunable electronic structures of germanium monochalcogenide nanosheets via light non-metallic atom functionalization: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 23080-23088.	2.8	18
44	Intrinsic ferromagnetism and valley polarization in hydrogenated group V transition-metal dinitride (MN₂H₂, M = V/Nb/Ta) nanosheets: insights from first-principles. Nanoscale, 2020, 12, 1002-1012.	5.6	17
45	Ground-state phase diagram of Na_xCoO₂: correlation of Na ordering with CoO₂stacking sequences. Journal of Physics Condensed Matter, 2009, 21, 035401.	1.8	15
46	Stereo Boron Nitride Nanoribbons with Junction-Dependent Electronic Structures from First-Principles. Journal of Physical Chemistry C, 2012, 116, 5995-6003.	3.1	15
47	First-principles study of pressure effects on and. Solid State Communications, 2009, 149, 2125-2129.	1.9	12
48	Structural, Electronic, and Magnetic Properties of the Semifluorinated Boron Nitride Bilayer: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 3114-3121.	3.1	12
49	Intrinsic magnetism and electronic structure of graphene-like Be₃C₂ nanoribbons and their Si, Ge analogues: a computational study. Journal of Materials Chemistry C, 2017, 5, 10728-10736.	5.5	11
50	Surface functionalization of molybdenum dinitride nanosheets by halogen and alkali atoms: a first-principles study. Journal of Materials Chemistry C, 2017, 5, 683-689.	5.5	10
51	Adsorption on the carbon nanotubes. Frontiers of Physics in China, 2006, 1, 317-322.	1.0	9
52	Electronic structure and topological features of tin-based binary nanosheets and their hydrogenated/fluorinated derivatives: A first-principles study. Applied Surface Science, 2016, 382, 1-9.	6.1	9
53	Tunable electronic and magnetic properties of graphene-like XYBe₃ (XY = BN, AlN, SiC, GeC) nanosheets with carrier doping: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 6830-6837.	2.8	9
54	Tunable Electronic Structures of Hydrogenated Zigzag and Armchair Dumbbell Silicene Nanosheets: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 23208-23216.	3.1	9

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55	Stable H-Terminated Edges, Variable Semiconducting Properties, and Solar Cell Applications of C₃N Nanoribbons: A First-Principles Study. ACS Omega, 2018, 3, 8777-8786. First-principles study of two-dimensional MoN2X2Y2 (X=B<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 722 Td (xmlns:mml="http:/	3.5	9
56		6.1	9
57	with peculiar electronic and magnetic properties. Applied Surface Science, 2022, 593, 153317. Electronic structure of fluorinated and hydrogenated beryllium monoxide nanostructures. Physica Status Solidi - Rapid Research Letters, 2012, 6, 83-85.	2.4	8
58	Stabilizing the isolated Sn2Bi nanosheet and tailoring its electronic structure by chemical functionalization: A computational study. Applied Physics Letters, 2019, 114, .	3.3	8
59	Structural stability and the electronic properties of a (SiH)₂O-formed siloxene sheet: a computational study. Physical Chemistry Chemical Physics, 2017, 19, 18030-18035.	2.8	7
60	Tunable magnetic and electronic properties of BN nanosheets with triangular defects: a first-principles study. Journal of Physics Condensed Matter, 2014, 26, 435302.	1.8	6
61	Lattice thermal conductivities and thermoelectric performances of binary tin-based sheets: A computational study. Applied Surface Science, 2017, 396, 1164-1169.	6.1	6
62	Large-Gap Quantum Spin Hall States in the Bilayer Hexagonal Structure of Rhenium and Technetium Dinitrides: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 25524-25530.	3.1	6
63	Ground states of diatomic molecules adsorbed on single-walled carbon nanotubes. Physical Review B, 2006, 74, .	3.2	5
64	Electronic properties of boron nanotubes with axial strain. Frontiers of Physics in China, 2009, 4, 383-388.	1.0	5
65	Stable puckered C₂N₂ nanosheet with giant anisotropic hole carrier mobility: insights from first-principles. Journal of Materials Chemistry C, 2020, 8, 15655-15663.	5.5	4
66	First-principles study of bilayer hexagonal structure of SN₂ nanosheet: a highly stable non-metal platform for the quantum anomalous Hall effect. Journal of Materials Chemistry C, 2021, 9, 5961-5969.	5.5	4
67	First-principles study of the triwing graphene nanoribbons: junction-dependent electronic structures and electric field modulations. Physical Chemistry Chemical Physics, 2012, 14, 2040.	2.8	3
68	Back Cover: Mechanical and electronic properties of stoichiometric silicene and germanene oxides from firstâ€principles (Phys. Status Solidi RRL 6/2013). Physica Status Solidi - Rapid Research Letters, 2013, 7, .	2.4	0