Yi Ding

List of Publications by Year in Descending Order

67 papers	3,211 citations	27 h-index	56 g-index
68 ext. papers	3,551 ext. citations	4 avg, IF	5.95 L-index

#	Paper	IF	Citations
67	First-principles study of two-dimensional MoN2X2Y2 (X=B~In, Y=N~Te) nanosheets: The IIIⅣVI analogues of MoSi2N4 with peculiar electronic and magnetic properties. *Applied Surface Science*, **2022**, 593, 153317	6.7	0
66	Switchable valley polarization and quantum anomalous Hall state in the VN2X2Y2 nanosheets (X = group-III and Y = group-VI elements). *Applied Physics Letters*, **2021**, 119, 193101	3.4	1
65	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	7.1	1
64	Computational Exploration of Stable 4d/5d Transition-Metal MSi2N4 (M = Y□d and Hf□g) Nanosheets and Their Versatile Electronic and Magnetic Properties. *Journal of Physical Chemistry C*, **2021**, 125, 19580-19591	3.8	3
63	Intrinsic ferromagnetism and valley polarization in hydrogenated group V transition-metal dinitride (MNH, M = V/Nb/Ta) nanosheets: insights from first-principles. *Nanoscale*, **2020**, 12, 1002-1012	7.7	9
62	Stable puckered C2N2 nanosheet with giant anisotropic hole carrier mobility: insights from first-principles. *Journal of Materials Chemistry C*, **2020**, 8, 15655-15663	7.1	1
61	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	3.8	3
60	Stabilizing the isolated Sn2Bi nanosheet and tailoring its electronic structure by chemical functionalization: A computational study. *Applied Physics Letters*, **2019**, 114, 073103	3.4	8
59	Tunable electronic and magnetic properties of graphene-like XYBe (XY = BN, AlN, SiC, GeC) nanosheets with carrier doping: a first-principles study. *Physical Chemistry Chemical Physics*, **2018**, 20, 6830-6837	3.6	5
58	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	7.1	16
57	Stable H-Terminated Edges, Variable Semiconducting Properties, and Solar Cell Applications of CN Nanoribbons: A First-Principles Study. *ACS Omega*, **2018**, 3, 8777-8786	3.9	6
56	Tunable Electronic Structures of Hydrogenated Zigzag and Armchair Dumbbell Silicene Nanosheets: A Computational Study. *Journal of Physical Chemistry C*, **2018**, 122, 23208-23216	3.8	8
55	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	3.8	15
54	Structural stability and the electronic properties of a (SiH)O-formed siloxene sheet: a computational study. *Physical Chemistry Chemical Physics*, **2017**, 19, 18030-18035	3.6	5
53	Lattice thermal conductivities and thermoelectric performances of binary tin-based sheets: A computational study. *Applied Surface Science*, **2017**, 396, 1164-1169	6.7	6
52	Surface functionalization of molybdenum dinitride nanosheets by halogen and alkali atoms: a first-principles study. *Journal of Materials Chemistry C*, **2017**, 5, 683-689	7.1	8
51	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	7.1	9

50	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	7.1	24
49	An enzyme–copper nanoparticle hybrid catalyst prepared from disassembly of an enzyme–inorganic nanocrystal three-dimensional nanostructure. *RSC Advances*, **2016**, 6, 20772-20776	3.7	26
48	Enhanced piezoelectricity and half-metallicity of fluorinated AlN nanosheets and nanoribbons: a first-principles study. *Journal of Materials Chemistry C*, **2016**, 4, 1517-1526	7.1	16
47	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	6.7	8
46	Highly active, stable and self-antimicrobial enzyme catalysts prepared by biomimetic mineralization of copper hydroxysulfate. *Nanoscale*, **2016**, 8, 17440-17445	7.7	52
45	Tunable electronic structures of germanium monochalcogenide nanosheets via light non-metallic atom functionalization: a first-principles study. *Physical Chemistry Chemical Physics*, **2016**, 18, 23080-8	3.6	16
44	Electronic Structure and Carrier Mobilities of Arsenene and Antimonene Nanoribbons: A First-Principle Study. *Nanoscale Research Letters*, **2015**, 10, 955	5	117
43	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	3.8	167
42	The electronic structures of group-V-group-IV hetero-bilayer structures: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 27769-76	3.6	45
41	Hydrogen-induced stabilization and tunable electronic structures of penta-silicene: a computational study. *Journal of Materials Chemistry C*, **2015**, 3, 11341-11348	7.1	65
40	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	32
39	Quasi-Free-Standing Features of Stanene/Stanane on InSe and GaTe Nanosheets: A Computational Study. *Journal of Physical Chemistry C*, **2015**, 119, 27848-27854	3.8	22
38	Unusual structural and electronic properties of porous silicene and germanene: insights from first-principles calculations. *Nanoscale Research Letters*, **2015**, 10, 13	5	22
37	Electronic structures of reconstructed zigzag silicene nanoribbons. *Applied Physics Letters*, **2014**, 104, 083111	3.4	40
36	First-principles study of the electronic and magnetic properties of 4-8 line-defect-embedded BN sheets decorated with transition metals. *Annalen Der Physik*, **2014**, 526, 415-422	2.6	16
35	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
34	Anisotropic elastic behaviour and one-dimensional metal in phosphorene. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 939-942	2.5	24
33	Geometric and Electronic Structures of Two-Dimensional SiC3 Compound. *Journal of Physical Chemistry C*, **2014**, 118, 4509-4515	3.8	63

32	Electronic structures of silicene/GaS heterosheets. *Applied Physics Letters*, **2013**, 103, 043114	3.4	91
31	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	3.8	185
30	Strain-induced self-doping in silicene and germanene from first-principles. *Solid State Communications*, **2013**, 155, 6-11	1.6	114
29	Mechanical and electronic properties of stoichiometric silicene and germanene oxides from first-principles. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 410-413	2.5	33
28	Structural, Electronic, and Magnetic Properties of the Semifluorinated Boron Nitride Bilayer: A First-Principles Study. *Journal of Physical Chemistry C*, **2013**, 117, 3114-3121	3.8	11
27	Electronic structures of zigzag silicene nanoribbons with asymmetric sp2–sp3 edges. *Applied Physics Letters*, **2013**, 102, 143115	3.4	67
26	First-principles study of the triwing graphene nanoribbons: junction-dependent electronic structures and electric field modulations. *Physical Chemistry Chemical Physics*, **2012**, 14, 2040-9	3.6	3
25	Electronic structures of silicene fluoride and hydride. *Applied Physics Letters*, **2012**, 100, 083102	3.4	150
24	Stereo Boron Nitride Nanoribbons with Junction-Dependent Electronic Structures from First-Principles. *Journal of Physical Chemistry C*, **2012**, 116, 5995-6003	3.8	12
23	Electronic structures of zigzag SiC nanoribbons with asymmetric hydrogen-terminations. *Applied Physics Letters*, **2012**, 101, 013102	3.4	39
22	Electronic structure of fluorinated and hydrogenated beryllium monoxide nanostructures. *Physica Status Solidi - Rapid Research Letters*, **2012**, 6, 83-85	2.5	7
21	Electronic structures of Fe-terminated armchair boron nitride nanoribbons. *Applied Physics Letters*, **2011**, 99, 053123	3.4	22
20	First-principles study of half-metallicity in semi-hydrogenated BC3, BC5, BC7, and B-doped graphone sheets. *Nanoscale Research Letters*, **2011**, 6, 190	5	20
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	3.8	47
18	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	2.8	495
17	Electronic structures of graphane sheets with foreign atom substitutions. *Applied Physics Letters*, **2011**, 98, 163104	3.4	31
16	Fluorination-induced half-metallicity in zigzag boron nitride nanoribbons: First-principles calculations. *Physical Review B*, **2010**, 81,	3.3	62
15	Electronic structures of fully fluorinated and semifluorinated zinc oxide sheets. *Applied Physics Letters*, **2010**, 96, 213117	3.4	24

14	Structural, Electronic, and Magnetic Properties of Defects in the BC3 Sheet from First Principles. *Journal of Physical Chemistry C*, **2010**, 114, 12416-12421	3.8	32
13	Electronic structures of BC3 nanoribbons. *Applied Physics Letters*, **2009**, 94, 073111	3.4	50
12	Ground-state phase diagram of Na(x)CoO(2): correlation of Na ordering with CoO(2) stacking sequences. *Journal of Physics Condensed Matter*, **2009**, 21, 035401	1.8	15
11	Electronic properties of boron nanotubes with axial strain. *Frontiers of Physics in China*, **2009**, 4, 383-388		5
10	Electronic and magnetic properties of 3d transition-metal selenides from first principles. *Solid State Communications*, **2009**, 149, 505-509	1.6	19
9	First-principles study of pressure effects on and. *Solid State Communications*, **2009**, 149, 2125-2129	1.6	11
8	Tuning Electronic Properties of Hydro-Boron□Carbon Compounds by Hydrogen and Boron Contents: A First Principles Study. *Journal of Physical Chemistry C*, **2009**, 113, 18468-18472	3.8	33
7	Electronic structures of silicon nanoribbons. *Applied Physics Letters*, **2009**, 95, 083115	3.4	259
6	Electronic properties of graphene nanoribbons embedded in boron nitride sheets. *Applied Physics Letters*, **2009**, 95, 123105	3.4	111
5	The stabilities of boron nitride nanoribbons with different hydrogen-terminated edges. *Applied Physics Letters*, **2009**, 94, 233107	3.4	70
4	Electronic structures of boron nanoribbons. *Applied Physics Letters*, **2008**, 93, 043107	3.4	39
3	Ab initio prediction of stable boron sheets and boron nanotubes: Structure, stability, and electronic properties. *Physical Review B*, **2008**, 77,	3.3	280
2	Adsorption on the carbon nanotubes. *Frontiers of Physics in China*, **2006**, 1, 317-322		5
1	Ground states of diatomic molecules adsorbed on single-walled carbon nanotubes. *Physical Review B*, **2006**, 74,	3.3	4