Xiao-Bao Yang

List of Publications by Year
in descending order

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116 papers	3,822 citations	159525 30 h-index	133188 59 g-index
117 all docs	117 docs citations	117 times ranked	4594 citing authors

#	Article	IF	Citations
1	Ab initioprediction of stable boron sheets and boron nanotubes: Structure, stability, and electronic properties. Physical Review B, 2008, 77, .	1.1	315
2	Band-Gap Modulation in Single Bi³⁺-Doped Yttriumâ€“Scandiumâ€“Niobium Vanadates for Color Tuning over the Whole Visible Spectrum. Chemistry of Materials, 2016, 28, 2692-2703.	3.2	246
3	Effects of organic cations on the defect physics of tin halide perovskites. Journal of Materials Chemistry A, 2017, 5, 15124-15129.	5.2	213
4	Photo and pH Stable, Highly-Luminescent Silicon Nanospheres and Their Bioconjugates for Immunofluorescent Cell Imaging. Journal of the American Chemical Society, 2009, 131, 4434-4438.	6.6	193
5	Highly Efficient and Stable Narrow-Band Red Phosphor Cs₂SiF₆:Mn⁴⁺ for High-Power Warm White LED Applications. ACS Photonics, 2017, 4, 2556-2565.	3.2	177
6	Red Photoluminescence from Bi³⁺ and the Influence of the Oxygen-Vacancy Perturbation in ScVO₄: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 7515-7522.	1.5	164
7	Broadly tuning Bi³⁺ emission via crystal field modulation in solid solution compounds (Y,Lu,Sc)VO₄:Bi for ultraviolet converted white LEDs. Journal of Materials Chemistry C, 2014, 2, 6068-6076.	2.7	164
8	Two-Dimensional Anti-Vanâ€™t Hoff/Le Bel Array AlB₆ with High Stability, Unique Motif, Triple Dirac Cones, and Superconductivity. Journal of the American Chemical Society, 2019, 141, 3630-3640.	6.6	154
9	Electronic properties of single-walled silicon nanotubes compared to carbon nanotubes. Physical Review B, 2005, 72, .	1.1	145
10	Enhanced Transformation of Cr(VI) by Heterocyclic-N within Nitrogen-Doped Biochar: Impact of Surface Modulatory Persistent Free Radicals (PFRs). Environmental Science & Technology, 2020, 54, 8123-8132.	4.6	107
11	The nucleation and growth of borophene on the Ag (111) surface. Nano Research, 2016, 9, 2616-2622.	5.8	86
12	Stable calcium adsorbates on carbon nanostructures: Applications for high-capacity hydrogen storage. Physical Review B, 2009, 79, .	1.1	74
13	Bright Green Emission from Self-Trapped Excitons Triggered by Sb³⁺ Doping in Rb₄CdCl₆. Chemistry of Materials, 2022, 34, 5717-5725.	3.2	72
14	Catalytic Reactivity of CuNi Alloys toward H₂O and CO Dissociation for an Efficient Waterâ€“Gas Shift: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 745-752.	1.5	71
15	One-dimensional CuO nanowire: synthesis, electrical, and optoelectronic devices application. Nanoscale Research Letters, 2014, 9, 637.	3.1	71
16	Transparent and flexible selenium nanobelt-based visible light photodetector. CrystEngComm, 2012, 14, 1942.	1.3	68
17	Monolayer hexagonal arsenene with tunable electronic structures and magnetic properties via impurity doping. Journal of Materials Chemistry C, 2016, 4, 362-370.	2.7	64
18	Surface Passivation and Transfer Doping of Silicon Nanowires. Angewandte Chemie - International Edition, 2009, 48, 9896-9900.	7.2	57

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19	Two-Dimensional Semiconducting Boron Monolayers. Journal of the American Chemical Society, 2017, 139, 17233-17236.	6.6	57
20	Theoretical search for half-Heusler topological insulators. Physical Review B, 2015, 91, .	1.1	54
21	Processing-dependence and the nature of the blue-shift of Bi³⁺-related photoemission in ScVO₄at elevated temperatures. Journal of Materials Chemistry C, 2014, 2, 9850-9857.	2.7	53
22	Stability of transition metals on Mg(0001) surfaces and their effects on hydrogen adsorption. International Journal of Hydrogen Energy, 2012, 37, 309-317.	3.8	48
23	Zeroâ€Dimensional Organic Copper(I) Iodide Hybrid with High Antiâ€Water Stability for Blueâ€Lightâ€Excitable Solidâ€State Lighting. Advanced Optical Materials, 2022, 10, .	3.6	48
24	Transition-metal dispersion on carbon-doped boron nitride nanostructures: Applications for high-capacity hydrogen storage. Physical Review B, 2012, 86, .	1.1	45
25	Electronic structures of boron nanoribbons. Applied Physics Letters, 2008, 93, .	1.5	40
26	Wavelengthâ€Tunability and Multiband Emission from Singleâ€Site Mn²⁺ Doped CaO Through Antiferromagnetic Coupling and Tailored Superexchange Reactions. Advanced Optical Materials, 2017, 5, 1700070.	3.6	40
27	A systematic first-principles study of surface energies, surface relaxation and Friedel oscillation of magnesium surfaces. Journal Physics D: Applied Physics, 2014, 47, 115305.	1.3	39
28	Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. Physical Chemistry Chemical Physics, 2017, 19, 29237-29243.	1.3	39
29	Ideal Nodal Line Semimetal in a Two-Dimensional Boron Bilayer. Journal of Physical Chemistry C, 2019, 123, 4977-4983.	1.5	35
30	Firstâ€Principles Calculations of Quantum Efficiency for Point Defects in Semiconductors: The Example of Yellow Luminance by GaN: C_N+O_N and GaN:C_N. Advanced Optical Materials, 2017, 5, 1700404.	3.6	33
31	Fullâ€Color Chemically Modulated gâ€C₃N₄ for Whiteâ€Lightâ€Emitting Device. Advanced Optical Materials, 2019, 7, 1900775.	3.6	33
32	Controllable hydrogen adsorption and desorption by strain modulation on Ti decorated defective graphene. International Journal of Hydrogen Energy, 2015, 40, 12063-12071.	3.8	30
33	Calculations of hydrogen coverage on single-walled carbon nanotubes: Dependence on nanotube size, temperature, and pressure. Physical Review B, 2006, 74, .	1.1	28
34	Surface Defects-Induced p-type Conduction of Silicon Nanowires. Journal of Physical Chemistry C, 2011, 115, 18453-18458.	1.5	28
35	Opening the Band Gap of Graphene via Fluorination for High-Performance Dual-Mode Photodetector Application. ACS Applied Materials & Interfaces, 2019, 11, 21702-21710.	4.0	28
36	Understanding the stable boron clusters: A bond model and first-principles calculations based on high-throughput screening. Journal of Chemical Physics, 2015, 142, 214307.	1.2	27

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37	First-Principles Study of Biaxial Strain Effect on Hydrogen Adsorbed Mg (0001) Surface. Journal of Physical Chemistry C, 2012, 116, 14943-14949.	1.5	24
38	First-principle prediction of robust half-metallic Te-based half-Heusler alloys. Journal of Magnetism and Magnetic Materials, 2014, 350, 119-123.	1.0	24
39	First-Principles Study of Optoelectronic Properties of the Noble Metal (Ag and Pd) Doped BiOX (X = F,) Tj ETQq1 1 0.784314 rgBT /Ov	1.6	24
40	Bonding differences between single iron atoms versus iron chains with carbon nanotubes: First-principles calculations. Physical Review B, 2007, 76, .	1.1	22
41	Theoretical study of hydrogen dissociation and diffusion on Nb and Ni co-doped Mg(0001): A synergistic effect. Surface Science, 2012, 606, L45-L49.	0.8	21
42	An electron compensation mechanism for the polymorphism of boron monolayers. Nanoscale, 2018, 10, 13410-13416.	2.8	19
43	Theoretical Study of Oxygen-Vacancy Distribution in In₂O₃. Journal of Physical Chemistry C, 2021, 125, 7077-7085.	1.5	19
44	Surface Dangling Bond-Mediated Molecules Doping of Germanium Nanowires. Journal of Physical Chemistry C, 2011, 115, 24293-24299.	1.5	18
45	Unveiling White Light Emission of a One-Dimensional Cu(I)-Based Organometallic Halide toward Single-Phase Light-Emitting Diode Applications. Journal of Physical Chemistry Letters, 2021, 12, 12345-12351.	2.1	17
46	High-coverage stable structures of potassium adsorbed on single-walled carbon nanotubes. Physical Review B, 2004, 69, .	1.1	16
47	Geometrical eigen-subspace framework based molecular conformation representation for efficient structure recognition and comparison. Journal of Chemical Physics, 2017, 146, 154108.	1.2	16
48	Tailoring Cluster Configurations Enables Tunable Broad-Band Luminescence in Glass. Chemistry of Materials, 2020, 32, 8653-8661.	3.2	16
49	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. Journal of Materials Chemistry C, 2020, 8, 2798-2805.	2.7	16
50	Metal-semiconductor and semiconductor-semiconductor transitions in carbon nanotubes induced by intercalating alkali atoms. Physical Review B, 2005, 71, .	1.1	15
51	The role of oxygen defects in a bismuth doped ScVO₄ matrix: tuning luminescence by hydrogen treatment. Journal of Materials Chemistry C, 2017, 5, 314-321.	2.7	15
52	Biased screening for multi-component materials with Structures of Alloy Generation And Recognition (SAGAR). Computational Materials Science, 2021, 193, 110386.	1.4	15
53	Heavy Mn²⁺-doped near-infrared photon upconversion luminescence in fluoride RbZnF₃:Yb³⁺,Mn²⁺ guided by dopant distribution simulation. Journal of Materials Chemistry C, 2020, 8, 12164-12172.	2.7	14
54	Ground states of adsorbates on single-walled carbon nanotubes. Physical Review B, 2003, 67, .	1.1	13

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55	Ground states of group-IV nanostructures: Magic structures of diamond and silicon nanocrystals. Physical Review B, 2011, 83, .	1.1	13
56	Modeling and stabilities of Mg/MgH2 interfaces: A first-principles investigation. AIP Advances, 2014, 4, .	0.6	13
57	Atom Classification Model for Total Energy Evaluation of Two-Dimensional Multicomponent Materials. Journal of Physical Chemistry A, 2020, 124, 4506-4511.	1.1	13
58	A Practical Criterion for Screening Stable Boron Nanostructures. Journal of Physical Chemistry C, 2017, 121, 11950-11955.	1.5	13
59	Tuning the polarization and magnetism in BiCoO3 by strain and oxygen vacancy effect: A first-principle study. Journal of Applied Physics, 2012, 111, 013901.	1.1	12
60	Theoretical study of tunable magnetism of two-dimensional MnSe₂ through strain, charge, and defect. Journal of Physics Condensed Matter, 2021, 33, 215803.	0.7	12
61	Theoretical study of the influence of Na on CO adsorption and dissociation on Pd(111): Long-range or short-range interactions between co-adsorbates?. Chemical Physics Letters, 2011, 511, 33-38.	1.2	11
62	Theoretical investigation of structural stability and electronic properties of hydrogenated silicon nanocrystals: Size, shape, and surface reconstruction. Physical Review B, 2012, 86, .	1.1	11
63	Theoretical study of strain induced magnetic transition of single-layer CrTe3. Journal of Applied Physics, 2020, 127, .	1.1	11
64	Interaction between NO and Na, O, S, Cl on Au and Pd(111) surfaces. Physical Chemistry Chemical Physics, 2011, 13, 14466.	1.3	10
65	Role of organic cations on hybrid halide perovskite CH3NH3PbI3 surfaces. Journal of Solid State Chemistry, 2018, 258, 488-494.	1.4	10
66	Adsorption on the carbon nanotubes. Frontiers of Physics in China, 2006, 1, 317-322.	1.0	9
67	An efficient algorithm for spatially-correlated random fields generation and its applications on the two-phase material. Solid State Communications, 2014, 182, 30-33.	0.9	9
68	Theoretical investigations of the interaction between transition-metal and benzoquinone: Metal dispersion and hydrogen storage. International Journal of Hydrogen Energy, 2016, 41, 11275-11283.	3.8	9
69	High-coverage stable structures of 3d transition metal intercalated bilayer graphene. Physical Chemistry Chemical Physics, 2016, 18, 14244-14251.	1.3	9
70	An intrinsic representation of atomic structure: From clusters to periodic systems. Journal of Chemical Physics, 2017, 147, 144106.	1.2	9
71	An extended cluster expansion for ground states of heterofullerenes. Scientific Reports, 2017, 7, 16211.	1.6	9
72	Tuning the decay of Mn2+ emission via magnetically coupling with Cr3+ in ZnGa2O4. Journal of Applied Physics, 2018, 124, 063108.	1.1	9

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73	Role of intrinsic defects on the persistent luminescence of pristine and Mn doped ZnGa2O4. Journal of Applied Physics, 2019, 125, .	1.1	9
74	Doping induced charge density wave in monolayer TiS2 and phonon-mediated superconductivity. Journal of Applied Physics, 2020, 127, 044301.	1.1	9
75	Tuning<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mi>p</mml:mi><mml:mo stretchy="false">/</mml:mo><mml:mi>n</mml:mi></mml:math>conductivity in wurtzite transition metal monoxide: Role of native defects in CoO and MnO. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2635-2639.	0.9	8
76	Motif based high-throughput structure prediction of superconducting monolayer titanium boride. Physical Chemistry Chemical Physics, 2020, 22, 16236-16243.	1.3	8
77	Surface structure and phase transition of K adsorption on Au(111): By ab initio atomistic thermodynamics. Journal of Chemical Physics, 2012, 136, 044510.	1.2	7
78	Stable sandwich structures of two-dimensional iron borides FeB_xalloy: a first-principles calculation. RSC Advances, 2017, 7, 30320-30326.	1.7	7
79	Structural stabilities and electronic properties of Mg28-nAln clusters: A first-principles study. AIP Advances, 2017, 7, 095023.	0.6	7
80	Adsorptionâ€Free Growth of Ultraâ€Thin Molybdenum Membranes with a Lowâ€Symmetry Rectangular Lattice Structure. Small, 2020, 16, 2001325.	5.2	7
81	All-boron planar ferromagnetic structures: from clusters to monolayers. Nanoscale, 2021, 13, 9881-9887.	2.8	7
82	Unconventional line defects engineering in two-dimensional boron monolayers. Physical Review Materials, 2021, 5, .	0.9	7
83	Toward ferromagnetic semimetal ground state with multiple Weyl nodes in van der Waals crystal MnSb₄Te₇. New Journal of Physics, 2022, 24, 043033.	1.2	7
84	Ground states of potassium adsorbate on single-walled carbon nanotubes. Computer Physics Communications, 2005, 169, 20-23.	3.0	5
85	Effect of biaxial strain on half-metallicity of transition metal alloyed zinc-blende ZnO and GaAs: a first-principles study. Journal Physics D: Applied Physics, 2011, 44, 205002.	1.3	5
86	Competition between Pauli Exclusion and H-Bonding: H2O and NH3 on Silicene. Journal of Physical Chemistry C, 2016, 120, 19151-19159.	1.5	5
87	Gap maximum of graphene nanoflakes: a first-principles study combined with the Monte Carlo tree search method. RSC Advances, 2017, 7, 37881-37886.	1.7	5
88	H-Bond Interaction-Enhanced Dissociation of H₂O on Si(100)-2Ã—1. Journal of Physical Chemistry C, 2014, 118, 24603-24610.	1.5	4
89	Theoretical investigations on diamondoids (CnHm, n = 10â€“41): Nomenclature, structural stabilities, and gap distributions. Journal of Chemical Physics, 2018, 148, 014306.	1.2	4
90	Theoretical investigations on stable structures of C60-nNn (n=2â€“12): Symmetry, model interaction, and global optimization. Carbon, 2019, 154, 140-149.	5.4	4

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91	Energy landscape of Au₁₃: a global view of structure transformation. Physical Chemistry Chemical Physics, 2020, 22, 4402-4406.	1.3	4
92	Coupling experiments with calculations to understand the thermodynamics evolution for the sorption of zwitterionic ciprofloxacin on oxidizing-aged pyrogenic chars in the aquatic system. Journal of Hazardous Materials, 2021, 411, 125101.	6.5	4
93	Minimum Vertex-type Sequence Indexing for Clusters on Square Lattice. Scientific Reports, 2017, 7, 392.	1.6	3
94	The electronic properties of CH₃NH₃PbI₃ perovskite surfaces tuned by inverted polarities of pyridine and ethylamine. Journal of Materials Chemistry C, 2018, 6, 6733-6738.	2.7	3
95	Insights into the unusual semiconducting behavior in low-dimensional boron. Nanoscale, 2019, 11, 7866-7874.	2.8	3
96	High-performance CdScInO thin-film transistors and their stability improvement under negative bias (illumination) temperature stress. Journal of Materials Chemistry C, 2019, 7, 13960-13965.	2.7	3
97	Theoretical investigation of V2xFe2(1-x)Zr and ScxY1-xFe2 (0<x<1) quasi-binary alloy: Stable structures, mechanical and electronical properties. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126658.	0.9	3
98	Structural stabilities and optical properties of Si Ge H nanocrystals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126597.	0.9	3
99	Theoretical investigations for MFe2 (M = Y, La) Laves alloy and hydrides HxMFe2: Structural stability, lattice thermodynamics, and elastic properties. Solid State Communications, 2021, 337, 114452.	0.9	3
100	Theoretical studies of geometry asymmetry in tellurium nanostructures: intrinsic dipole, charge separation, and semiconductorâ€“metal transition. RSC Advances, 2014, 4, 44004-44010.	1.7	2
101	CNT-graphene heterostructures: First-principle study of electrical and thermal conductions. , 2017, , .		2
102	Improving Negative-Bias-Temperature-Stress Stability for Thin-Film Transistors by Doping Mg Into ScInO Semiconductor. IEEE Transactions on Electron Devices, 2019, 66, 2620-2623.	1.6	2
103	Quasilattice-Conserved Optimization of the Atomic Structure of Decagonal Ael-Co-Ni Quasicrystals. Chinese Physics Letters, 2015, 32, 036102.	1.3	1
104	The structural evolution of hydrogenated silicon carbide nanocrystals: an approach from bond energy model, Wangâ€“Landau method and first-principles studies. Journal Physics D: Applied Physics, 2016, 49, 245305.	1.3	1
105	Energy gaps of graphene clusters: the first-principles calculations based on high-throughput screening. Molecular Simulation, 2017, 43, 558-562.	0.9	1
106	Mg-X (X = Ni, Pd, Ti, Nb) interface and atomic mixture effect: a first-principles study. Materials Research Express, 2019, 6, 016305.	0.8	1
107	Quantum Dynamics Simulation of Doublet Excitation and Magnetic Field Effect in Neutral Radical Materials. Journal of Physical Chemistry Letters, 2020, 11, 1194-1198.	2.1	1
108	Oxidation of amines and their derivatives with persulfate without activation: Impact of mineral oxides and stoichiometric efficiency. Chemical Engineering Journal, 2021, 426, 131930.	6.6	1

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109	Theoretical prediction of solution and order-disorder transition in alloy materials. Wuli Xuebao/Acta Physica Sinica, 2021, .	0.2	1
110	Possible high-spin states in hydrogenated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mn>60</mml:mn></mml:msub></mml:math> molecules. Physical Review B, 2021, 104, .	1.1	1
111	Determining ground states of alloys by a symmetry-based classification. Physical Review Materials, 2022, 6, .	0.9	1
112	Configuration Sensitivity of Electrocatalytic Oxygen Reduction Reaction on Nitrogen-Doped Graphene. Journal of Physical Chemistry Letters, 2022, 13, 6187-6193.	2.1	1
113	Theoretical studies of the passivantsâ€™ effect on the SixGe1-x nanowires: Composition profiles, diameter, shape, and electronic properties. Journal of Chemical Physics, 2013, 139, 154713.	1.2	0
114	Temperature effect on the structural stabilities and electronic properties of X22H28 (X=C, Si and Ge) nanocrystals: A first-principles study. AIP Advances, 2016, 6, 125112.	0.6	0
115	THE TRANSPORT BEHAVIOR OF TYPICAL METALLIC FISSION PRODUCTS IN HTGRS. The Proceedings of the International Conference on Nuclear Engineering (ICONE), 2019, 2019.27, 1300.	0.0	0
116	Theoretical study of magnetic phase transition in La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mfrac><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:mfrac></mml:mrow><mml:mn xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mfrac><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:mfrac></mml:mrow><mml:mn Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 432, 128010.	0.9	0