Shengbai Zhang

List of Publications by Year in descending order

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240 papers	22,518 citations	9756 73 h-index	8835 145 g-index
241 all docs	241 docs citations	241 times ranked	21208 citing authors

#	Article	IF	Citations
1	Chemical potential dependence of defect formation energies in GaAs: Application to Ga self-diffusion. Physical Review Letters, 1991, 67, 2339-2342.	2.9	1,472
2	Defect physics of theCuInSe2chalcopyrite semiconductor. Physical Review B, 1998, 57, 9642-9656.	1.1	1,264
3	Origin ofp-type doping difficulty in ZnO:â€ƒThe impurity perspective. Physical Review B, 2002, 66, .	1.1	1,068
4	MoS₂ Nanoribbons: High Stability and Unusual Electronic and Magnetic Properties. Journal of the American Chemical Society, 2008, 130, 16739-16744.	6.6	876
5	Hydrogen Storage in Novel Organometallic Buckyballs. Physical Review Letters, 2005, 94, 155504.	2.9	629
6	Doping by Large-Size-Mismatched Impurities: The Microscopic Origin of Arsenic- or Antimony-Dopedp-Type Zinc Oxide. Physical Review Letters, 2004, 92, 155504.	2.9	584
7	Chemical trends of defect formation and doping limit in II-VI semiconductors:â€ƒThe case of CdTe. Physical Review B, 2002, 66, .	1.1	548
8	Effects of Ga addition to CuInSe2 on its electronic, structural, and defect properties. Applied Physics Letters, 1998, 72, 3199-3201.	1.5	482
9	Strong Covalency-Induced Recombination Centers in Perovskite Solar Cell Material CH₃NH₃PbI₃. Journal of the American Chemical Society, 2014, 136, 14570-14575.	6.6	462
10	Evidence for Native-Defect Donors inn-Type ZnO. Physical Review Letters, 2005, 95, 225502.	2.9	460
11	A phenomenological model for systematization and prediction of doping limits in IIâ€“VI and Iâ€“IIIâ€“VI2 compounds. Journal of Applied Physics, 1998, 83, 3192-3196.	1.1	412
12	First-principles calculation of band offsets, optical bowings, and defects in CdS, CdSe, CdTe, and their alloys. Journal of Applied Physics, 2000, 87, 1304-1311.	1.1	406
13	Control of Doping by Impurity Chemical Potentials: Predictions forp-Type ZnO. Physical Review Letters, 2001, 86, 5723-5726.	2.9	362
14	First-principles study of native defects in anataseTiO2. Physical Review B, 2006, 73, .	1.1	346
15	Graphene Oxide as an Ideal Substrate for Hydrogen Storage. ACS Nano, 2009, 3, 2995-3000.	7.3	342
16	Reversible Lithiumâ€ion Insertion in Molybdenum Oxide Nanoparticles. Advanced Materials, 2008, 20, 3627-3632.	11.1	330
17	Effects of Na on the electrical and structural properties of CuInSe2. Journal of Applied Physics, 1999, 85, 7214-7218.	1.1	322
18	Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. Physical Review Letters, 1997, 78, 4059-4062.	2.9	303

#	Article	IF	Citations
19	Nanostructured Carbon Allotropes with Weyl-like Loops and Points. Nano Letters, 2015, 15, 6974-6978.	4.5	302
20	Hydrogenation: A Simple Approach To Realize Semiconductorâ^'Half-Metalâ^'Metal Transition in Boron Nitride Nanoribbons. Journal of the American Chemical Society, 2010, 132, 1699-1705.	6.6	277
21	Dopant and defect energetics: Si in GaAs. Physical Review B, 1993, 47, 6791-6794.	1.1	264
22	ZnO light-emitting diode grown by plasma-assisted metal organic chemical vapor deposition. Applied Physics Letters, 2006, 88, 173506.	1.5	261
23	Theoretical study of the effects of isovalent coalloying of Bi and N in GaAs. Physical Review B, 2002, 65, .	1.1	235
24	Nitrogen Solubility and Induced Defect Complexes in Epitaxial GaAs:N. Physical Review Letters, 2001, 86, 1789-1792.	2.9	228
25	Half metallicity along the edge of zigzag boron nitride nanoribbons. Physical Review B, 2008, 78, .	1.1	226
26	High-pressure phases of III-V zinc-blende semiconductors. Physical Review B, 1987, 35, 7604-7610.	1.1	220
27	Structure stability and carrier localization inCdX(X=S,Se,Te)semiconductors. Physical Review B, 2000, 62, 6944-6947.	1.1	212
28	Microscopic Origin of the Phenomenological Equilibrium â€œDoping Limit Ruleâ€•inn-Type III-V Semiconductors. Physical Review Letters, 2000, 84, 1232-1235.	2.9	204
29	One order of magnitude faster phase change at reduced power in Ti-Sb-Te. Nature Communications, 2014, 5, 4086.	5.8	195
30	Topological Insulator Thin Films of Bi₂Te₃ with Controlled Electronic Structure. Advanced Materials, 2011, 23, 2929-2932.	11.1	194
31	Revealing the biexciton and trion-exciton complexes in BN encapsulated WSe2. Nature Communications, 2018, 9, 3719.	5.8	175
32	Chalcogenide perovskites â€“ an emerging class of ionic semiconductors. Nano Energy, 2016, 22, 129-135.	8.2	174
33	The microscopic origin of the doping limits in semiconductors and wide-gap materials and recent developments in overcoming these limits: a review. Journal of Physics Condensed Matter, 2002, 14, R881-R903.	0.7	169
34	First-principles study of cation distribution in eighteen closed-shell AIIB2IIIO4 and AIVB2IIO4 spinel oxides. Physical Review B, 2001, 63, .	1.1	162
35	Elemental Ferroelectricity and Antiferroelectricity in Groupâ€V Monolayer. Advanced Functional Materials, 2018, 28, 1707383.	7.8	145
36	Hydrogen passivation effect in nitrogen-doped ZnO thin films. Applied Physics Letters, 2005, 86, 122107.	1.5	139

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37	Tunable spin states in the two-dimensional magnet CrI₃. Nanoscale, 2018, 10, 14298-14303.	2.8	136
38	Stability of graphene oxide phases from first-principles calculations. Physical Review B, 2010, 82, .	1.1	124
39	Experimental observation of quantum oscillation of surface chemical reactivities. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9204-9208.	3.3	123
40	Co and Pt Dualâ€Singleâ€Atoms with Oxygenâ€Coordinated Coâ€“Oâ€“Pt Dimer Sites for Ultrahigh Photocatalytic Hydrogen Evolution Efficiency. Advanced Materials, 2021, 33, e2003327.	11.1	123
41	Quasiparticle intepretation of photoemission spectra and optical properties of GaAs(110). Physical Review Letters, 1989, 63, 2112-2115.	2.9	120
42	Native defects in second-generation topological insulators: Effect of spin-orbit interaction on Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	117
43	Discovering lead-free perovskite solar materials with a split-anion approach. Nanoscale, 2016, 8, 6284-6289.	2.8	116
44	Surface dimerization induced CuPtB versus CuPtA ordering of GaInP alloys. Applied Physics Letters, 1995, 67, 3141-3143.	1.5	112
45	Artificial nanocluster crystal: Lattice of identical Al clusters. Applied Physics Letters, 2002, 80, 3186-3188.	1.5	112
46	Na Adsorption on theSi(111)â"(7Ã—7)Surface: From Two-Dimensional Gas to Nanocluster Array. Physical Review Letters, 2003, 91, 126101.	2.9	110
47	New twinning route in face-centered cubic nanocrystalline metals. Nature Communications, 2017, 8, 2142.	5.8	110
48	Ultrahigh Photocatalytic CO₂ Reduction Efficiency and Selectivity Manipulation by Singleâ€Tungstenâ€Atom Oxide at the Atomic Step of TiO₂. Advanced Materials, 2022, 34, e2109074.	11.1	107
49	Wiring-Up Hydrogenase with Single-Walled Carbon Nanotubes. Nano Letters, 2007, 7, 3528-3534.	4.5	106
50	Fabrication and structural analysis of Al, Ga, and In nanocluster crystals. Physical Review B, 2002, 66, .	1.1	104
51	Three-dimensional Pentagon Carbon with a genesis of emergent fermions. Nature Communications, 2017, 8, 15641.	5.8	104
52	The role of collective motion in the ultrafast charge transfer in van der Waals heterostructures. Nature Communications, 2016, 7, 11504.	5.8	103
53	Confinement, surface, and chemisorption effects on the optical properties of Si quantum wires. Physical Review B, 1994, 50, 14405-14415.	1.1	102
54	Two-Dimensional Transition Metal Honeycomb Realized: Hf on Ir(111). Nano Letters, 2013, 13, 4671-4674.	4.5	102

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55	Interactions between nitrogen, hydrogen, and gallium vacancies inGaAs1â^'xNxalloys. Physical Review B, 2003, 67, .	1.1	99
56	Breakdown of the band-gap-common-cation rule:â€,â€,The origin of the small band gap of InN. Physical Review B, 2003, 67, .	1.1	97
57	Compensation in Al-Doped ZnO by Al-Related Acceptor Complexes: Synchrotron X-Ray Absorption Spectroscopy and Theory. Physical Review Letters, 2013, 110, 055502.	2.9	92
58	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). Solid State Communications, 1988, 66, 585-588.	0.9	91
59	Reconstruction and energetics of the polar (112) and(1Â¯1Â¯2Â¯)versus the nonpolar (220) surfaces ofCuInSe2. Physical Review B, 2002, 65, .	1.1	89
60	Element-resolved atomic structure imaging of rocksalt Ge2Sb2Te5 phase-change material. Applied Physics Letters, 2016, 108, .	1.5	89
61	Boron-Based Organometallic Nanostructures:â€‰ Hydrogen Storage Properties and Structure Stability. Nano Letters, 2008, 8, 157-161.	4.5	88
62	Method of linear combination of structural motifs for surface and step energy calculations: Application to GaAs(001). Physical Review B, 1996, 53, 1343-1356.	1.1	87
63	First-principles study of transparentp-type conductiveSrCu2O2and related compounds. Physical Review B, 2002, 65, .	1.1	85
64	Defect properties of CuInSe2 and CuGaSe2. Journal of Physics and Chemistry of Solids, 2005, 66, 1994-1999.	1.9	84
65	Control of conduction type in Al- and N-codoped ZnO thin films. Applied Physics Letters, 2005, 86, 202106.	1.5	83
66	Surface-reconstruction-enhanced solubility of N, P, As, and Sb in III-V semiconductors. Applied Physics Letters, 1997, 71, 677-679.	1.5	82
67	Effect of Spin State on the Dihydrogen Binding Strength to Transition Metal Centers in Metal-Organic Frameworks. Journal of the American Chemical Society, 2007, 129, 12606-12607.	6.6	82
68	Amphoteric Phosphorus Doping for Stable pâ€Type ZnO. Advanced Materials, 2007, 19, 3333-3337.	11.1	80
69	Band structure and stability of zinc-blende-based semiconductor polytypes. Physical Review B, 1999, 59, R2478-R2481.	1.1	79
70	Formation of extended hydrogen complexes in silicon. Physical Review B, 1991, 43, 12142-12145.	1.1	78
71	The Role of Ionic Liquid Electrolyte in an Aluminumâ€“Graphite Electrochemical Cell. ACS Energy Letters, 2017, 2, 689-693.	8.8	78
72	Borderline Magic Clustering: The Fabrication of Tetravalent Pb Cluster Arrays onSi(111)â^'(7Ã—7)Surfaces. Physical Review Letters, 2004, 93, 116103.	2.9	77

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73	Microscopic structure of hydrogenâ€“shallow-donor complexes in crystalline silicon. Physical Review B, 1990, 41, 3882-3884.	1.1	75
74	Electronic structure of semiconductor quantum films. Physical Review B, 1993, 48, 11204-11219.	1.1	73
75	Accurate and efficient calculation of van der Waals interactions within density functional theory by local atomic potential approach. Journal of Chemical Physics, 2008, 129, 154102.	1.2	73
76	Structural and electronic properties of the Al-GaAs(110) interface. Physical Review B, 1986, 34, 768-772.	1.1	72
77	Stability ofDXcenters inAlxGa1â^'xAs alloys. Physical Review B, 1990, 42, 7174-7177.	1.1	71
78	Impurity-bound small polarons in ZnO: Hybrid density functional calculations. Physical Review B, 2009, 80, .	1.1	71
79	First-principles calculations of a robust two-dimensional boron honeycomb sandwiching a triangular molybdenum layer. Physical Review B, 2014, 90, .	1.1	70
80	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. Physical Review B, 1989, 40, 3162-3168.	1.1	69
81	Size- and Surface-dependent Stability, Electronic Properties, and Potential as Chemical Sensors: Computational Studies on One-dimensional ZnO Nanostructures. Journal of Physical Chemistry C, 2008, 112, 13926-13931.	1.5	67
82	Dynamic Jahn-Teller Effect in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>NV</mml:mi><mml:mo>â^'</mml:mo></mml:msup></mml:math>Center in Diamond. Physical Review Letters, 2011, 107, 146403.	2.9	67
83	Quasiparticle band gap of organic-inorganic hybrid perovskites: Crystal structure, spin-orbit coupling, and self-energy effects. Physical Review B, 2016, 93, .	1.1	67
84	p-type behavior in nominally undoped ZnO thin films by oxygen plasma growth. Applied Physics Letters, 2006, 88, 262103.	1.5	66
85	Comparative Study of Carbon and BN Nanographenes: Ground Electronic States and Energy Gap Engineering. Journal of Physical Chemistry C, 2008, 112, 12677-12682.	1.5	66
86	Stability and Band-Gap Tuning of the Chalcogenide Perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BaZrS</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></ in Raman and Optical Investigations at High Pressures. Physical Review Applied, 2017, 8, .	1.5	65
87	Energetics of the As vacancy in GaAs: The stability of the 3+ charge state. Physical Review B, 1994, 50, 4962-4964.	1.1	64
88	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. Chemistry of Materials, 2016, 28, 5022-5028.	3.2	63
89	Optimizing photoelectrochemical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m chemical codoping. Physical Review B, 2010, 82, .	1.1	62
90	Modification of Defect Structures in Graphene by Electron Irradiation: Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2012, 116, 16070-16079.	1.5	61

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91	Atomic-Scale Magnetism of Cr-Doped Bi₂Se₃ Thin Film Topological Insulators. ACS Nano, 2015, 9, 10237-10243.	7.3	54
92	Machine Learning Augmented Discovery of Chalcogenide Double Perovskites for Photovoltaics. Advanced Theory and Simulations, 2019, 2, 1800173.	1.3	54
93	Ti-Alloying of BaZrS₃ Chalcogenide Perovskite for Photovoltaics. ACS Omega, 2020, 5, 18579-18583.	1.6	54
94	Direct Atom-by-Atom Chemical Identification of Nanostructures and Defects of Topological Insulators. Nano Letters, 2013, 13, 2851-2856.	4.5	53
95	Ultrahigh Photocatalytic Rate at a Singleâ€Metalâ€Atomâ€Oxide. Advanced Materials, 2019, 31, e1903491.	11.1	53
96	Titanium-decorated graphene oxide for carbon monoxide capture and separation. Physical Chemistry Chemical Physics, 2011, 13, 21126.	1.3	52
97	An Environmentally Stable and Leadâ€Free Chalcogenide Perovskite. Advanced Functional Materials, 2020, 30, 2001387.	7.8	52
98	Electron-Rich Driven Electrochemical Solid-State Amorphization in Liâ€“Si Alloys. Nano Letters, 2013, 13, 4511-4516.	4.5	51
99	Emergence of Nontrivial Lowâ€Energy Dirac Fermions in Antiferromagnetic EuCd₂As₂. Advanced Materials, 2020, 32, e1907565.	11.1	51
100	Multivalency-Induced Band Gap Opening at MoS₂ Edges. Chemistry of Materials, 2015, 27, 3326-3331.	3.2	50
101	Tip size effect on the appearance of a STM image for complex surfaces:â€ƒTheory versus experiment forSi(111)â^'(7Ã—7). Physical Review B, 2004, 70, .	1.1	49
102	Identification of magnetic dopants on the surfaces of topological insulators: Experiment and theory for Fe on Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Te<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>(111). Physical Review B, 2012, 85, .	1.1	49
103	A class of topological nodal rings and its realization in carbon networks. Physical Review B, 2018, 97, .	1.1	49
104	Regioselectivity control of graphene functionalization by ripples. Physical Chemistry Chemical Physics, 2011, 13, 19449.	1.3	46
105	Mapping the 3D surface potential in Bi2Se3. Nature Communications, 2013, 4, 2277.	5.8	46
106	Chalcogenide perovskite BaZrS3 thin-film electronic and optoelectronic devices by low temperature processing. Nano Energy, 2021, 85, 105959.	8.2	46
107	Crystalline Liquid and Rubber-Like Behavior in Cu Nanowires. Nano Letters, 2013, 13, 3812-3816.	4.5	45
108	Photoinduced Vacancy Ordering and Phase Transition in MoTe₂. Nano Letters, 2019, 19, 3612-3617.	4.5	43

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109	Highâ€Throughput Screening for Phaseâ€Change Memory Materials. Advanced Functional Materials, 2021, 31, 2009803.	7.8	43
110	Origin of high thermal stability of amorphous Ge1Cu2Te3 alloy: A significant Cu-bonding reconfiguration modulated by Te lone-pair electrons for crystallization. Acta Materialia, 2015, 90, 88-93.	3.8	42
111	Epitaxial Growth of Two-Dimensional Insulator Monolayer Honeycomb BeO. ACS Nano, 2021, 15, 2497-2505.	7.3	42
112	The crystalline/amorphous contact in Cu₂O/Ta₂O₅ heterostructures: increasing its sunlight-driven overall water splitting efficiency. Journal of Materials Chemistry A, 2017, 5, 2732-2738.	5.2	41
113	Bipolar Doping by Intrinsic Defects and Magnetic Phase Instability in Monolayer CrI₃. Chemistry of Materials, 2020, 32, 1545-1552.	3.2	41
114	Semi-Dirac semimetal in silicene oxide. Physical Chemistry Chemical Physics, 2017, 19, 3820-3825.	1.3	40
115	A two-step dry process for Cs₂SnI₆ perovskite thin film. Materials Research Letters, 2017, 5, 540-546.	4.1	40
116	Evolution of structural properties and formation of N-N split interstitials inGaAs1â^'xNxalloys. Physical Review B, 2005, 71, .	1.1	39
117	Impurity doping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Formation energies and defect levels from first-principles calculations. Physical Review B, 2010, 82, .	1.1	39
118	Vertical/Planar Growth and Surface Orientation of Bi₂Te₃ and Bi₂Se₃ Topological Insulator Nanoplates. Nano Letters, 2015, 15, 3147-3152.	4.5	39
119	Accuracy of density functional theory methods for weakly bonded systems: The case of dihydrogen binding on metal centers. Physical Review B, 2010, 82, .	1.1	38
120	A novel two-dimensional MgB₆ crystal: metal-layer stabilized boron kagome lattice. Physical Chemistry Chemical Physics, 2015, 17, 1093-1098.	1.3	38
121	Directional Forces by Momentumless Excitation and Order-to-Order Transition in Peierls-Distorted Solids: The Case of GeTe. Physical Review Letters, 2018, 120, 185701.	2.9	38
122	Stabilization mechanisms of polar surfaces: ZnO surfaces. Physical Review B, 2008, 78, .	1.1	37
123	Stacking Fault Enriching the Electronic and Transport Properties of Few-Layer Phosphorenes and Black Phosphorus. Nano Letters, 2016, 16, 1317-1322.	4.5	37
124	Homobenzene: Homoaromaticity and Homoantiaromaticity in Cycloheptatrienes. Journal of Physical Chemistry A, 2008, 112, 10586-10594.	1.1	36
125	Theory ofMnsupersaturation inSiandGe. Physical Review B, 2004, 70, .	1.1	35
126	Hydrogen in ZnO revisited: Bond center versus antibonding site. Physical Review B, 2008, 78, .	1.1	35

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127	Open-Shell Singlet Character of Stable Derivatives of Nonacene, Hexacene and Teranthene. Organic Letters, 2011, 13, 3316-3319.	2.4	35
128	Spin-Triplet Excitonic Insulator: The Case of Semihydrogenated Graphene. Physical Review Letters, 2020, 124, 166401.	2.9	35
129	Hydrogen pairs and local vibrational frequencies in H-irradiatedGaAs1âˆ’yNy. Physical Review B, 2005, 72, .	1.1	33
130	Regulating energy transfer of excited carriers and the case for excitation-induced hydrogen dissociation on hydrogenated graphene. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 908-911.	3.3	32
131	Time-dependent density-functional theory molecular-dynamics study on amorphization of Sc-Sb-Te alloy under optical excitation. Npj Computational Materials, 2020, 6, .	3.5	32
132	Achieving Ferromagnetism in Single-Crystalline ZnS Wurtzite Nanowires via Chromium Doping. Journal of Physical Chemistry C, 2010, 114, 12099-12103.	1.5	31
133	Metalâ€“Insulator Transition of Geâ€“Sbâ€“Te Superlattice: An Electron Counting Model Study. IEEE Nanotechnology Magazine, 2018, 17, 140-146.	1.1	31
134	Nanoscale Behavior and Manipulation of the Phase Transition in Singleâ€Crystal Cu₂Se. Advanced Materials, 2019, 31, e1804919.	11.1	31
135	Structure and sources of disorder in poly(3-hexylthiophene) crystals investigated by density functional calculations with van der Waals interactions. Physical Review B, 2011, 83, .	1.1	30
136	Theoretical Insights into the Structures of Graphene Oxide and Its Chemical Conversions Between Graphene. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2406-2422.	0.4	30
137	Local structure ofCuIn3Se5:X-ray absorption fine structure study and first-principles calculations. Physical Review B, 2003, 68, .	1.1	29
138	Endohedral Metalloborofullerenes La2@B80 and Sc3N@B80: A Density Functional Theory Prediction. Journal of Physical Chemistry A, 2009, 113, 11613-11618.	1.1	29
139	Ab initiocalculations predicting the existence of an oxidized calcium dihydrogen complex to store molecular hydrogen in densities up to 100 g/L. Physical Review B, 2009, 79, .	1.1	29
140	Half-Excitonic Insulator: A Single-Spin Bose-Einstein Condensate. Physical Review Letters, 2019, 122, 236402.	2.9	29
141	Method for defect stability diagram fromab initiocalculations: A case study of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	28
142	Molecular doping of ZnO by ammonia: a possible shallow acceptor. Journal of Materials Chemistry C, 2015, 3, 339-344.	2.7	28
143	Charged defects in two-dimensional semiconductors of arbitrary thickness and geometry: Formulation and application to few-layer black phosphorus. Physical Review B, 2017, 96, .	1.1	28
144	Electronic structure of identical metal cluster arrays onSi(111)â˜7Ã—7surfaces. Physical Review B, 2005, 72, .	1.1	27

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145	Band Alignment and the Built-in Potential of Solids. Physical Review Letters, 2018, 121, 196802.	2.9	27
146	Semimetal or Semiconductor: The Nature of High Intrinsic Electrical Conductivity in TiS₂. Journal of Physical Chemistry Letters, 2019, 10, 6996-7001.	2.1	27
147	Ab initiostructural characterization of a hydrogen-covered diamond (001) surface. Physical Review B, 2004, 70, .	1.1	26
148	Self-Assembly of Linear Arrays of Semiconductor Nanoparticles on Carbon Single-Walled Nanotubesâ€. Journal of Physical Chemistry B, 2006, 110, 25153-25157.	1.2	26
149	A Nanoscale Jigsawâ€Puzzle Approach to Large Ï€â€Conjugated Systems. Angewandte Chemie - International Edition, 2010, 49, 6764-6767.	7.2	26
150	DXcenters in GaAs and GaSb. Physical Review B, 2005, 72, .	1.1	25
151	Role of nano in catalysis: Palladium catalyzed hydrogen desorption from nanosized magnesium hydride. Nano Energy, 2013, 2, 742-748.	8.2	25
152	Realizing an intrinsic excitonic insulator by decoupling exciton binding energy from the minimum band gap. Physical Review B, 2018, 98, .	1.1	25
153	Defect tolerance in chalcogenide perovskite photovoltaic material BaZrS3. Science China Materials, 2021, 64, 2976-2986.	3.5	25
154	van der Waals epitaxy of CdS thin films on single-crystalline graphene. Applied Physics Letters, 2017, 110, .	1.5	24
155	Graphite-like surface reconstructions on C{111} and their implication forn-type diamond. Physical Review B, 2002, 66, .	1.1	22
156	Atomic scale high-angle annular dark field STEM analysis of the N configuration in dilute nitrides of GaAs. Physical Review B, 2009, 80, .	1.1	22
157	Structures and lattice energies of molecular crystals using density functional theory: Assessment of a local atomic potential approach. Chemical Physics Letters, 2012, 550, 94-98.	1.2	22
158	Direct observation of Pt nanocrystal coalescence induced by electron-excitation-enhanced van der Waals interactions. Nano Research, 2014, 7, 308-314.	5.8	22
159	Enhanced dihydrogen adsorption in symmetry-lowered metalâ€“porphyrin-containing frameworks. Physical Chemistry Chemical Physics, 2009, 11, 11400.	1.3	21
160	Interactions between Al12X (X = Al, C, N and P) nanoparticles and DNA nucleobases/base pairs: implications for nanotoxicity. Journal of Molecular Modeling, 2012, 18, 559-568.	0.8	21
161	Enhancing the ambient stability of few-layer black phosphorus by surface modification. RSC Advances, 2018, 8, 14676-14683.	1.7	21
162	Realization of semiconducting layered multiferroic heterojunctions via asymmetrical magnetoelectric coupling. Physical Review B, 2021, 103, .	1.1	21

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163	Band structures and native defects of ammonia borane. Physical Review B, 2009, 80, .	1.1	20
164	Correlated High-Pressure Phase Sequence of VO₂ under Strong Compression. Journal of Physical Chemistry Letters, 2018, 9, 2388-2393.	2.1	20
165	Excitation to defect-bound band edge states in two-dimensional semiconductors and its effect on carrier transport. Npj Computational Materials, 2019, 5, .	3.5	20
166	Realization of AlSb in the Double-Layer Honeycomb Structure: A Robust Class of Two-Dimensional Material. ACS Nano, 2021, 15, 8184-8191.	7.3	20
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