Shengbai Zhang

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

235 papers	19,196 citations	70 h-index	135 g-index
241 ext. papers	20,889 ext. citations	7.2 avg, IF	6.76 L-index

#	Paper	IF	Citations
235	Defect tolerance in CsPbI3: reconstruction of the potential energy landscape and band degeneracy in spin□rbit coupling. *Journal of Materials Chemistry A*, **2022**, 10, 3018-3024	13	3
234	Defects in Statically Unstable Solids: The Case for Cubic Perovskite □CsPbI3. *Chinese Physics Letters* , **2022**, 39, 046101	1.8	1
233	Ultrahigh Photocatalytic CO Reduction Efficiency and Selectivity Manipulation by Single-Tungsten-Atom Oxide at the Atomic Step of TiO.. *Advanced Materials*, **2022**, e2109074	24	7
232	Dative epitaxy of commensurate monocrystalline covalent-van der Waals moir□supercrystal.. *Advanced Materials*, **2022**, e2200117	24	6
231	High-Stability Light-Element Magnetic Superatoms Determined by Hund's Rule.. *Journal of Physical Chemistry Letters*, **2022**, 2632-2637	6.4	0
230	Realization of AlSb in the Double-Layer Honeycomb Structure: A Robust Class of Two-Dimensional Material. *ACS Nano*, **2021**, 15, 8184-8191	16.7	4
229	High-Throughput Screening for Phase-Change Memory Materials. *Advanced Functional Materials*, **2021**, 31, 2009803	15.6	15
228	Realization of semiconducting layered multiferroic heterojunctions via asymmetrical magnetoelectric coupling. *Physical Review B*, **2021**, 103,	3.3	5
227	Orientation-Controlled Large-Area Epitaxial PbI Thin Films with Tunable Optical Properties. *ACS Applied Materials & Interfaces*, **2021**, 13, 32450-32460	9.5	3
226	Chalcogenide perovskite BaZrS3 thin-film electronic and optoelectronic devices by low temperature processing. *Nano Energy*, **2021**, 85, 105959	17.1	13
225	Epitaxial Growth of Two-Dimensional Insulator Monolayer Honeycomb BeO. *ACS Nano*, **2021**, 15, 2497-2505	17	13
224	Co and Pt Dual-Single-Atoms with Oxygen-Coordinated Co-O-Pt Dimer Sites for Ultrahigh Photocatalytic Hydrogen Evolution Efficiency. *Advanced Materials*, **2021**, 33, e2003327	24	42
223	Remote Passivation in Two-Dimensional Materials: The Case of the Monolayer-Bilayer Lateral Junction of MoSe. *Journal of Physical Chemistry Letters*, **2021**, 12, 8046-8052	6.4	0
222	Mexican-hat potential energy surface in two-dimensional III2-VI3 materials and the importance of entropy barrier in ultrafast reversible ferroelectric phase change. *Applied Physics Reviews*, **2021**, 8, 031413	17.3	1
221	Ligand-Assisted Charge-Transfer Mechanism: The Case of CdSe/Cysteine/MoS Heterostructures.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12329-12335	6.4	0
220	Ultrafast processes in photochromic material YHxOy studied by excited-state density functional theory simulation. *Science China Materials*, **2020**, 63, 1579-1587	7.1	9
219	Emergence of Nontrivial Low-Energy Dirac Fermions in Antiferromagnetic EuCd As. *Advanced Materials*, **2020**, 32, e1907565	24	14

218	Bipolar Doping by Intrinsic Defects and Magnetic Phase Instability in Monolayer CrI3. *Chemistry of Materials*, **2020**, 32, 1545-1552	9.6	13
217	Time-dependent density-functional theory molecular-dynamics study on amorphization of Sc-Sb-Te alloy under optical excitation. *Npj Computational Materials*, **2020**, 6,	10.9	14
216	An Environmentally Stable and Lead-Free Chalcogenide Perovskite. *Advanced Functional Materials*, **2020**, 30, 2001387	15.6	23
215	Spin-Triplet Excitonic Insulator: The Case of Semihydrogenated Graphene. *Physical Review Letters*, **2020**, 124, 166401	7.4	9
214	Phase Transition in a Memristive Suspended MoS Monolayer Probed by Opto- and Electro-Mechanics. *ACS Nano*, **2020**, 14, 13611-13618	16.7	5
213	Carrier Dynamics and Transfer across the CdS/MoS Interface upon Optical Excitation. *Journal of Physical Chemistry Letters*, **2020**, 11, 6544-6550	6.4	7
212	Polarity- and Pressure-Dependent Hydrogen Dynamics on ZnO Polar Surfaces Revealed by Near-Ambient-Pressure X-ray Photoelectron Spectroscopy. *Journal of Physical Chemistry C*, **2020**, 124, 25431-25436	3.8	4
211	Ti-Alloying of BaZrS Chalcogenide Perovskite for Photovoltaics. *ACS Omega*, **2020**, 5, 18579-18583	3.9	20
210	Anisotropic band structure of TiS3 nanoribbon revealed by polarized photocurrent spectroscopy. *Applied Physics Letters*, **2020**, 117, 073101	3.4	1
209	Octahedron rotation evolution in 2D perovskites and its impact on optoelectronic properties: the case of Ba$_2$ZrS$_3$ chalcogenides. *Materials Horizons*, **2020**, 7, 2985-2993	14.4	8
208	Vector potential and surface magnetic field in magnetoelectric antiferromagnetic materials. *Physical Review B*, **2020**, 102,	3.3	1
207	Optical subpicosecond nonvolatile switching and electron-phonon coupling in ferroelectric materials. *Physical Review B*, **2020**, 102,	3.3	4
206	Semimetal or Semiconductor: The Nature of High Intrinsic Electrical Conductivity in TiS. *Journal of Physical Chemistry Letters*, **2019**, 10, 6996-7001	6.4	10
205	Understanding the origin of bandgap problem in transition and post-transition metal oxides. *Journal of Chemical Physics*, **2019**, 151, 124703	3.9	3
204	Excitation to defect-bound band edge states in two-dimensional semiconductors and its effect on carrier transport. *Npj Computational Materials*, **2019**, 5,	10.9	13
203	Half-Excitonic Insulator: A Single-Spin Bose-Einstein Condensate. *Physical Review Letters*, **2019**, 122, 236402	7.4	10
202	Long-range magnetic order stabilized by acceptors. *Physical Review B*, **2019**, 99,	3.3	3
201	Photoinduced Vacancy Ordering and Phase Transition in MoTe. *Nano Letters*, **2019**, 19, 3612-3617	11.5	30

200	Machine Learning Augmented Discovery of Chalcogenide Double Perovskites for Photovoltaics. *Advanced Theory and Simulations*, **2019**, 2, 1800173	3.5	30
199	Ultrahigh Photocatalytic Rate at a Single-Metal-Atom-Oxide. *Advanced Materials*, **2019**, 31, e1903491	24	29
198	Spontaneous symmetry lowering of Si (001) towards two-dimensional ferro/antiferroelectric behavior. *Physical Review Materials*, **2019**, 3,	3.2	5
197	Nanoscale Behavior and Manipulation of the Phase Transition in Single-Crystal Cu Se. *Advanced Materials*, **2019**, 31, e1804919	24	17
196	Formation mechanism of twin domain boundary in 2D materials: The case for WTe2. *Nano Research*, **2019**, 12, 569-573	10	4
195	Elemental Ferroelectricity and Antiferroelectricity in Group-V Monolayer. *Advanced Functional Materials*, **2018**, 28, 1707383	15.6	86
194	Correlated High-Pressure Phase Sequence of VO under Strong Compression. *Journal of Physical Chemistry Letters*, **2018**, 9, 2388-2393	6.4	13
193	Enhancing the ambient stability of few-layer black phosphorus by surface modification.. *RSC Advances*, **2018**, 8, 14676-14683	3.7	15
192	Intercalated Chevrel Phase Mo6S8 as a Janus Material for Energy Generation and Storage. *ACS Applied Energy Materials*, **2018**, 1, 440-446	6.1	10
191	Metal□nsulator Transition of Ge$_3$Sb$_2$□e Superlattice: An Electron Counting Model Study. *IEEE Nanotechnology Magazine*, **2018**, 17, 140-146	2.6	26
190	Directional Forces by Momentumless Excitation and Order-to-Order Transition in Peierls-Distorted Solids: The Case of GeTe. *Physical Review Letters*, **2018**, 120, 185701	7.4	21
189	A class of topological nodal rings and its realization in carbon networks. *Physical Review B*, **2018**, 97,	3.3	32
188	Stochasticity in materials structure, properties, and processing-A review. *Applied Physics Reviews*, **2018**, 5,	17.3	10
187	Tuning the structures of two-dimensional cuprous oxide confined on Au(111). *Nano Research*, **2018**, 11, 5957-5967	10	7
186	Doping-induced antiferromagnetic bicollinear insulating state and superconducting temperature of monolayer FeSe systems. *Physical Review B*, **2018**, 98,	3.3	2
185	Realizing an intrinsic excitonic insulator by decoupling exciton binding energy from the minimum band gap. *Physical Review B*, **2018**, 98,	3.3	12
184	Nexus networks in carbon honeycombs. *Physical Review Materials*, **2018**, 2,	3.2	13
183	Band Alignment and the Built-in Potential of Solids. *Physical Review Letters*, **2018**, 121, 196802	7.4	17

182	Electronic fingerprints of Cr and V dopants in the topological insulator Sb2Te3. *Physical Review B*, **2018**, 98,	3.3	13
181	Electrical properties and structural transition of Ge2Sb2Te5 adjusted by rare-earth element Gd for nonvolatile phase-change memory. *Journal of Applied Physics*, **2018**, 124, 145107	2.5	8
180	Revealing the biexciton and trion-exciton complexes in BN encapsulated WSe. *Nature Communications*, **2018**, 9, 3719	17.4	105
179	Erratum to Metal Insulator Transition of GeSbTe Superlattice: An Electron Counting Model Study [Jan 18 140-146]. *IEEE Nanotechnology Magazine*, **2018**, 17, 614-614	2.6	
178	Red phosphorus in its two-dimensional limit: novel clathrates with varying band gaps and superior chemical stabilities. *Nanoscale*, **2018**, 10, 13969-13975	7.7	4
177	Tunable spin states in the two-dimensional magnet CrI. *Nanoscale*, **2018**, 10, 14298-14303	7.7	90
176	Semi-Dirac semimetal in silicene oxide. *Physical Chemistry Chemical Physics*, **2017**, 19, 3820-3825	3.6	19
175	The Role of Ionic Liquid Electrolyte in an Aluminum Graphite Electrochemical Cell. *ACS Energy Letters*, **2017**, 2, 689-693	20.1	57
174	van der Waals epitaxy of CdS thin films on single-crystalline graphene. *Applied Physics Letters*, **2017**, 110, 153104	3.4	23
173	Three-dimensional Pentagon Carbon with a genesis of emergent fermions. *Nature Communications*, **2017**, 8, 15641	17.4	81
172	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	13	30
171	Charged defects in two-dimensional semiconductors of arbitrary thickness and geometry: Formulation and application to few-layer black phosphorus. *Physical Review B*, **2017**, 96,	3.3	20
170	Stability and Band-Gap Tuning of the Chalcogenide Perovskite BaZrS3 in Raman and Optical Investigations at High Pressures. *Physical Review Applied*, **2017**, 8,	4.3	38
169	A two-step dry process for Cs2SnI6 perovskite thin film. *Materials Research Letters*, **2017**, 5, 540-546	7.4	27
168	New twinning route in face-centered cubic nanocrystalline metals. *Nature Communications*, **2017**, 8, 2142	17.4	75
167	Enhanced van der Waals epitaxy via electron transfer enabled interfacial dative bond formation. *Physical Review Materials*, **2017**, 1,	3.2	4
166	Discovering lead-free perovskite solar materials with a split-anion approach. *Nanoscale*, **2016**, 8, 6284-9	7.7	97
165	Phonon-Enabled Carrier Transport of Localized States at Non-Polar Semiconductor Surfaces: A First-Principles-Based Prediction. *Journal of Physical Chemistry Letters*, **2016**, 7, 3548-53	6.4	5

164	Nonlinear Electron-Lattice Interactions in a Wurtzite Semiconductor Enabled via Strongly Correlated Oxide. *Advanced Materials*, **2016**, 28, 8975-8982	24	9
163	Quasiparticle band gap of organic-inorganic hybrid perovskites: Crystal structure, spin-orbit coupling, and self-energy effects. *Physical Review B*, **2016**, 93,	3.3	53
162	Stability investigations on the non-vdW-exfoliated surfaces of the topological insulator Bi2Te3: A first-principles study. *Physical Review B*, **2016**, 93,	3.3	5
161	Solvent-Based Atomistic Theory for Doping Colloidal-Synthesized Quantum Dots via Cation Exchange. *Journal of Physical Chemistry C*, **2016**, 120, 27085-27090	3.8	6
160	The role of collective motion in the ultrafast charge transfer in van der Waals heterostructures. *Nature Communications*, **2016**, 7, 11504	17.4	79
159	Stacking Fault Enriching the Electronic and Transport Properties of Few-Layer Phosphorenes and Black Phosphorus. *Nano Letters*, **2016**, 16, 1317-22	11.5	35
158	Chalcogenide perovskites an emerging class of ionic semiconductors. *Nano Energy*, **2016**, 22, 129-135	17.1	104
157	Kinetics stabilized doping: computational optimization of carbon-doped anatase TiO2 for visible-light driven water splitting. *Physical Chemistry Chemical Physics*, **2016**, 18, 2776-83	3.6	13
156	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. *Chemistry of Materials*, **2016**, 28, 5022-5028	9.6	51
155	Manipulation of Optical Transmittance by Ordered-Oxygen-Vacancy in Epitaxial LaBaCoO Thin Films. *Scientific Reports*, **2016**, 6, 37496	4.9	6
154	Communication: Effect of accidental mode degeneracy on Raman intensity in 2D materials: Hybrid functional study of bilayer phosphorene. *Journal of Chemical Physics*, **2016**, 145, 021102	3.9	5
153	Element-resolved atomic structure imaging of rocksalt Ge2Sb2Te5 phase-change material. *Applied Physics Letters*, **2016**, 108, 191902	3.4	72
152	Possible n/p-type conductivity of two-dimensional graphene oxide by boron and nitrogen doping: Evaluated via constrained excitation. *Applied Physics Letters*, **2016**, 109, 203113	3.4	4
151	Anisotropic Strain Induced Directional Metallicity in Highly Epitaxial LaBaCoO Thin Films on (110) NdGaO. *Scientific Reports*, **2016**, 6, 37337	4.9	5
150	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	8.4	34
149	Multivalency-Induced Band Gap Opening at MoS2 Edges. *Chemistry of Materials*, **2015**, 27, 3326-3331	9.6	39
148	Vertical/Planar Growth and Surface Orientation of Bi2Te3 and Bi2Se3 Topological Insulator Nanoplates. *Nano Letters*, **2015**, 15, 3147-52	11.5	30
147	Nanostructured Carbon Allotropes with Weyl-like Loops and Points. *Nano Letters*, **2015**, 15, 6974-8	11.5	248

146	Atomic-Scale Magnetism of Cr-Doped Bi2Se3 Thin Film Topological Insulators. *ACS Nano*, **2015**, 9, 10237-43	13.7	46
145	Single-Crystal CdTe Homojunction Structures for Solar Cell Applications. *Journal of Electronic Materials*, **2015**, 44, 3118-3123	1.9	6
144	A novel two-dimensional MgB6 crystal: metal-layer stabilized boron kagome lattice. *Physical Chemistry Chemical Physics*, **2015**, 17, 1093-8	3.6	29
143	Molecular doping of ZnO by ammonia: a possible shallow acceptor. *Journal of Materials Chemistry C*, **2015**, 3, 339-344	7.1	24
142	Absolute redox potential of liquid water: a first-principles theory. *Chemical Science*, **2014**, 5, 1216-1220	9.4	7
141	One order of magnitude faster phase change at reduced power in Ti-Sb-Te. *Nature Communications*, **2014**, 5, 4086	17.4	158
140	The new phase [Tl$_5$Sb$_5$Se$_8$][Sn$_5$Sb$_5$Se$_8$]: a naturally formed semiconducting heterostructure with two-dimensional conductance. *Journal of the American Chemical Society*, **2014**, 136, 11079-84	16.4	10
139	Strong covalency-induced recombination centers in perovskite solar cell material CH3NH3PbI3. *Journal of the American Chemical Society*, **2014**, 136, 14570-5	16.4	374
138	Observation of Coulomb repulsion between Cu intercalants in CuxBi2Se3. *Physical Review B*, **2014**, 89,	3.3	8
137	First-principles calculations of a robust two-dimensional boron honeycomb sandwiching a triangular molybdenum layer. *Physical Review B*, **2014**, 90,	3.3	59
136	Direct observation of Pt nanocrystal coalescence induced by electron-excitation-enhanced van der Waals interactions. *Nano Research*, **2014**, 7, 308-314	10	19
135	Mapping the 3D surface potential in Bi$_2$Se$_3$. *Nature Communications*, **2013**, 4, 2277	17.4	43
134	Crystalline liquid and rubber-like behavior in Cu nanowires. *Nano Letters*, **2013**, 13, 3812-6	11.5	39
133	Two-dimensional transition metal honeycomb realized: Hf on Ir(111). *Nano Letters*, **2013**, 13, 4671-4	11.5	89
132	Electron-rich driven electrochemical solid-state amorphization in Li-Si alloys. *Nano Letters*, **2013**, 13, 4511-6	11.5	45
131	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, 908-11	11.5	29
130	Role of nano in catalysis: Palladium catalyzed hydrogen desorption from nanosized magnesium hydride. *Nano Energy*, **2013**, 2, 742-748	17.1	21
129	Compensation in Al-doped ZnO by Al-related acceptor complexes: synchrotron x-ray absorption spectroscopy and theory. *Physical Review Letters*, **2013**, 110, 055502	7.4	86

128	Direct atom-by-atom chemical identification of nanostructures and defects of topological insulators. *Nano Letters*, **2013**, 13, 2851-6	11.5	48
127	Electronic Structure and Mobility of Alkylated and Nonalkylated Organic Semiconductors: Role of van der Waals Interactions. *Applied Physics Express*, **2013**, 6, 071601	2.4	7
126	Interactions between AlX (X = Al, C, N and P) nanoparticles and DNA nucleobases/base pairs: implications for nanotoxicity. *Journal of Molecular Modeling*, **2012**, 18, 559-68	2	17
125	Bond maximization of graphene in hydrogen addition reactions. *Nanoscale*, **2012**, 4, 1171-6	7.7	13
124	Method for defect stability diagram from ab initio calculations: A case study of SrTiO3. *Physical Review B*, **2012**, 86,	3.3	27
123	Identification of magnetic dopants on the surfaces of topological insulators: Experiment and theory for Fe on Bi2Te3(111). *Physical Review B*, **2012**, 85,	3.3	47
122	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	2.5	19
121	Modification of Defect Structures in Graphene by Electron Irradiation: Ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2012**, 116, 16070-16079	3.8	55
120	Native defects in second-generation topological insulators: Effect of spin-orbit interaction on Bi2Se3. *Physical Review B*, **2012**, 86,	3.3	97
119	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. *Physical Review B*, **2012**, 85,	3.3	15
118	Dynamic Jahn-Teller effect in the NV(-) center in diamond. *Physical Review Letters*, **2011**, 107, 146403	7.4	49
117	Theoretical Insights into the Structures of Graphene Oxide and Its Chemical Conversions Between Graphene. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 2406-2422	0.3	28
116	Topological insulator thin films of Bi2Te3 with controlled electronic structure. *Advanced Materials*, **2011**, 23, 2929-32	24	172
115	Titanium-decorated graphene oxide for carbon monoxide capture and separation. *Physical Chemistry Chemical Physics*, **2011**, 13, 21126-31	3.6	48
114	Altering the spin state of transition metal centers in metal-organic frameworks by molecular hydrogen adsorption: a first-principles study. *Physical Chemistry Chemical Physics*, **2011**, 13, 5042-6	3.6	9
113	Regioselectivity control of graphene functionalization by ripples. *Physical Chemistry Chemical Physics*, **2011**, 13, 19449-53	3.6	39
112	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,	3.3	30
111	Open-shell singlet character of stable derivatives of nonacene, hexacene and teranthene. *Organic Letters*, **2011**, 13, 3316-9	6.2	33

110	Charged dopants in semiconductor nanowires under partially periodic boundary conditions. *Physical Review B*, **2011**, 83,	3.3	10
109	Optimizing photoelectrochemical properties of TiO2 by chemical codoping. *Physical Review B*, **2010**, 82,	3.3	57
108	Self-purification in Si nanocrystals: An energetics study. *Physical Review B*, **2010**, 82,	3.3	17
107	Hydrogenation: a simple approach to realize semiconductor-half-metal-metal transition in boron nitride nanoribbons. *Journal of the American Chemical Society*, **2010**, 132, 1699-705	16.4	254
106	Impurity doping in SiO2: Formation energies and defect levels from first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	31
105	Accuracy of density functional theory methods for weakly bonded systems: The case of dihydrogen binding on metal centers. *Physical Review B*, **2010**, 82,	3.3	34
104	Stability of graphene oxide phases from first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	113
103	Achieving Ferromagnetism in Single-Crystalline ZnS Wurtzite Nanowires via Chromium Doping. *Journal of Physical Chemistry C*, **2010**, 114, 12099-12103	3.8	27
102	A nanoscale jigsaw-puzzle approach to large π-conjugated systems. *Angewandte Chemie - International Edition*, **2010**, 49, 6764-7	16.4	25
101	Band structures and native defects of ammonia borane. *Physical Review B*, **2009**, 80,	3.3	20
100	Atomic scale high-angle annular dark field STEM analysis of the N configuration in dilute nitrides of GaAs. *Physical Review B*, **2009**, 80,	3.3	20
99	Impurity-bound small polarons in ZnO: Hybrid density functional calculations. *Physical Review B*, **2009**, 80,	3.3	68
98	Unexpected Coulomb binding between Ca and H+ in ZnO. *Journal of Vacuum Science & Technology B*, **2009**, 27, 1601		
97	Activated dissociation of O2 on Pb(111) surfaces by Pb adatoms. *Physical Review B*, **2009**, 80,	3.3	7
96	Endohedral metalloborofullerenes La2@B80 and Sc3N@B80: a density functional theory prediction. *Journal of Physical Chemistry A*, **2009**, 113, 11613-8	2.8	28
95	Graphene oxide as an ideal substrate for hydrogen storage. *ACS Nano*, **2009**, 3, 2995-3000	16.7	301
94	Enhanced dihydrogen adsorption in symmetry-lowered metal-porphyrin-containing frameworks. *Physical Chemistry Chemical Physics*, **2009**, 11, 11400-3	3.6	21
93	Ab initio calculations 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,	3.3	28

92	Half metallicity along the edge of zigzag boron nitride nanoribbons. *Physical Review B*, **2008**, 78,	3.3	211
91	Boron-based organometallic nanostructures: hydrogen storage properties and structure stability. *Nano Letters*, **2008**, 8, 157-61	11.5	83
90	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	3.9	70
89	MoS2 nanoribbons: high stability and unusual electronic and magnetic properties. *Journal of the American Chemical Society*, **2008**, 130, 16739-44	16.4	772
88	Comparative Study of Carbon and BN Nanographenes: Ground Electronic States and Energy Gap Engineering. *Journal of Physical Chemistry C*, **2008**, 112, 12677-12682	3.8	63
87	Homobenzene: homoaromaticity and homoantiaromaticity in cycloheptatrienes. *Journal of Physical Chemistry A*, **2008**, 112, 10586-94	2.8	31
86	Polarization driven covalently-bonded octahedral-twinning and backbone-peripheral-helical nanoarchitectures. *Nano Letters*, **2008**, 8, 2258-64	11.5	13
85	Stabilization mechanisms of polar surfaces: ZnO surfaces. *Physical Review B*, **2008**, 78,	3.3	36
84	Hydrogen in ZnO revisited: Bond center versus antibonding site. *Physical Review B*, **2008**, 78,	3.3	34
83	Reversible Lithium-Ion Insertion in Molybdenum Oxide Nanoparticles. *Advanced Materials*, **2008**, 20, 3627-3632	24	304
82	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	3.8	63
81	Wiring-up hydrogenase with single-walled carbon nanotubes. *Nano Letters*, **2007**, 7, 3528-34	11.5	91
80	Amphoteric Phosphorus Doping for Stable p-Type ZnO. *Advanced Materials*, **2007**, 19, 3333-3337	24	76
79	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, 12606-7	16.4	77
78	Experimental observation of quantum oscillation of surface chemical reactivities. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 9204-8	11.5	113
77	Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage. *Materials Research Society Symposia Proceedings*, **2007**, 1041, 1		
76	Nontrivial Tuning of the Hydrogen-Binding Energy to Fullerenes with Endohedral Metal Dopants. *Journal of Physical Chemistry C*, **2007**, 111, 13275-13279	3.8	9
75	5-7-5 line defects on As$_2$Si(100): A general stress-relief mechanism for V/IV surfaces. *Physical Review B*, **2006**, 74,	3.3	15

74	Dihydrogen bonding, p-type conductivity, and origin of change in work function of hydrogenated diamond (001) surfaces. *Physical Review B*, **2006**, 74,	3.3	9
73	ZnO light-emitting diode grown by plasma-assisted metal organic chemical vapor deposition. *Applied Physics Letters*, **2006**, 88, 173506	3.4	239
72	First-principles study of native defects in anatase TiO2. *Physical Review B*, **2006**, 73,	3.3	307
71	p-type behavior in nominally undoped ZnO thin films by oxygen plasma growth. *Applied Physics Letters*, **2006**, 88, 262103	3.4	62
70	Self-assembly of linear arrays of semiconductor nanoparticles on carbon single-walled nanotubes. *Journal of Physical Chemistry B*, **2006**, 110, 25153-7	3.4	24
69	Evidence for native-defect donors in n-type ZnO. *Physical Review Letters*, **2005**, 95, 225502	7.4	420
68	Hydrogen passivation effect in nitrogen-doped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 122107	3.4	134
67	DX centers in GaAs and GaSb. *Physical Review B*, **2005**, 72,	3.3	20
66	Defect properties of CuInSe2 and CuGaSe2. *Journal of Physics and Chemistry of Solids*, **2005**, 66, 1994-1999	3.9	73
65	Hydrogen storage in novel organometallic buckyballs. *Physical Review Letters*, **2005**, 94, 155504	7.4	568
64	Control of conduction type in Al- and N-codoped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 202106	3.4	81
63	Evolution of structural properties and formation of N-N split interstitials in GaAs1−xNx alloys. *Physical Review B*, **2005**, 71,	3.3	39
62	Electronic structure of identical metal cluster arrays on Si(111)77 surfaces. *Physical Review B*, **2005**, 72,	3.3	25
61	Hydrogen pairs and local vibrational frequencies in H-irradiated GaAs1−yNy. *Physical Review B*, **2005**, 72,	3.3	30
60	Identification of Ga-interstitial defects in GaNyP1−y and AlxGa1−xNyP1−y. *Physical Review B*, **2004**, 70,	3.3	18
59	Theory of Mn supersaturation in Si and Ge. *Physical Review B*, **2004**, 70,	3.3	34
58	Borderline magic clustering: the fabrication of tetravalent Pb cluster arrays on Si(111)-(7x7) surfaces. *Physical Review Letters*, **2004**, 93, 116103	7.4	73
57	Spin driving reconstructions on the GaAs(001):Mn surface. *Physical Review B*, **2004**, 69,	3.3	16

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