# Shengbai Zhang

## List of Publications by Citations



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|---|---|---|---|
| 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 | Chemical potential dependence of defect formation energies in GaAs: Application to Ga self-diffusion. *Physical Review Letters*, **1991**, 67, 2339-2342 | 7.4 | 1269 |
| 234 | Defect physics of the CuInSe2 chalcopyrite semiconductor. *Physical Review B*, **1998**, 57, 9642-9656 | 3.3 | 1128 |
| 233 | Origin of p-type doping difficulty in ZnO: The impurity perspective. *Physical Review B*, **2002**, 66, | 3.3 | 998 |
| 232 | MoS2 nanoribbons: high stability and unusual electronic and magnetic properties. *Journal of the American Chemical Society*, **2008**, 130, 16739-44 | 16.4 | 772 |
| 231 | Hydrogen storage in novel organometallic buckyballs. *Physical Review Letters*, **2005**, 94, 155504 | 7.4 | 568 |
| 230 | Doping by large-size-mismatched impurities: the microscopic origin of arsenic- or antimony-doped p-type zinc oxide. *Physical Review Letters*, **2004**, 92, 155504 | 7.4 | 549 |
| 229 | Chemical trends of defect formation and doping limit in II-VI semiconductors: The case of CdTe. *Physical Review B*, **2002**, 66, | 3.3 | 463 |
| 228 | Evidence for native-defect donors in n-type ZnO. *Physical Review Letters*, **2005**, 95, 225502 | 7.4 | 420 |
| 227 | Effects of Ga addition to CuInSe2 on its electronic, structural, and defect properties. *Applied Physics Letters*, **1998**, 72, 3199-3201 | 3.4 | 420 |
| 226 | Strong covalency-induced recombination centers in perovskite solar cell material CH3NH3PbI3. *Journal of the American Chemical Society*, **2014**, 136, 14570-5 | 16.4 | 374 |
| 225 | A phenomenological model for systematization and prediction of doping limits in II-VI and I-III-VI2 compounds. *Journal of Applied Physics*, **1998**, 83, 3192-3196 | 2.5 | 372 |
| 224 | 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 | 2.5 | 360 |
| 223 | Control of doping by impurity Cchemical potentials: predictions for p-type ZnO. *Physical Review Letters*, **2001**, 86, 5723-6 | 7.4 | 339 |
| 222 | First-principles study of native defects in anatase TiO2. *Physical Review B*, **2006**, 73, | 3.3 | 307 |
| 221 | Reversible Lithium-Ion Insertion in Molybdenum Oxide Nanoparticles. *Advanced Materials*, **2008**, 20, 3627-3632 | 21 | 304 |
| 220 | Graphene oxide as an ideal substrate for hydrogen storage. *ACS Nano*, **2009**, 3, 2995-3000 | 16.7 | 301 |
| 219 | Effects of Na on the electrical and structural properties of CuInSe2. *Journal of Applied Physics*, **1999**, 85, 7214-7218 | 2.5 | 283 |

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|---|---|---|---|
| 218 | Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. *Physical Review Letters*, **1997**, 78, 4059-4062 | 7.4 | 264 |
| 217 | 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 |
| 216 | Nanostructured Carbon Allotropes with Weyl-like Loops and Points. *Nano Letters*, **2015**, 15, 6974-8 | 11.5 | 248 |
| 215 | Dopant and defect energetics: Si in GaAs. *Physical Review B*, **1993**, 47, 6791-6794 | 3.3 | 248 |
| 214 | ZnO light-emitting diode grown by plasma-assisted metal organic chemical vapor deposition. *Applied Physics Letters*, **2006**, 88, 173506 | 3.4 | 239 |
| 213 | Theoretical study of the effects of isovalent coalloying of Bi and N in GaAs. *Physical Review B*, **2002**, 65, | 3.3 | 219 |
| 212 | Half metallicity along the edge of zigzag boron nitride nanoribbons. *Physical Review B*, **2008**, 78, | 3.3 | 211 |
| 211 | Nitrogen solubility and induced defect complexes in epitaxial GaAs:N. *Physical Review Letters*, **2001**, 86, 1789-92 | 7.4 | 208 |
| 210 | Structure stability and carrier localization in CdX(X=S,Se,Te) semiconductors. *Physical Review B*, **2000**, 62, 6944-6947 | 3.3 | 192 |
| 209 | High-pressure phases of III-V zinc-blende semiconductors. *Physical Review B*, **1987**, 35, 7604-7610 | 3.3 | 184 |
| 208 | Microscopic origin of the phenomenological equilibrium "Doping limit Rule" in n-type III-V semiconductors. *Physical Review Letters*, **2000**, 84, 1232-5 | 7.4 | 180 |
| 207 | Topological insulator thin films of Bi2Te3 with controlled electronic structure. *Advanced Materials*, **2011**, 23, 2929-32 | 24 | 172 |
| 206 | One order of magnitude faster phase change at reduced power in Ti-Sb-Te. *Nature Communications*, **2014**, 5, 4086 | 17.4 | 158 |
| 205 | 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 | 1.8 | 155 |
| 204 | First-principles study of cation distribution in eighteen closed-shell AIIB2IIIO4 and AIVB2IIO4 spinel oxides. *Physical Review B*, **2001**, 63, | 3.3 | 148 |
| 203 | Hydrogen passivation effect in nitrogen-doped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 122107 | 3.4 | 134 |
| 202 | Stability of graphene oxide phases from first-principles calculations. *Physical Review B*, **2010**, 82, | 3.3 | 113 |
| 201 | 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 |

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|---|---|---|---|
| 200 | Quasiparticle intepretation of photoemission spectra and optical properties of GaAs(110). *Physical Review Letters*, **1989**, 63, 2112-2115 | 7.4 | 113 |
| 199 | Artificial nanocluster crystal: Lattice of identical Al clusters. *Applied Physics Letters*, **2002**, 80, 3186-3188 | 3.4 | 108 |
| 198 | Na adsorption on the Si111-(7 x 7) surface: from two-dimensional gas to nanocluster array. *Physical Review Letters*, **2003**, 91, 126101 | 7.4 | 105 |
| 197 | Revealing the biexciton and trion-exciton complexes in BN encapsulated WSe. *Nature Communications*, **2018**, 9, 3719 | 17.4 | 105 |
| 196 | Chalcogenide perovskites an emerging class of ionic semiconductors. *Nano Energy*, **2016**, 22, 129-135 | 17.1 | 104 |
| 195 | Surface dimerization induced CuPtB versus CuPtA ordering of GaInP alloys. *Applied Physics Letters*, **1995**, 67, 3141-3143 | 3.4 | 104 |
| 194 | Fabrication and structural analysis of Al, Ga, and In nanocluster crystals. *Physical Review B*, **2002**, 66, | 3.3 | 102 |
| 193 | Discovering lead-free perovskite solar materials with a split-anion approach. *Nanoscale*, **2016**, 8, 6284-9 | 7.7 | 97 |
| 192 | Native defects in second-generation topological insulators: Effect of spin-orbit interaction on Bi2Se3. *Physical Review B*, **2012**, 86, | 3.3 | 97 |
| 191 | Confinement, surface, and chemisorption effects on the optical properties of Si quantum wires. *Physical Review B*, **1994**, 50, 14405-14415 | 3.3 | 95 |
| 190 | Breakdown of the band-gap-common-cation rule: The origin of the small band gap of InN. *Physical Review B*, **2003**, 67, | 3.3 | 93 |
| 189 | Wiring-up hydrogenase with single-walled carbon nanotubes. *Nano Letters*, **2007**, 7, 3528-34 | 11.5 | 91 |
| 188 | Tunable spin states in the two-dimensional magnet CrI. *Nanoscale*, **2018**, 10, 14298-14303 | 7.7 | 90 |
| 187 | Two-dimensional transition metal honeycomb realized: Hf on Ir(111). *Nano Letters*, **2013**, 13, 4671-4 | 11.5 | 89 |
| 186 | Quasiparticle calculation of valence band offset of AlAs-GaAs(001). *Solid State Communications*, **1988**, 66, 585-588 | 1.6 | 88 |
| 185 | Elemental Ferroelectricity and Antiferroelectricity in Group-V Monolayer. *Advanced Functional Materials*, **2018**, 28, 1707383 | 15.6 | 86 |
| 184 | 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 |
| 183 | Boron-based organometallic nanostructures: hydrogen storage properties and structure stability. *Nano Letters*, **2008**, 8, 157-61 | 11.5 | 83 |

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|---|---|---|---|
| 182 | Interactions between nitrogen, hydrogen, and gallium vacancies in GaAs1□Nx alloys. *Physical Review B*, **2003**, 67, | 3.3 | 83 |
| 181 | First-principles study of transparent p-type conductive SrCu2O2 and related compounds. *Physical Review B*, **2002**, 65, | 3.3 | 83 |
| 180 | Method of linear combination of structural motifs for surface and step energy calculations: Application to GaAs(001). *Physical Review B*, **1996**, 53, 1343-1356 | 3.3 | 83 |
| 179 | Reconstruction and energetics of the polar (112) and (1□1□2□) versus the nonpolar (220) surfaces of CuInSe2. *Physical Review B*, **2002**, 65, | 3.3 | 82 |
| 178 | Three-dimensional Pentagon Carbon with a genesis of emergent fermions. *Nature Communications*, **2017**, 8, 15641 | 17.4 | 81 |
| 177 | Control of conduction type in Al- and N-codoped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 202106 | 3.4 | 81 |
| 176 | The role of collective motion in the ultrafast charge transfer in van der Waals heterostructures. *Nature Communications*, **2016**, 7, 11504 | 17.4 | 79 |
| 175 | Surface-reconstruction-enhanced solubility of N, P, As, and Sb in III-V semiconductors. *Applied Physics Letters*, **1997**, 71, 677-679 | 3.4 | 78 |
| 174 | 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 |
| 173 | Amphoteric Phosphorus Doping for Stable p-Type ZnO. *Advanced Materials*, **2007**, 19, 3333-3337 | 24 | 76 |
| 172 | New twinning route in face-centered cubic nanocrystalline metals. *Nature Communications*, **2017**, 8, 2142 | 17.4 | 75 |
| 171 | Band structure and stability of zinc-blende-based semiconductor polytypes. *Physical Review B*, **1999**, 59, R2478-R2481 | 3.3 | 75 |
| 170 | Microscopic structure of hydrogen-shallow-donor complexes in crystalline silicon. *Physical Review B*, **1990**, 41, 3882-3884 | 3.3 | 74 |
| 169 | Borderline magic clustering: the fabrication of tetravalent Pb cluster arrays on Si(111)-(7x7) surfaces. *Physical Review Letters*, **2004**, 93, 116103 | 7.4 | 73 |
| 168 | Defect properties of CuInSe2 and CuGaSe2. *Journal of Physics and Chemistry of Solids*, **2005**, 66, 1994-1999 | 3.9 | 73 |
| 167 | Formation of extended hydrogen complexes in silicon. *Physical Review B*, **1991**, 43, 12142-12145 | 3.3 | 73 |
| 166 | Element-resolved atomic structure imaging of rocksalt Ge2Sb2Te5 phase-change material. *Applied Physics Letters*, **2016**, 108, 191902 | 3.4 | 72 |
| 165 | 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 |

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|---|---|---|---|
| 164 | Stability of DX centers in AlxGa1-xAs alloys. *Physical Review B*, **1990**, 42, 7174-7177 | 3.3 | 69 |
| 163 | Structural and electronic properties of the Al-GaAs(110) interface. *Physical Review B*, **1986**, 34, 768-772 | 3.3 | 69 |
| 162 | Impurity-bound small polarons in ZnO: Hybrid density functional calculations. *Physical Review B*, **2009**, 80, | 3.3 | 68 |
| 161 | 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 |
| 160 | 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 |
| 159 | p-type behavior in nominally undoped ZnO thin films by oxygen plasma growth. *Applied Physics Letters*, **2006**, 88, 262103 | 3.4 | 62 |
| 158 | Electronic structure of semiconductor quantum films. *Physical Review B*, **1993**, 48, 11204-11219 | 3.3 | 61 |
| 157 | Energetics of the As vacancy in GaAs: The stability of the 3+ charge state. *Physical Review B*, **1994**, 50, 4962-4964 | 3.3 | 60 |
| 156 | First-principles calculations of a robust two-dimensional boron honeycomb sandwiching a triangular molybdenum layer. *Physical Review B*, **2014**, 90, | 3.3 | 59 |
| 155 | Evaluation of quasiparticle energies for semiconductors without inversion symmetry. *Physical Review B*, **1989**, 40, 3162-3168 | 3.3 | 58 |
| 154 | The Role of Ionic Liquid Electrolyte in an Aluminum□Graphite Electrochemical Cell. *ACS Energy Letters*, **2017**, 2, 689-693 | 20.1 | 57 |
| 153 | Optimizing photoelectrochemical properties of TiO2 by chemical codoping. *Physical Review B*, **2010**, 82, | 3.3 | 57 |
| 152 | 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 |
| 151 | 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 |
| 150 | Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. *Chemistry of Materials*, **2016**, 28, 5022-5028 | 9.6 | 51 |
| 149 | Dynamic Jahn-Teller effect in the NV(-) center in diamond. *Physical Review Letters*, **2011**, 107, 146403 | 7.4 | 49 |
| 148 | Direct atom-by-atom chemical identification of nanostructures and defects of topological insulators. *Nano Letters*, **2013**, 13, 2851-6 | 11.5 | 48 |
| 147 | Titanium-decorated graphene oxide for carbon monoxide capture and separation. *Physical Chemistry Chemical Physics*, **2011**, 13, 21126-31 | 3.6 | 48 |

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|---|---|---|---|
| 146 | 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 |
| 145 | Atomic-Scale Magnetism of Cr-Doped Bi2Se3 Thin Film Topological Insulators. *ACS Nano*, **2015**, 9, 10237-43 | 13.7 | 46 |
| 144 | Electron-rich driven electrochemical solid-state amorphization in Li-Si alloys. *Nano Letters*, **2013**, 13, 4511-6 | 11.5 | 45 |
| 143 | Mapping the 3D surface potential in Bi2Se3. *Nature Communications*, **2013**, 4, 2277 | 17.4 | 43 |
| 142 | Tip size effect on the appearance of a STM image for complex surfaces: Theory versus experiment for Si(111)(7×7). *Physical Review B*, **2004**, 70, | 3.3 | 43 |
| 141 | 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 |
| 140 | Multivalency-Induced Band Gap Opening at MoS2 Edges. *Chemistry of Materials*, **2015**, 27, 3326-3331 | 9.6 | 39 |
| 139 | Crystalline liquid and rubber-like behavior in Cu nanowires. *Nano Letters*, **2013**, 13, 3812-6 | 11.5 | 39 |
| 138 | Regioselectivity control of graphene functionalization by ripples. *Physical Chemistry Chemical Physics*, **2011**, 13, 19449-53 | 3.6 | 39 |
| 137 | Evolution of structural properties and formation of N-N split interstitials in GaAs1−xNx alloys. *Physical Review B*, **2005**, 71, | 3.3 | 39 |
| 136 | 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 |
| 135 | Stabilization mechanisms of polar surfaces: ZnO surfaces. *Physical Review B*, **2008**, 78, | 3.3 | 36 |
| 134 | Stacking Fault Enriching the Electronic and Transport Properties of Few-Layer Phosphorenes and Black Phosphorus. *Nano Letters*, **2016**, 16, 1317-22 | 11.5 | 35 |
| 133 | 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 |
| 132 | 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 |
| 131 | Hydrogen in ZnO revisited: Bond center versus antibonding site. *Physical Review B*, **2008**, 78, | 3.3 | 34 |
| 130 | Theory of Mn supersaturation in Si and Ge. *Physical Review B*, **2004**, 70, | 3.3 | 34 |
| 129 | Open-shell singlet character of stable derivatives of nonacene, hexacene and teranthene. *Organic Letters*, **2011**, 13, 3316-9 | 6.2 | 33 |

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|---|---|---|---|
| 128 | A class of topological nodal rings and its realization in carbon networks. *Physical Review B*, **2018**, 97, | 3.3 | 32 |
| 127 | Impurity doping in SiO2: Formation energies and defect levels from first-principles calculations. *Physical Review B*, **2010**, 82, | 3.3 | 31 |
| 126 | Homobenzene: homoaromaticity and homoantiaromaticity in cycloheptatrienes. *Journal of Physical Chemistry A*, **2008**, 112, 10586-94 | 2.8 | 31 |
| 125 | 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 |
| 124 | Photoinduced Vacancy Ordering and Phase Transition in MoTe. *Nano Letters*, **2019**, 19, 3612-3617 | 11.5 | 30 |
| 123 | Machine Learning Augmented Discovery of Chalcogenide Double Perovskites for Photovoltaics. *Advanced Theory and Simulations*, **2019**, 2, 1800173 | 3.5 | 30 |
| 122 | Vertical/Planar Growth and Surface Orientation of Bi2Te3 and Bi2Se3 Topological Insulator Nanoplates. *Nano Letters*, **2015**, 15, 3147-52 | 11.5 | 30 |
| 121 | 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 |
| 120 | Hydrogen pairs and local vibrational frequencies in H-irradiated GaAs1□Ny. *Physical Review B*, **2005**, 72, | 3.3 | 30 |
| 119 | A novel two-dimensional MgB6 crystal: metal-layer stabilized boron kagome lattice. *Physical Chemistry Chemical Physics*, **2015**, 17, 1093-8 | 3.6 | 29 |
| 118 | Ultrahigh Photocatalytic Rate at a Single-Metal-Atom-Oxide. *Advanced Materials*, **2019**, 31, e1903491 | 24 | 29 |
| 117 | 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 |
| 116 | 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 |
| 115 | Endohedral metalloborofullerenes La2@B80 and Sc3N@B80: a density functional theory prediction. *Journal of Physical Chemistry A*, **2009**, 113, 11613-8 | 2.8 | 28 |
| 114 | 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 |
| 113 | A two-step dry process for Cs2SnI6 perovskite thin film. *Materials Research Letters*, **2017**, 5, 540-546 | 7.4 | 27 |
| 112 | Method for defect stability diagram from ab initio calculations: A case study of SrTiO3. *Physical Review B*, **2012**, 86, | 3.3 | 27 |
| 111 | Achieving Ferromagnetism in Single-Crystalline ZnS Wurtzite Nanowires via Chromium Doping. *Journal of Physical Chemistry C*, **2010**, 114, 12099-12103 | 3.8 | 27 |

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|---|---|---|---|
| 110 | Metal□nsulator Transition of Ge□Sb□Te Superlattice: An Electron Counting Model Study. *IEEE Nanotechnology Magazine*, **2018**, 17, 140-146 | 2.6 | 26 |
| 109 | A nanoscale jigsaw-puzzle approach to large □-conjugated systems. *Angewandte Chemie - International Edition*, **2010**, 49, 6764-7 | 16.4 | 25 |
| 108 | Ab initio structural characterization of a hydrogen-covered diamond (001) surface. *Physical Review B*, **2004**, 70, | 3.3 | 25 |
| 107 | Electronic structure of identical metal cluster arrays on Si(111)□□ surfaces. *Physical Review B*, **2005**, 72, | 3.3 | 25 |
| 106 | Molecular doping of ZnO by ammonia: a possible shallow acceptor. *Journal of Materials Chemistry C*, **2015**, 3, 339-344 | 7.1 | 24 |
| 105 | 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 |
| 104 | Local structure of CuIn3Se5: X-ray absorption fine structure study and first-principles calculations. *Physical Review B*, **2003**, 68, | 3.3 | 24 |
| 103 | van der Waals epitaxy of CdS thin films on single-crystalline graphene. *Applied Physics Letters*, **2017**, 110, 153104 | 3.4 | 23 |
| 102 | An Environmentally Stable and Lead-Free Chalcogenide Perovskite. *Advanced Functional Materials*, **2020**, 30, 2001387 | 15.6 | 23 |
| 101 | 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 |
| 100 | Role of nano in catalysis: Palladium catalyzed hydrogen desorption from nanosized magnesium hydride. *Nano Energy*, **2013**, 2, 742-748 | 17.1 | 21 |
| 99 | Enhanced dihydrogen adsorption in symmetry-lowered metal-porphyrin-containing frameworks. *Physical Chemistry Chemical Physics*, **2009**, 11, 11400-3 | 3.6 | 21 |
| 98 | 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 |
| 97 | Band structures and native defects of ammonia borane. *Physical Review B*, **2009**, 80, | 3.3 | 20 |
| 96 | 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 |
| 95 | DX centers in GaAs and GaSb. *Physical Review B*, **2005**, 72, | 3.3 | 20 |
| 94 | Ti-Alloying of BaZrS Chalcogenide Perovskite for Photovoltaics. *ACS Omega*, **2020**, 5, 18579-18583 | 3.9 | 20 |
| 93 | Semi-Dirac semimetal in silicene oxide. *Physical Chemistry Chemical Physics*, **2017**, 19, 3820-3825 | 3.6 | 19 |

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|---|---|---|---|
| 92 | Direct observation of Pt nanocrystal coalescence induced by electron-excitation-enhanced van der Waals interactions. *Nano Research*, **2014**, 7, 308-314 | 10 | 19 |
| 91 | 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 |
| 90 | Graphite-like surface reconstructions on C{111} and their implication for n-type diamond. *Physical Review B*, **2002**, 66, | 3.3 | 19 |
| 89 | Identification of Ga-interstitial defects in GaNyP1− and AlxGa1−NyP1−. *Physical Review B*, **2004**, 70, | 3.3 | 18 |
| 88 | 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 |
| 87 | Self-purification in Si nanocrystals: An energetics study. *Physical Review B*, **2010**, 82, | 3.3 | 17 |
| 86 | Nanoscale Behavior and Manipulation of the Phase Transition in Single-Crystal Cu Se. *Advanced Materials*, **2019**, 31, e1804919 | 24 | 17 |
| 85 | Band Alignment and the Built-in Potential of Solids. *Physical Review Letters*, **2018**, 121, 196802 | 7.4 | 17 |
| 84 | Spin driving reconstructions on the GaAs(001):Mn surface. *Physical Review B*, **2004**, 69, | 3.3 | 16 |
| 83 | Relativistic screened orbital radii. *Physical Review B*, **1987**, 36, 5861-5867 | 3.3 | 16 |
| 82 | Enhancing the ambient stability of few-layer black phosphorus by surface modification.. *RSC Advances*, **2018**, 8, 14676-14683 | 3.7 | 15 |
| 81 | Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. *Physical Review B*, **2012**, 85, | 3.3 | 15 |
| 80 | 5-7-5 line defects on AsSi(100): A general stress-relief mechanism for V/IV surfaces. *Physical Review B*, **2006**, 74, | 3.3 | 15 |
| 79 | High-Throughput Screening for Phase-Change Memory Materials. *Advanced Functional Materials*, **2021**, 31, 2009803 | 15.6 | 15 |
| 78 | Emergence of Nontrivial Low-Energy Dirac Fermions in Antiferromagnetic EuCd As. *Advanced Materials*, **2020**, 32, e1907565 | 24 | 14 |
| 77 | 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 |
| 76 | 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 |
| 75 | Bipolar Doping by Intrinsic Defects and Magnetic Phase Instability in Monolayer CrI3. *Chemistry of Materials*, **2020**, 32, 1545-1552 | 9.6 | 13 |

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|---|---|---|---|
| 74 | Correlated High-Pressure Phase Sequence of VO under Strong Compression. *Journal of Physical Chemistry Letters*, **2018**, 9, 2388-2393 | 6.4 | 13 |
| 73 | 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 |
| 72 | Bond maximization of graphene in hydrogen addition reactions. *Nanoscale*, **2012**, 4, 1171-6 | 7.7 | 13 |
| 71 | Polarization driven covalently-bonded octahedral-twinning and backbone-peripheral-helical nanoarchitectures. *Nano Letters*, **2008**, 8, 2258-64 | 11.5 | 13 |
| 70 | Nexus networks in carbon honeycombs. *Physical Review Materials*, **2018**, 2, | 3.2 | 13 |
| 69 | Chalcogenide perovskite BaZrS3 thin-film electronic and optoelectronic devices by low temperature processing. *Nano Energy*, **2021**, 85, 105959 | 17.1 | 13 |
| 68 | Epitaxial Growth of Two-Dimensional Insulator Monolayer Honeycomb BeO. *ACS Nano*, **2021**, 15, 2497-2505 | 15.7 | 13 |
| 67 | Electronic fingerprints of Cr and V dopants in the topological insulator Sb2Te3. *Physical Review B*, **2018**, 98, | 3.3 | 13 |
| 66 | Realizing an intrinsic excitonic insulator by decoupling exciton binding energy from the minimum band gap. *Physical Review B*, **2018**, 98, | 3.3 | 12 |
| 65 | Theory of Be-induced defects in Si. *Physical Review B*, **1990**, 42, 11252-11260 | 3.3 | 12 |
| 64 | Semimetal or Semiconductor: The Nature of High Intrinsic Electrical Conductivity in TiS. *Journal of Physical Chemistry Letters*, **2019**, 10, 6996-7001 | 6.4 | 10 |
| 63 | Half-Excitonic Insulator: A Single-Spin Bose-Einstein Condensate. *Physical Review Letters*, **2019**, 122, 236402 | 7.4 | 10 |
| 62 | Intercalated Chevrel Phase Mo6S8 as a Janus Material for Energy Generation and Storage. *ACS Applied Energy Materials*, **2018**, 1, 440-446 | 6.1 | 10 |
| 61 | Stochasticity in materials structure, properties, and processing-A review. *Applied Physics Reviews*, **2018**, 5, | 17.3 | 10 |
| 60 | The new phase [TlSbSe][SnSbSe] a naturally formed semiconducting heterostructure with two-dimensional conductance. *Journal of the American Chemical Society*, **2014**, 136, 11079-84 | 16.4 | 10 |
| 59 | Charged dopants in semiconductor nanowires under partially periodic boundary conditions. *Physical Review B*, **2011**, 83, | 3.3 | 10 |
| 58 | Ultrafast processes in photochromic material YHxOy studied by excited-state density functional theory simulation. *Science China Materials*, **2020**, 63, 1579-1587 | 7.1 | 9 |
| 57 | Spin-Triplet Excitonic Insulator: The Case of Semihydrogenated Graphene. *Physical Review Letters*, **2020**, 124, 166401 | 7.4 | 9 |

| | | | |
|---|---|---|---|
| 56 | Nonlinear Electron-Lattice Interactions in a Wurtzite Semiconductor Enabled via Strongly Correlated Oxide. *Advanced Materials*, **2016**, 28, 8975-8982 | 24 | 9 |
| 55 | 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 |
| 54 | 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 |
| 53 | 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 |
| 52 | Defect tolerance in chalcogenide perovskite photovoltaic material BaZrS3. *Science China Materials*,1 | 7.1 | 9 |
| 51 | Observation of Coulomb repulsion between Cu intercalants in CuxBi2Se3. *Physical Review B*, **2014**, 89, | 3.3 | 8 |
| 50 | Octahedron rotation evolution in 2D perovskites and its impact on optoelectronic properties: the case of Ba2rS chalcogenides. *Materials Horizons*, **2020**, 7, 2985-2993 | 14.4 | 8 |
| 49 | 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 |
| 48 | Tuning the structures of two-dimensional cuprous oxide confined on Au(111). *Nano Research*, **2018**, 11, 5957-5967 | 10 | 7 |
| 47 | Absolute redox potential of liquid water: a first-principles theory. *Chemical Science*, **2014**, 5, 1216-1220 | 9.4 | 7 |
| 46 | 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 |
| 45 | Activated dissociation of O2 on Pb(111) surfaces by Pb adatoms. *Physical Review B*, **2009**, 80, | 3.3 | 7 |
| 44 | Carrier Dynamics and Transfer across the CdS/MoS Interface upon Optical Excitation. *Journal of Physical Chemistry Letters*, **2020**, 11, 6544-6550 | 6.4 | 7 |
| 43 | 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 |
| 42 | Single-Crystal CdTe Homojunction Structures for Solar Cell Applications. *Journal of Electronic Materials*, **2015**, 44, 3118-3123 | 1.9 | 6 |
| 41 | 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 |
| 40 | Zhang and Zunger Reply:. *Physical Review Letters*, **1997**, 79, 3313-3313 | 7.4 | 6 |
| 39 | Physics of defects and hydrogen in dilute nitrides. *IEE Proceedings: Optoelectronics*, **2004**, 151, 369-377 | | 6 |

| | | | |
|---|---|---|---|
| 38 | Manipulation of Optical Transmittance by Ordered-Oxygen-Vacancy in Epitaxial LaBaCoO Thin Films. *Scientific Reports*, **2016**, 6, 37496 | 4.9 | 6 |
| 37 | Dative epitaxy of commensurate monocrystalline covalent-van der Waals moiré supercrystal.. *Advanced Materials*, **2022**, e2200117 | 24 | 6 |
| 36 | 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 |
| 35 | 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 |
| 34 | Spontaneous symmetry lowering of Si (001) towards two-dimensional ferro/antiferroelectric behavior. *Physical Review Materials*, **2019**, 3, | 3.2 | 5 |
| 33 | Phase Transition in a Memristive Suspended MoS Monolayer Probed by Opto- and Electro-Mechanics. *ACS Nano*, **2020**, 14, 13611-13618 | 16.7 | 5 |
| 32 | Realization of semiconducting layered multiferroic heterojunctions via asymmetrical magnetoelectric coupling. *Physical Review B*, **2021**, 103, | 3.3 | 5 |
| 31 | 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 |
| 30 | Anisotropic Strain Induced Directional Metallicity in Highly Epitaxial LaBaCoO Thin Films on (110) NdGaO. *Scientific Reports*, **2016**, 6, 37337 | 4.9 | 5 |
| 29 | Enhanced van der Waals epitaxy via electron transfer enabled interfacial dative bond formation. *Physical Review Materials*, **2017**, 1, | 3.2 | 4 |
| 28 | 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 |
| 27 | Optical subpicosecond nonvolatile switching and electron-phonon coupling in ferroelectric materials. *Physical Review B*, **2020**, 102, | 3.3 | 4 |
| 26 | 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 |
| 25 | 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 |
| 24 | Formation mechanism of twin domain boundary in 2D materials: The case for WTe2. *Nano Research*, **2019**, 12, 569-573 | 10 | 4 |
| 23 | 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 |
| 22 | Understanding the origin of bandgap problem in transition and post-transition metal oxides. *Journal of Chemical Physics*, **2019**, 151, 124703 | 3.9 | 3 |
| 21 | Long-range magnetic order stabilized by acceptors. *Physical Review B*, **2019**, 99, | 3.3 | 3 |

| | | | |
|---|---|---|---|
| 20 | 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 |
| 19 | Orientation-Controlled Large-Area Epitaxial PbI Thin Films with Tunable Optical Properties. *ACS Applied Materials & Interfaces*, **2021**, 13, 32450-32460 | 9.5 | 3 |
| 18 | Doping-induced antiferromagnetic bicollinear insulating state and superconducting temperature of monolayer FeSe systems. *Physical Review B*, **2018**, 98, | 3.3 | 2 |
| 17 | An Insulating Overlayer for GaAs. *Materials Research Society Symposia Proceedings*, **1991**, 221, 301 | | 1 |
| 16 | Bipolar Doping by Intrinsic Defects and Magnetic Phase Instability in Monolayer CrI3 | | 1 |
| 15 | Anisotropic band structure of TiS3 nanoribbon revealed by polarized photocurrent spectroscopy. *Applied Physics Letters*, **2020**, 117, 073101 | 3.4 | 1 |
| 14 | Vector potential and surface magnetic field in magnetoelectric antiferromagnetic materials. *Physical Review B*, **2020**, 102, | 3.3 | 1 |
| 13 | 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 |
| 12 | Defects in Statically Unstable Solids: The Case for Cubic Perovskite □CsPbI3. *Chinese Physics Letters* , **2022**, 39, 046101 | 1.8 | 1 |
| 11 | 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 |
| 10 | High-Stability Light-Element Magnetic Superatoms Determined by Hund's Rule.. *Journal of Physical Chemistry Letters*, **2022**, 2632-2637 | 6.4 | 0 |
| 9 | Ligand-Assisted Charge-Transfer Mechanism: The Case of CdSe/Cysteine/MoS Heterostructures.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12329-12335 | 6.4 | 0 |
| 8 | Unexpected Coulomb binding between Ca and H+ in ZnO. *Journal of Vacuum Science & Technology B* , **2009**, 27, 1601 | | |
| 7 | Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage. *Materials Research Society Symposia Proceedings*, **2007**, 1041, 1 | | |
| 6 | Quadruple-period ordering in MBE GaAsSb alloys. *Materials Research Society Symposia Proceedings*, **2003**, 794, 49 | | |
| 5 | Theory ofDX Centers in AlxGa1-x Alloys. *Materials Research Society Symposia Proceedings*, **1989**, 163, 765 | | |
| 4 | Theoretical Study of a New Transition Sequence in III-V Compounds: High-Pressure Phases of InSb. *Materials Research Society Symposia Proceedings*, **1990**, 193, 89 | | |
| 3 | Peculiar Doping Behavior of Si:Be.. *Materials Research Society Symposia Proceedings*, **1990**, 209, 119 | | |

| | | |
|---|---|---|
| 2 | 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 |
| 1 | Mixed Chalcogenide-Halides for Stable, Lead-Free and Defect-Tolerant Photovoltaics: Computational Screening and Experimental Validation of CuBiSCl 2 with Ideal Band Gap. *Advanced Functional Materials*,2112682 | 15.6 |