# Peihong Zhang

## List of Publications by Year in descending order

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Version: 2024-02-01

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|---|---|---|---|
| 90 papers | 4,454 citations | 81839 39 h-index | 106281 65 g-index |
| 90 all docs | 90 docs citations | 90 times ranked | 6274 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Defect-Induced Intrinsic Magnetism in Wide-Gap III Nitrides. Physical Review Letters, 2008, 100, 117204. | 2.9 | 328 |
| 2 | Chalcogenide Perovskites for Photovoltaics. Nano Letters, 2015, 15, 581-585. | 4.5 | 249 |
| 3 | Plastic Deformations of Carbon Nanotubes. Physical Review Letters, 1998, 81, 5346-5349. | 2.9 | 231 |
| 4 | Quasiparticle Band Gap of ZnO: High Accuracy from the Conventional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msup><mml:msup><mml:mi>W</mml:mi><mml:mn> Physical Review Letters, 2010, 105, 146401. | 2.9 | 212 |
| 5 | High intrinsic carrier mobility and photon absorption in the perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>. Physical Chemistry Chemical Physics, 2015, 17, 11516-11520. | 1.3 | 182 |
| 6 | Gapping by Squashing: Metal-Insulator and Insulator-Metal Transitions in Collapsed Carbon Nanotubes. Physical Review Letters, 2000, 84, 2453-2456. | 2.9 | 121 |
| 7 | Discovering lead-free perovskite solar materials with a split-anion approach. Nanoscale, 2016, 8, 6284-6289. | 2.8 | 116 |
| 8 | Computational design of direct-bandgap semiconductors that lattice-match silicon. Nature, 2001, 409, 69-71. | 13.7 | 110 |
| 9 | Smallest Nanotube: Breaking the Symmetry ofsp3Bonds in Tubular Geometries. Physical Review Letters, 2001, 87, 125502. | 2.9 | 102 |
| 10 | Theory of sodium ordering inNaxCoO2. Physical Review B, 2005, 71, . | 1.1 | 102 |
| 11 | Comparative study of structural and electronic properties of Cu-based multinary semiconductors. Physical Review B, 2011, 84, . | 1.1 | 95 |
| 12 | Theoretical insights into the uranyl adsorption behavior on vanadium carbide MXene. Applied Surface Science, 2017, 426, 572-578. | 3.1 | 83 |
| 13 | Doping effects on the electronic and structural properties ofCoO2: AnLSDA+Ustudy. Physical Review B, 2004, 70, . | 1.1 | 77 |
| 14 | Prediction that Uniaxial Tension alongâŸ¨111âŸ©Produces a Direct Band Gap in Germanium. Physical Review Letters, 2009, 102, 156401. | 2.9 | 74 |
| 15 | Theory ofB2OandBeB2Nanotubes: New Semiconductors and Metals in One Dimension. Physical Review Letters, 2002, 89, 056403. | 2.9 | 70 |
| 16 | Prediction of MXene based 2D tunable band gap semiconductors: GW quasiparticle calculations. Nanoscale, 2019, 11, 3993-4000. | 2.8 | 69 |
| 17 | Collective stabilization of hydrogen chemisorption on graphenic surfaces. Physical Review B, 2003, 68, . | 1.1 | 68 |
| 18 | Unconventional magnetism in semiconductors: Role of localized acceptor states. Physical Review B, 2010, 81, . | 1.1 | 67 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Structural properties and quasiparticle band structures of Cu-based quaternary semiconductors for photovoltaic applications. Journal of Applied Physics, 2012, 111, . | 1.1 | 67 |
| 21 | 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 |
| 22 | Fermi Surface ofNaxCoO2. Physical Review Letters, 2004, 93, 236402. | 2.9 | 66 |
| 23 | Quasiparticle energy of semicoredelectrons inZnS: CombinedLDA+UandGWapproach. Physical Review B, 2006, 74, . | 1.1 | 65 |
| 24 | Screened Coulomb interaction of localized electrons in solids from first principles. Physical Review B, 2012, 85, . | 1.1 | 62 |
| 25 | Hole-lattice coupling and photoinduced insulator-metal transition in VO<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>. Physical Review B, 2013, 88, . | 1.1 | 62 |
| 26 | Room temperature ferromagnetism in Mn-doped CdS nanorods. Applied Physics Letters, 2008, 93, . | 1.5 | 61 |
| 27 | Speeding up GW Calculations to Meet the Challenge of Large Scale Quasiparticle Predictions. Scientific Reports, 2016, 6, 36849. | 1.6 | 60 |
| 28 | Electronic structure of antifluorite Cu2X (X = S, Se, Te) within the modified Becke-Johnson potential plus an on-site Coulomb U. Journal of Chemical Physics, 2014, 140, 074702. | 1.2 | 58 |
| 29 | Nucleation of Carbon Nanotubes without Pentagonal Rings. Physical Review Letters, 1999, 83, 1791-1794. | 2.9 | 53 |
| 30 | VO<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>: Orbital competition, magnetism, and phase stability. Physical Review B, 2012, 86, . | 1.1 | 53 |
| 31 | Electronic properties of energy harvesting Cu-chalcogenides: pâ€“d hybridization and d-electron localization. Computational Materials Science, 2015, 108, 239-249. | 1.4 | 49 |
| 32 | Plastic deformations of boron-nitride nanotubes: An unexpected weakness. Physical Review B, 2000, 62, 11050-11053. | 1.1 | 45 |
| 33 | Grapheneâ€“ferromagnet interfaces: hybridization, magnetization and charge transfer. Nanoscale, 2013, 5, 1902. | 2.8 | 45 |
| 34 | Defect-induced magnetism in nitride and oxide nanowires: Surface effects and quantum confinement. Physical Review B, 2010, 82, . | 1.1 | 44 |
| 35 | Screened Coulomb interactions of localized electrons in transition metals and transition-metal oxides. Physical Review B, 2012, 86, . | 1.1 | 44 |
| 36 | Near-edge band structures and band gaps of Cu-based semiconductors predicted by the modified Becke-Johnson potential plus an on-site Coulomb U. Journal of Chemical Physics, 2013, 139, 184706. | 1.2 | 43 |

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|---|---|---|---|
| 37 | Synthesis of Layerâ€Tunable Graphene: A Combined Kinetic Implantation and Thermal Ejection Approach. Advanced Functional Materials, 2015, 25, 3666-3675. | 7.8 | 43 |
| 38 | Prediction of a multicenter-bonded solid boron hydride for hydrogen storage. Physical Review B, 2011, 83, . | 1.1 | 42 |
| 39 | Emptying and filling a tunnel bronze. Chemical Science, 2015, 6, 1712-1718. | 3.7 | 42 |
| 40 | Electron-Phonon Renormalization in Cuprate Superconductors. Physical Review Letters, 2007, 98, 067005. | 2.9 | 41 |
| 41 | Prediction of Ti3C2O2 MXene as an effective capturer of formaldehyde. Applied Surface Science, 2019, 469, 770-774. | 3.1 | 40 |
| 42 | An X-ray Absorption Spectroscopy Study of the Cathodic Discharge of Ag<sub>2</sub>VO<sub>2</sub>PO<sub>4</sub>: Geometric and Electronic Structure Characterization of Intermediate phases and Mechanistic Insights. Journal of Physical Chemistry C, 2011, 115, 14437-14447. | 1.5 | 39 |
| 43 | On the applicability of hybrid functionals for predicting fundamental properties of metals. Solid State Communications, 2016, 234-235, 10-13. | 0.9 | 36 |
| 44 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>quasiparticle corrections to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:mo>â^•</mml:mo><mml:mi> structure of bcc hydrogen. Physical Review B, 2008, 77, . | 1.1 | 34 |
| 45 | Flexible crystalline Î²-Ga<sub>2</sub>O<sub>3</sub>solar-blind photodetectors. Journal of Materials Chemistry C, 2020, 8, 14732-14739. | 2.7 | 34 |
| 46 | Hole Extraction by Design in Photocatalytic Architectures Interfacing CdSe Quantum Dots with Topochemically Stabilized Tin Vanadium Oxide. Journal of the American Chemical Society, 2018, 140, 17163-17174. | 6.6 | 33 |
| 47 | Splitting of the zone-center phonon in MnO and NiO. Solid State Communications, 2007, 142, 504-508. | 0.9 | 31 |
| 48 | Quasiparticle band structures of CuCl, CuBr, AgCl, and AgBr: The extreme case. Physical Review B, 2018, 98, . | 1.1 | 30 |
| 49 | The Middle Road Less Taken: Electronic-Structure-Inspired Design of Hybrid Photocatalytic Platforms for Solar Fuel Generation. Accounts of Chemical Research, 2019, 52, 645-655. | 7.6 | 29 |
| 50 | Carrier-dopant exchange interactions in Mn-doped PbS colloidal quantum dots. Applied Physics Letters, 2012, 101, 062410. | 1.5 | 28 |
| 51 | Charge Disproportionation and Voltageâ€Induced Metalâ€“Insulator Transitions Evidenced in Î²â€Pb<sub>x</sub>V<sub>2</sub>O<sub>5</sub> Nanowires. Advanced Functional Materials, 2013, 23, 153-160. | 7.8 | 28 |
| 52 | Semimetal or Semiconductor: The Nature of High Intrinsic Electrical Conductivity in TiS<sub>2</sub>. Journal of Physical Chemistry Letters, 2019, 10, 6996-7001. | 2.1 | 27 |
| 53 | Theory of Oxygen-Boron Vacancy Defect in Cubic Boron Nitride: A Diamond<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mi>NV</mml:mi></mml:mrow><mml:mrow><mml:mo>â^’</mml:mo></mml:mrow><mml:mo> Center. Physical Review Letters, 2014, 113, 136401. | 2.9 | 25 |
| 54 | Defect tolerance in chalcogenide perovskite photovoltaic material BaZrS3. Science China Materials, 2021, 64, 2976-2986. | 3.5 | 25 |

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|---|---|---|---|
| 55 | Discovery of elusive structures of multifunctional transition-metal borides. Nanoscale, 2016, 8, 1055-1065. | 2.8 | 24 |
| 56 | Engineering the Near-Edge Electronic Structure of SnSe through Strains. Physical Review Applied, 2017, 8, . | 1.5 | 23 |
| 57 | Tunable Type-II <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Bi</mml:mi><mml:mi>VO</mml:mi></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow><mml:mi mathvariant="normal">g</mml:mi></mml:mrow></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> Heterojunctions for Photocatalytic Water Splitting. Physical Review Applied, 2021, | 1.5 | 23 |
| 58 | Nonlocal Screening, Electron-Phonon Coupling, and Phonon Renormalization in Metals. Physical Review Letters, 2005, 94, 225502. | 2.9 | 22 |
| 59 | Phonon-Assisted Crossover from a Nonmagnetic Peierls Insulator to a Magnetic Stoner Metal. Physical Review Letters, 2014, 113, 176401. | 2.9 | 22 |
| 60 | Selective electrochemical reactivity of rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> the suppression of metal-insulator transition. Physical Review B, 2016, 93, . | 1.1 | 22 |
| 61 | High-Fidelity Transfer of Chemical Vapor Deposition Grown 2D Transition Metal Dichalcogenides via Substrate Decoupling and Polymer/Small Molecule Composite. ACS Nano, 2020, 14, 7370-7379. | 7.3 | 22 |
| 62 | Theory of the color change of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Na</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> a function of Na-charge doping. Physical Review B, 2009, 79, . | 1.1 | 21 |
| 63 | Quasiparticle electronic structure of honeycomb C <sub>3</sub> N: from monolayer to bulk. 2D Materials, 2019, 6, 015018. | 2.0 | 20 |
| 64 | Electric Polarization Switching on an Atomically Thin Metallic Oxide. Nano Letters, 2021, 21, 144-150. | 4.5 | 19 |
| 65 | Prediction of protected band edge states and dielectric tunable quasiparticle and excitonic properties of monolayer MoSi2N4. Npj Computational Materials, 2022, 8, . | 3.5 | 19 |
| 66 | Rare earth chalcogenide Ce3Te4 as high efficiency high temperature thermoelectric material. Applied Physics Letters, 2011, 98, . | 1.5 | 18 |
| 67 | Difficulty in predicting shallow defects with hybrid functionals: Implication of the long-range exchange interaction. Physical Review B, 2013, 88, . | 1.1 | 18 |
| 68 | Pinning down high-performance Cu-chalcogenides as thin-film solar cell absorbers: A successive screening approach. Journal of Chemical Physics, 2016, 144, 194706. | 1.2 | 18 |
| 69 | Electronic Phase Transitions of Î´-Ag<sub>x</sub>V<sub>2</sub>O<sub>5</sub> Nanowires: Interplay between Geometric and Electronic Structures. Journal of Physical Chemistry C, 2014, 118, 21235-21243. | 1.5 | 17 |
| 70 | Ab Initiocalculations of phonon splitting in antiferromagneticZnCr2O4. Physical Review B, 2007, 75, . | 1.1 | 15 |
| 71 | Anisotropic polaron localization and spontaneous symmetry breaking: Comparison of cation-site acceptors in GaN and ZnO. Physical Review B, 2014, 90, . | 1.1 | 15 |
| 72 | Tuning the Deoxygenation of Bulk-Dissolved Oxygen in Copper. Journal of Physical Chemistry C, 2018, 122, 8254-8261. | 1.5 | 15 |

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| 73 | Charging-assisted hydrogen release mechanism in layered boron hydride. Physical Review B, 2011, 84, . | 1.1 | 13 |
| 74 | Theory of metastable group-IV alloys formed from CVD precursors. Physical Review B, 2001, 64, . | 1.1 | 12 |
| 75 | Theory of the electronic structure of alternating<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mg</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and graphene layered structures. Physical Review B, 2008, 77, . | 1.1 | 12 |
| 76 | Diamond nanowires with nitrogen vacancy under a transverse electric field. Physical Review B, 2015, 91, . | 1.1 | 11 |
| 77 | Giant Narrow-Band Optical Absorption and Distinctive Excitonic Structures of Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub> | 1.5 | 11 |
| 78 | Phonon instability and pressure-induced isostructural semiconductor-semimetal transition of monoclinic VO2. Physical Review B, 2016, 94, . | 1.1 | 10 |
| 79 | Optimizing the Dopant and Carrier Concentration of Ca5Al2Sb6 for High Thermoelectric Efficiency. Scientific Reports, 2016, 6, 29550. | 1.6 | 10 |
| 80 | Remarkable Band-Gap Renormalization via Dimensionality of the Layered Material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">B</mml:mi></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2020, 14, . | 1.5 | 9 |
| 81 | Combined subsampling and analytical integration for efficient large-scale GW calculations for 2D systems. Npj Computational Materials, 2020, 6, . | 3.5 | 9 |
| 82 | Electronâ€“phonon renormalization and phonon anharmonicity in metals. Solid State Communications, 2008, 148, 151-154. | 0.9 | 6 |
| 83 | Electrode Reaction Mechanism of Ag<sub>2</sub>VO<sub>2</sub>PO<sub>4</sub> Cathode. Chemistry of Materials, 2016, 28, 3428-3434. | 3.2 | 6 |
| 84 | Ab initio study of thermodynamically consistent equation of state of warm dense aluminum plasma. Physics of Plasmas, 2016, 23, 092710. | 0.7 | 4 |
| 85 | Isosymmetric phase transitions, ultrahigh ductility, and topological nodal lines in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mo>â^’</mml:mo><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi | 1.1 | 4 |
| 86 | Quasiparticle band structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m : A combined <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml: | 1.1 | 4 |
| 87 | perovskite oxides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrZr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BaZr | 1.1 | 3 |
| 88 | Thermoelectric probe of defect state induced by ionic liquid gating in vanadium dioxide. Applied Physics Letters, 2020, 116, 193502. | 1.5 | 2 |
| 89 | Numerical methods for efficient GW calculations and the applications in low-dimensional systems. Electronic Structure, 0, , . | 1.0 | 1 |
| 90 | Graphene: Synthesis of Layer-Tunable Graphene: A Combined Kinetic Implantation and Thermal Ejection Approach (Adv. Funct. Mater. 24/2015). Advanced Functional Materials, 2015, 25, 3796-3796. | 7.8 | 0 |