Peihong Zhang

List of Publications by Year in descending order

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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	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:m	3.5	11
2	Prediction of protected band edge states and dielectric tunable quasiparticle and excitonic properties of monolayer MoSi2N4. Npj Computational Materials, 2022, 8, .	3.5	19
3	Electric Polarization Switching on an Atomically Thin Metallic Oxide. Nano Letters, 2021, 21, 144-150.	4.5	19
4	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:r	1.1	4
5	Defect tolerance in chalcogenide perovskite photovoltaic material BaZrS3. Science China Materials, 2021, 64, 2976-2986.	3.5	25
6	Quasiparticle band structures of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r 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 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>â^’</mml:mi><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	3
7	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, .	1.1	4
8	Combined subsampling and analytical integration for efficient large-scale GW calculations for 2D systems. Npj Computational Materials, 2020, 6, .	1.5	9
9	Flexible crystalline Î²-Ga₂O₃solar-blind photodetectors. Journal of Materials Chemistry C, 2020, 8, 14732-14739.	3.5	9
10	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.	2.7	34
11	Thermoelectric probe of defect state induced by ionic liquid gating in vanadium dioxide. Applied Physics Letters, 2020, 116, 193502.	7.3	22
12	Semimetal or Semiconductor: The Nature of High Intrinsic Electrical Conductivity in TiS₂. Journal of Physical Chemistry Letters, 2019, 10, 6996-7001.	1.5	2
13	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:mrow><mml:mi mathvariant="normal">g</mml:mi></mml:mrow></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> Prediction of MXene based 2D tunable band gap semiconductors: GW quasiparticle calculations. Nanoscale, 2019, 11, 3993-4000.	2.1	27
14	Quasiparticle electronic structure of honeycomb C ₃ N: from monolayer to bulk. 2D Materials, 2019, 6, 015018.	1.5	23
15	Prediction of Ti3C2O2 MXene as an effective capturer of formaldehyde. Applied Surface Science, 2019, 469, 770-774.	2.8	69
16	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.	2.0	20
17		3.1	40
18		7.6	29

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19	Tuning the Deoxygenation of Bulk-Dissolved Oxygen in Copper. Journal of Physical Chemistry C, 2018, 122, 8254-8261.	1.5	15
20	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
21	Quasiparticle band structures of CuCl, CuBr, AgCl, and AgBr: The extreme case. Physical Review B, 2018, 98, .	1.1	30
22	Engineering the Near-Edge Electronic Structure of SnSe through Strains. Physical Review Applied, 2017, 8, .	1.5	23
23	Theoretical insights into the uranyl adsorption behavior on vanadium carbide MXene. Applied Surface Science, 2017, 426, 572-578.	3.1	83
24	Phonon instability and pressure-induced isostructural semiconductor-semimetal transition of monoclinic VO2. Physical Review B, 2016, 94, .	1.1	10
25	Optimizing the Dopant and Carrier Concentration of Ca5Al2Sb6 for High Thermoelectric Efficiency. Scientific Reports, 2016, 6, 29550.	1.6	10
26	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
27	Ab initio study of thermodynamically consistent equation of state of warm dense aluminum plasma. Physics of Plasmas, 2016, 23, 092710.	0.7	4
28	Electrode Reaction Mechanism of Ag₂VO₂PO₄ Cathode. Chemistry of Materials, 2016, 28, 3428-3434.	3.2	6
29	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
30	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 the suppression of metal-insulator transition. Physical Review B, 2016, 93, .	1.1	22
31	Speeding up GW Calculations to Meet the Challenge of Large Scale Quasiparticle Predictions. Scientific Reports, 2016, 6, 36849.	1.6	60
32	Discovery of elusive structures of multifunctional transition-metal borides. Nanoscale, 2016, 8, 1055-1065.	2.8	24
33	On the applicability of hybrid functionals for predicting fundamental properties of metals. Solid State Communications, 2016, 234-235, 10-13.	0.9	36
34	Discovering lead-free perovskite solar materials with a split-anion approach. Nanoscale, 2016, 8, 6284-6289.	2.8	116
35	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
36	Synthesis of Layerâ€Tunable Graphene: A Combined Kinetic Implantation and Thermal Ejection Approach. Advanced Functional Materials, 2015, 25, 3666-3675.	7.8	43

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37	Chalcogenide Perovskites for Photovoltaics. Nano Letters, 2015, 15, 581-585.	4.5	249
38	Electronic properties of energy harvesting Cu-chalcogenides: pâ€“d hybridization and d-electron localization. Computational Materials Science, 2015, 108, 239-249.	1.4	49
39	High intrinsic carrier mobility and photon absorption in the perovskite CH₃NH₃PbI₃. Physical Chemistry Chemical Physics, 2015, 17, 11516-11520.	1.3	182
40	Diamond nanowires with nitrogen vacancy under a transverse electric field. Physical Review B, 2015, 91, .	1.1	11
41	Emptying and filling a tunnel bronze. Chemical Science, 2015, 6, 1712-1718.	3.7	42
42	Anisotropic polaron localization and spontaneous symmetry breaking: Comparison of cation-site acceptors in GaN and ZnO. Physical Review B, 2014, 90, .	1.1	15
43	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
44	Phonon-Assisted Crossover from a Nonmagnetic Peierls Insulator to a Magnetic Stoner Metal. Physical Review Letters, 2014, 113, 176401.	2.9	22
45	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:mo>n Center. Physical Review Letters, 2014, 113, 136401.	2.9	25
46	Electronic Phase Transitions of Î´-Ag_xV₂O₅ Nanowires: Interplay between Geometric and Electronic Structures. Journal of Physical Chemistry C, 2014, 118, 21235-21243.	1.5	17
47	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
48	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
49	Difficulty in predicting shallow defects with hybrid functionals: Implication of the long-range exchange interaction. Physical Review B, 2013, 88, .	1.1	18
50	Grapheneâ€“ferromagnet interfaces: hybridization, magnetization and charge transfer. Nanoscale, 2013, 5, 1902.	2.8	45
51	Charge Disproportionation and Voltageâ€Induced Metalâ€“Insulator Transitions Evidenced in Î²â€²Pb_xV₂O₅ Nanowires. Advanced Functional Materials, 2013, 23, 153-160.	7.8	28
52	Screened Coulomb interactions of localized electrons in transition metals and transition-metal oxides. Physical Review B, 2012, 86, .	1.1	44
53	Screened Coulomb interaction of localized electrons in solids from first principles. Physical Review B, 2012, 85, .	1.1	62
54	Carrier-dopant exchange interactions in Mn-doped PbS colloidal quantum dots. Applied Physics Letters, 2012, 101, 062410.	1.5	28

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55	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
56	Structural properties and quasiparticle band structures of Cu-based quaternary semiconductors for photovoltaic applications. Journal of Applied Physics, 2012, 111, .	1.1	67
57	An X-ray Absorption Spectroscopy Study of the Cathodic Discharge of Ag₂VO₂PO₄: Geometric and Electronic Structure Characterization of Intermediate phases and Mechanistic Insights. Journal of Physical Chemistry C, 2011, 115, 14437-14447.	1.5	39
58	Comparative study of structural and electronic properties of Cu-based multinary semiconductors. Physical Review B, 2011, 84, .	1.1	95
59	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
60	Charging-assisted hydrogen release mechanism in layered boron hydride. Physical Review B, 2011, 84, .	1.1	13
61	Prediction of a multicenter-bonded solid boron hydride for hydrogen storage. Physical Review B, 2011, 83, .	1.1	42
62	Rare earth chalcogenide Ce3Te4 as high efficiency high temperature thermoelectric material. Applied Physics Letters, 2011, 98, .	1.5	18
63	Unconventional magnetism in semiconductors: Role of localized acceptor states. Physical Review B, 2010, 81, .	1.1	67
64	Defect-induced magnetism in nitride and oxide nanowires: Surface effects and quantum confinement. Physical Review B, 2010, 82, .	1.1	44
65	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
66	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> a function of Na-charge doping. Physical Review B, 2009, 79, .	1.1	21
67	Prediction that Uniaxial Tension alongâŸ¨111âŸ©Produces a Direct Band Gap in Germanium. Physical Review Letters, 2009, 102, 156401.	2.9	74
68	Electronâ€“phonon renormalization and phonon anharmonicity in metals. Solid State Communications, 2008, 148, 151-154.	0.9	6
69	Defect-Induced Intrinsic Magnetism in Wide-Gap III Nitrides. Physical Review Letters, 2008, 100, 117204.	2.9	328
70	<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
71	Room temperature ferromagnetism in Mn-doped CdS nanorods. Applied Physics Letters, 2008, 93, .	1.5	61
72	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

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73	Electron-Phonon Renormalization in Cuprate Superconductors. Physical Review Letters, 2007, 98, 067005.	2.9	41
74	Ab Initiocalculations of phonon splitting in antiferromagneticZnCr2O4. Physical Review B, 2007, 75, .	1.1	15
75	Splitting of the zone-center phonon in MnO and NiO. Solid State Communications, 2007, 142, 504-508.	0.9	31
76	Quasiparticle energy of semicoredelectrons inZnS: CombinedLDA+UandGWapproach. Physical Review B, 2006, 74, .	1.1	65
77	Nonlocal Screening, Electron-Phonon Coupling, and Phonon Renormalization in Metals. Physical Review Letters, 2005, 94, 225502.	2.9	22
78	Theory of sodium ordering inNaxCoO2. Physical Review B, 2005, 71, .	1.1	102
79	Doping effects on the electronic and structural properties ofCoO2: AnLSDA+Ustudy. Physical Review B, 2004, 70, .	1.1	77
80	Fermi Surface ofNaxCoO2. Physical Review Letters, 2004, 93, 236402.	2.9	66
81	Collective stabilization of hydrogen chemisorption on graphenic surfaces. Physical Review B, 2003, 68, .	1.1	68
82	Theory ofB2OandBeB2Nanotubes: New Semiconductors and Metals in One Dimension. Physical Review Letters, 2002, 89, 056403.	2.9	70
83	Computational design of direct-bandgap semiconductors that lattice-match silicon. Nature, 2001, 409, 69-71.	13.7	110
84	Smallest Nanotube: Breaking the Symmetry ofsp3Bonds in Tubular Geometries. Physical Review Letters, 2001, 87, 125502.	2.9	102
85	Theory of metastable group-IV alloys formed from CVD precursors. Physical Review B, 2001, 64, .	1.1	12
86	Plastic deformations of boron-nitride nanotubes: An unexpected weakness. Physical Review B, 2000, 62, 11050-11053.	1.1	45
87	Gapping by Squashing: Metal-Insulator and Insulator-Metal Transitions in Collapsed Carbon Nanotubes. Physical Review Letters, 2000, 84, 2453-2456.	2.9	121
88	Nucleation of Carbon Nanotubes without Pentagonal Rings. Physical Review Letters, 1999, 83, 1791-1794.	2.9	53
89	Plastic Deformations of Carbon Nanotubes. Physical Review Letters, 1998, 81, 5346-5349.	2.9	231
90	Numerical methods for efficient GW calculations and the applications in low-dimensional systems. Electronic Structure, 0, , .	1.0	1