Shang-Peng Gao

List of Publications by Year
in descending order

64 papers	3,741 citations	236925 25 h-index	123424 61 g-index
64 all docs	64 docs citations	64 times ranked	5322 citing authors

#	Article	IF	Citations
1	Anionic Redox Regulated via Metalâ€“Ligand Combinations in Layered Sulfides. Advanced Materials, 2022, 34, e2107353.	21.0	11
2	Electronic and catalytic properties of carbon nitride derivatives tuned by building blocks and linkages. International Journal of Hydrogen Energy, 2022, 47, 8761-8775.	7.1	5
3	Exciton Emissions in Bilayer WSe₂ Tuned by the Ferroelectric Polymer. Journal of Physical Chemistry Letters, 2022, 13, 1636-1643.	4.6	3
4	Ultrastable Zinc Anode by Simultaneously Manipulating Solvation Sheath and Inducing Oriented Deposition with PEG Stability Promoter. Small, 2022, 18, e2103345.	10.0	39
5	Anomalous Redox Features Induced by Strong Covalency in Layered NaTi _{1â^' y} V _y S ₂ Cathodes for Naâ€ion Batteries. Angewandte Chemie - International Edition, 2022, , .	13.8	2
6	Depolarization of Few-Layer III-V and II-VI Materials through Symmetric Rumpling. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
7	Layer-dependent band gaps and dielectric constants of ultrathin fluorite crystals. Journal of Physics and Chemistry of Solids, 2021, 148, 109738.	4.0	8
8	Superior-Performance Aqueous Zinc-Ion Batteries Based on the In Situ Growth of MnO₂ Nanosheets on V₂CT_X MXene. ACS Nano, 2021, 15, 2971-2983.	14.6	205
9	A method to restore the intrinsic dielectric functions of 2D materials in periodic calculations. Nanoscale, 2021, 13, 17057-17067.	5.6	11
10	Zn²⁺-Intercalated V₂O₅Â·nH₂O derived from V₂CT_x MXene for hyper-stable zinc-ion storage. Journal of Materials Chemistry A, 2021, 9, 17994-18005.	10.3	34
11	Electronic and optical properties of ultrathin cerium dioxide: A many-body GW-BSE investigation. Computational Materials Science, 2021, 198, 110696.	3.0	6
12	Density Functional Theory Study of ZnIn₂S₄ and CdIn₂S₄ Polymorphs Using Fullâ€Potential Linearized Augmented Plane Wave Method and Modified Beckeâ€“Johnson Potential. Physica Status Solidi (B): Basic Research, 2020, 257, 1900485.	1.5	19
13	Tunable electronic properties and Schottky barrier in a graphene/WSe₂ heterostructure under out-of-plane strain and an electric field. Physical Chemistry Chemical Physics, 2020, 22, 23699-23706.	2.8	27
14	Synthesis of Honeycombâ€Structured Beryllium Oxide via Graphene Liquid Cells. Angewandte Chemie, 2020, 132, 15864-15870.	2.0	0
15	Synthesis of Honeycombâ€Structured Beryllium Oxide via Graphene Liquid Cells. Angewandte Chemie - International Edition, 2020, 59, 15734-15740.	13.8	18
16	Etchingâ€Doping Sedimentation Equilibrium Strategy: Accelerating Kinetics on Hollow Rhâ€Doped CoFeâ€Layered Double Hydroxides for Water Splitting. Advanced Functional Materials, 2020, 30, 2003556.	14.9	117
17	A black Phosphorus/BiVO4(010) heterostructure for promising photocatalytic performance: First-principles study. Journal of Physics and Chemistry of Solids, 2020, 143, 109466.	4.0	18
18	Peculiar bond characters of fivefold coordinated octet compound crystals. Chemical Science, 2020, 11, 4340-4350.	7.4	7

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19	Stability, electronic structures, and band alignment of two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>II</mml:mi><mml:mi>A</mml:mi></mml:msub></mml:ma -IV- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> materials. Physical Review Materials, 2020, 4, .	2.4	8
20	Structures and characteristics of atomically thin ZrO₂from monolayer to bilayer and two-dimensional ZrO₂â€“MoS₂heterojunction. RSC Advances, 2019, 9, 32984-32994.	3.6	25
21	First-principles study of structural, vibrational, and electronic properties of trigonally bonded II-IV-N2. Computational Materials Science, 2019, 158, 88-97.	3.0	6
22	Stability and electronic properties of GaN phases with inversion symmetry to inherently inhibit polarization. Physical Review Materials, 2019, 3, .	2.4	11
23	Large-scale controlled synthesis of porous two-dimensional nanosheets for the hydrogen evolution reaction through a chemical pathway. Nanoscale, 2018, 10, 6168-6176.	5.6	23
24	Phonon dispersions, band structures, and dielectric functions of BeO and BeS polymorphs. Journal of Physics and Chemistry of Solids, 2018, 118, 242-247.	4.0	16
25	Hierarchical Macroâ€“Mesoporous Polymeric Carbon Nitride Microspheres with Narrow Bandgap for Enhanced Photocatalytic Hydrogen Production. Advanced Materials Interfaces, 2018, 5, 1801241.	3.7	21
26	A honeycomb-like monolayer of HfO₂ and the calculation of static dielectric constant eliminating the effect of vacuum spacing. Physical Chemistry Chemical Physics, 2018, 20, 26453-26462.	2.8	29
27	Layer-Dependent Chemically Induced Phase Transition of Two-Dimensional MoS₂. Nano Letters, 2018, 18, 3435-3440.	9.1	69
28	A general strategy for the functionalization of two-dimensional metal chalcogenides. Nanoscale, 2018, 10, 10657-10663.	5.6	9
29	Insight into the hydrogen evolution reaction of nickel dichalcogenide nanosheets: activities related to non-metal ligands. Nanoscale, 2017, 9, 5538-5544.	5.6	97
30	Bottom-up Approach Design, Band Structure, and Lithium Storage Properties of Atomically Thin Î³-FeOOH Nanosheets. ACS Applied Materials & Interfaces, 2016, 8, 21334-21342.	8.0	49
31	Edge preference and band gap characters of MoS2 and WS2 nanoribbons. Surface Science, 2016, 653, 107-112.	1.9	51
32	Band Gap Characters and Ferromagnetic/Antiferromagnetic Coupling in Group-IV Monolayers Tuned by Chemical Species and Hydrogen Adsorption Configurations. Nanoscale Research Letters, 2015, 10, 1040.	5.7	46
33	Tuning the electronic structure of silicene and germanene by biaxial strain and electric field. Physical Review B, 2015, 91, .	3.2	137
34	Effect of configuration and biaxial strain to electronic structure of half-fluorinated graphene. Surface Science, 2015, 635, 78-84.	1.9	13
35	Oneâ€Step Selfâ€Assembly Fabrication of High Quality Ni_xMg_{1â€x}O Bowlâ€Shaped Array Film and Its Enhanced Photocurrent by Mg,²⁺ Doping. Advanced Functional Materials, 2015, 25, 3256-3263.	14.9	13
36	Band gaps and dielectric functions of cubic and hexagonal diamond polytypes calculated by many-body perturbation theory. Physica Status Solidi (B): Basic Research, 2015, 252, 235-242.	1.5	11

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37	The Stability, Electronic Structure, and Optical Property of TiO₂ Polymorphs. Journal of Physical Chemistry C, 2014, 118, 11385-11396.	3.1	223
38	Theoretical ELNES fingerprints of BC2N polytypes. Computational Materials Science, 2013, 68, 335-341.	3.0	1
39	Band structures for Ge3N4 polymorphs studied by DFT-LDA and GWA. Computational Materials Science, 2013, 67, 292-295.	3.0	14
40	Structure and electronic structure of S-doped graphitic C ₃ N ₄ investigated by density functional theory. Chinese Physics B, 2012, 21, 107101.	1.4	38
41	Crystal structures and band gap characters of h-BN polytypes predicted by the dispersion corrected DFT and GW method. Solid State Communications, 2012, 152, 1817-1820.	1.9	59
42	Band gap of C3N4 in the GW approximation. International Journal of Hydrogen Energy, 2012, 37, 11072-11080.	7.1	208
43	Cubic, wurtzite, and 4H-BN band structures calculated using GW methods and maximally localized Wannier functions interpolation. Computational Materials Science, 2012, 61, 266-269.	3.0	29
44	GW calculations of the band gaps of BC2N polytypes. European Physical Journal B, 2012, 85, 1.	1.5	5
45	ELNES for boron, carbon, and nitrogen K-edges with different chemical environments in layered materials studied by density functional theory. Ultramicroscopy, 2012, 112, 61-68.	1.9	15
46	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
47	Ab initiocalculation of ELNES/XANES of BeO polymorphs. Physica Status Solidi (B): Basic Research, 2010, 247, 2190-2194.	1.5	9
48	Electronic structure of oxide fuels from experiment and first principles calculations. Journal of Physics: Conference Series, 2010, 241, 012062.	0.4	5
49	Core-level spectroscopy calculation and the plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104203.	1.8	78
50	First-principles calculation of spectral features, chemical shift and absolute threshold of ELNES and XANES using a plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104204.	1.8	88
51	Development of electron energy-loss spectroscopy for nanoscience. Micron, 2008, 39, 658-665.	2.2	7
52	Theory of core-hole effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math>core-level spectroscopy of the first-row elements. Physical Review B, 2008, 77, .	3.2	102
53	Sub-Nanometer Au Monolayer-Protected Clusters Exhibiting Molecule-like Electronic Behavior:Â Quantitative High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy and Electrochemical Characterization of Clusters with Precise Atomic Stoichiometry. Journal of Physical Chemistry B, 2006, 110, 12874-12883.	2.6	107
54	Metal Core Bonding Motifs of Monodisperse Icosahedral Au13and Larger Au Monolayer-Protected Clusters As Revealed by X-ray Absorption Spectroscopy and Transmission Electron Microscopy. Journal of Physical Chemistry B, 2006, 110, 14564-14573.	2.6	81

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55	Theoretical electron energy-loss spectroscopy and its application in materials research. Microscopy (Oxford, England), 2005, 54, 293-298.	1.5	5
56	Identification of polymorphs of sp3 bonded carbon and boron nitride using core-level absorption spectroscopy. Chemical Physics Letters, 2004, 400, 413-418.	2.6	21
57	Anisotropic spectroscopy of nitrogen K-edge in group-III nitrides. Applied Physics Letters, 2004, 84, 2784-2786.	3.3	22
58	Unoccupied electronic states inCaB6studied by density functional theory and EELS measurements. Physical Review B, 2004, 69, .	3.2	19
59	Dendrite-Assisted Growth of Silicon Nanowires in Electroless Metal Deposition. Advanced Functional Materials, 2003, 13, 127-132.	14.9	356
60	A Simple Method To Synthesize Nanowires. Chemistry of Materials, 2002, 14, 3564-3568.	6.7	183
61	Synthesis of Large-Area Silicon Nanowire Arrays via Self-Assembling Nanoelectrochemistry. Advanced Materials, 2002, 14, 1164.	21.0	686
62	Isolating and identifying the ELNES signal of CN nanocrystals embedded in an amorphous matrix. Chemical Physics Letters, 2002, 352, 12-19.	2.6	10
63	Cluster model calculation of N near K-edge energy-loss fine structures in hexagonal GaN crystal. Science in China Series A: Mathematics, 2001, 44, 1602-1607.	0.5	1
64	Anomalous Redox Features Induced by Strong Covalency in Layered NaTi _{1â” y} V _y S ₂ Cathodes for Naâ€ion Batteries. Angewandte Chemie, 0, , .	2.0	0