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	Synthesis of Large-Area Silicon Nanowire Arrays via Self-Assembling Nanoelectrochemistry. Advanced Materials, 2002, 14, 1164.	21.0	686
2	Dendrite-Assisted Growth of Silicon Nanowires in Electroless Metal Deposition. Advanced Functional Materials, 2003, 13, 127-132.	14.9	356
3	The Stability, Electronic Structure, and Optical Property of TiO₂ Polymorphs. Journal of Physical Chemistry C, 2014, 118, 11385-11396.	3.1	223
4	Band gap of C3N4 in the GW approximation. International Journal of Hydrogen Energy, 2012, 37, 11072-11080.	7.1	208
5	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
6	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
7	A Simple Method To Synthesize Nanowires. Chemistry of Materials, 2002, 14, 3564-3568.	6.7	183
8	Tuning the electronic structure of silicene and germanene by biaxial strain and electric field. Physical Review B, 2015, 91, .	3.2	137
9	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
10	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
11	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
12	Insight into the hydrogen evolution reaction of nickel dichalcogenide nanosheets: activities related to non-metal ligands. Nanoscale, 2017, 9, 5538-5544.	5.6	97
13	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
14	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
15	Core-level spectroscopy calculation and the plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104203.	1.8	78
16	Layer-Dependent Chemically Induced Phase Transition of Two-Dimensional MoS₂. Nano Letters, 2018, 18, 3435-3440.	9.1	69
17	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
18	Edge preference and band gap characters of MoS2 and WS2 nanoribbons. Surface Science, 2016, 653, 107-112.	1.9	51

#	Article	IF	Citations
19	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
20	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
21	Ultrastable Zinc Anode by Simultaneously Manipulating Solvation Sheath and Inducing Oriented Deposition with PEG Stability Promoter. Small, 2022, 18, e2103345.	10.0	39
22	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
23	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
24	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
25	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
26	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
27	Structures and characteristics of atomically thin ZrO₂from monolayer to bilayer and two-dimensional ZrO₂â€“MoS₂heterojunction. RSC Advances, 2019, 9, 32984-32994.	3.6	25
28	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
29	Anisotropic spectroscopy of nitrogen K-edge in group-III nitrides. Applied Physics Letters, 2004, 84, 2784-2786.	3.3	22
30	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
31	Hierarchical Macroâ€“Mesoporous Polymeric Carbon Nitride Microspheres with Narrow Bandgap for Enhanced Photocatalytic Hydrogen Production. Advanced Materials Interfaces, 2018, 5, 1801241.	3.7	21
32	Unoccupied electronic states inCaB6studied by density functional theory and EELS measurements. Physical Review B, 2004, 69, .	3.2	19
33	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
34	Synthesis of Honeycombâ€Structured Beryllium Oxide via Graphene Liquid Cells. Angewandte Chemie - International Edition, 2020, 59, 15734-15740.	13.8	18
35	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
36	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

#	Article	IF	Citations
37	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
38	Band structures for Ge3N4 polymorphs studied by DFT-LDA and GWA. Computational Materials Science, 2013, 67, 292-295.	3.0	14
39	Effect of configuration and biaxial strain to electronic structure of half-fluorinated graphene. Surface Science, 2015, 635, 78-84.	1.9	13
40	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
41	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
42	A method to restore the intrinsic dielectric functions of 2D materials in periodic calculations. Nanoscale, 2021, 13, 17057-17067.	5.6	11
43	Stability and electronic properties of GaN phases with inversion symmetry to inherently inhibit polarization. Physical Review Materials, 2019, 3, .	2.4	11
44	Anionic Redox Regulated via Metalâ€“Ligand Combinations in Layered Sulfides. Advanced Materials, 2022, 34, e2107353.	21.0	11
45	Isolating and identifying the ELNES signal of CN nanocrystals embedded in an amorphous matrix. Chemical Physics Letters, 2002, 352, 12-19.	2.6	10
46	Ab initiocalculation of ELNES/XANES of BeO polymorphs. Physica Status Solidi (B): Basic Research, 2010, 247, 2190-2194.	1.5	9
47	A general strategy for the functionalization of two-dimensional metal chalcogenides. Nanoscale, 2018, 10, 10657-10663.	5.6	9
48	Layer-dependent band gaps and dielectric constants of ultrathin fluorite crystals. Journal of Physics and Chemistry of Solids, 2021, 148, 109738.	4.0	8
49	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
50	Development of electron energy-loss spectroscopy for nanoscience. Micron, 2008, 39, 658-665.	2.2	7
51	Peculiar bond characters of fivefold coordinated octet compound crystals. Chemical Science, 2020, 11, 4340-4350.	7.4	7
52	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
53	Electronic and optical properties of ultrathin cerium dioxide: A many-body GW-BSE investigation. Computational Materials Science, 2021, 198, 110696.	3.0	6
54	Theoretical electron energy-loss spectroscopy and its application in materials research. Microscopy (Oxford, England), 2005, 54, 293-298.	1.5	5

#	Article	IF	Citations
55	Electronic structure of oxide fuels from experiment and first principles calculations. Journal of Physics: Conference Series, 2010, 241, 012062.	0.4	5
56	GW calculations of the band gaps of BC2N polytypes. European Physical Journal B, 2012, 85, 1.	1.5	5
57	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
58	Exciton Emissions in Bilayer WSe₂ Tuned by the Ferroelectric Polymer. Journal of Physical Chemistry Letters, 2022, 13, 1636-1643.	4.6	3
59	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
60	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
61	Theoretical ELNES fingerprints of BC2N polytypes. Computational Materials Science, 2013, 68, 335-341.	3.0	1
62	Synthesis of Honeycombâ€Structured Beryllium Oxide via Graphene Liquid Cells. Angewandte Chemie, 2020, 132, 15864-15870.	2.0	0
63	Depolarization of Few-Layer III-V and II-VI Materials through Symmetric Rumpling. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
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