Hai-bo Shu

List of Publications by Year
in descending order

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107 papers	3,598 citations	126858 33 h-index	149623 56 g-index
108 all docs	108 docs citations	108 times ranked	5770 citing authors

#	Article	IF	Citations
1	Heteroepitaxial growth and interface band alignment in a large-mismatch CsPbI₃/GaN heterojunction. Journal of Materials Chemistry C, 2022, 10, 1984-1990.	2.7	10
2	Polarizationâ€Induced Bandâ€Alignment Transition and Nonvolatile pâ€n Junctions in 2D Van der Waals Heterostructures. Advanced Electronic Materials, 2022, 8, .	2.6	9
3	Spacer Cation Engineering of Two-Dimensional Hybrid Perovskites with Tunable Band Alignment and Optoelectronic Properties. Journal of Physical Chemistry C, 2022, 126, 8408-8416.	1.5	10
4	Hierarchical computational screening of layered lead-free metal halide perovskites for optoelectronic applications. Journal of Materials Chemistry A, 2021, 9, 6476-6486.	5.2	15
5	2D-VN2 MXene as a novel anode material for Li, Na and K ion batteries: Insights from the first-principles calculations. Journal of Colloid and Interface Science, 2021, 593, 51-58.	5.0	35
6	Epitaxial growth of wafer scale antioxidant single-crystal graphene on twinned Pt(111). Carbon, 2021, 181, 225-233.	5.4	12
7	Intrinsic point defects in halide double perovskite Cs2NaBiCl6 insight from first-principles. Thin Solid Films, 2021, 732, 138781.	0.8	4
8	Strong intrinsic room-temperature ferromagnetism in freestanding non-van der Waals ultrathin 2D crystals. Nature Communications, 2021, 12, 5688.	5.8	61
9	Intrinsic Polarization-Induced Enhanced Ferromagnetism and Self-Doped pâ€“n Junctions in CrBr₃/GaN van der Waals Heterostructures. ACS Applied Materials & Interfaces, 2021, 13, 8764-8773.	4.0	19
10	In Situ Visualization of Optoelectronic Behavior of Grain Boundaries in Monolayer WSe₂ at the Nanoscale. Journal of Physical Chemistry C, 2021, 125, 26883-26891.	1.5	20
11	Intriguing electronic structures and carrier mobilities of two-dimensional GaN nanosheets: Thickness and surface effects. Computational Materials Science, 2020, 172, 109337.	1.4	13
12	Sulfur-Driven Transition from Vertical to Lateral Growth of 2D SnSâ€“SnS₂ Heterostructures and Their Band Alignments. Journal of Physical Chemistry C, 2020, 124, 27820-27828.	1.5	11
13	Ultrafast nucleation and growth of high-quality monolayer MoSe₂ crystals via vapor-liquid-solid mechanism. Nanotechnology, 2020, 31, 335601.	1.3	20
14	Synergistic enhancement effect of MoO3@Ag hybrid nanostructures for boosting selective detection sensitivity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 241, 118611.	2.0	13
15	Chemical vapor deposition growth and characterization of graphite-like film. Materials Research Express, 2020, 7, 015609.	0.8	2
16	Intrinsic point defects in lead-free organic inorganic hybrid double perovskite (OIHDP) (MA)2KBiCl6. Organic Electronics, 2020, 81, 105668.	1.4	6
17	Defect Passivation and Photoluminescence Enhancement of Monolayer MoS₂ Crystals through Sodium Halide-Assisted Chemical Vapor Deposition Growth. ACS Applied Materials & Interfaces, 2020, 12, 9563-9571.	4.0	52
18	Interface and polarization effects induced Schottky-barrier-free contacts in two-dimensional MXene/GaN heterojunctions. Journal of Materials Chemistry C, 2020, 8, 7350-7357.	2.7	34

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19	Electronic and optical properties of layered Ruddlesden Popper hybrid X2(MA)n-1SnnI3n+1 perovskite insight by first principles. Journal of Physics and Chemistry of Solids, 2020, 144, 109510.	1.9	3
20	Electron-injection driven phase transition in two-dimensional transition metal dichalcogenides. Journal of Materials Chemistry C, 2020, 8, 4432-4440.	2.7	31
21	Total absorption of WO3/WS2 stacked thin films in middle infrared light. Infrared Physics and Technology, 2019, 103, 103098.	1.3	2
22	Electrochemical Lithiation Mechanism of Two-Dimensional Transition-Metal Dichalcogenide Anode Materials: Intercalation versus Conversion Reactions. Journal of Physical Chemistry C, 2019, 123, 2139-2146.	1.5	47
23	Effect of surface intrinsic defects on the structural stability and electronic properties of the all-inorganic halide perovskite CsPbI3(0â€¯0â€¯1) film. Chemical Physics Letters, 2019, 734, 136719.	1.2	19
24	Negative electron affinity driven broadband absorption of Cs3+nPbnSb2I9+3n/GaN van der Waals heterostructures. Journal of Materials Chemistry A, 2019, 7, 22346-22352.	5.2	5
25	Thickness-Dependent Phase Stability and Electronic Properties of GaN Nanosheets and MoS₂/GaN van der Waals Heterostructures. Journal of Physical Chemistry C, 2019, 123, 3861-3867.	1.5	38
26	First-principles explorations of Li2S@V2CT hybrid structure as cathode material for lithiumâ€‘sulfur battery. Applied Surface Science, 2019, 489, 677-683.	3.1	39
27	Tuning the photoluminescence of large Ti3C2Tx MXene flakes. Ceramics International, 2019, 45, 11468-11474.	2.3	22
28	Fe, N co-doped graphene as a multi-functional anchor material for lithium-sulfur battery. Journal of Physics and Chemistry of Solids, 2019, 126, 280-286.	1.9	41
29	Unveiling the Growth Mechanism of MoS₂ with Chemical Vapor Deposition: From Two-Dimensional Planar Nucleation to Self-Seeding Nucleation. Crystal Growth and Design, 2018, 18, 1012-1019.	1.4	92
30	The effect of solvent environment toward optimization of SERS sensors for pesticides detection from chemical enhancement aspects. Sensors and Actuators B: Chemical, 2018, 256, 721-728.	4.0	51
31	Nonstoichiometry induced broadband tunable photoluminescence of monolayer WSe₂. Chemical Communications, 2018, 54, 743-746.	2.2	12
32	Enhanced Electrocatalytic Hydrogen Evolution from Large-Scale, Facile-Prepared, Highly Crystalline WTe₂ Nanoribbons with Weyl Semimetallic Phase. ACS Applied Materials & Interfaces, 2018, 10, 458-467.	4.0	64
33	Interface Synergistic Effect from Layered Metal Sulfides of MoS₂/SnS₂ van der Waals Heterojunction with Enhanced Li-Ion Storage Performance. Journal of Physical Chemistry C, 2018, 122, 24600-24608.	1.5	32
34	Semiconducting edges and flake-shape evolution of monolayer GaSe: role of edge reconstructions. Nanoscale, 2018, 10, 12133-12140.	2.8	10
35	Hierarchical MoO₃/SnS₂ coreâ€“shell nanowires with enhanced electrochemical performance for lithium-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 17171-17179.	1.3	32
36	Design rules of heteroatom-doped graphene to achieve high performance lithiumâ€“sulfur batteries: Both strong anchoring and catalysing based on first principles calculation. Journal of Colloid and Interface Science, 2018, 529, 426-431.	5.0	50

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37	Intriguing electronic and optical properties of two-dimensional Janus transition metal dichalcogenides. Physical Chemistry Chemical Physics, 2018, 20, 18571-18578.	1.3	141
38	Is borophene a suitable anode material for sodium ion battery?. Journal of Alloys and Compounds, 2017, 704, 152-159.	2.8	62
39	Design of a silver nanoparticle for sensitive surface enhanced Raman spectroscopy detection of carmine dye. Food Chemistry, 2017, 237, 974-980.	4.2	61
40	Electrocatalytic Activity and Design Principles of Heteroatom-Doped Graphene Catalysts for Oxygen-Reduction Reaction. Journal of Physical Chemistry C, 2017, 121, 14434-14442.	1.5	49
41	Efficient electron transfer kuramite Cu3SnS4 nanosheet thin film towards platinum-free cathode in dye-sensitized solar cells. Journal of Power Sources, 2017, 341, 60-67.	4.0	39
42	The Role of Intrinsic Defects in Electrocatalytic Activity of Monolayer VS₂ Basal Planes for the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2017, 121, 1530-1536.	1.5	93
43	Interface effect on electronic and optical properties of antimonene/GaAs van der Waals heterostructures. Journal of Materials Chemistry C, 2017, 5, 9687-9693.	2.7	29
44	Capture the growth kinetics of CVD growth of two-dimensional MoS2. Npj 2D Materials and Applications, 2017, 1, .	3.9	115
45	Defect Engineering in MoSe₂ for the Hydrogen Evolution Reaction: From Point Defects to Edges. ACS Applied Materials & Interfaces, 2017, 9, 42688-42698.	4.0	171
46	Borophene as Efficient Sulfur Hosts for Lithiumâ€“Sulfur Batteries: Suppressing Shuttle Effect and Improving Conductivity. Journal of Physical Chemistry C, 2017, 121, 15549-15555.	1.5	97
47	Unveiling the atomic structure and electronic properties of atomically thin boron sheets on an Ag(111) surface. Nanoscale, 2016, 8, 16284-16291.	2.8	59
48	Impact of Surface Point Defects on Electronic Properties and p-Type Doping of GaAs Nanowires. Journal of Physical Chemistry C, 2016, 120, 22088-22095.	1.5	13
49	Facile Preparation of Single MoS₂ Atomic Crystals with Highly Tunable Photoluminescence by Morphology and Atomic Structure. Crystal Growth and Design, 2016, 16, 7094-7101.	1.4	8
50	Band structures and spatial carrier confinement in GaAs/GaP core-shell nanowires: Core/shell composition and size effects. Journal of Alloys and Compounds, 2016, 682, 571-578.	2.8	7
51	Interfacial structure, ferroelectric stability, and magnetoelectric effect of magnetoelectric junction FeCo/BaTiO3/FeCo with alloy electrode. Journal of Materials Science, 2016, 51, 3297-3302.	1.7	3
52	First-principles study of the origin of magnetism induced by intrinsic defects in monolayer MoS2. Applied Surface Science, 2016, 361, 199-205.	3.1	61
53	Electronic and magnetic properties of germanene: Surface functionalization and strain effects. Solid State Communications, 2016, 226, 19-24.	0.9	36
54	The effect of lithium adsorption on the formation of 1T-MoS2 phase based on first-principles calculation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 1767-1771.	0.9	16

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55	The capacity fading mechanism and improvement of cycling stability in MoS₂-based anode materials for lithium-ion batteries. Nanoscale, 2016, 8, 2918-2926.	2.8	168
56	Invisible growth of microstructural defects in graphene chemical vapor deposition on copper foil. Carbon, 2016, 96, 237-242.	5.4	43
57	Crystal Phase and Facet Effects on the Structural Stability and Electronic Properties of GaP Nanowires. Journal of Physical Chemistry C, 2015, 119, 12030-12036.	1.5	8
58	Doping properties of MoS 2 /ZnO (0001) heterojunction ruled by interfacial micro-structure: From first principles. Solid State Communications, 2015, 204, 67-71.	0.9	23
59	Role of Chemical Potential in Flake Shape and Edge Properties of Monolayer MoS₂. Journal of Physical Chemistry C, 2015, 119, 4294-4301.	1.5	178
60	Evolution of morphology and microstructure of GaAs/GaSb nanowire heterostructures. Nanoscale Research Letters, 2015, 10, 108.	3.1	3
61	Layer-Dependent Dopant Stability and Magnetic Exchange Coupling of Iron-Doped MoS₂ Nanosheets. ACS Applied Materials & Interfaces, 2015, 7, 7534-7541.	4.0	90
62	Atomic Mechanism of Electrocatalytically Active Coâ€“N Complexes in Graphene Basal Plane for Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2015, 7, 27405-27413.	4.0	139
63	What are the active carbon species during graphene chemical vapor deposition growth?. Nanoscale, 2015, 7, 1627-1634.	2.8	89
64	Temperature-dependent nitrogen configuration of N-doped graphene by chemical vapor deposition. Carbon, 2015, 81, 814-820.	5.4	45
65	Synthesis and characterization of flower-like MoS2 microspheres by hydrothermal method. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 016102.	0.2	5
66	Vacancy effect on the doping of silicon nanowires: A first-principles study. Chinese Physics B, 2014, 23, 067304.	0.7	8
67	Crystal facet effect on structural stability and electronic properties of wurtzite InP nanowires. Journal of Applied Physics, 2014, 115, .	1.1	6
68	Two-dimensional silicene nucleation on a Ag(111) surface: structural evolution and the role of surface diffusion. Physical Chemistry Chemical Physics, 2014, 16, 304-310.	1.3	30
69	Ab initioinvestigation of the structural and electronic properties of amorphous HgTe. Journal of Physics Condensed Matter, 2014, 26, 045503.	0.7	0
70	The structural and electronic properties of amorphous HgCdTe from first-principles calculations. Journal Physics D: Applied Physics, 2014, 47, 025304.	1.3	2
71	The edge termination controlled kinetics in graphene chemical vapor deposition growth. Chemical Science, 2014, 5, 4639-4645.	3.7	41
72	The influence of unintentional Au impurities on the doping properties of Si nanowires. Solid State Communications, 2014, 183, 8-12.	0.9	5

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73	First principles study on molecule doping in MoS2 monolayer. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 117101.	0.2	8
74	Quantum confinement effect on electronic and optical properties of SnS. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 067101.	0.2	1
75	Phase Separation Induced by Au Catalysts in Ternary InGaAs Nanowires. Nano Letters, 2013, 13, 643-650.	4.5	79
76	Strain driven enhancement of ferroelectricity and magnetoelectric effect in multiferroic tunnel junction. Physical Chemistry Chemical Physics, 2013, 15, 14770.	1.3	10
77	Role of Chemical Potential in Tuning Equilibrium Crystal Shape and Electronic Properties of Wurtzite GaAs Nanowires. Journal of Physical Chemistry C, 2013, 117, 23349-23356.	1.5	15
78	Theoretical and Experimental Investigations on the Growth of SnS van der Waals Epitaxies on Graphene Buffer Layer. Crystal Growth and Design, 2013, 13, 4755-4759.	1.4	18
79	Band-offset effect on localization of carriers and p-type doping of InAs/GaAs coreâ€“shell nanowires. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1464-1468.	0.9	6
80	Band gap tuning in HgTe through uniaxial strains. Solid State Communications, 2013, 166, 1-5.	0.9	3
81	Enhancement of the accuracy of the simplified modal method for designing a subwavelength triangular grooves grating. Optics Letters, 2013, 38, 10.	1.7	14
82	Structural, electronic, and optical properties of hydrogenated few-layer silicene: Size and stacking effects. Journal of Applied Physics, 2013, 114, .	1.1	26
83	Effect of Molecular Passivation on the Doping of InAs Nanowires. Journal of Physical Chemistry C, 2012, 116, 17928-17933.	1.5	16
84	Edge Structural Stability and Kinetics of Graphene Chemical Vapor Deposition Growth. ACS Nano, 2012, 6, 3243-3250.	7.3	179
85	Magic Carbon Clusters in the Chemical Vapor Deposition Growth of Graphene. Journal of the American Chemical Society, 2012, 134, 2970-2975.	6.6	138
86	Towards ultra small noble metal nanoparticles: testing Jellium model for ligand protected copper and silver M13 core nanoparticles. Physical Chemistry Chemical Physics, 2011, 13, 3274.	1.3	10
87	First-Principles Study of the Doping of InAs Nanowires: Role of Surface Dangling Bonds. Journal of Physical Chemistry C, 2011, 115, 14449-14454.	1.5	30
88	Effect of Electrodes on Geometric and Transport Properties of the Graphene-Based Nanomolecular Devices. Journal of Nanoscience and Nanotechnology, 2011, 11, 10778-10781.	0.9	0
89	Transport properties of graphene nanoribbonâ€based molecular devices. Journal of Computational Chemistry, 2011, 32, 737-741.	1.5	8
90	The finiteâ€size effect on the transport properties in edgeâ€modified graphene nanoribbonâ€based molecular devices. Journal of Computational Chemistry, 2011, 32, 1753-1759.	1.5	4

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91	Structural, electronic and magnetic properties of Ag_nFe clusters (nâ©½ 15): local magnetic moment interacting with delocalized electrons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 035102.	0.6	13
92	Tailoring electronic properties of InAs nanowires by surface functionalization. Journal of Applied Physics, 2011, 110, 103713.	1.1	13
93	Surfactant Effect of Au on Ga Adsorption on GaAs(0001) Surface. Journal of Nanoscience and Nanotechnology, 2010, 10, 7351-7354.	0.9	0
94	Preferential adsorption of gallium on GaAs(111)B surfaces during the initial growth of Au-assisted GaAs nanowires. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 3247-3253.	0.9	3
95	Spatial confinement of carriers and tunable band structures in InAs/InP-coreâ€“shell nanowires. Chemical Physics Letters, 2010, 495, 261-265.	1.2	22
96	Thermodynamic phase diagram for hydrogen on polar InP(111)B surfaces. Journal of Applied Physics, 2010, 107, 063516.	1.1	7
97	First-Principles Study of Initial Growth of InP Nanowires: Self-Catalytic Effect and Nucleation Mechanism of In Adatoms. Journal of Physical Chemistry C, 2010, 114, 10195-10201.	1.5	5
98	Catalytic effect and nucleation stability of Au on GaAs(111)B surface. Journal of Applied Physics, 2010, 108, 013526.	1.1	5
99	Effects of electrode contact on geometry structure and transport properties of the graphene-based nanomolecule Devices. , 2010, , .		0
100	Structural Stability and Electronic Properties of InAs Nanowires and Nanotubes: Effects of Surface and Size. Journal of Physical Chemistry C, 2010, 114, 17514-17518.	1.5	20
101	The geometric structure influence on the ferromagnetism in Carbon-doped anatase : First-principles study. Solid State Communications, 2009, 149, 1717-1721.	0.9	15
102	Bonding mechanism and relaxation energy of (): First-principles study. Journal of Physics and Chemistry of Solids, 2009, 70, 707-712.	1.9	8
103	Effect of Mn doping on the microstructures and dielectric properties of Bi3.15Nd0.85Ti3O12 thin films. Thin Solid Films, 2008, 516, 8240-8243.	0.8	16
104	Effects of lattice strain and ion displacement on the bonding mechanism of the ferroelectric perovskite material BaTiO3: first-principles study. Journal of Physics Condensed Matter, 2007, 19, 276213.	0.7	4
105	Ferroelectric and dielectric properties of Nd3+â‹•Zr4+ cosubstituted Bi4Ti3O12 thin films. Applied Physics Letters, 2007, 90, 102906.	1.5	13
106	Rapid Wafer-Scale Growth of MoS2(1â€“x)Se2x Alloy Monolayers with Tunable Compositions and Optical Properties for High-Performance Photodetectors. ACS Applied Nano Materials, 0, , .	2.4	5
107	Structural Stability and Optoelectronic Properties of Lead-Free Halide Perovskite CsSnBr3 by Introducing Transition-Metal Dopants. Journal of Electronic Materials, 0, , 1.	1.0	2