# Hai-bo Shu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8008240/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 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 | Edge Structural Stability and Kinetics of Graphene Chemical Vapor Deposition Growth. ACS Nano, 2012, 6, 3243-3250. | 7.3 | 179 |
| 2 | Role of Chemical Potential in Flake Shape and Edge Properties of Monolayer MoS<sub>2</sub>. Journal of Physical Chemistry C, 2015, 119, 4294-4301. | 1.5 | 178 |
| 3 | Defect Engineering in MoSe<sub>2</sub> for the Hydrogen Evolution Reaction: From Point Defects to Edges. ACS Applied Materials & Interfaces, 2017, 9, 42688-42698. | 4.0 | 171 |
| 4 | The capacity fading mechanism and improvement of cycling stability in MoS<sub>2</sub>-based anode materials for lithium-ion batteries. Nanoscale, 2016, 8, 2918-2926. | 2.8 | 168 |
| 5 | Intriguing electronic and optical properties of two-dimensional Janus transition metal dichalcogenides. Physical Chemistry Chemical Physics, 2018, 20, 18571-18578. | 1.3 | 141 |
| 6 | 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 |
| 7 | Magic Carbon Clusters in the Chemical Vapor Deposition Growth of Graphene. Journal of the American Chemical Society, 2012, 134, 2970-2975. | 6.6 | 138 |
| 8 | Capture the growth kinetics of CVD growth of two-dimensional MoS2. Npj 2D Materials and Applications, 2017, 1, . | 3.9 | 115 |
| 9 | 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 |
| 10 | The Role of Intrinsic Defects in Electrocatalytic Activity of Monolayer VS<sub>2</sub> Basal Planes for the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2017, 121, 1530-1536. | 1.5 | 93 |
| 11 | Unveiling the Growth Mechanism of MoS<sub>2</sub> with Chemical Vapor Deposition: From Two-Dimensional Planar Nucleation to Self-Seeding Nucleation. Crystal Growth and Design, 2018, 18, 1012-1019. | 1.4 | 92 |
| 12 | Layer-Dependent Dopant Stability and Magnetic Exchange Coupling of Iron-Doped MoS<sub>2</sub> Nanosheets. ACS Applied Materials & Interfaces, 2015, 7, 7534-7541. | 4.0 | 90 |
| 13 | What are the active carbon species during graphene chemical vapor deposition growth?. Nanoscale, 2015, 7, 1627-1634. | 2.8 | 89 |
| 14 | Phase Separation Induced by Au Catalysts in Ternary InGaAs Nanowires. Nano Letters, 2013, 13, 643-650. | 4.5 | 79 |
| 15 | Enhanced Electrocatalytic Hydrogen Evolution from Large-Scale, Facile-Prepared, Highly Crystalline WTe<sub>2</sub> Nanoribbons with Weyl Semimetallic Phase. ACS Applied Materials & Interfaces, 2018, 10, 458-467. | 4.0 | 64 |
| 16 | Is borophene a suitable anode material for sodium ion battery?. Journal of Alloys and Compounds, 2017, 704, 152-159. | 2.8 | 62 |
| 17 | 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 |
| 18 | Design of a silver nanoparticle for sensitive surface enhanced Raman spectroscopy detection of carmine dye. Food Chemistry, 2017, 237, 974-980. | 4.2 | 61 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Strong intrinsic room-temperature ferromagnetism in freestanding non-van der Waals ultrathin 2D crystals. Nature Communications, 2021, 12, 5688. | 5.8 | 61 |
| 20 | 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 |
| 21 | Defect Passivation and Photoluminescence Enhancement of Monolayer MoS<sub>2</sub> Crystals through Sodium Halide-Assisted Chemical Vapor Deposition Growth. ACS Applied Materials & Interfaces, 2020, 12, 9563-9571. | 4.0 | 52 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | Temperature-dependent nitrogen configuration of N-doped graphene by chemical vapor deposition. Carbon, 2015, 81, 814-820. | 5.4 | 45 |
| 27 | Invisible growth of microstructural defects in graphene chemical vapor deposition on copper foil. Carbon, 2016, 96, 237-242. | 5.4 | 43 |
| 28 | The edge termination controlled kinetics in graphene chemical vapor deposition growth. Chemical Science, 2014, 5, 4639-4645. | 3.7 | 41 |
| 29 | 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 |
| 30 | 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 |
| 31 | 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 |
| 32 | Thickness-Dependent Phase Stability and Electronic Properties of GaN Nanosheets and MoS<sub>2</sub>/GaN van der Waals Heterostructures. Journal of Physical Chemistry C, 2019, 123, 3861-3867. | 1.5 | 38 |
| 33 | Electronic and magnetic properties of germanene: Surface functionalization and strain effects. Solid State Communications, 2016, 226, 19-24. | 0.9 | 36 |
| 34 | 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 |
| 35 | 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 |
| 36 | Interface Synergistic Effect from Layered Metal Sulfides of MoS<sub>2</sub>/SnS<sub>2</sub> van der Waals Heterojunction with Enhanced Li-Ion Storage Performance. Journal of Physical Chemistry C, 2018, 122, 24600-24608. | 1.5 | 32 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Hierarchical MoO<sub>3</sub>/SnS<sub>2</sub> coreâ€“shell nanowires with enhanced electrochemical performance for lithium-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 17171-17179. | 1.3 | 32 |
| 38 | Electron-injection driven phase transition in two-dimensional transition metal dichalcogenides. Journal of Materials Chemistry C, 2020, 8, 4432-4440. | 2.7 | 31 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | Structural, electronic, and optical properties of hydrogenated few-layer silicene: Size and stacking effects. Journal of Applied Physics, 2013, 114, . | 1.1 | 26 |
| 43 | 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 |
| 44 | Spatial confinement of carriers and tunable band structures in InAs/InP-coreâ€“shell nanowires. Chemical Physics Letters, 2010, 495, 261-265. | 1.2 | 22 |
| 45 | Tuning the photoluminescence of large Ti3C2Tx MXene flakes. Ceramics International, 2019, 45, 11468-11474. | 2.3 | 22 |
| 46 | 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 |
| 47 | Ultrafast nucleation and growth of high-quality monolayer MoSe<sub>2</sub> crystals via vapor-liquid-solid mechanism. Nanotechnology, 2020, 31, 335601. | 1.3 | 20 |
| 48 | In Situ Visualization of Optoelectronic Behavior of Grain Boundaries in Monolayer WSe<sub>2</sub> at the Nanoscale. Journal of Physical Chemistry C, 2021, 125, 26883-26891. | 1.5 | 20 |
| 49 | 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 |
| 50 | Intrinsic Polarization-Induced Enhanced Ferromagnetism and Self-Doped pâ€“n Junctions in CrBr<sub>3</sub>/GaN van der Waals Heterostructures. ACS Applied Materials & Interfaces, 2021, 13, 8764-8773. | 4.0 | 19 |
| 51 | 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 |
| 52 | 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 |
| 53 | Effect of Molecular Passivation on the Doping of InAs Nanowires. Journal of Physical Chemistry C, 2012, 116, 17928-17933. | 1.5 | 16 |
| 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | The geometric structure influence on the ferromagnetism in Carbon-doped anatase : First-principles study. Solid State Communications, 2009, 149, 1717-1721. | 0.9 | 15 |
| 56 | 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 |
| 57 | 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 |
| 58 | Enhancement of the accuracy of the simplified modal method for designing a subwavelength triangular grooves grating. Optics Letters, 2013, 38, 10. | 1.7 | 14 |
| 59 | Ferroelectric and dielectric properties of Nd3+âˆ•Zr4+ cosubstituted Bi4Ti3O12 thin films. Applied Physics Letters, 2007, 90, 102906. | 1.5 | 13 |
| 60 | Structural, electronic and magnetic properties of Ag<sub>n</sub>Fe 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 |
| 61 | Tailoring electronic properties of InAs nanowires by surface functionalization. Journal of Applied Physics, 2011, 110, 103713. | 1.1 | 13 |
| 62 | 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 |
| 63 | Intriguing electronic structures and carrier mobilities of two-dimensional GaN nanosheets: Thickness and surface effects. Computational Materials Science, 2020, 172, 109337. | 1.4 | 13 |
| 64 | 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 |
| 65 | Nonstoichiometry induced broadband tunable photoluminescence of monolayer WSe<sub>2</sub>. Chemical Communications, 2018, 54, 743-746. | 2.2 | 12 |
| 66 | Epitaxial growth of wafer scale antioxidant single-crystal graphene on twinned Pt(111). Carbon, 2021, 181, 225-233. | 5.4 | 12 |
| 67 | Sulfur-Driven Transition from Vertical to Lateral Growth of 2D SnSâ€“SnS<sub>2</sub> Heterostructures and Their Band Alignments. Journal of Physical Chemistry C, 2020, 124, 27820-27828. | 1.5 | 11 |
| 68 | 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 |
| 69 | Strain driven enhancement of ferroelectricity and magnetoelectric effect in multiferroic tunnel junction. Physical Chemistry Chemical Physics, 2013, 15, 14770. | 1.3 | 10 |
| 70 | Semiconducting edges and flake-shape evolution of monolayer GaSe: role of edge reconstructions. Nanoscale, 2018, 10, 12133-12140. | 2.8 | 10 |
| 71 | Heteroepitaxial growth and interface band alignment in a large-mismatch CsPbI<sub>3</sub>/GaN heterojunction. Journal of Materials Chemistry C, 2022, 10, 1984-1990. | 2.7 | 10 |
| 72 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Polarizationâ€Induced Bandâ€Alignment Transition and Nonvolatile pâ€n Junctions in 2D Van der Waals Heterostructures. Advanced Electronic Materials, 2022, 8, . | 2.6 | 9 |
| 74 | Bonding mechanism and relaxation energy of (): First-principles study. Journal of Physics and Chemistry of Solids, 2009, 70, 707-712. | 1.9 | 8 |
| 75 | Transport properties of graphene nanoribbonâ€based molecular devices. Journal of Computational Chemistry, 2011, 32, 737-741. | 1.5 | 8 |
| 76 | Vacancy effect on the doping of silicon nanowires: A first-principles study. Chinese Physics B, 2014, 23, 067304. | 0.7 | 8 |
| 77 | 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 |
| 78 | Facile Preparation of Single MoS<sub>2</sub> Atomic Crystals with Highly Tunable Photoluminescence by Morphology and Atomic Structure. Crystal Growth and Design, 2016, 16, 7094-7101. | 1.4 | 8 |
| 79 | First principles study on molecule doping in MoS2 monolayer. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 117101. | 0.2 | 8 |
| 80 | Thermodynamic phase diagram for hydrogen on polar InP(111)B surfaces. Journal of Applied Physics, 2010, 107, 063516. | 1.1 | 7 |
| 81 | 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 |
| 82 | 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 |
| 83 | Crystal facet effect on structural stability and electronic properties of wurtzite InP nanowires. Journal of Applied Physics, 2014, 115, . | 1.1 | 6 |
| 84 | Intrinsic point defects in lead-free organic inorganic hybrid double perovskite (OIHDP) (MA)2KBiCl6. Organic Electronics, 2020, 81, 105668. | 1.4 | 6 |
| 85 | 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 |
| 86 | Catalytic effect and nucleation stability of Au on GaAs(111)B surface. Journal of Applied Physics, 2010, 108, 013526. | 1.1 | 5 |
| 87 | The influence of unintentional Au impurities on the doping properties of Si nanowires. Solid State Communications, 2014, 183, 8-12. | 0.9 | 5 |
| 88 | 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 |
| 89 | 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 |
| 90 | Synthesis and characterization of flower-like MoS2 microspheres by hydrothermal method. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 016102. | 0.2 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | 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 |
| 92 | 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 |
| 93 | Intrinsic point defects in halide double perovskite Cs2NaBiCl6 insight from first-principles. Thin Solid Films, 2021, 732, 138781. | 0.8 | 4 |
| 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 | Band gap tuning in HgTe through uniaxial strains. Solid State Communications, 2013, 166, 1-5. | 0.9 | 3 |
| 96 | Evolution of morphology and microstructure of GaAs/GaSb nanowire heterostructures. Nanoscale Research Letters, 2015, 10, 108. | 3.1 | 3 |
| 97 | 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 |
| 98 | 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 |
| 99 | The structural and electronic properties of amorphous HgCdTe from first-principles calculations. Journal Physics D: Applied Physics, 2014, 47, 025304. | 1.3 | 2 |
| 100 | Total absorption of WO3/WS2 stacked thin films in middle infrared light. Infrared Physics and Technology, 2019, 103, 103098. | 1.3 | 2 |
| 101 | Chemical vapor deposition growth and characterization of graphite-like film. Materials Research Express, 2020, 7, 015609. | 0.8 | 2 |
| 102 | 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 |
| 103 | Quantum confinement effect on electronic and optical properties of SnS. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 067101. | 0.2 | 1 |
| 104 | Surfactant Effect of Au on Ga Adsorption on GaAs(0001) Surface. Journal of Nanoscience and Nanotechnology, 2010, 10, 7351-7354. | 0.9 | 0 |
| 105 | Effects of electrode contact on geometry structure and transport properties of the graphene-based nanomolecule Devices. , 2010, , . | | 0 |
| 106 | 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 |
| 107 | Ab initioinvestigation of the structural and electronic properties of amorphous HgTe. Journal of Physics Condensed Matter, 2014, 26, 045503. | 0.7 | 0 |