

# Jingsong Huang

## List of Publications by Year in descending order

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90  
papers

6,339  
citations

87723

38  
h-index

64668

79  
g-index

98  
all docs

98  
docs citations

98  
times ranked

9148  
citing authors

| #  | ARTICLE  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | Ultrathin Planar Graphene Supercapacitors. <i>Nano Letters</i> , 2011, 11, 1423-1427.  | 4.5  | 1,145     |
| 2  | A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes. <i>Chemistry - A European Journal</i> , 2008, 14, 6614-6626.   | 1.7  | 545       |
| 3  | Theoretical Model for Nanoporous Carbon Supercapacitors. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 520-524.   | 7.2  | 526       |
| 4  | A physical catalyst for the electrolysis of nitrogen to ammonia. <i>Science Advances</i> , 2018, 4, e1700336.  | 4.7  | 264       |
| 5  | Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores. <i>ACS Nano</i> , 2011, 5, 9044-9051.   | 7.3  | 188       |
| 6  | Ion Distribution in Electrified Micropores and Its Role in the Anomalous Enhancement of Capacitance. <i>ACS Nano</i> , 2010, 4, 2382-2390.   | 7.3  | 183       |
| 7  | Chemical nature of ferroelastic twin domains in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite. <i>Nature Materials</i> , 2018, 17, 1013-1019.  | 13.3 | 183       |
| 8  | The importance of ion size and electrode curvature on electrical double layers in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1152-1161.   | 1.3  | 173       |
| 9  | Intermolecular Covalent $\pi$ - $\pi$ Bonding Interaction Indicated by Bond Distances, Energy Bands, and Magnetism in Biphenalenyl Biradicaloid Molecular Crystal. <i>Journal of the American Chemical Society</i> , 2007, 129, 1634-1643. | 6.6  | 145       |
| 10 | Curvature effects in carbon nanomaterials: Exohedral versus endohedral supercapacitors. <i>Journal of Materials Research</i> , 2010, 25, 1525-1531.  | 1.2  | 142       |
| 11 | Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. <i>Chemical Physics Letters</i> , 2004, 390, 110-115.   | 1.2  | 137       |
| 12 | Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope. <i>Science</i> , 2019, 363, 525-528.   | 6.0  | 124       |
| 13 | Boron Nitride Nanoribbons Become Metallic. <i>Nano Letters</i> , 2011, 11, 3267-3273.  | 4.5  | 120       |
| 14 | Structure and dynamics of electrical double layers in organic electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5468.   | 1.3  | 107       |
| 15 | Tracking ion intercalation into layered Ti <sub>3</sub> C <sub>2</sub> MXene films across length scales. <i>Energy and Environmental Science</i> , 2020, 13, 2549-2558.  | 15.6 | 100       |
| 16 | A $\sigma$ -counter-charge layer in generalized solvents framework for electrical double layers in neat and hybrid ionic liquid electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14723.                                | 1.3  | 90        |
| 17 | Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 36-42.   | 2.1  | 78        |
| 18 | Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1732-1737.  | 2.1  | 77        |

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|----|--|-----|-----------|
| 19 | Validation of intermolecular transfer integral and bandwidth calculations for organic molecular materials. <i>Journal of Chemical Physics</i> , 2005, 122, 234707.   | 1.2 | 76        |
| 20 | Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine. <i>Advanced Functional Materials</i> , 2017, 27, 1700749.   | 7.8 | 74        |
| 21 | Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ . <i>Journal of Physical Chemistry C</i> , 2015, 119, 1136-1145.  | 1.5 | 73        |
| 22 | Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. <i>2D Materials</i> , 2017, 4, 021016.   | 2.0 | 72        |
| 23 | A theoretical and experimental study on manipulating the structure and properties of carbon nanotubes using substitutional dopants. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 97-118.                             | 1.0 | 70        |
| 24 | Duality of the interfacial thermal conductance in graphene-based nanocomposites. <i>Carbon</i> , 2014, 75, 169-177.  | 5.4 | 67        |
| 25 | Thermodynamics and Kinetics of Gas Storage in Porous Liquids. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7195-7200.   | 1.2 | 64        |
| 26 | Crystal packing of TCNQ anion $\pi$ -radicals governed by intermolecular covalent $\pi$ - $\pi$ bonding: DFT calculations and statistical analysis of crystal structures. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2625. | 1.3 | 61        |
| 27 | Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. <i>Nanoscale</i> , 2014, 6, 449-456.  | 2.8 | 59        |
| 28 | Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. <i>Nature Communications</i> , 2017, 8, 14815.   | 5.8 | 58        |
| 29 | Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors. <i>Journal of Materials Research</i> , 2010, 25, 1469-1475.  | 1.2 | 53        |
| 30 | Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18012-18016.  | 1.5 | 53        |
| 31 | Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. <i>Journal of Chemical Physics</i> , 2015, 142, 244703.  | 1.2 | 51        |
| 32 | Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 22-30.  | 2.1 | 51        |
| 33 | Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. <i>Journal of Physical Chemistry C</i> , 2014, 118, 16236-16245.  | 1.5 | 48        |
| 34 | Non-Transition-Metal Catalytic System for $\text{N}_2$ Reduction to $\text{NH}_3$ : A Density Functional Theory Study of Al-Doped Graphene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 570-576.                           | 2.1 | 43        |
| 35 | Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors. <i>Journal of the American Chemical Society</i> , 2003, 125, 13334-13335.   | 6.6 | 42        |
| 36 | Structure and Electronic Properties of Edge-Functionalized Armchair Boron Nitride Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15675-15681.  | 1.5 | 40        |

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|----|---|-----|-----------|
| 37 | Theoretical Analysis of Intermolecular Covalent $\pi$ - $\pi$ Bonding and Magnetic Properties of Phenalenyl and spiro-Biphenalenyl Radical $\pi$ -Dimers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6304-6315.              | 1.1 | 39        |
| 38 | A Novel and Functional Single-Layer Sheet of ZnSe. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 1458-1464.  | 4.0 | 38        |
| 39 | A dicyanobenzoquinone based cathode material for rechargeable lithium and sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 17888-17895.   | 5.2 | 35        |
| 40 | Fluxional $\sigma$ -bonds of 2,5,8-tri-tert-butyl-1,3-diazaphenalenyl dimers: stepwise [3,3], [5,5] and [7,7] sigmatropic rearrangements via $\pi$ -dimer intermediates. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5084. | 1.3 | 32        |
| 41 | Pancake $\pi$ - $\pi$ Bonding Goes Double: Unexpected $4e$ /All-Sites Bonding in Boron- and Nitrogen-Doped Phenalenyls. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2318-2325.  | 2.1 | 32        |
| 42 | Nitrogen Doping Enables Covalent-Like $\pi$ - $\pi$ Bonding between Graphenes. <i>Nano Letters</i> , 2015, 15, 5482-5491.   | 4.5 | 31        |
| 43 | Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured $2H\text{-NbTe}_2$ on Graphene for Enhanced Photoresponse. <i>Advanced Electronic Materials</i> , 2017, 3, 1700024.  | 2.6 | 31        |
| 44 | One-Dimensional Metallic Conducting Pathway of Cyclohexyl-Substituted Spiro-Biphenalenyl Neutral Radical Molecular Crystal. <i>Journal of the American Chemical Society</i> , 2006, 128, 1418-1419.                                   | 6.6 | 28        |
| 45 | Dynamics of electrical double layer formation in room-temperature ionic liquids under constant-current charging conditions. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 284109.  | 0.7 | 28        |
| 46 | Benzotrifuranone: Synthesis, Structure, and Access to Polycyclic Heteroaromatics. <i>Organic Letters</i> , 2009, 11, 4314-4317.   | 2.4 | 27        |
| 47 | Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence. <i>ACS Nano</i> , 2020, 14, 5090-5098.   | 7.3 | 27        |
| 48 | Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25817-25825.   | 1.5 | 26        |
| 49 | Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15447-15455.   | 1.5 | 26        |
| 50 | Effects of partial La filling and Sb vacancy defects on $\text{CoS}_3$ skutterudites. <i>Physical Review B</i> , 2017, 95, .  | 1.1 | 26        |
| 51 | MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane. <i>ACS Nano</i> , 2021, 15, 6233-6242.   | 7.3 | 26        |
| 52 | Electronic Structures and Charge Transport Properties of the Organic Semiconductor Bis[1,2,5]thiadiazolo-p-quinobis(1,3-dithiole), BTQBT, and Its Derivatives. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12891-12898.       | 1.2 | 23        |
| 53 | Structure and charging kinetics of electrical double layers at large electrode voltages. <i>Microfluidics and Nanofluidics</i> , 2010, 8, 703-708.  | 1.0 | 23        |
| 54 | Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24335-24344.                                | 1.5 | 23        |

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|----|--|------|-----------|
| 55 | Reply to: On the ferroelectricity of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskites. <i>Nature Materials</i> , 2019, 18, 1051-1053.  | 13.3 | 21        |
| 56 | Stepwise Cope Rearrangement of Cyclo-biphenalenyl via an Unusual Multicenter Covalent $\pi$ -Bonded Intermediate. <i>Journal of the American Chemical Society</i> , 2006, 128, 7277-7286.        | 6.6  | 20        |
| 57 | Selectively Deuterated Poly( $\mu$ -caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties. <i>Macromolecules</i> , 2018, 51, 9393-9404.                         | 2.2  | 20        |
| 58 | Strain-Induced Chemical Gradient and Polarization in Metal Halide Perovskites. <i>Advanced Electronic Materials</i> , 2020, 6, 1901235.  | 2.6  | 19        |
| 59 | Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800172.  | 1.3  | 18        |
| 60 | Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2320-2326.   | 2.1  | 18        |
| 61 | Direct writing of heterostructures in single atomically precise graphene nanoribbons. <i>Physical Review Materials</i> , 2019, 3, .  | 0.9  | 18        |
| 62 | Cyclo-biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism. <i>Chemistry of Materials</i> , 2011, 23, 874-885.                            | 3.2  | 17        |
| 63 | Electric Field Effects on the Intermolecular Interactions in Water Whiskers: Insight from Structures, Energetics, and Properties. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2083-2090. | 1.1  | 17        |
| 64 | Ab Initio Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nanocomposite Coating Applications. <i>ACS Applied Nano Materials</i> , 2018, 1, 2029-2035.   | 2.4  | 17        |
| 65 | Deuteration as a Means to Tune Crystallinity of Conducting Polymers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4333-4340.  | 2.1  | 16        |
| 66 | Multicomponent Gas Storage in Organic Cage Molecules. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12426-12433.   | 1.5  | 15        |
| 67 | Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond. <i>Journal of Energy Chemistry</i> , 2021, 63, 285-293.               | 7.1  | 15        |
| 68 | Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111). <i>Chemical Communications</i> , 2019, 55, 11848-11851.  | 2.2  | 14        |
| 69 | Electro-Induced Dewetting and Concomitant Ionic Current Avalanche in Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3120-3126.   | 2.1  | 13        |
| 70 | Solvate Ionic Liquids at Electrified Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 32151-32161.  | 4.0  | 13        |
| 71 | On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. <i>Chemical Science</i> , 2021, 12, 15637-15644.  | 3.7  | 11        |
| 72 | Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26007-26018.  | 1.5  | 9         |

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|----|--|------|-----------|
| 73 | Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. <i>Npj Computational Materials</i> , 2019, 5, .   | 3.5  | 9         |
| 74 | Hydrogen diffusion studies of microcrystalline and crystalline LaNi <sub>3.94</sub> Si <sub>0.54</sub> films. <i>Journal of Alloys and Compounds</i> , 1995, 231, 297-301.   | 2.8  | 8         |
| 75 | Theoretical investigations of electrical transport properties in CoSb <sub>3</sub> skutterudites under hydrostatic loadings. <i>Rare Metals</i> , 2018, 37, 316-325.   | 3.6  | 8         |
| 76 | Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22494-22503.  | 1.5  | 8         |
| 77 | Short communication: Hydrogen diffusion studies of microcrystalline LaNi <sub>3.94</sub> Si <sub>0.54</sub> films using the electrochemical permeation technique*1. <i>International Journal of Hydrogen Energy</i> , 1995, 20, 849-851. | 3.8  | 3         |
| 78 | Modern Theories of Carbon-Based Electrochemical Capacitors: A Short Review. , 2010, , .  |      | 3         |
| 79 | Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278.  |      | 3         |
| 80 | Molecular Heterogeneity of Polystyrene-Modified Fullerene Core Stars. <i>Macromolecules</i> , 2013, 46, 7451-7457.   | 2.2  | 3         |
| 81 | A computational workflow for designing silicon donor qubits. <i>Nanotechnology</i> , 2016, 27, 424002.   | 1.3  | 3         |
| 82 | Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25712.  | 1.0  | 3         |
| 83 | Ionic liquids-mediated interactions between nanorods. <i>Journal of Chemical Physics</i> , 2017, 147, 134704.  | 1.2  | 2         |
| 84 | Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. <i>Langmuir</i> , 2018, 34, 14552-14561.   | 1.6  | 2         |
| 85 | A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. <i>Journal of Computational Chemistry</i> , 2019, 40, 532-542.                              | 1.5  | 2         |
| 86 | Computational modeling of carbon nanostructures for energy storage applications. , 2010, , .   |      | 1         |
| 87 | Perovskites: Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine (Adv. Funct. Mater. 26/2017). <i>Advanced Functional Materials</i> , 2017, 27, .  | 7.8  | 1         |
| 88 | Geometry aids green carbon electrochemistry. <i>Nature Catalysis</i> , 2018, 1, 903-904.   | 16.1 | 1         |
| 89 | Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy. <i>Microscopy and Microanalysis</i> , 2019, 25, 1088-1089.   | 0.2  | 0         |
| 90 | From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. <i>Theoretical and Computational Chemistry</i> , 2022, , 61-86.   | 0.2  | 0         |