

# Jingsong Huang

## List of Publications by Year in descending order

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90  
papers

6,339  
citations

87888

38  
h-index

64796

79  
g-index

98  
all docs

98  
docs citations

98  
times ranked

9148  
citing authors

#	ARTICLE	IF	CITATIONS
1	Ultrathin Planar Graphene Supercapacitors. Nano Letters, 2011, 11, 1423-1427.	9.1	1,145
2	A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes. Chemistry - A European Journal, 2008, 14, 6614-6626.	3.3	545
3	Theoretical Model for Nanoporous Carbon Supercapacitors. Angewandte Chemie - International Edition, 2008, 47, 520-524.	13.8	526
4	A physical catalyst for the electrolysis of nitrogen to ammonia. Science Advances, 2018, 4, e1700336.	10.3	264
5	Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores. ACS Nano, 2011, 5, 9044-9051.	14.6	188
6	Ion Distribution in Electrified Micropores and Its Role in the Anomalous Enhancement of Capacitance. ACS Nano, 2010, 4, 2382-2390.	14.6	183
7	Chemical nature of ferroelastic twin domains in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite. Nature Materials, 2018, 17, 1013-1019.	27.5	183
8	The importance of ion size and electrode curvature on electrical double layers in ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 1152-1161.	2.8	173
9	Intermolecular Covalent $\pi$ - $\pi$ Bonding Interaction Indicated by Bond Distances, Energy Bands, and Magnetism in Biphenalenyl Biradicaloid Molecular Crystal. Journal of the American Chemical Society, 2007, 129, 1634-1643.	13.7	145
10	Curvature effects in carbon nanomaterials: Exohedral versus endohedral supercapacitors. Journal of Materials Research, 2010, 25, 1525-1531.	2.6	142
11	Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. Chemical Physics Letters, 2004, 390, 110-115.	2.6	137
12	Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope. Science, 2019, 363, 525-528.	12.6	124
13	Boron Nitride Nanoribbons Become Metallic. Nano Letters, 2011, 11, 3267-3273.	9.1	120
14	Structure and dynamics of electrical double layers in organic electrolytes. Physical Chemistry Chemical Physics, 2010, 12, 5468.	2.8	107
15	Tracking ion intercalation into layered Ti <sub>3</sub> C <sub>2</sub> MXene films across length scales. Energy and Environmental Science, 2020, 13, 2549-2558.	30.8	100
16	A $\pi$ -counter-charge layer in generalized solvents framework for electrical double layers in neat and hybrid ionic liquid electrolytes. Physical Chemistry Chemical Physics, 2011, 13, 14723.	2.8	90
17	Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging. Journal of Physical Chemistry Letters, 2016, 7, 36-42.	4.6	78
18	Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores. Journal of Physical Chemistry Letters, 2012, 3, 1732-1737.	4.6	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.	3.0	76
20	Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine. <i>Advanced Functional Materials</i> , 2017, 27, 1700749.	14.9	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.	3.1	73
22	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. <i>2D Materials</i> , 2017, 4, 021016.	4.4	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.	2.0	70
24	Duality of the interfacial thermal conductance in graphene-based nanocomposites. <i>Carbon</i> , 2014, 75, 169-177.	10.3	67
25	Thermodynamics and Kinetics of Gas Storage in Porous Liquids. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7195-7200.	2.6	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.	2.8	61
27	Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. <i>Nanoscale</i> , 2014, 6, 449-456.	5.6	59
28	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. <i>Nature Communications</i> , 2017, 8, 14815.	12.8	58
29	Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors. <i>Journal of Materials Research</i> , 2010, 25, 1469-1475.	2.6	53
30	Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18012-18016.	3.1	53
31	Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. <i>Journal of Chemical Physics</i> , 2015, 142, 244703.	3.0	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.	4.6	51
33	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. <i>Journal of Physical Chemistry C</i> , 2014, 118, 16236-16245.	3.1	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.	4.6	43
35	Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors. <i>Journal of the American Chemical Society</i> , 2003, 125, 13334-13335.	13.7	42
36	Structure and Electronic Properties of Edge-Functionalized Armchair Boron Nitride Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15675-15681.	3.1	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.	2.5	39
38	A Novel and Functional Single-Layer Sheet of ZnSe. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 1458-1464.	8.0	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.	10.3	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.	2.8	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.	4.6	32
42	Nitrogen Doping Enables Covalent-Like $\pi$ - $\pi$ Bonding between Graphenes. <i>Nano Letters</i> , 2015, 15, 5482-5491.	9.1	31
43	Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured $2\text{H-TaS}_2$ on Graphene for Enhanced Photoresponse. <i>Advanced Electronic Materials</i> , 2017, 3, 1700024.	5.1	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.	13.7	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.	1.8	28
46	Benzotrifuranone: Synthesis, Structure, and Access to Polycyclic Heteroaromatics. <i>Organic Letters</i> , 2009, 11, 4314-4317.	4.6	27
47	Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence. <i>ACS Nano</i> , 2020, 14, 5090-5098.	14.6	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.	3.1	26
49	Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15447-15455.	3.1	26
50	Effects of partial La filling and Sb vacancy defects on $\text{CoS}_3$ skutterudites. <i>Physical Review B</i> , 2017, 95, .	3.2	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.	14.6	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.	2.6	23
53	Structure and charging kinetics of electrical double layers at large electrode voltages. <i>Microfluidics and Nanofluidics</i> , 2010, 8, 703-708.	2.2	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.	3.1	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.	27.5	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.	13.7	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.	4.8	20
58	Strain-Induced Chemical Gradient and Polarization in Metal Halide Perovskites. <i>Advanced Electronic Materials</i> , 2020, 6, 1901235.	5.1	19
59	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800172.	2.8	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.	4.6	18
61	Direct writing of heterostructures in single atomically precise graphene nanoribbons. <i>Physical Review Materials</i> , 2019, 3, .	2.4	18
62	Cyclo-biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism. <i>Chemistry of Materials</i> , 2011, 23, 874-885.	6.7	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.	2.5	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.	5.0	17
65	Deuteration as a Means to Tune Crystallinity of Conducting Polymers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4333-4340.	4.6	16
66	Multicomponent Gas Storage in Organic Cage Molecules. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12426-12433.	3.1	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.	12.9	15
68	Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111). <i>Chemical Communications</i> , 2019, 55, 11848-11851.	4.1	14
69	Electro-Induced Dewetting and Concomitant Ionic Current Avalanche in Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3120-3126.	4.6	13
70	Solvate Ionic Liquids at Electrified Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 32151-32161.	8.0	13
71	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. <i>Chemical Science</i> , 2021, 12, 15637-15644.	7.4	11
72	Ab Initio Predictions of Hexagonal Zr(B <sub>2</sub> C <sub>2</sub> N <sub>2</sub> ) Polymorphs for Coherent Interface Design. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26007-26018.	3.1	9

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73	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. Npj Computational Materials, 2019, 5, .	8.7	9
74	Hydrogen diffusion studies of microcrystalline and crystalline LaNi <sub>3.94</sub> Si <sub>0.54</sub> films. Journal of Alloys and Compounds, 1995, 231, 297-301.	5.5	8
75	Theoretical investigations of electrical transport properties in CoSb <sub>3</sub> skutterudites under hydrostatic loadings. Rare Metals, 2018, 37, 316-325.	7.1	8
76	Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 22494-22503.	3.1	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. International Journal of Hydrogen Energy, 1995, 20, 849-851.	7.1	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. Macromolecules, 2013, 46, 7451-7457.	4.8	3
81	A computational workflow for designing silicon donor qubits. Nanotechnology, 2016, 27, 424002.	2.6	3
82	Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. International Journal of Quantum Chemistry, 2018, 118, e25712.	2.0	3
83	Ionic liquids-mediated interactions between nanorods. Journal of Chemical Physics, 2017, 147, 134704.	3.0	2
84	Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. Langmuir, 2018, 34, 14552-14561.	3.5	2
85	A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. Journal of Computational Chemistry, 2019, 40, 532-542.	3.3	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)). Advanced Functional Materials, 2017, 27, .	14.9	1
88	Geometry aids green carbon electrochemistry. Nature Catalysis, 2018, 1, 903-904.	34.4	1
89	Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy. Microscopy and Microanalysis, 2019, 25, 1088-1089.	0.4	0
90	From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. Theoretical and Computational Chemistry, 2022, , 61-86.	0.4	0