Jingsong Huang

List of Publications by Year
in descending order

90	6,339	87723 38	64668 79
papers	citations	h-index	g-index

98	98	98	9148
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. Theoretical and Computational Chemistry, 2022, , 61-86.	0.2	0
2	MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane. ACS Nano, 2021, 15, 6233-6242.	7.3	26
3	Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions. Journal of Physical Chemistry Letters, 2021, 12, 2320-2326.	2.1	18
4	Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond. Journal of Energy Chemistry, 2021, 63, 285-293.	7.1	15
5	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. Chemical Science, 2021, 12, 15637-15644.	3.7	11
6	Tracking ion intercalation into layered Ti₃C₂ MXene films across length scales. Energy and Environmental Science, 2020, 13, 2549-2558.	15.6	100
7	Strainâ€“Chemical Gradient and Polarization in Metal Halide Perovskites. Advanced Electronic Materials, 2020, 6, 1901235.	2.6	19
8	Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence. ACS Nano, 2020, 14, 5090-5098.	7.3	27
9	A dicyanobenzoquinone based cathode material for rechargeable lithium and sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 17888-17895.	5.2	35
10	Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy. Microscopy and Microanalysis, 2019, 25, 1088-1089.	0.2	0
11	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. Npj Computational Materials, 2019, 5, .	3.5	9
12	Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111). Chemical Communications, 2019, 55, 11848-11851.	2.2	14
13	Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope. Science, 2019, 363, 525-528.	6.0	124
14	Reply to: On the ferroelectricity of CH3NH3PbI3 perovskites. Nature Materials, 2019, 18, 1051-1053.	13.3	21
15	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. Advanced Theory and Simulations, 2019, 2, 1800172.	1.3	18
16	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.	1.5	2
17	Direct writing of heterostructures in single atomically precise graphene nanoribbons. Physical Review Materials, 2019, 3, .	0.9	18
18	Ab Initio Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nanocomposite Coating Applications. ACS Applied Nano Materials, 2018, 1, 2029-2035.	2.4	17

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19	Theoretical investigations of electrical transport properties in CoSb3 skutterudites under hydrostatic loadings. Rare Metals, 2018, 37, 316-325.	3.6	8
20	Non-Transition-Metal Catalytic System for N₂ Reduction to NH₃: AÂDensity Functional Theory Study of Al-Doped Graphene. Journal of Physical Chemistry Letters, 2018, 9, 570-576.	2.1	43
21	A physical catalyst for the electrolysis of nitrogen to ammonia. Science Advances, 2018, 4, e1700336.	4.7	264
22	Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes. Langmuir, 2018, 34, 14552-14561.	1.6	2
23	Selectively Deuterated Poly(Îµ-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties. Macromolecules, 2018, 51, 9393-9404.	2.2	20
24	Geometry aids green carbon electrochemistry. Nature Catalysis, 2018, 1, 903-904.	16.1	1
25	Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. International Journal of Quantum Chemistry, 2018, 118, e25712.	1.0	3
26	Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 22494-22503.	1.5	8
27	Solvate Ionic Liquids at Electrified Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 32151-32161.	4.0	13
28	Chemical nature of ferroelastic twin domains in CH3NH3PbI3 perovskite. Nature Materials, 2018, 17, 1013-1019.	13.3	183
29	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. 2D Materials, 2017, 4, 021016.	2.0	72
30	Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2Hâ€/1Tâ€²â€MoS₂ on Graphene for Enhanced Photoresponse. Advanced Electronic Materials, 2017, 3, 1700024.	2.6	31
31	Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€"Inorganic Perovskites by Chlorine. Advanced Functional Materials, 2017, 27, 1700749.	7.8	74
32	Multicomponent Gas Storage in Organic Cage Molecules. Journal of Physical Chemistry C, 2017, 121, 12426-12433.	1.5	15
33	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. Nature Communications, 2017, 8, 14815.	5.8	58
34	Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design. Journal of Physical Chemistry C, 2017, 121, 26007-26018.	1.5	9
35	Ionic liquids-mediated interactions between nanorods. Journal of Chemical Physics, 2017, 147, 134704.	1.2	2
36	Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers. Journal of Physical Chemistry C, 2017, 121, 24335-24344.	1.5	23

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37	Deuteration as a Means to Tune Crystallinity of Conducting Polymers. Journal of Physical Chemistry Letters, 2017, 8, 4333-4340.	2.1	16
38	Perovskites: Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine (Adv. Funct. Mater. 26/2017). Advanced Functional Materials, 2017, 27, .	7.8	1
39	Effects of partial La filling and Sb vacancy defects on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CoS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> skutterudites. Physical Review B, 2017, 95, .	1.1	26
40	Thermodynamics and Kinetics of Gas Storage in Porous Liquids. Journal of Physical Chemistry B, 2016, 120, 7195-7200.	1.2	64
41	A computational workflow for designing silicon donor qubits. Nanotechnology, 2016, 27, 424002.	1.3	3
42	Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging. Journal of Physical Chemistry Letters, 2016, 7, 36-42.	2.1	78
43	Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. Journal of Chemical Physics, 2015, 142, 244703.	1.2	51
44	Pancake Ï€â€“Ï€ Bonding Goes Double: Unexpected 4e/All-Sites Bonding in Boron- and Nitrogen-Doped Phenalenyls. Journal of Physical Chemistry Letters, 2015, 6, 2318-2325.	2.1	32
45	Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study. Journal of Physical Chemistry Letters, 2015, 6, 22-30.	2.1	51
46	A Novel and Functional Single-Layer Sheet of ZnSe. ACS Applied Materials & Interfaces, 2015, 7, 1458-1464.	4.0	38
47	Electric Field Effects on the Intermolecular Interactions in Water Whiskers: Insight from Structures, Energetics, and Properties. Journal of Physical Chemistry A, 2015, 119, 2083-2090.	1.1	17
48	Nitrogen Doping Enables Covalent-Like Ï€â€“Ï€ Bonding between Graphenes. Nano Letters, 2015, 15, 5482-5491.	4.5	31
49	Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite CH₃NH₃PbI₃. Journal of Physical Chemistry C, 2015, 119, 1136-1145.	1.5	73
50	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
51	Duality of the interfacial thermal conductance in graphene-based nanocomposites. Carbon, 2014, 75, 169-177.	5.4	67
52	Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. Nanoscale, 2014, 6, 449-456.	2.8	59
53	Dynamics of electrical double layer formation in room-temperature ionic liquids under constant-current charging conditions. Journal of Physics Condensed Matter, 2014, 26, 284109.	0.7	28
54	Electro-Induced Dewetting and Concomitant Ionic Current Avalanche in Nanopores. Journal of Physical Chemistry Letters, 2013, 4, 3120-3126.	2.1	13

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55	Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2013, 117, 25817-25825.	1.5	26
56	Molecular Heterogeneity of Polystyrene-Modified Fullerene Core Stars. Macromolecules, 2013, 46, 7451-7457.	2.2	3
57	Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons. Journal of Physical Chemistry C, 2013, 117, 15447-15455.	1.5	26
58	Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores. Journal of Physical Chemistry Letters, 2012, 3, 1732-1737.	2.1	77
59	Structure and Electronic Properties of Edge-Functionalized Armchair Boron Nitride Nanoribbons. Journal of Physical Chemistry C, 2012, 116, 15675-15681.	1.5	40
60	Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278.		3
61	The importance of ion size and electrode curvature on electrical double layers in ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 1152-1161.	1.3	173
62	Cyclo-biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism. Chemistry of Materials, 2011, 23, 874-885.	3.2	17
63	Boron Nitride Nanoribbons Become Metallic. Nano Letters, 2011, 11, 3267-3273.	4.5	120
64	Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores. ACS Nano, 2011, 5, 9044-9051.	7.3	188
65	Ultrathin Planar Graphene Supercapacitors. Nano Letters, 2011, 11, 1423-1427.	4.5	1,145
66	A â€œcounter-charge layer in generalized solventsâ€• framework for electrical double layers in neat and hybrid ionic liquid electrolytes. Physical Chemistry Chemical Physics, 2011, 13, 14723.	1.3	90
67	Structure and charging kinetics of electrical double layers at large electrode voltages. Microfluidics and Nanofluidics, 2010, 8, 703-708.	1.0	23
68	Effect of diffuse layer and pore shapes in mesoporous carbon supercapacitors. Journal of Materials Research, 2010, 25, 1469-1475.	1.2	53
69	Computational modeling of carbon nanostructures for energy storage applications. , 2010, , .		1
70	Modern Theories of Carbon-Based Electrochemical Capacitors: A Short Review. , 2010, , .		3
71	Ion Distribution in Electrified Micropores and Its Role in the Anomalous Enhancement of Capacitance. ACS Nano, 2010, 4, 2382-2390.	7.3	183
72	Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors. Journal of Physical Chemistry C, 2010, 114, 18012-18016.	1.5	53

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73	Curvature effects in carbon nanomaterials: Exohedral versus endohedral supercapacitors. Journal of Materials Research, 2010, 25, 1525-1531.	1.2	142
74	Fluxional Ïƒ-bonds of 2,5,8-tri-tert-butyl-1,3-diazaphenalenyl dimers: stepwise [3,3], [5,5] and [7,7] sigmatropic rearrangements viaÏ€-dimer intermediates. Physical Chemistry Chemical Physics, 2010, 12, 5084.	1.3	32
75	Structure and dynamics of electrical double layers in organic electrolytes. Physical Chemistry Chemical Physics, 2010, 12, 5468.	1.3	107
76	A theoretical and experimental study on manipulating the structure and properties of carbon nanotubes using substitutional dopants. International Journal of Quantum Chemistry, 2009, 109, 97-118.	1.0	70
77	Benzotrifuranone: Synthesis, Structure, and Access to Polycyclic Heteroaromatics. Organic Letters, 2009, 11, 4314-4317.	2.4	27
78	A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes. Chemistry - A European Journal, 2008, 14, 6614-6626.	1.7	545
79	Theoretical Model for Nanoporous Carbon Supercapacitors. Angewandte Chemie - International Edition, 2008, 47, 520-524.	7.2	526
80	Crystal packing of TCNQ anion Ï€-radicals governed by intermolecular covalent Ï€â€“Ï€ bonding: DFT calculations and statistical analysis of crystal structures. Physical Chemistry Chemical Physics, 2008, 10, 2625.	1.3	61
81	Intermolecular Covalent Ï€âˆ’Ï€ 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.	6.6	145
82	Theoretical Analysis of Intermolecular Covalent Ï€âˆ’Ï€ Bonding and Magnetic Properties of Phenalenyl and spiro-Biphenalenyl Radical Ï€-Dimers. Journal of Physical Chemistry A, 2007, 111, 6304-6315.	1.1	39
83	Stepwise Cope Rearrangement of Cyclo-biphenalenyl via an Unusual Multicenter Covalent Ï€-Bonded Intermediate. Journal of the American Chemical Society, 2006, 128, 7277-7286.	6.6	20
84	One-Dimensional Metallic Conducting Pathway of Cyclohexyl-Substituted Spiro-Biphenalenyl Neutral Radical Molecular Crystal. Journal of the American Chemical Society, 2006, 128, 1418-1419.	6.6	28
85	Electronic Structures and Charge Transport Properties of the Organic Semiconductor Bis[1,2,5]thiadiazolo-p-quinobis(1,3-dithiole), BTQBT, and Its Derivatives. Journal of Physical Chemistry B, 2005, 109, 12891-12898.	1.2	23
86	Validation of intermolecular transfer integral and bandwidth calculations for organic molecular materials. Journal of Chemical Physics, 2005, 122, 234707.	1.2	76
87	Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. Chemical Physics Letters, 2004, 390, 110-115.	1.2	137
88	Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors. Journal of the American Chemical Society, 2003, 125, 13334-13335.	6.6	42
89	Short communication: Hydrogen diffusion studies of microcrystalline LaNi3.94 Si0.54 films using the electrochemical permeation technique*1. International Journal of Hydrogen Energy, 1995, 20, 849-851.	3.8	3
90	Hydrogen diffusion studies of microcrystalline and crystalline LaNi3.94Si0.54 films. Journal of Alloys and Compounds, 1995, 231, 297-301.	2.8	8