Hao Ren

List of Publications by Year
in descending order

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76	2,283	304602	233338
papers	citations	22 h-index	45 g-index

77	77	77	3307
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Highly efficient photocatalytic reduction of nitrogen into ammonia by single Ru atom catalyst supported by BeO monolayer. Chinese Chemical Letters, 2022, 33, 399-403.	4.8	13
2	Understanding the oxygen-vacancy-related catalytic cycle for H2 oxidation on ceria-based SOFC anode and the promotion effect of lanthanide doping from theoretical perspectives. Applied Surface Science, 2022, 576, 151803.	3.1	6
3	Carbon Dot Blinking Fingerprint Uncovers Native Membrane Receptor Organizations via Deep Learning. Analytical Chemistry, 2022, 94, 3914-3921.	3.2	6
4	Effective Tuning of the Performance of Conductive Silicon Compound by Few-Layered Graphene Additives. Nanomaterials, 2022, 12, 907.	1.9	0
5	A Novel Lattice Boltzmann Scheme with Single Extended Force Term for Electromagnetic Wave Propagating in One-Dimensional Plasma Medium. Electronics (Switzerland), 2022, 11, 882.	1.8	2
6	Machine learning recognition of protein secondary structures based on two-dimensional spectroscopic descriptors. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2202713119.	3.3	16
7	A New Lattice Boltzmann Scheme for Photonic Bandgap and Defect Mode Simulation in One-Dimensional Plasma Photonic Crystals. Photonics, 2022, 9, 464.	0.9	0
8	High-performance aluminum-polyaniline battery based on the interaction between aluminum ion and -NH groups. Science China Materials, 2021, 64, 318-328.	3.5	31
9	Density functional theory study of thiophene desulfurization and conversion of desulfurization products on the Ni(111) surface and Ni₅₅ cluster: implication for the mechanism of reactive adsorption desulfurization over Ni/ZnO catalysts. Catalysis Science and Technology, 2021, 11, 1615-1625.	2.1	12
10	Deep-Learning-Assisted Single-Molecule Tracking on a Live Cell Membrane. Analytical Chemistry, 2021, 93, 8810-8816.	3.2	18
11	ZnO monolayer supported single atom catalysts for efficient nitrogen electroreduction to ammonia. Applied Surface Science, 2021, 555, 149682.	3.1	15
12	A machine learning vibrational spectroscopy protocol for spectrum prediction and spectrum-based structure recognition. Fundamental Research, 2021, 1, 488-494.	1.6	19
13	Analysis of the Influence of Silicone Rubber Aging on the Transmission Parameters of Terahertz Waves. Energies, 2021, 14, 4238.	1.6	5
14	Computational design of photoswitchable anion receptors: Red-shifted and bistable di-ortho-fluoro di-ortho-chloro azobenzene derivatives. Chemical Physics, 2021, 548, 111246.	0.9	2
15	Structural insights of catalytic intermediates in dialumene based CO2 capture: Evidences from theoretical resonance Raman spectra. Chinese Chemical Letters, 2021, 32, 2469-2473.	4.8	10
16	Ultrafast stimulated resonance Raman signatures of lithium polysulfides for shuttling effect characterization: An ab initio study. Journal of Chemical Physics, 2021, 155, 174301.	1.2	2
17	Data-Driven Design of Nanopore Graphene for Water Desalination. Journal of Physical Chemistry C, 2021, 125, 27685-27692.	1.5	12
18	Mo doping induced metallic CoSe for enhanced electrocatalytic hydrogen evolution. Applied Catalysis B: Environmental, 2020, 268, 118467.	10.8	93

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19	High performance aluminum ion battery using polyaniline/ordered mesoporous carbon composite. Journal of Power Sources, 2020, 477, 228702.	4.0	33
20	Controllable Substitution of S Radicals on Triazine Covalent Framework to Expedite Degradation of Polysulfides. Small, 2020, 16, e2004631.	5.2	19
21	Î²-Hydrogen of Polythiophene Induced Aluminum Ion Storage for High-Performance Al-Polythiophene Batteries. ACS Applied Materials & Interfaces, 2020, 12, 46065-46072.	4.0	31
22	Adsorption and dehydrogenation of C₂â€“C₆n-alkanes over a Pt catalyst: a theoretical study on the size effects of alkane molecules and Pt substrates. Physical Chemistry Chemical Physics, 2020, 22, 21835-21843.	1.3	18
23	Lithium and Sodium Adsorption on Monolayer Tellurene. Journal of Physical Chemistry C, 2020, 124, 28074-28082.	1.5	4
24	Temperatureâ€Mediated Engineering of Graphdiyne Framework Enabling Highâ€Performance Potassium Storage. Advanced Functional Materials, 2020, 30, 2003039.	7.8	62
25	Theoretical investigation on H2 oxidation mechanisms over pristine and Sm-doped CeO2(1â€¯1â€¯1) surfaces. Applied Surface Science, 2020, 511, 145388.	3.1	12
26	First principles study of ferroelectric hexagonal compounds RInO3 (R = Dy, Er, and Ho): electronic structure, optical and dielectric properties. RSC Advances, 2020, 10, 4080-4086.	1.7	4
27	Controllably Enriched Oxygen Vacancies through Polymer Assistance in Titanium Pyrophosphate as a Super Anode for Na/K-Ion Batteries. ACS Nano, 2019, 13, 9227-9236.	7.3	94
28	Modulation of Inverse Spinel Fe₃O₄ by Phosphorus Doping as an Industrially Promising Electrocatalyst for Hydrogen Evolution. Advanced Materials, 2019, 31, e1905107.	11.1	225
29	Diabatic Hamiltonian construction in van der Waals heterostructure complexes. Journal of Materials Chemistry A, 2019, 7, 27484-27492.	5.2	6
30	Efficient energy gap tuning for T-carbon via single atomic doping. Chemical Physics, 2019, 518, 69-73.	0.9	13
31	Structural Modulation of Co Catalyzed Carbon Nanotubes with Cuâ€“Co Bimetal Active Center to Inspire Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2019, 11, 3937-3945.	4.0	51
32	Combined thermodynamic and kinetic analysis of GroEL interacting with CXCR4 transmembrane peptides. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1576-1583.	1.1	0
33	Extracting pulmonary surfactants to form inverse micelles on suspended graphene nanosheets. Environmental Science: Nano, 2018, 5, 130-140.	2.2	19
34	Stabilizing Effect of Inherent Knots on Proteins Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2018, 115, 1681-1689.	0.2	11
35	NBNâ€Doped Conjugated Polycyclic Aromatic Hydrocarbons as an AIEgen Class for Extremely Sensitive Detection of Explosives. Angewandte Chemie, 2018, 130, 15736-15742.	1.6	17
36	NBNâ€Doped Conjugated Polycyclic Aromatic Hydrocarbons as an AIEgen Class for Extremely Sensitive Detection of Explosives. Angewandte Chemie - International Edition, 2018, 57, 15510-15516.	7.2	67

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37	Chemical identification of the amyloid peptide aggregation-prone Al(III)-peptide complexes by resonance Raman signatures: A computational study. Chemical Physics, 2018, 513, 1-6.	0.9	5
38	An amorphous tin-based nanohybrid for ultra-stable sodium storage. Journal of Materials Chemistry A, 2018, 6, 18920-18927.	5.2	22
39	Role of Lipid Coating in the Transport of Nanodroplets across the Pulmonary Surfactant Layer Revealed by Molecular Dynamics Simulations. Langmuir, 2018, 34, 9054-9063.	1.6	24
40	â€œDryâ€•NiCo2O4 nanorods for electrochemical non-enzymatic glucose sensing. Chinese Journal of Chemical Physics, 2018, 31, 799-805.	0.6	5
41	Electronic and transport properties of 2H 1â^'x 1T x MoS 2 hybrid structure: A first-principle study. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 91, 178-184.	1.3	7
42	Transport of nanoparticles across pulmonary surfactant monolayer: a molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 17568-17576.	1.3	32
43	First principles studies on electronic and transport properties of edge contact graphene-MoS2 heterostructure. Computational Materials Science, 2017, 133, 137-144.	1.4	23
44	A first principles study of the interaction between two-dimensional black phosphorus and Al₂O₃dielectric. RSC Advances, 2017, 7, 13777-13783.	1.7	5
45	High-Density Super-Resolution Localization Imaging with Blinking Carbon Dots. Analytical Chemistry, 2017, 89, 11831-11838.	3.2	51
46	Interaction pathways between soft lipid nanodiscs and plasma membranes: A molecular modeling study. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2096-2105.	1.4	9
47	Identifying Cu(<scp>ii</scp>)â€“amyloid peptide binding intermediates in the early stages of aggregation by resonance Raman spectroscopy: a simulation study. Physical Chemistry Chemical Physics, 2017, 19, 31103-31112.	1.3	10
48	Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. Physical Chemistry Chemical Physics, 2017, 19, 32389-32397.	1.3	12
49	Stable folding intermediates prevent fast interconversion between the closed and open states of Mad2 through its denatured state. Protein Engineering, Design and Selection, 2016, 29, gzv056.	1.0	5
50	Visible and Near-Infrared Dual-Emission Carbogenic Small Molecular Complex with High RNA Selectivity and Renal Clearance for Nucleolus and Tumor Imaging. ACS Applied Materials & Interfaces, 2016, 8, 28529-28537.	4.0	39
51	Strong Fermi level pinning induces a high rectification ratio and negative differential resistance in hydrogen bonding bridged single cytidine pair junctions. Physical Chemistry Chemical Physics, 2016, 18, 26586-26594.	1.3	14
52	Chaperonin-enhanced Escherichia coli cell-free expression of functional CXCR4. Journal of Biotechnology, 2016, 231, 193-200.	1.9	8
53	How transmembrane peptides insert and orientate in biomembranes: a combined experimental and simulation study. Physical Chemistry Chemical Physics, 2016, 18, 17483-17494.	1.3	11
54	An Ultraâ€High Fluorescence Enhancement and High Throughput Assay for Revealing Expression and Internalization of Chemokine Receptor CXCR4. Chemistry - A European Journal, 2016, 22, 5863-5867.	1.7	6

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55	Gas adsorption on MoS₂/WS₂ in-plane heterojunctions and the Iâ€“V response: a first principles study. RSC Advances, 2016, 6, 17494-17503.	1.7	56
56	The electronic structure, mechanical flexibility and carrier mobility of black arsenicâ€“phosphorus monolayers: a first principles study. Physical Chemistry Chemical Physics, 2016, 18, 9779-9787.	1.3	50
57	Electronic and transport properties of graphene with grain boundaries. RSC Advances, 2016, 6, 1090-1097.	1.7	14
58	Energy gap engineering of polymeric carbon nitride nanosheets for matching with NaYF₄:Yb,Tm: enhanced visible-near infrared photocatalytic activity. Chemical Communications, 2016, 52, 453-456.	2.2	43
59	Folding of newly translated membrane protein CCR5 is assisted by the chaperonin GroEL-GroES. Scientific Reports, 2015, 5, 17037.	1.6	13
60	Simulations of two-dimensional infrared and stimulated resonance Raman spectra of photoactive yellow protein. Chemical Physics, 2013, 422, 63-72.	0.9	2
61	Two-dimensional stimulated resonance Raman spectroscopy study of the Trp-cage peptide folding. Physical Chemistry Chemical Physics, 2013, 15, 19457.	1.3	17
62	Time Resolved Photoelectron Spectroscopy of Thioflavin T Photoisomerization: A Simulation Study. Journal of Physical Chemistry A, 2013, 117, 6096-6104.	1.1	20
63	Multiple Core and Vibronic Coupling Effects in Attosecond Stimulated X-Ray Raman Spectroscopy. Journal of Chemical Theory and Computation, 2013, 9, 5479-5489.	2.3	12
64	Twoâ€dimensional stimulated ultraviolet resonance Raman spectra of tyrosine and tryptophan: a simulation study. Journal of Raman Spectroscopy, 2013, 44, 544-559.	1.2	27
65	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146.	1.5	103
66	Deep UV Resonance Raman Spectroscopy of Î²-Sheet Amyloid Fibrils: A QM/MM Simulation. Journal of Physical Chemistry B, 2011, 115, 13955-13962.	1.2	14
67	Electronic structure of bismuth telluride quasi-two-dimensional crystal: A first principles study. Applied Physics Letters, 2011, 98, .	1.5	19
68	Identifying configuration and orientation of adsorbed molecules by inelastic electron tunneling spectra. Journal of Chemical Physics, 2010, 133, 064702.	1.2	6
69	Important Structural Factors Controlling the Conductance of DNA Pairs in Molecular Junctions. Journal of Physical Chemistry C, 2010, 114, 14240-14242.	1.5	11
70	Simulation of inelastic electronic tunneling spectra of adsorbates from first principles. Journal of Chemical Physics, 2009, 130, 134707.	1.2	12
71	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	1.5	219
72	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2008, 129, 074704.	1.2	182

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73	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. Chinese Journal of Chemical Physics, 2007, 20, 489-494.	0.6	8
74	Switching mechanism of photochromic diarylethene derivatives molecular junctions. Journal of Chemical Physics, 2007, 127, 094705.	1.2	44
75	Tuning the electronic structure of graphene nanoribbons through chemical edge modification: A theoretical study. Physical Review B, 2007, 75, .	1.1	156
76	Single quintuple bond [PhCrCrPh] molecule as a possible molecular switch. Journal of Chemical Physics, 2006, 125, 184713.	1.2	19