Hao Ren

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Modulation of Inverse Spinel Fe ₃ O ₄ by Phosphorus Doping as an Industrially Promising Electrocatalyst for Hydrogen Evolution. Advanced Materials, 2019, 31, e1905107.	11.1	225
2	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	1,5	219
3	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2008, 129, 074704.	1.2	182
4	Tuning the electronic structure of graphene nanoribbons through chemical edge modification: A theoretical study. Physical Review B, 2007, 75, .	1.1	156
5	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146.	1.5	103
6	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
7	Mo doping induced metallic CoSe for enhanced electrocatalytic hydrogen evolution. Applied Catalysis B: Environmental, 2020, 268, 118467.	10.8	93
8	NBNâ€Doped Conjugated Polycyclic Aromatic Hydrocarbons as an AlEgen Class for Extremely Sensitive Detection of Explosives. Angewandte Chemie - International Edition, 2018, 57, 15510-15516.	7.2	67
9	Temperatureâ€Mediated Engineering of Graphdiyne Framework Enabling Highâ€Performance Potassium Storage. Advanced Functional Materials, 2020, 30, 2003039.	7.8	62
10	Gas adsorption on MoS ₂ /WS ₂ in-plane heterojunctions and the l–V response: a first principles study. RSC Advances, 2016, 6, 17494-17503.	1.7	56
11	High-Density Super-Resolution Localization Imaging with Blinking Carbon Dots. Analytical Chemistry, 2017, 89, 11831-11838.	3.2	51
12	Structural Modulation of Co Catalyzed Carbon Nanotubes with Cu–Co Bimetal Active Center to Inspire Oxygen Reduction Reaction. ACS Applied Materials & Diterfaces, 2019, 11, 3937-3945.	4.0	51
13	The electronic structure, mechanical flexibility and carrier mobility of black arsenic–phosphorus monolayers: a first principles study. Physical Chemistry Chemical Physics, 2016, 18, 9779-9787.	1.3	50
14	Switching mechanism of photochromic diarylethene derivatives molecular junctions. Journal of Chemical Physics, 2007, 127, 094705.	1.2	44
15	Energy gap engineering of polymeric carbon nitride nanosheets for matching with NaYF ₄ :Yb,Tm: enhanced visible-near infrared photocatalytic activity. Chemical Communications, 2016, 52, 453-456.	2.2	43
16	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 & Emp; Interfaces, 2016, 8, 28529-28537.	4.0	39
17	High performance aluminum ion battery using polyaniline/ordered mesoporous carbon composite. Journal of Power Sources, 2020, 477, 228702.	4.0	33
18	Transport of nanoparticles across pulmonary surfactant monolayer: a molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 17568-17576.	1.3	32

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19	\hat{l}^2 -Hydrogen of Polythiophene Induced Aluminum Ion Storage for High-Performance Al-Polythiophene Batteries. ACS Applied Materials & Samp; Interfaces, 2020, 12, 46065-46072.	4.0	31
20	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
21	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
22	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
23	First principles studies on electronic and transport properties of edge contact graphene-MoS2 heterostructure. Computational Materials Science, 2017, 133, 137-144.	1.4	23
24	An amorphous tin-based nanohybrid for ultra-stable sodium storage. Journal of Materials Chemistry A, 2018, 6, 18920-18927.	5.2	22
25	Time Resolved Photoelectron Spectroscopy of Thioflavin T Photoisomerization: A Simulation Study. Journal of Physical Chemistry A, 2013, 117, 6096-6104.	1.1	20
26	Single quintuple bond [PhCrCrPh] molecule as a possible molecular switch. Journal of Chemical Physics, 2006, 125, 184713.	1.2	19
27	Electronic structure of bismuth telluride quasi-two-dimensional crystal: A first principles study. Applied Physics Letters, 2011, 98, .	1.5	19
28	Extracting pulmonary surfactants to form inverse micelles on suspended graphene nanosheets. Environmental Science: Nano, 2018, 5, 130-140.	2.2	19
29	Controllable Substitution of S Radicals on Triazine Covalent Framework to Expedite Degradation of Polysulfides. Small, 2020, 16, e2004631.	5.2	19
30	A machine learning vibrational spectroscopy protocol for spectrum prediction and spectrum-based structure recognition. Fundamental Research, 2021, 1, 488-494.	1.6	19
31	Adsorption and dehydrogenation of C ₂ –C ₆ <i>n</i> -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
32	Deep-Learning-Assisted Single-Molecule Tracking on a Live Cell Membrane. Analytical Chemistry, 2021, 93, 8810-8816.	3.2	18
33	Two-dimensional stimulated resonance Raman spectroscopy study of the Trp-cage peptide folding. Physical Chemistry Chemical Physics, 2013, 15, 19457.	1.3	17
34	NBNâ€Doped Conjugated Polycyclic Aromatic Hydrocarbons as an AlEgen Class for Extremely Sensitive Detection of Explosives. Angewandte Chemie, 2018, 130, 15736-15742.	1.6	17
35	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
36	ZnO monolayer supported single atom catalysts for efficient nitrogen electroreduction to ammonia. Applied Surface Science, 2021, 555, 149682.	3.1	15

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37	Deep UV Resonance Raman Spectroscopy of \hat{l}^2 -Sheet Amyloid Fibrils: A QM/MM Simulation. Journal of Physical Chemistry B, 2011, 115, 13955-13962.	1.2	14
38	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
39	Electronic and transport properties of graphene with grain boundaries. RSC Advances, 2016, 6, 1090-1097.	1.7	14
40	Folding of newly translated membrane protein CCR5 is assisted by the chaperonin GroEL-GroES. Scientific Reports, 2015, 5, 17037.	1.6	13
41	Efficient energy gap tuning for T-carbon via single atomic doping. Chemical Physics, 2019, 518, 69-73.	0.9	13
42	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
43	Simulation of inelastic electronic tunneling spectra of adsorbates from first principles. Journal of Chemical Physics, 2009, 130, 134707.	1.2	12
44	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
45	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
46	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
47	Density functional theory study of thiophene desulfurization and conversion of desulfurization products on the Ni(111) surface and Ni ₅₅ cluster: implication for the mechanism of reactive adsorption desulfurization over Ni/ZnO catalysts. Catalysis Science and Technology, 2021, 11, 1615-1625.	2.1	12
48	Data-Driven Design of Nanopore Graphene for Water Desalination. Journal of Physical Chemistry C, 2021, 125, 27685-27692.	1.5	12
49	Important Structural Factors Controlling the Conductance of DNA Pairs in Molecular Junctions. Journal of Physical Chemistry C, 2010, 114, 14240-14242.	1.5	11
50	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
51	Stabilizing Effect of Inherent Knots on Proteins Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2018, 115, 1681-1689.	0.2	11
52	Identifying Cu(<scp>ii</scp>)–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
53	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
54	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

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55	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. Chinese Journal of Chemical Physics, 2007, 20, 489-494.	0.6	8
56	Chaperonin-enhanced Escherichia coli cell-free expression of functional CXCR4. Journal of Biotechnology, 2016, 231, 193-200.	1.9	8
57	Electronic and transport properties of 2H $1\hat{a}^*x$ 1T x MoS 2 hybrid structure: A first-principle study. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 91, 178-184.	1.3	7
58	Identifying configuration and orientation of adsorbed molecules by inelastic electron tunneling spectra. Journal of Chemical Physics, 2010, 133, 064702.	1.2	6
59	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
60	Diabatic Hamiltonian construction in van der Waals heterostructure complexes. Journal of Materials Chemistry A, 2019, 7, 27484-27492.	5.2	6
61	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
62	Carbon Dot Blinking Fingerprint Uncovers Native Membrane Receptor Organizations via Deep Learning. Analytical Chemistry, 2022, 94, 3914-3921.	3.2	6
63	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
64	A first principles study of the interaction between two-dimensional black phosphorus and Al ₂ O ₃ dielectric. RSC Advances, 2017, 7, 13777-13783.	1.7	5
65	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
66	Analysis of the Influence of Silicone Rubber Aging on the Transmission Parameters of Terahertz Waves. Energies, 2021, 14, 4238.	1.6	5
67	"Dry―NiCo2O4 nanorods for electrochemical non-enzymatic glucose sensing. Chinese Journal of Chemical Physics, 2018, 31, 799-805.	0.6	5
68	Lithium and Sodium Adsorption on Monolayer Tellurene. Journal of Physical Chemistry C, 2020, 124, 28074-28082.	1.5	4
69	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
70	Simulations of two-dimensional infrared and stimulated resonance Raman spectra of photoactive yellow protein. Chemical Physics, 2013, 422, 63-72.	0.9	2
71	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
72	Ultrafast stimulated resonance Raman signatures of lithium polysulfides for shuttling effect characterization: An <i>ab initio</i> study. Journal of Chemical Physics, 2021, 155, 174301.	1.2	2

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73	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
74	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
75	Effective Tuning of the Performance of Conductive Silicon Compound by Few-Layered Graphene Additives. Nanomaterials, 2022, 12, 907.	1.9	O
76	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