Jing

List of Publications by Year
in descending order

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84	2,711	201385 27	205818 48
papers	citations	h-index	g-index

88	88	88	3614
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. Physical Chemistry Chemical Physics, 2022, 24, 1326-1337.	1.3	18
2	Surface Stability and Morphology of Calcium Phosphate Tuned by pH Values and Lactic Acid Additives: Theoretical and Experimental Study. ACS Applied Materials & Interfaces, 2022, 14, 4836-4851.	4.0	16
3	Discovery of Electronic Structure and Interfacial Interaction Features in Catalytic Activity. Langmuir, 2022, 38, 3959-3968.	1.6	2
4	Identification of Single-Molecule Catecholamine Enantiomers Using a Programmable Nanopore. ACS Nano, 2022, 16, 6615-6624.	7.3	24
5	Single-Atom Tailoring of Two-Dimensional Atomic Crystals Enables Highly Efficient Detection and Pattern Recognition of Chemical Vapors. ACS Sensors, 2022, 7, 1533-1543.	4.0	16
6	Transition orbital projection approach for excited state tracking. Journal of Chemical Physics, 2022, 156, .	1.2	2
7	In Situ Synthesis of Organopolysulfides Enabling Spatial and Kinetic Co-Mediation of Sulfur Chemistry. ACS Nano, 2022, 16, 9163-9171.	7.3	13
8	Boosting the performance of single-atom catalysts via external electric field polarization. Nature Communications, 2022, 13, .	5.8	52
9	Nitrogen reduction reaction energy and pathways in metal-zeolites: deep learning and explainable machine learning with local acidity and hydrogen bonding features. Journal of Materials Chemistry A, 2022, 10, 14976-14988.	5.2	14
10	Batch-Scale Synthesis of Nanoparticle-Agminated Three-Dimensional Porous Cu@Cu₂O Microspheres for Highly Selective Electrocatalysis of Nitrate to Ammonia. Environmental Science & Technology, 2022, 56, 10299-10307.	4.6	37
11	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. Accounts of Chemical Research, 2021, 54, 169-181.	7.6	36
12	Near-Infrared-Responsive Photo-Driven Nitrogen Fixation Enabled by Oxygen Vacancies and Sulfur Doping in Black TiO_{2â€“<i>x</i>}S_{<i>y</i>} Nanoplatelets. ACS Applied Materials & Interfaces, 2021, 13, 4975-4983.	4.0	48
13	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. Journal of Physical Chemistry B, 2021, 125, 518-527.	1.2	4
14	Missing-Linker 2D Conductive Metal Organic Frameworks for Rapid Gas Detection. ACS Sensors, 2021, 6, 429-438.	4.0	34
15	Dual Intrareticular Oxidation of Mixed-Ligand Metalâ€“Organic Frameworks for Stepwise Electrochemiluminescence. Journal of the American Chemical Society, 2021, 143, 3049-3053.	6.6	81
16	Transferable Multilevel Attention Neural Network for Accurate Prediction of Quantum Chemistry Properties via Multitask Learning. Journal of Chemical Information and Modeling, 2021, 61, 1066-1082.	2.5	63
17	Shear viscosity prediction of alcohols, hydrocarbons, halogenated, carbonyl, nitrogen-containing, and sulfur compounds using the variable force fields. Journal of Chemical Physics, 2021, 154, 074502.	1.2	5
18	Nonradiative Triplet Loss Suppressed in Organic Photovoltaic Blends with Fluoridated Nonfullerene Acceptors. Journal of the American Chemical Society, 2021, 143, 4359-4366.	6.6	60

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19	Simultaneous Optimization of Donor/Acceptor Pairs and Device Specifications for Nonfullerene Organic Solar Cells Using a QSPR Model with Morphological Descriptors. Journal of Physical Chemistry Letters, 2021, 12, 4980-4986.	2.1	16
20	Role of Graphite Felt Electrode and Electron Delocalization of Cinnamate Ester in Electrochemical Hydrogenation Reaction. Journal of Physical Chemistry C, 2021, 125, 13871-13879.	1.5	3
21	In(III) Metalâ€“Organic Framework Incorporated with Enzyme-Mimicking Nickel Bis(dithiolene) Ligand for Highly Selective CO₂ Electroreduction. Journal of the American Chemical Society, 2021, 143, 14071-14076.	6.6	54
22	Chemically Self-Charging Aqueous Zinc-Organic Battery. Journal of the American Chemical Society, 2021, 143, 15369-15377.	6.6	109
23	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. Npj Computational Materials, 2021, 7, .	3.5	19
24	Heterochelation boosts sodium storage in Ï€-d conjugated coordination polymers. Energy and Environmental Science, 2021, 14, 6514-6525.	15.6	24
25	Programmable nano-reactors for stochastic sensing. Nature Communications, 2021, 12, 5811.	5.8	29
26	Layer or Tube? Uncovering Key Factors Determining the Rolling-up of Layered Coordination Polymers. Journal of the American Chemical Society, 2021, 143, 17587-17598.	6.6	10
27	Photodriven Catalytic Hydrogenation of CO₂ to CH₄ with Nearly 100% Selectivity over Ag₂₅ Clusters. Nano Letters, 2021, 21, 8693-8700.	4.5	27
28	Observing halogen-bond-assisted electron transport in high-performance polymer solar cells. Applied Physics Letters, 2021, 119, 183302.	1.5	4
29	Molecular Origin of the Biologically Accelerated Mineralization of Hydroxyapatite on Bacterial Cellulose for More Robust Nanocomposites. Nano Letters, 2021, 21, 10292-10300.	4.5	19
30	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. Chemical Science, 2021, 12, 14987-15006.	3.7	16
31	Effect of the Defect Modulator and Ligand Length of Metalâ€“Organic Frameworks on Carbon Dioxide Photoreduction. ACS Applied Materials & Interfaces, 2021, 13, 61578-61586.	4.0	21
32	Molecular Design of Fused-Ring Phenazine Derivatives for Long-Cycling Alkaline Redox Flow Batteries. ACS Energy Letters, 2020, 5, 411-417.	8.8	136
33	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. Chemical Science, 2020, 11, 8000-8004.	3.7	22
34	Formation of a mixed-valence Cu(<scp>i</scp>)/Cu(<scp>ii</scp>) metalâ€“organic framework with the full light spectrum and high selectivity of CO₂ photoreduction into CH₄. Chemical Science, 2020, 11, 10143-10148.	3.7	40
35	A low symmetry cluster meets a low symmetry ligand to sharply boost MOF thermal stability. Chemical Communications, 2020, 56, 11985-11988.	2.2	19
36	Ligand Effects of BrettPhos and RuPhos on Rate-Limiting Steps in Buchwaldâ€“Hartwig Amination Reaction Due to the Modulation of Steric Hindrance and Electronic Structure. ACS Omega, 2020, 5, 21385-21391.	1.6	11

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37	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. Journal of Physical Chemistry A, 2020, 124, 5007-5014.	1.1	23
38	Cooperative Multipoint Recognition of Sialic Acid by Benzoboroxole-Based Receptors Bearing Cationic Hydrogen-Bond Donors. Journal of Organic Chemistry, 2020, 85, 8330-8338.	1.7	12
39	Superlubricity of Fullerene Derivatives Induced by Hostâ€“Guest Assembly. ACS Applied Materials & Interfaces, 2020, 12, 18924-18933.	4.0	27
40	Promoting Z-to-E Thermal Isomerization of Azobenzene Derivatives by Noncovalent Interaction with Phosphorene: Theoretical Prediction and Experimental Study. Journal of Physical Chemistry C, 2020, 124, 15961-15968.	1.5	3
41	Competitive Selection of Conformation Chirality of Water-Soluble Pillar[5]arene Induced by Amino Acid Derivatives. Organic Letters, 2020, 22, 2266-2270.	2.4	56
42	Toward Stable Lithium Plating/Stripping by Successive Desolvation and Exclusive Transport of Li Ions. ACS Applied Materials & Interfaces, 2020, 12, 10461-10470.	4.0	50
43	Zeolite Adsorption Isotherms Predicted by Pore Channel and Local Environmental Descriptors: Feature Learning on DFT Binding Strength. Journal of Physical Chemistry C, 2020, 124, 9314-9328.	1.5	12
44	A Two-Ended Data-Driven Accelerated Sampling Method for Exploring the Transition Pathways between Two Known States of Protein. Journal of Chemical Theory and Computation, 2020, 16, 4631-4640.	2.3	9
45	Chelation-assisted formation of multi-yolkâ€“shell Co₄N@carbon nanoboxes for self-discharge-suppressed high-performance Liâ€“SeS₂ batteries. Journal of Materials Chemistry A, 2019, 7, 20302-20309.	5.2	29
46	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. Journal of Materials Chemistry A, 2019, 7, 17480-17488.	5.2	80
47	Cyclometalated Iridium(III) Complexes Incorporating Aromatic Phosphonate Ligands: Syntheses, Structures, and Tunable Optical Properties. ACS Omega, 2019, 4, 16543-16550.	1.6	11
48	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of N-Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. ACS Catalysis, 2019, 9, 10142-10151.	5.5	42
49	Unlocking the action mechanisms of molecular nonlinear optical absorption for optical conjugated polymers under aggregation states. Polymer Chemistry, 2019, 10, 114-124.	1.9	9
50	An excellent example illustrating the fluorescence sensing property of cobaltâ€“organic frameworks. Dalton Transactions, 2019, 48, 2285-2289.	1.6	22
51	Linking inhibitor motions to proteolytic stability of sunflower trypsin inhibitor-1. RSC Advances, 2019, 9, 13776-13786.	1.7	3
52	Selectivity control of Pd(PMe₃)₄-catalyzed hydrogenation of internal alkynes to E-alkenes by reaction time and water content in formic acid. Dalton Transactions, 2019, 48, 10033-10042.	1.6	4
53	van der Waals Epitaxial Growth and Interfacial Passivation of Two-Dimensional Single-Crystalline Few-Layer Gray Arsenic Nanoflakes. Chemistry of Materials, 2019, 31, 4524-4535.	3.2	41
54	Planar versus Nonplanar Pd Clusters: Stability and CO Oxidation Activity of Pd Clusters with and without TiO₂(110) Substrate. Journal of Physical Chemistry C, 2019, 123, 13739-13747.	1.5	6

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55	Tuning the liquid-phase exfoliation of arsenic nanosheets by interaction with various solvents. Physical Chemistry Chemical Physics, 2019, 21, 12087-12090.	1.3	25
56	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 4072-4081.	1.3	19
57	Hydrogen Bonding Promoted Tautomerism between Azo and Hydrazone Forms in Calcon with Multistimuli Responsiveness and Biocompatibility. Journal of Chemical Information and Modeling, 2019, 59, 2110-2122.	2.5	8
58	A Dataâ€Đriven Accelerated Sampling Method for Searching Functional States of Proteins. Advanced Theory and Simulations, 2019, 2, 1800171.	1.3	6
59	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. Electronic Structure, 2019, 1, 044003.	1.0	8
60	Oxazolidine Transient Bases as Molecular Platforms for Testing Dynamic CO₂ Capture in Biochemical Systems. ACS Omega, 2018, 3, 2883-2894.	1.6	10
61	Synergistic steric pairing effects of terfluorenes with ternary side groups on Î²-conformation transition: experiments and computations. Journal of Materials Chemistry C, 2018, 6, 1551-1561.	2.7	7
62	Hydrogen Evolution Reaction in Alkaline Media: Alpha- or Beta-Nickel Hydroxide on the Surface of Platinum?. ACS Energy Letters, 2018, 3, 237-244.	8.8	230
63	Molecular Quantum Dot Cellular Automata Based on Diboryl Monoradical Anions. Journal of Physical Chemistry C, 2018, 122, 2454-2460.	1.5	30
64	Dual Role of a Photocatalyst: Generation of Ni(0) Catalyst and Promotion of Catalytic Câ€“N Bond Formation. ACS Catalysis, 2018, 8, 1456-1463.	5.5	69
65	Unexpected solvent effects on the UV/Vis absorption spectra of o -cresol in toluene and benzene: in contrast with non-aromatic solvents. Royal Society Open Science, 2018, 5, 171928.	1.1	16
66	Oxygen Species on Nitrogen-Doped Carbon Nanosheets as Efficient Active Sites for Multiple Electrocatalysis. ACS Applied Materials & Interfaces, 2018, 10, 11678-11688.	4.0	58
67	The effect of electrostatic field on the catalytic properties of platinum clusters confined in zeolite for hydrogenation. Catalysis Science and Technology, 2018, 8, 6384-6395.	2.1	18
68	Surface modification of porous PLGA scaffolds with plasma for preventing dimensional shrinkage and promoting scaffoldâ€“cell/tissue interactions. Journal of Materials Chemistry B, 2018, 6, 7605-7613.	2.9	25
69	Atomic Substitution Enabled Synthesis of Vacancy-Rich Two-Dimensional Black TiO_{2â€“x} Nanoflakes for High-Performance Rechargeable Magnesium Batteries. ACS Nano, 2018, 12, 12492-12502.	7.3	116
70	Role of Synergistic Câ€“HÂ·Â·Â·N and Câ€“HÂ·Â·Â·O H-Bonding Interactions in Self-Assemblies of a Phthalocyanine Derivative and Several Pyridine Derivatives. Journal of Physical Chemistry C, 2018, 122, 24158-24163.	1.5	10
71	Oxygen Vacancy Engineering Promoted Photocatalytic Ammonia Synthesis on Ultrathin Two-Dimensional Bismuth Oxybromide Nanosheets. Nano Letters, 2018, 18, 7372-7377.	4.5	308
72	Catalytic enantioselective synthesis of cyclopropanes featuring vicinal all-carbon quaternary stereocenters with a CH₂F group; study of the influence of Câ€“Fâ‹¯Hâ€“N interactions on reactivity. Organic Chemistry Frontiers, 2018, 5, 2960-2968.	2.3	30

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73	On-Demand Electrical Switching of Antibodyâ€“Antigen Binding on Surfaces. ACS Applied Bio Materials, 2018, 1, 738-747.	2.3	5
74	Theoretical Investigations on the Roles of Intramolecular Structure Distortion versus Irregular Intermolecular Packing in Optical Spectra of 6T Nanoparticles. Chemistry of Materials, 2017, 29, 2513-2520.	3.2	19
75	Polarization Effects on the Cellulose Dissolution in Ionic Liquids: Molecular Dynamics Simulations with Polarization Model and Integrated Tempering Enhanced Sampling Method. Journal of Physical Chemistry B, 2017, 121, 4319-4332.	1.2	10
76	Prediction on the light-assisted exfoliation of multilayered arsenene by the photo-isomerization of azobenzene. Nanoscale, 2017, 9, 7006-7011.	2.8	40
77	The Peculiar Role of the Au₃ Unit in Au_m Clusters: Ïƒ-Aromaticity of the Au₅Zn⁺ Ion. Inorganic Chemistry, 2017, 56, 5793-5803.	1.9	27
78	Tuning the collective switching behavior of azobenzene/Au hybrid materials: flexible versus rigid azobenzene backbones and Au(111) surfaces versus curved Au nanoparticles. Nanoscale, 2017, 9, 16700-16710.	2.8	13
79	A pair of 3D enantiotopic zinc(ii) complexes based on two asymmetric achiral ligands. Dalton Transactions, 2017, 46, 14779-14784.	1.6	12
80	A light-driven modulation of electric conductance through the adsorption of azobenzene onto silicon-doped- and pyridine-like N3-vacancy graphene. Nanoscale, 2017, 9, 19017-19025.	2.8	5
81	Aggregation-induced visible light absorption makes reactant 1,2-diisocyanoarenes act as photosensitizers in double radical isocyanide insertions. Physical Chemistry Chemical Physics, 2017, 19, 31443-31451.	1.3	6
82	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 5231-5239.	2.3	28
83	Unconventional Oâ€“HÂ·Â·Â·C Hydrogen Bonding and Effects of Conformational Changes on Infrared Spectroscopy of o-Cresol in Solutions. Journal of Physical Chemistry A, 2016, 120, 10196-10206.	1.1	3
84	Enhanced Electron Transfer and Spin Flip through Spinâ€“Orbital Couplings in Organic/Inorganic Heterojunctions: A Nonadiabatic Surface Hopping Simulation. Journal of Physical Chemistry Letters, 0, , 4840-4848.	2.1	5