

List of Publications by Year in descending order

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Oxygen Vacancy Engineering Promoted Photocatalytic Ammonia Synthesis on Ultrathin Two-Dimensional Bismuth Oxybromide Nanosheets. <i>Nano Letters</i> , 2018, 18, 7372-7377.	9.1	308
2	Hydrogen Evolution Reaction in Alkaline Media: Alpha- or Beta-Nickel Hydroxide on the Surface of Platinum?. <i>ACS Energy Letters</i> , 2018, 3, 237-244.	17.4	230
3	Molecular Design of Fused-Ring Phenazine Derivatives for Long-Cycling Alkaline Redox Flow Batteries. <i>ACS Energy Letters</i> , 2020, 5, 411-417.	17.4	136
4	Atomic Substitution Enabled Synthesis of Vacancy-Rich Two-Dimensional Black TiO ₂ Nanoflakes for High-Performance Rechargeable Magnesium Batteries. <i>ACS Nano</i> , 2018, 12, 12492-12502.	14.6	116
5	Chemically Self-Charging Aqueous Zinc-Organic Battery. <i>Journal of the American Chemical Society</i> , 2021, 143, 15369-15377.	13.7	109
6	Dual Intrareticular Oxidation of Mixed-Ligand Metal-Organic Frameworks for Stepwise Electrochemiluminescence. <i>Journal of the American Chemical Society</i> , 2021, 143, 3049-3053.	13.7	81
7	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. <i>Journal of Materials Chemistry A</i> , 2019, 7, 17480-17488.	10.3	80
8	Dual Role of a Photocatalyst: Generation of Ni(0) Catalyst and Promotion of Catalytic C-N Bond Formation. <i>ACS Catalysis</i> , 2018, 8, 1456-1463.	11.2	69
9	Transferable Multilevel Attention Neural Network for Accurate Prediction of Quantum Chemistry Properties via Multitask Learning. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1066-1082.	5.4	63
10	Nonradiative Triplet Loss Suppressed in Organic Photovoltaic Blends with Fluoridated Nonfullerene Acceptors. <i>Journal of the American Chemical Society</i> , 2021, 143, 4359-4366.	13.7	60
11	Oxygen Species on Nitrogen-Doped Carbon Nanosheets as Efficient Active Sites for Multiple Electrocatalysis. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 11678-11688.	8.0	58
12	Competitive Selection of Conformation Chirality of Water-Soluble Pillar[5]arene Induced by Amino Acid Derivatives. <i>Organic Letters</i> , 2020, 22, 2266-2270.	4.6	56
13	In(III) Metal-Organic Framework Incorporated with Enzyme-Mimicking Nickel Bis(dithiolene) Ligand for Highly Selective CO ₂ Electroreduction. <i>Journal of the American Chemical Society</i> , 2021, 143, 14071-14076.	13.7	54
14	Boosting the performance of single-atom catalysts via external electric field polarization. <i>Nature Communications</i> , 2022, 13, .	12.8	52
15	Toward Stable Lithium Plating/Stripping by Successive Desolvation and Exclusive Transport of Li Ions. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 10461-10470.	8.0	50
16	Near-Infrared-Responsive Photo-Driven Nitrogen Fixation Enabled by Oxygen Vacancies and Sulfur Doping in Black TiO ₂ S Nanoplatelets. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 4975-4983.	8.0	48
17	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of N-Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. <i>ACS Catalysis</i> , 2019, 9, 10142-10151.	11.2	42
18	van der Waals Epitaxial Growth and Interfacial Passivation of Two-Dimensional Single-Crystalline Few-Layer Gray Arsenic Nanoflakes. <i>Chemistry of Materials</i> , 2019, 31, 4524-4535.	6.7	41

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19	Prediction on the light-assisted exfoliation of multilayered arsenene by the photo-isomerization of azobenzene. <i>Nanoscale</i> , 2017, 9, 7006-7011.	5.6	40
20	Formation of a mixed-valence Cu(ⁱ)/Cu(ⁱⁱ) metal-organic framework with the full light spectrum and high selectivity of CO ₂ photoreduction into CH ₄ . <i>Chemical Science</i> , 2020, 11, 10143-10148.	7.4	40
21	Batch-Scale Synthesis of Nanoparticle-Agminated Three-Dimensional Porous Cu@Cu ₂ O Microspheres for Highly Selective Electrocatalysis of Nitrate to Ammonia. <i>Environmental Science & Technology</i> , 2022, 56, 10299-10307.	10.0	37
22	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. <i>Accounts of Chemical Research</i> , 2021, 54, 169-181.	15.6	36
23	Missing-Linker 2D Conductive Metal Organic Frameworks for Rapid Gas Detection. <i>ACS Sensors</i> , 2021, 6, 429-438.	7.8	34
24	Molecular Quantum Dot Cellular Automata Based on Diboryl Monoradical Anions. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2454-2460.	3.1	30
25	Catalytic enantioselective synthesis of cyclopropanes featuring vicinal all-carbon quaternary stereocenters with a CH ₂ F group; study of the influence of C-H...N interactions on reactivity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2960-2968.	4.5	30
26	Chelation-assisted formation of multi-yolk-shell Co ₄ N@carbon nanoboxes for self-discharge-suppressed high-performance Li-SeS ₂ batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20302-20309.	10.3	29
27	Programmable nano-reactors for stochastic sensing. <i>Nature Communications</i> , 2021, 12, 5811.	12.8	29
28	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5231-5239.	5.3	28
29	The Peculiar Role of the Au ₃ Unit in Au _m Clusters: π -Aromaticity of the Au ₅ Zn ⁺ Ion. <i>Inorganic Chemistry</i> , 2017, 56, 5793-5803.	4.0	27
30	Superlubricity of Fullerene Derivatives Induced by Host-Guest Assembly. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 18924-18933.	8.0	27
31	Photodriven Catalytic Hydrogenation of CO ₂ to CH ₄ with Nearly 100% Selectivity over Ag ₂₅ Clusters. <i>Nano Letters</i> , 2021, 21, 8693-8700.	9.1	27
32	Surface modification of porous PLGA scaffolds with plasma for preventing dimensional shrinkage and promoting scaffold-cell/tissue interactions. <i>Journal of Materials Chemistry B</i> , 2018, 6, 7605-7613.	5.8	25
33	Tuning the liquid-phase exfoliation of arsenic nanosheets by interaction with various solvents. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12087-12090.	2.8	25
34	Heterochelation boosts sodium storage in π -d conjugated coordination polymers. <i>Energy and Environmental Science</i> , 2021, 14, 6514-6525.	30.8	24
35	Identification of Single-Molecule Catecholamine Enantiomers Using a Programmable Nanopore. <i>ACS Nano</i> , 2022, 16, 6615-6624.	14.6	24
36	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5007-5014.	2.5	23

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37	An excellent example illustrating the fluorescence sensing property of cobalt-organic frameworks. Dalton Transactions, 2019, 48, 2285-2289.	3.3	22
38	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. Chemical Science, 2020, 11, 8000-8004.	7.4	22
39	Effect of the Defect Modulator and Ligand Length of Metal-Organic Frameworks on Carbon Dioxide Photoreduction. ACS Applied Materials & Interfaces, 2021, 13, 61578-61586.	8.0	21
40	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.	6.7	19
41	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.	2.8	19
42	A low symmetry cluster meets a low symmetry ligand to sharply boost MOF thermal stability. Chemical Communications, 2020, 56, 11985-11988.	4.1	19
43	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. Npj Computational Materials, 2021, 7, .	8.7	19
44	Molecular Origin of the Biologically Accelerated Mineralization of Hydroxyapatite on Bacterial Cellulose for More Robust Nanocomposites. Nano Letters, 2021, 21, 10292-10300.	9.1	19
45	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.	4.1	18
46	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.	2.8	18
47	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.	2.4	16
48	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.	4.6	16
49	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. Chemical Science, 2021, 12, 14987-15006.	7.4	16
50	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.	8.0	16
51	Single-Atom Tailoring of Two-Dimensional Atomic Crystals Enables Highly Efficient Detection and Pattern Recognition of Chemical Vapors. ACS Sensors, 2022, 7, 1533-1543.	7.8	16
52	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.	10.3	14
53	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.	5.6	13
54	In Situ Synthesis of Organopolysulfides Enabling Spatial and Kinetic Co-Mediation of Sulfur Chemistry. ACS Nano, 2022, 16, 9163-9171.	14.6	13

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55	A pair of 3D enantiotopic zinc(ii) complexes based on two asymmetric achiral ligands. Dalton Transactions, 2017, 46, 14779-14784.	3.3	12
56	Cooperative Multipoint Recognition of Sialic Acid by Benzoboroxole-Based Receptors Bearing Cationic Hydrogen-Bond Donors. Journal of Organic Chemistry, 2020, 85, 8330-8338.	3.2	12
57	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.	3.1	12
58	Cyclometalated Iridium(III) Complexes Incorporating Aromatic Phosphonate Ligands: Syntheses, Structures, and Tunable Optical Properties. ACS Omega, 2019, 4, 16543-16550.	3.5	11
59	Ligand Effects of BrettPhos and RuPhos on Rate-Limiting Steps in Buchwald-Hartwig Amination Reaction Due to the Modulation of Steric Hindrance and Electronic Structure. ACS Omega, 2020, 5, 21385-21391.	3.5	11
60	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.	2.6	10
61	Oxazolidine Transient Bases as Molecular Platforms for Testing Dynamic CO ₂ Capture in Biochemical Systems. ACS Omega, 2018, 3, 2883-2894.	3.5	10
62	Role of Synergistic C-H...N and C-H...O H-Bonding Interactions in Self-Assemblies of a Phthalocyanine Derivative and Several Pyridine Derivatives. Journal of Physical Chemistry C, 2018, 122, 24158-24163.	3.1	10
63	Layer or Tube? Uncovering Key Factors Determining the Rolling-up of Layered Coordination Polymers. Journal of the American Chemical Society, 2021, 143, 17587-17598.	13.7	10
64	Unlocking the action mechanisms of molecular nonlinear optical absorption for optical conjugated polymers under aggregation states. Polymer Chemistry, 2019, 10, 114-124.	3.9	9
65	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.	5.3	9
66	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.	5.4	8
67	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. Electronic Structure, 2019, 1, 044003.	2.8	8
68	Synergistic steric pairing effects of terfluorenes with ternary side groups on π^2 -conformation transition: experiments and computations. Journal of Materials Chemistry C, 2018, 6, 1551-1561.	5.5	7
69	Aggregation-induced visible light absorption makes reactant 1,2-diisocyanobenzenes act as photosensitizers in double radical isocyanide insertions. Physical Chemistry Chemical Physics, 2017, 19, 31443-31451.	2.8	6
70	Planar versus Nonplanar Pd Clusters: Stability and CO Oxidation Activity of Pd Clusters with and without TiO ₂ (110) Substrate. Journal of Physical Chemistry C, 2019, 123, 13739-13747.	3.1	6
71	A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins. Advanced Theory and Simulations, 2019, 2, 1800171.	2.8	6
72	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.	5.6	5

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73	On-Demand Electrical Switching of Antibody–Antigen Binding on Surfaces. ACS Applied Bio Materials, 2018, 1, 738-747.	4.6	5
74	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.	3.0	5
75	Enhanced Electron Transfer and Spin Flip through Spin–Orbital Couplings in Organic/Inorganic Heterojunctions: A Nonadiabatic Surface Hopping Simulation. Journal of Physical Chemistry Letters, 2019, 10, 4840-4848.	4.6	5
76	Selectivity control of Pd(PMe ₃) ₄ -catalyzed hydrogenation of internal alkynes to <i>E</i> -alkenes by reaction time and water content in formic acid. Dalton Transactions, 2019, 48, 10033-10042.	3.3	4
77	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. Journal of Physical Chemistry B, 2021, 125, 518-527.	2.6	4
78	Observing halogen-bond-assisted electron transport in high-performance polymer solar cells. Applied Physics Letters, 2021, 119, 183302.	3.3	4
79	Unconventional O–H···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.	2.5	3
80	Linking inhibitor motions to proteolytic stability of sunflower trypsin inhibitor-1. RSC Advances, 2019, 9, 13776-13786.	3.6	3
81	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.	3.1	3
82	Role of Graphite Felt Electrode and Electron Delocalization of Cinnamate Ester in Electrochemical Hydrogenation Reaction. Journal of Physical Chemistry C, 2021, 125, 13871-13879.	3.1	3
83	Discovery of Electronic Structure and Interfacial Interaction Features in Catalytic Activity. Langmuir, 2022, 38, 3959-3968.	3.5	2
84	Transition orbital projection approach for excited state tracking. Journal of Chemical Physics, 2022, 156, .	3.0	2