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List of Publications by Year in Descending Order

75 papers	1,345 citations	19 h-index	33 g-index
88 ext. papers	2,003 ext. citations	8.5 avg, IF	5.08 L-index

#	Paper	IF	Citations
75	Observing halogen-bond-assisted electron transport in high-performance polymer solar cells. *Applied Physics Letters*, **2021**, 119, 183302	3.4	1
74	Molecular Origin of the Biologically Accelerated Mineralization of Hydroxyapatite on Bacterial Cellulose for More Robust Nanocomposites. *Nano Letters*, **2021**,	11.5	9
73	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning.. *Chemical Science*, **2021**, 12, 14987-15006	9.4	3
72	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. *Physical Chemistry Chemical Physics*, **2021**,	3.6	4
71	Programmable nano-reactors for stochastic sensing. *Nature Communications*, **2021**, 12, 5811	17.4	3
70	Layer or Tube? Uncovering Key Factors Determining the Rolling-up of Layered Coordination Polymers. *Journal of the American Chemical Society*, **2021**, 143, 17587-17598	16.4	1
69	Photodriven Catalytic Hydrogenation of CO to CH with Nearly 100% Selectivity over Ag Clusters. *Nano Letters*, **2021**, 21, 8693-8700	11.5	4
68	Nonradiative Triplet Loss Suppressed in Organic Photovoltaic Blends with Fluoridated Nonfullerene Acceptors. *Journal of the American Chemical Society*, **2021**, 143, 4359-4366	16.4	24
67	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	6.4	7
66	Role of Graphite Felt Electrode and Electron Delocalization of Cinnamate Ester in Electrochemical Hydrogenation Reaction. *Journal of Physical Chemistry C*, **2021**, 125, 13871-13879	3.8	3
65	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	24.3	11
64	Near-Infrared-Responsive Photo-Driven Nitrogen Fixation Enabled by Oxygen Vacancies and Sulfur Doping in Black TiOS Nanoplatelets. *ACS Applied Materials & Interfaces*, **2021**, 13, 4975-4983	9.5	19
63	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. *Journal of Physical Chemistry B*, **2021**, 125, 518-527	3.4	1
62	Missing-Linker 2D Conductive Metal Organic Frameworks for Rapid Gas Detection. *ACS Sensors*, **2021**, 6, 429-438	9.2	9
61	Dual Intrareticular Oxidation of Mixed-Ligand Metal-Organic Frameworks for Stepwise Electrochemiluminescence. *Journal of the American Chemical Society*, **2021**, 143, 3049-3053	16.4	26
60	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	6.1	19
59	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	3.9	2

58	In(III) Metal-Organic Framework Incorporated with Enzyme-Mimicking Nickel Bis(dithiolene) Ligand for Highly Selective CO Electroreduction. *Journal of the American Chemical Society*, **2021**, 143, 14071-14076	16.4	14
57	Chemically Self-Charging Aqueous Zinc-Organic Battery. *Journal of the American Chemical Society*, **2021**, 143, 15369-15377	16.4	16
56	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. *Npj Computational Materials*, **2021**, 7,	10.9	4
55	Effect of the Defect Modulator and Ligand Length of Metal-Organic Frameworks on Carbon Dioxide Photoreduction.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61578-61586	9.5	1
54	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	2.8	13
53	Cooperative Multipoint Recognition of Sialic Acid by Benzoboroxole-Based Receptors Bearing Cationic Hydrogen-Bond Donors. *Journal of Organic Chemistry*, **2020**, 85, 8330-8338	4.2	4
52	Superlubricity of Fullerene Derivatives Induced by Host-Guest Assembly. *ACS Applied Materials & Interfaces*, **2020**, 12, 18924-18933	9.5	12
51	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	3.8	1
50	Competitive Selection of Conformation Chirality of Water-Soluble Pillar[5]arene Induced by Amino Acid Derivatives. *Organic Letters*, **2020**, 22, 2266-2270	6.2	28
49	Toward Stable Lithium Plating/Stripping by Successive Desolvation and Exclusive Transport of Li Ions. *ACS Applied Materials & Interfaces*, **2020**, 12, 10461-10470	9.5	27
48	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	3.8	4
47	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	6.4	4
46	Molecular Design of Fused-Ring Phenazine Derivatives for Long-Cycling Alkaline Redox Flow Batteries. *ACS Energy Letters*, **2020**, 5, 411-417	20.1	67
45	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. *Chemical Science*, **2020**, 11, 8000-8004	9.4	10
44	Formation of a mixed-valence Cu(i)/Cu(ii) metal-organic framework with the full light spectrum and high selectivity of CO photoreduction into CH. *Chemical Science*, **2020**, 11, 10143-10148	9.4	18
43	A low symmetry cluster meets a low symmetry ligand to sharply boost MOF thermal stability. *Chemical Communications*, **2020**, 56, 11985-11988	5.8	10
42	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	3.9	5
41	Cyclometalated Iridium(III) Complexes Incorporating Aromatic Phosphonate Ligands: Syntheses, Structures, and Tunable Optical Properties. *ACS Omega*, **2019**, 4, 16543-16550	3.9	5

40	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of N-Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. *ACS Catalysis*, **2019**, 9, 10142-10151	13.1	25
39	Unlocking the action mechanisms of molecular nonlinear optical absorption for optical conjugated polymers under aggregation states. *Polymer Chemistry*, **2019**, 10, 114-124	4.9	7
38	An excellent example illustrating the fluorescence sensing property of cobalt-organic frameworks. *Dalton Transactions*, **2019**, 48, 2285-2289	4.3	14
37	Linking inhibitor motions to proteolytic stability of sunflower trypsin inhibitor-1.. *RSC Advances*, **2019**, 9, 13776-13786	3.7	2
36	Selectivity control of Pd(PMe)-catalyzed hydrogenation of internal alkynes to E-alkenes by reaction time and water content in formic acid. *Dalton Transactions*, **2019**, 48, 10033-10042	4.3	3
35	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	9.6	23
34	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	3.8	4
33	Tuning the liquid-phase exfoliation of arsenic nanosheets by interaction with various solvents. *Physical Chemistry Chemical Physics*, **2019**, 21, 12087-12090	3.6	18
32	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	3.6	11
31	Chelation-assisted formation of multi-yolk□shell Co4N@carbon nanoboxes for self-discharge-suppressed high-performance Li□SeS2 batteries. *Journal of Materials Chemistry A*, **2019**, 7, 20302-20309	13	22
30	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. *Journal of Materials Chemistry A*, **2019**, 7, 17480-17488	13	50
29	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	6.1	3
28	A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins. *Advanced Theory and Simulations*, **2019**, 2, 1800171	3.5	4
27	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. *Electronic Structure*, **2019**, 1, 044003	2.6	6
26	Oxazolidine Transient Bases as Molecular Platforms for Testing Dynamic CO Capture in Biochemical Systems. *ACS Omega*, **2018**, 3, 2883-2894	3.9	8
25	Synergistic steric pairing effects of terfluorenes with ternary side groups on □conformation transition: experiments and computations. *Journal of Materials Chemistry C*, **2018**, 6, 1551-1561	7.1	5
24	Hydrogen Evolution Reaction in Alkaline Media: Alpha- or Beta-Nickel Hydroxide on the Surface of Platinum?. *ACS Energy Letters*, **2018**, 3, 237-244	20.1	148
23	Molecular Quantum Dot Cellular Automata Based on Diboryl Monoradical Anions. *Journal of Physical Chemistry C*, **2018**, 122, 2454-2460	3.8	27

22	Dual Role of a Photocatalyst: Generation of Ni(0) Catalyst and Promotion of Catalytic C N Bond Formation. *ACS Catalysis*, **2018**, 8, 1456-1463	13.1	43
21	Unexpected solvent effects on the UV/Vis absorption spectra of -cresol in toluene and benzene: in contrast with non-aromatic solvents. *Royal Society Open Science*, **2018**, 5, 171928	3.3	9
20	Oxygen Species on Nitrogen-Doped Carbon Nanosheets as Efficient Active Sites for Multiple Electrocatalysis. *ACS Applied Materials & Interfaces*, **2018**, 10, 11678-11688	9.5	42
19	On-Demand Electrical Switching of Antibody-Antigen Binding on Surfaces.. *ACS Applied Bio Materials*, **2018**, 1, 738-747	4.1	2
18	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	5.5	9
17	Surface modification of porous PLGA scaffolds with plasma for preventing dimensional shrinkage and promoting scaffold-cell/tissue interactions. *Journal of Materials Chemistry B*, **2018**, 6, 7605-7613	7.3	19
16	Atomic Substitution Enabled Synthesis of Vacancy-Rich Two-Dimensional Black TiO Nanoflakes for High-Performance Rechargeable Magnesium Batteries. *ACS Nano*, **2018**, 12, 12492-12502	16.7	85
15	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	3.8	5
14	Oxygen Vacancy Engineering Promoted Photocatalytic Ammonia Synthesis on Ultrathin Two-Dimensional Bismuth Oxybromide Nanosheets. *Nano Letters*, **2018**, 18, 7372-7377	11.5	200
13	Catalytic enantioselective synthesis of cyclopropanes featuring vicinal all-carbon quaternary stereocenters with a CH2F group; study of the influence of C F?H N interactions on reactivity. *Organic Chemistry Frontiers*, **2018**, 5, 2960-2968	5.2	25
12	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	9.6	17
11	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	3.4	7
10	Prediction on the light-assisted exfoliation of multilayered arsenene by the photo-isomerization of azobenzene. *Nanoscale*, **2017**, 9, 7006-7011	7.7	30
9	The Peculiar Role of the Au Unit in Au Clusters: Aromaticity of the AuZn Ion. *Inorganic Chemistry*, **2017**, 56, 5793-5803	5.1	20
8	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	7.7	9
7	A pair of 3D enantiotopic zinc(ii) complexes based on two asymmetric achiral ligands. *Dalton Transactions*, **2017**, 46, 14779-14784	4.3	7
6	A light-driven modulation of electric conductance through the adsorption of azobenzene onto silicon-doped- and pyridine-like N-vacancy graphene. *Nanoscale*, **2017**, 9, 19017-19025	7.7	5
5	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	3.6	5

4	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	6.4	14
3	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	2.8	2
2	Heterochelation boosts sodium storage in □d conjugated coordination polymers. *Energy and Environmental Science*,	35.4	4
1	Enhanced Electron Transfer and Spin Flip through Spin□Orbital Couplings in Organic/Inorganic Heterojunctions: A Nonadiabatic Surface Hopping Simulation. *Journal of Physical Chemistry Letters*,4840-4848	6.4	0