Jun Zhang

List of Publications by Year
in descending order

27 papers	2,086 citations	567281 15 h-index	552781 26 g-index
31 all docs	31 docs citations	31 times ranked	1446 citing authors

#	Article	IF	Citations
1	Functionalization of Electrodes with Tunable [EMIM]_x[Cl]_{x+1}^{â€“} Ionic Liquid Clusters for Electrochemical Separations. Chemistry of Materials, 2022, 34, 2612-2623.	6.7	5
2	Selective Catalytic Reduction of NO_x with NH₃ over Cu/SSZ-13: Elucidating Dynamics of Cu Active Sites with In Situ UVâ€“Vis Spectroscopy and DFT Calculations. Journal of Physical Chemistry C, 2022, 126, 8720-8733.	3.1	20
3	Atom typing using graph representation learning: How do models learn chemistry?. Journal of Chemical Physics, 2022, 156, .	3.0	7
4	Global optimization of chemical cluster structures: Methods, applications, and challenges. International Journal of Quantum Chemistry, 2021, 121, e26553.	2.0	31
5	Graphene Oxide as a Pb(II) Separation Medium: Has Part of the Story Been Overlooked?. Jacs Au, 2021, 1, 766-776.	7.9	9
6	Efficient evaluation of electrostatic potential with computerized optimized code. Physical Chemistry Chemical Physics, 2021, 23, 20323-20328.	2.8	664
7	Ligand control of low-frequency electron paramagnetic resonance linewidth in Cr(iii) complexes. Dalton Transactions, 2021, 50, 5342-5350.	3.3	5
8	Structure and Stability of the Ionic Liquid Clusters [EMIM]_n[BF₄]_{n+1}^{â€“} (n = 1â€“9): Implications for Electrochemical Separations. Journal of Physical Chemistry Letters, 2020, 11, 6844-6851.	4.6	12
9	NWPEsSe: An Adaptive-Learning Global Optimization Algorithm for Nanosized Cluster Systems. Journal of Chemical Theory and Computation, 2020, 16, 3947-3958.	5.3	47
10	General Protocol for the Accurate Prediction of Molecular ¹³C/¹H NMR Chemical Shifts via Machine Learning Augmented DFT. Journal of Chemical Information and Modeling, 2020, 60, 3746-3754.	5.4	53
11	Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts. Journal of Catalysis, 2020, 386, 30-38.	6.2	22
12	<scp>libreta</scp>: Computerized Optimization and Code Synthesis for Electron Repulsion Integral Evaluation. Journal of Chemical Theory and Computation, 2018, 14, 572-587.	5.3	89
13	Origins of the enantioselectivity of a palladium catalyst with BINOLâ€“phosphoric acid ligands. Organic and Biomolecular Chemistry, 2018, 16, 8064-8071.	2.8	14
14	Structures and energetics of hydrated deprotonated cis-pinonic acid anion clusters and their atmospheric relevance. Physical Chemistry Chemical Physics, 2017, 19, 10676-10684.	2.8	17
15	A Theoretical Study on Methane Câ€”H Bond Activation by Bare [FeO]^{+/0/â€“}. Journal of Physical Chemistry A, 2017, 121, 3501-3514.	2.5	16
16	The first water coordination sphere of lanthanide(iii) motexafins (Ln-Motex2+, Ln = La, Gd, Lu) and its effects on structures, reduction potentials and UV-vis absorption spectra. Theoretical studies. Physical Chemistry Chemical Physics, 2017, 19, 20160-20171.	2.8	9
17	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. Journal of the American Chemical Society, 2016, 138, 11368-11377.	13.7	85
18	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO₂]⁺ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. Journal of the American Chemical Society, 2016, 138, 7973-7981.	13.7	90

#	Article	IF	Citations
19	Global optimization of clusters of rigid molecules using the artificial bee colony algorithm. Physical Chemistry Chemical Physics, 2016, 18, 3003-3010.	2.8	292
20	Third-Order Incremental Dual-Basis Set Zero-Buffer Approach for Large High-Spin Open-Shell Systems. Journal of Chemical Theory and Computation, 2015, 11, 962-968.	5.3	10
21	ABCluster: the artificial bee colony algorithm for cluster global optimization. Physical Chemistry Chemical Physics, 2015, 17, 24173-24181.	2.8	415
22	Approaching the complete basis set limit of CCSD(T) for large systems by the third-order incremental dual-basis set zero-buffer F12 method. Journal of Chemical Physics, 2014, 140, 044114.	3.0	12
23	Actinoid(III) Hydrationâ€"First Principle Gibbs Energies of Hydration Using High Level Correlation Methods. Journal of Chemical Theory and Computation, 2014, 10, 5593-5598.	5.3	30
24	Dispersion Interaction Stabilizes Sterically Hindered Double Fullerenes. Chemistry - A European Journal, 2014, 20, 13909-13912.	3.3	21
25	Understanding Lanthanoid(III) Hydration Structure and Kinetics by Insights from Energies and Wave functions. Inorganic Chemistry, 2014, 53, 7700-7708.	4.0	82
26	Third-Order Incremental Dual-Basis Set Zero-Buffer Approach: An Accurate and Efficient Way To Obtain CCSD and CCSD(T) Energies. Journal of Chemical Theory and Computation, 2013, 9, 2992-3003.	5.3	29
27	Tailored Computational Approaches to Interrogate Heavy Element Chemistry and Structure in Condensed Phase. ACS Symposium Series, 0, , 219-245.	0.5	0