Yi-Pei Li

List of Publications by Year
in descending order

22 papers	1,508 citations	471061 17 h-index	642321 23 g-index
23 all docs	23 docs citations	23 times ranked	1548 citing authors

#	Article	IF	Citations
1	Unveiling the elusive role of tetraethyl orthosilicate hydrolysis in ionic-liquid-templated zeolite synthesis. Materials Today Chemistry, 2022, 23, 100658.	1.7	2
2	Rational synthesis of ruthenium-based metallo-supramolecular polymers as heterogeneous catalysts for catalytic transfer hydrogenation of carbonyl compounds. Applied Catalysis B: Environmental, 2022, 312, 121383.	10.8	10
3	Dielsâ€“Alder Conversion of Acrylic Acid and 2,5â€Dimethylfuran to paraâ€Xylene Over Heterogeneous Biâ€BTC Metalâ€Organic Framework Catalysts Under Mild Conditions. Angewandte Chemie - International Edition, 2021, 60, 624-629.	7.2	27
4	Dielsâ€“Alder Conversion of Acrylic Acid and 2,5â€Dimethylfuran to paraâ€Xylene Over Heterogeneous Biâ€BTC Metalâ€Organic Framework Catalysts Under Mild Conditions. Angewandte Chemie, 2021, 133, 634-639.	1.6	8
5	Quantum Mechanical Calculations for Biomass Valorization over Metalâ€Organic Frameworks (MOFs). Chemistry - an Asian Journal, 2021, 16, 1049-1056.	1.7	7
6	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
7	Understanding the Catalytic Activity of Microporous and Mesoporous Zeolites in Cracking by Experiments and Simulations. Catalysts, 2021, 11, 1114.	1.6	7
8	Learning to Optimize Molecular Geometries Using Reinforcement Learning. Journal of Chemical Theory and Computation, 2021, 17, 818-825.	2.3	19
9	Proton-Conductive Cerium-Based Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2021, 13, 55358-55366.	4.0	23
10	Synergistic effects of Pt-embedded, MIL-53-derived catalysts (Pt@Al2O3) and NaBH4 for water-mediated hydrogenolysis of biomass-derived furfural to 1,5-pentanediol at near-ambient temperature. Journal of Catalysis, 2020, 390, 46-56.	3.1	43
11	Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. Journal of Chemical Information and Modeling, 2020, 60, 2697-2717.	2.5	113
12	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. Proceedings of the Combustion Institute, 2019, 37, 363-371.	2.4	62
13	Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach. Journal of Physical Chemistry A, 2019, 123, 5826-5835.	1.1	72
14	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. Journal of Physical Chemistry A, 2019, 123, 2142-2152.	1.1	42
15	Unimolecular Reaction Pathways of a Î³-Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. Journal of the American Chemical Society, 2018, 140, 1035-1048.	6.6	82
16	Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA. ACS Catalysis, 2016, 6, 5052-5061.	5.5	18
17	Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2861-2870.	2.3	38
18	Propene Metathesis over Supported Tungsten Oxide Catalysts: A Study of Active Site Formation. ACS Catalysis, 2016, 6, 7728-7738.	5.5	60

#	Article	IF	Citations
19	Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 1840-1850.	1.5	110
20	Experimental and Theoretical Study of n-Butanal Self-Condensation over Ti Species Supported on Silica. ACS Catalysis, 2014, 4, 2908-2916.	5.5	34
21	Computational Study of p-Xylene Synthesis from Ethylene and 2,5-Dimethylfuran Catalyzed by H-BEA. Journal of Physical Chemistry C, 2014, 118, 22090-22095.	1.5	64
22	Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. ACS Catalysis, 2014, 4, 1537-1545.	5.5	148