

Yi-Pei Li

List of Publications by Year in descending order

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Version: 2024-02-01

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	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
2	Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. <i>ACS Catalysis</i> , 2014, 4, 1537-1545.	5.5	148
3	Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2697-2717.	2.5	113
4	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. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1840-1850.	1.5	110
5	Unimolecular Reaction Pathways of a $\hat{1}^3$ -Keto-hydroperoxide from Combined Application of Automated Reaction Discovery Methods. <i>Journal of the American Chemical Society</i> , 2018, 140, 1035-1048.	6.6	82
6	Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5826-5835.	1.1	72
7	Computational Study of <i>p</i> -Xylene Synthesis from Ethylene and 2,5-Dimethylfuran Catalyzed by H-BEA. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22090-22095.	1.5	64
8	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 363-371.	2.4	62
9	Propene Metathesis over Supported Tungsten Oxide Catalysts: A Study of Active Site Formation. <i>ACS Catalysis</i> , 2016, 6, 7728-7738.	5.5	60
10	Synergistic effects of Pt-embedded, MIL-53-derived catalysts (Pt@Al ₂ O ₃) and NaBH ₄ for water-mediated hydrogenolysis of biomass-derived furfural to 1,5-pentanediol at near-ambient temperature. <i>Journal of Catalysis</i> , 2020, 390, 46-56.	3.1	43
11	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2142-2152.	1.1	42
12	Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2861-2870.	2.3	38
13	Experimental and Theoretical Study of <i>n</i> -Butanal Self-Condensation over Ti Species Supported on Silica. <i>ACS Catalysis</i> , 2014, 4, 2908-2916.	5.5	34
14	Diels-Alder Conversion of Acrylic Acid and 2,5-Dimethylfuran to <i>p</i> -Xylene Over Heterogeneous Bi-BTC Metal-Organic Framework Catalysts Under Mild Conditions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 624-629.	7.2	27
15	Proton-Conductive Cerium-Based Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 55358-55366.	4.0	23
16	Learning to Optimize Molecular Geometries Using Reinforcement Learning. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 818-825.	2.3	19
17	Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA. <i>ACS Catalysis</i> , 2016, 6, 5052-5061.	5.5	18
18	Rational synthesis of ruthenium-based metallo-supramolecular polymers as heterogeneous catalysts for catalytic transfer hydrogenation of carbonyl compounds. <i>Applied Catalysis B: Environmental</i> , 2022, 312, 121383.	10.8	10

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19	Diels–Alder Conversion of Acrylic Acid and 2,5-Dimethylfuran to <i>para</i> -Xylene Over Heterogeneous Bi–BTC Metal–Organic Framework Catalysts Under Mild Conditions. <i>Angewandte Chemie</i> , 2021, 133, 634-639.	1.6	8
20	Quantum Mechanical Calculations for Biomass Valorization over Metal–Organic Frameworks (MOFs). <i>Chemistry - an Asian Journal</i> , 2021, 16, 1049-1056.	1.7	7
21	Understanding the Catalytic Activity of Microporous and Mesoporous Zeolites in Cracking by Experiments and Simulations. <i>Catalysts</i> , 2021, 11, 1114.	1.6	7
22	Unveiling the elusive role of tetraethyl orthosilicate hydrolysis in ionic-liquid-templated zeolite synthesis. <i>Materials Today Chemistry</i> , 2022, 23, 100658.	1.7	2