Seonah Kim

List of Publications by Year in descending order

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44 papers	2,286 citations	257450 24 h-index	233421 45 g-index
47 all docs	47 docs citations	47 times ranked	3214 citing authors

#	Article	IF	Citations
1	Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. Journal of Physical Chemistry Letters, 2011, 2, 2846-2852.	4.6	318
2	A Mechanistic Investigation of Acid-Catalyzed Cleavage of Aryl-Ether Linkages: Implications for Lignin Depolymerization in Acidic Environments. ACS Sustainable Chemistry and Engineering, 2014, 2, 472-485.	6.7	317
3	Quantum mechanical calculations suggest that lytic polysaccharide monooxygenases use a copper-oxyl, oxygen-rebound mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 149-154.	7.1	210
4	Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research. ACS Catalysis, 2018, 8, 770-784.	11.2	161
5	Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. Nature Communications, 2020, 11, 2328.	12.8	128
6	Measuring and predicting sooting tendencies of oxygenates, alkanes, alkenes, cycloalkanes, and aromatics on a unified scale. Combustion and Flame, 2018, 190, 349-364.	5.2	122
7	Structural and Electronic Snapshots during the Transition from a Cu(II) to Cu(I) Metal Center of a Lytic Polysaccharide Monooxygenase by X-ray Photoreduction. Journal of Biological Chemistry, 2014, 289, 18782-18792.	3.4	99
8	Through-Space Ultrafast Photoinduced Electron Transfer Dynamics of a C₇₀-Encapsulated Bisporphyrin Covalent Organic Polyhedron in a Low-Dielectric Medium. Journal of the American Chemical Society, 2017, 139, 4286-4289.	13.7	58
9	Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. Green Chemistry, 2018, 20, 567-582.	9.0	55
10	Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. Scientific Data, 2020, 7, 244.	5.3	49
11	Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. Accounts of Chemical Research, 2021, 54, 827-836.	15.6	47
12	Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate. Proceedings of the Combustion Institute, 2019, 37, 419-428.	3.9	45
13	Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. Journal of Physical Chemistry A, 2015, 119, 3604-3614.	2.5	44
14	Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5 zeolite. Catalysis Today, 2018, 312, 73-81.	4.4	44
15	A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. Energy & Fuels, 2017, 31, 9983-9990.	5.1	42
16	Prediction of Hydroxymethylfurfural Yield in Glucose Conversion through Investigation of Lewis Acid and Organic Solvent Effects. ACS Catalysis, 2020, 10, 14707-14721.	11.2	41
17	Sooting tendencies of co-optima test gasolines and their surrogates. Proceedings of the Combustion Institute, 2019, 37, 961-968.	3.9	39
18	Performance-advantaged ether diesel bioblendstock production by a priori design. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26421-26430.	7.1	39

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19	In-situ hydrogenation of bio-oil/bio-oil phenolic compounds with secondary alcohols over a synthesized mesoporous Ni/CeO2 catalyst. Chemical Engineering Journal, 2020, 382, 122912.	12.7	38
20	Crystal structure of glycoside hydrolase family 127 Î²-l-arabinofuranosidase from Bifidobacterium longum. Biochemical and Biophysical Research Communications, 2014, 447, 32-37.	2.1	35
21	Structural and molecular dynamics studies of a C1â€•oxidizing lytic polysaccharide monooxygenase from Heterobasidion irregulare reveal amino acids important for substrate recognition. FEBS Journal, 2018, 285, 2225-2242.	4.7	35
22	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. Wiley Interdisciplinary Reviews: Energy and Environment, 2018, 7, e297.	4.1	30
23	Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen. Green Chemistry, 2020, 22, 2403-2418.	9.0	26
24	Diffusion of Biomass Pyrolysis Products in H-ZSM-5 by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 500-510.	3.1	25
25	Tailoring diesel bioblendstock from integrated catalytic upgrading of carboxylic acids: a â€œfuel property firstâ€•approach. Green Chemistry, 2019, 21, 5813-5827.	9.0	25
26	A perspective on biomass-derived biofuels: From catalyst design principles to fuel properties. Journal of Hazardous Materials, 2020, 400, 123198.	12.4	23
27	Furan Production from Glycoaldehyde over HZSM-5. ACS Sustainable Chemistry and Engineering, 2016, 4, 2615-2623.	6.7	19
28	Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules. Journal of Physical Chemistry A, 2017, 121, 5475-5486.	2.5	16
29	Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence ratio. Combustion and Flame, 2020, 214, 103-115.	5.2	16
30	Carbocation Stability in H-ZSM5 at High Temperature. Journal of Physical Chemistry A, 2015, 119, 11397-11405.	2.5	14
31	Isotopic Studies for Tracking Biogenic Carbon during Co-processing of Biomass and Vacuum Gas Oil. ACS Sustainable Chemistry and Engineering, 2020, 8, 2652-2664.	6.7	14
32	Exploring Low-Temperature Dehydrogenation at Ionic Cu Sites in Beta Zeolite To Enable Alkane Recycle in Dimethyl Ether Homologation. ACS Catalysis, 2017, 7, 3662-3667.	11.2	13
33	Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. Proceedings of the Combustion Institute, 2019, 37, 1083-1090.	3.9	13
34	Chemical kinetic basis of synergistic blending for research octane number. Fuel, 2022, 307, 121865.	6.4	13
35	Theoretical Determination of Size Effects in Zeolite-Catalyzed Alcohol Dehydration. Catalysts, 2019, 9, 700.	3.5	11
36	Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers. Journal of Physical Chemistry A, 2020, 124, 4290-4304.	2.5	11

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37	Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers. Proceedings of the Combustion Institute, 2021, 38, 1143-1151.	3.9	10
38	Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors. Scientific Reports, 2018, 8, 12826.	3.3	9
39	Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. Proceedings of the Combustion Institute, 2021, 38, 1327-1334.	3.9	7
40	Understanding how chemical structure affects ignition-delay-time <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mi>Ï•</mml:mi></mml:math>-sensitivity. Combustion and Flame, 2021, 225, 377-387.	5.2	7
41	Toward rational design of supported vanadia catalysts of lignin conversion to phenol. Chemical Engineering Journal, 2022, 446, 136965.	12.7	4
42	Predicting Catalytic Pyrolysis Aromatic Selectivity from Pyrolysis Vapor Composition Using Mass Spectra Coupled with Statistical Analysis. ACS Sustainable Chemistry and Engineering, 2022, 10, 234-244.	6.7	3
43	Connecting cation site location to alkane dehydrogenation activity in Ni/BEA catalysts. Journal of Catalysis, 2022, 413, 264-273.	6.2	3
44	Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components. Energy & Fuels, 2019, 33, 10290-10296.	5.1	2