

# Seonah Kim

## List of Publications by Year in descending order

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44  
papers

2,286  
citations

257101

24  
h-index

233125

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. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2846-2852.	2.1	318
2	A Mechanistic Investigation of Acid-Catalyzed Cleavage of Aryl-Ether Linkages: Implications for Lignin Depolymerization in Acidic Environments. <i>ACS Sustainable Chemistry and Engineering</i> , 2014, 2, 472-485.	3.2	317
3	Quantum mechanical calculations suggest that lytic polysaccharide monoxygenases use a copper-oxyl, oxygen-rebound mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 149-154.	3.3	210
4	Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research. <i>ACS Catalysis</i> , 2018, 8, 770-784.	5.5	161
5	Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. <i>Nature Communications</i> , 2020, 11, 2328.	5.8	128
6	Measuring and predicting sooting tendencies of oxygenates, alkanes, alkenes, cycloalkanes, and aromatics on a unified scale. <i>Combustion and Flame</i> , 2018, 190, 349-364.	2.8	122
7	Structural and Electronic Snapshots during the Transition from a Cu(II) to Cu(I) Metal Center of a Lytic Polysaccharide Monoxygenase by X-ray Photoreduction. <i>Journal of Biological Chemistry</i> , 2014, 289, 18782-18792.	1.6	99
8	Through-Space Ultrafast Photoinduced Electron Transfer Dynamics of a C <sub>70</sub> -Encapsulated Bisporphyrin Covalent Organic Polyhedron in a Low-Dielectric Medium. <i>Journal of the American Chemical Society</i> , 2017, 139, 4286-4289.	6.6	58
9	Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. <i>Green Chemistry</i> , 2018, 20, 567-582.	4.6	55
10	Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. <i>Scientific Data</i> , 2020, 7, 244.	2.4	49
11	Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. <i>Accounts of Chemical Research</i> , 2021, 54, 827-836.	7.6	47
12	Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 419-428.	2.4	45
13	Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3604-3614.	1.1	44
14	Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5 zeolite. <i>Catalysis Today</i> , 2018, 312, 73-81.	2.2	44
15	A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. <i>Energy &amp; Fuels</i> , 2017, 31, 9983-9990.	2.5	42
16	Prediction of Hydroxymethylfurfural Yield in Glucose Conversion through Investigation of Lewis Acid and Organic Solvent Effects. <i>ACS Catalysis</i> , 2020, 10, 14707-14721.	5.5	41
17	Sooting tendencies of co-optima test gasolines and their surrogates. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 961-968.	2.4	39
18	Performance-advantaged ether diesel bioblendstock production by a priori design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 26421-26430.	3.3	39

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19	In-situ hydrogenation of bio-oil/bio-oil phenolic compounds with secondary alcohols over a synthesized mesoporous Ni/CeO <sub>2</sub> catalyst. <i>Chemical Engineering Journal</i> , 2020, 382, 122912.	6.6	38
20	Crystal structure of glycoside hydrolase family 127 $\beta$ -l-arabinofuranosidase from <i>Bifidobacterium longum</i> . <i>Biochemical and Biophysical Research Communications</i> , 2014, 447, 32-37.	1.0	35
21	Structural and molecular dynamics studies of a C1 $\alpha$ -oxidizing lytic polysaccharide monooxygenase from <i>Heterobasidium irregulare</i> reveal amino acids important for substrate recognition. <i>FEBS Journal</i> , 2018, 285, 2225-2242.	2.2	35
22	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. <i>Wiley Interdisciplinary Reviews: Energy and Environment</i> , 2018, 7, e297.	1.9	30
23	Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen. <i>Green Chemistry</i> , 2020, 22, 2403-2418.	4.6	26
24	Diffusion of Biomass Pyrolysis Products in H-ZSM-5 by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 500-510.	1.5	25
25	Tailoring diesel bioblendstock from integrated catalytic upgrading of carboxylic acids: a $\text{CO}_2$ -fuel property first approach. <i>Green Chemistry</i> , 2019, 21, 5813-5827.	4.6	25
26	A perspective on biomass-derived biofuels: From catalyst design principles to fuel properties. <i>Journal of Hazardous Materials</i> , 2020, 400, 123198.	6.5	23
27	Furan Production from Glycoaldehyde over HZSM-5. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 2615-2623.	3.2	19
28	Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5475-5486.	1.1	16
29	Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence ratio. <i>Combustion and Flame</i> , 2020, 214, 103-115.	2.8	16
30	Carbocation Stability in H-ZSM5 at High Temperature. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11397-11405.	1.1	14
31	Isotopic Studies for Tracking Biogenic Carbon during Co-processing of Biomass and Vacuum Gas Oil. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 2652-2664.	3.2	14
32	Exploring Low-Temperature Dehydrogenation at Ionic Cu Sites in Beta Zeolite To Enable Alkane Recycle in Dimethyl Ether Homologation. <i>ACS Catalysis</i> , 2017, 7, 3662-3667.	5.5	13
33	Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 1083-1090.	2.4	13
34	Chemical kinetic basis of synergistic blending for research octane number. <i>Fuel</i> , 2022, 307, 121865.	3.4	13
35	Theoretical Determination of Size Effects in Zeolite-Catalyzed Alcohol Dehydration. <i>Catalysts</i> , 2019, 9, 700.	1.6	11
36	Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4290-4304.	1.1	11

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37	Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1143-1151.	2.4	10
38	Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors. <i>Scientific Reports</i> , 2018, 8, 12826.	1.6	9
39	Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1327-1334.	2.4	7
40	Understanding how chemical structure affects ignition-delay-time $\tau_{\text{ign}}$ -sensitivity. <i>Combustion and Flame</i> , 2021, 225, 377-387.	2.8	7
41	Toward rational design of supported vanadia catalysts of lignin conversion to phenol. <i>Chemical Engineering Journal</i> , 2022, 446, 136965.	6.6	4
42	Predicting Catalytic Pyrolysis Aromatic Selectivity from Pyrolysis Vapor Composition Using Mass Spectra Coupled with Statistical Analysis. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 234-244.	3.2	3
43	Connecting cation site location to alkane dehydrogenation activity in Ni/BEA catalysts. <i>Journal of Catalysis</i> , 2022, 413, 264-273.	3.1	3
44	Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components. <i>Energy &amp; Fuels</i> , 2019, 33, 10290-10296.	2.5	2