

## Seonah Kim PhD

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### Research Interests:

- Material Design of Catalytic Upgrading of Biomass into (Bio)Fuels and Platform Chemicals
- Design Principles for Sustainable Chemistry: Mechanism-Driven Discovery of Biopolymer Upgrading
- Data-Driven Design of Green Chemical Properties

### Professional Appointments

Associate Professor, Colorado State University	2021 – present
Affiliated Scientist, National Renewable Energy Laboratory	2021 – present
Senior Scientist/Staff Scientist, National Renewable Energy Laboratory	2011 – 2020
Staff Scientist, National Renewable Energy Laboratory	2012 – 2015
Research Associate, National Renewable Energy Laboratory	2012 – 2012
Postdoctoral Associate, National Renewable Energy Laboratory	2011 – 2012
Postdoctoral Associate, University of California, Los Angeles (Advisor: Prof. Kendall N. Houk)	2008 – 2011
Research Associate, University of Utah (Advisor: Dr. Julio Facelli)	2007 – 2008
Research Assistant, University of Florida	2003 – 2007

### Education

Computational Chemistry (Physical Chemistry), University of Florida	2003 – 2007
• PhD with Dr. Adrian E. Roitberg	
Computer Science, University of Houston	1999 – 2003
• MS with Dr. B. Montgomery Pettitt	

### Publications

At CSU:

[77] *Sooting Tendency of Substituted Aromatic Oxygenates: The Role of Functional Groups and Positional Isomerism in Vanillin Isomers*, Hojin Junga, Jaeyoung Chob, Yeonjoon Kimc, Zhanhong Xiangd, Sabari Kumara, Piper Barnardd, Charles S. McEnallyd, Lisa D. Pfefferled, Seonah Kim, Proc. Comb. Inst. (in review, 2023)

[76] *Experimental and numerical study of the decomposition, product spectrum, and sooting properties of adamantane fuels*, Ga-Un Jeong, Zhanhong Xiang, Sabari Kumar, Collin Hansen, Adri van Duin, Seonah Kim, Charles S. McEnally, Lisa D. Pfefferle, Yuan Xuan, Proc. Comb. Inst. (in review, 2023)

[75] *Simple and efficient enantioselective  $\alpha$ -deuteration method of  $\alpha$ -amino acids without external chiral sources*, Soojun Park, Jae Hyun Kim, Dongjun Kim, Yeonjoon Kim, Seonah Kim, Sanghee Kim (in revision, 2023)

[74] *Design Green Chemicals by Predicting Vaporization Properties Using Explainable Graph Attention Networks*, Yeonjoon Kim, Hojin Jung, Keunhong Jeong, Jaeyoung Cho, Robert L. McCormick, Peter C. St. John, Seonah Kim†, *Green Chemistry* (in revision 2023)

[73] *Designing solvent systems in chemical processes using self-evolving solubility databases and graph neural networks*. Yeonjoon Kim, Hojin Jung, Sabari Kumar, Alex Claiborne, Robert S. Paton, Seonah Kim. ChemRxiv preprint.

DOI: 10.26434/chemrxiv-2022-sq34x, Chem. Sci. (accepted, 2023, *ChemSci Pick of the Week*, Jan. 3, 2024 and 2024 Chemical Science HOT Article Collection).

[72] *Expansion of bond dissociation prediction with machine learning to medicinally and environmentally relevant chemical space*, Shree Sowndarya S. V., Yeonjoon Kim, Seonah Kim, Peter C. St. John, and Robert S. Paton, *Digital Discovery*, 2, 1900 (2023).

[71] *Effect of the  $\beta$ -hydroxy group on ester reactivity: Combustion kinetics of methyl hexanoate and methyl 3-hydroxyhexanoate*, Samah Y. Mohamed, Nimal Naser, Gina Fioroni, Jon Luecke, Yeonjoon Kim, Peter C. St. John, Robert McCormick, Seonah Kim, *Combustion and Flame*, 258, 113071 (2023)

[70] *A Machine Learning Model for Automated Prediction of Bio-Oil Composition from Molecular Beam Mass Spectra*. Mohammed Jabed, Yeonjoon Kim, Clark Yarbrough, Anne Harman-Ware, Jessica Olstad, Reinhard Seiser, Cheyenne Paeper, Anne Starace, Seonah Kim, *ACS Sustainable Chemistry and Engineering*, 11, 32, 11912-11923 (2023).

[69] *Designing high-performance fuels through graph neural networks for predicting cetane number of multicomponent surrogate mixtures*. Yeonjoon Kim, Sabari Kumar, Jaeyoung Cho, Nimal Naser, Wonjong Ko, Peter C. St. John, Robert L. McCormick, Seonah Kim, SAE Technical Paper No. 2023-32-0052 (2023).

[68] *Short and Scalable Synthesis of Cynandione A*, Seoungwoo Kang, Yeonjoon Kim, Seonah Kim, Juyoung Ko, and Jae Hyun Kim, *Organic & Biomolecular Chemistry*, 21, 9, 1868-1871 (2023).

[67] *A comprehensive experimental and kinetic modeling study of di-isobutylene isomers- Part 2*, Nitin Lokachari, Goutham Kukkadapu, Brian D. Etz, Gina M. Fioroni, Seonah Kim, Mathias Steglich, Andras Bodi, Patrick Hemberger, Sergey S. Matveev, Anna Thomas, Hwasup Song, Guillaume Vanhove, Kuiwen Zhang, Guillaume Dayma, Maxence Lailliau, Zeynep Serinyel, Alexander A. Konnov, Philippe Dagaut, William J. Pitz, Henry J. Curran, *Comb. Flame*, 251, 112547 (2023).

[66] *Experimental and computational studies of the production of 1,3-butadiene from bio-2,3-butanediol using SiO<sub>2</sub>-supported H<sub>3</sub>PO<sub>4</sub> derivatives*, Juan V. Alegre-Requena, Glenn R. Hafenstine, Xiangchen Huo, Yanfei Guan, Jim Stunkel, Frederick G. Baddour, Kinga A. Unocic, Bruno C. Klein, Ryan E. Davis, Robert S. Paton, Derek R. Vardon<sup>†</sup> Seonah Kim<sup>†</sup>, *Chem. Eng. J.*, 466, 143346 (2023).

[65] *Sooting tendencies of terpenes and hydrogenated terpenes as sustainable transportation biofuels*, Junqing Zhu, Juan V. Alegre-Requena, Patrick Cherry, Dominic Curtis, Benjamin G. Harvey, Mohamed A. Jabed, Seonah Kim, Charles S. McEnally, Lisa D. Pfefferle, Josanne-Dee Woodroffe, *Proc. Comb. Inst.*, 39, 1, 877-887 (2023).

[64] *Enhancing  $\phi$ -sensitivity of ignition delay times through dilution of fuel-air mixture*, Jaeyoung Cho, Jon Luecke, Mohammad J Rahimi, Yeonjoon Kim, Bradley T Zigler, Seonah Kim<sup>†</sup>, *Proc. Comb. Inst.*, 39, 4, 4939-4947 (2023).

[63] *Physics-informed graph neural networks for predicting cetane number with systematic data quality analysis*, Yeonjoon Kim, Jaeyoung Cho, Nimal Naser, Sabari Kumar, Keunhong Jeong, Robert L. McCormick, Peter C. St. John, Seonah Kim<sup>†</sup>, *Proc. Comb. Inst.*, 39, 4, 4969-4978 (2023).

[62] *A comprehensive experimental and kinetic modeling study of di-isobutylene isomers: Part 1*, Nitin Lokachari, Goutham Kukkadapu, Hwasup Song, Guillaume Vanhove, Guillaume Dayma, Zeynep Serinyel, Kuiwen Zhang, Roland Dauphin, Brian Etz, Seonah Kim, Mathias Steglich, Andras Bodi, Gina Fioroni, Patrick Hemberger, Sergey S. Matveev, Alexander A. Konnov, Philippe Dagaut, Scott W Wagnon, William J. Pitz, Henry J. Curran, *Combustion and Flame*, 251, 112301 (2023).

[61] *Toward rational design of supported vanadia catalysts of lignin conversion to phenol via deoxygenation reaction*, Yeonjoon Kim, Mohammed A. Jabed, David M. Price, Dmitri Kilin, Seonah Kim<sup>†</sup>, *Chem. Eng. J.* 446, 136965 (2022)

[60] *Bioderived ether design for low emission and high reactivity transport fuels*, Jaeyoung Cho, Yeonjoon Kim, Brian D. Etz, Gina M. Fioroni, Nimal Naser, Junqing Zhu, Zhanhong Xiang, Cameron Hays, Juan V. Alegre-Requena, Peter C. St John, Bradley T. Zigler, Charles S. McEnally, Lisa D. Pfefferle, Robert L. McCormick, Seonah Kim<sup>†</sup>, *Sustainable Energy & Fuels*, 6, 3975-3988 (2022).

[59] *Predicting catalytic pyrolysis aromatic selectivity from Pyrolysis Vapor Composition using Mass Spectra Coupled with Statistical Analysis*, Anne K. Starace, David D. Lee, Kristen T. Hietala, Yeonjoon Kim, Seonah Kim, Anne E. Harman-Ware and Daniel L. Carpenter, *ACS Sustainable Chem. Eng.* 10, 234-244 (2022).

[58] *Chemical kinetic basis of synergistic blending for research octane number*, Gina M. Fioroni, Mohammed J. Rahimi, Charles K. Westbrook, Scott W. Wagnon, William J. Pitz, Seonah Kim and Robert L. McCormick, *Fuel* 307, 121865 (2022).

[57] *Connecting cation site location to alkane dehydrogenation activity in Ni/BEA catalysts*, Carrie A. Farberow; Evan C. Wegener; Anurag Kumar; Jacob Miller; Daniel P. Dupuis; Seonah Kim; Daniel A. Ruddy, *J. of Catalysis* 413, 264-273 (2022).

*Before CSU:*

[56] *Elucidating the chemical pathways of soot precursor formation during combustion of 1- and 2-phenylethanol*, Brian D. Etz, Gina M. Fioroni, Richard A. Messerly, Mohammad J. Rahimi, Peter C. St. John, David J. Robichaud, Earl D. Christensen, Brian P. Beekley, Charles S. McEnally, Lisa D. Pfefferle, Yuan Xuan, Shubham Vyas, Robert S. Paton, Robert L. McCormick, Seonah Kim<sup>†</sup>, *Proc. Comb. Inst.* 38, 1, 1327-1334 (2021). († denotes corresponding author)

[55] *Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers*, Yeonjoon Kim, Brian D. Etz, Peter C. St. John, Gina M. Fioroni, Richard A. Messerly, Shubham Vyas, Brian P. Beekley, Facheng Guo, Charles S. McEnally, Lisa D. Pfefferle, Robert L. McCormick, Seonah Kim<sup>†</sup>, *Proc. Comb. Inst.* 38, 1, 1143-1151 (2021). († denotes corresponding author)

[54] *"The importance of engineered and learned molecular representations in predicting organic reactivity, selectivity and chemical properties"*, Liliana Gallegos, Guilian Luchini, Peter C. St. John, Seonah Kim, Robert S. Paton, *Accounts of Chemical Research*, 54, 4, 827-836 (2021)

[53] *Understanding how chemical structure affects ignition-delay-time  $\phi$ -sensitivity*, Richard A. Messerly, Jon H. Luecke, Peter C. St. John, Brian D. Etz, Yeonjoon Kim, Bradley T. Zigler, Robert L. McCormick, Seonah Kim<sup>†</sup>, *Combustion & Flame*, 225, 377-387 (2021) († denotes corresponding author)

[52] *Prediction of Hydroxymethylfurfural Yield in Glucose Conversion through Investigation of Lewis Acid and Organic Solvent Effects*, Yeonjoon Kim, Ashutosh Mittal, David J. Robichaud, Heidi M. Pilath, Brian D. Etz, Peter C. St. John, David K. Johnson<sup>†</sup>, and Seonah Kim<sup>†</sup>, *ACS Catalysis*, 10, 24, 14707-14721 (2020). († denotes corresponding author)

[51] *Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules*, Peter St. John<sup>†</sup>, Yanfei Guan, Yeonjoon Kim, Brian D. Etz, Seonah Kim<sup>†</sup>, Robert S. Paton<sup>†</sup>, *Scientific Data*, 7, 244 (2020) († denotes corresponding author)

[50] *A perspective on biomass-derived biofuels: from catalyst design principles to fuel properties*, Yeonjoon Kim, Anna E. Thomas, David J. Robichaud, Kristiina Iisa, Peter C. St. John, Brian D. Etz, Gina M. Fioroni, Abhijit Dutta, Robert L. McCormick, Calvin Mukarakate<sup>†</sup>, Seonah Kim<sup>†</sup>, *J. Haz. Mat.*, 400, 5, 123198 (2020) († denotes corresponding author)

[49] *Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers*, Hyunguk Kwon, Brian D. Etz, Matthew J. Montgomery, Richard Messerly, Sharmin Shabnam, Shubham Vyas, Adri C. T. van Duin, Charles S. McEnally, Lisa D. Pfefferle, Seonah Kim<sup>†</sup>, and Yuan Xuan<sup>†</sup>, *J. Phys. Chem. A*, 124, 4290-4304 (2020) († denotes corresponding author)

[48] *Prediction of gas-phase homolytic bond dissociation energies at near chemical accuracy with sub-second computational cost*, Peter C. St. John<sup>†</sup>, Yanfei Guan, Yeonjoon Kim, Seonah Kim<sup>†</sup>, Robert S. Paton<sup>†</sup>, 10.26434/chemrxiv.10052048 (2019) and *Nature Comm.*, 11, 2328 (2020) (<sup>†</sup> denotes corresponding author)

[47] *Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen*, Kristiina Iisa, Yeonjoon Kim, Kellene A. Orton, David J. Robichaud, Rui Katahira, Michael J. Watson, Mark R. Nimlos, Joshua A. Schaidle, Calvin Mukarakate<sup>†</sup>, and Seonah Kim<sup>†</sup>, *Green Chem.*, 22, 2403-2418 (2020) (<sup>†</sup> denotes corresponding author, cover page, 2020 Green Chemistry Hot Articles)

[46] *Isotopic Studies for Tracking Biogenic Carbon during Co-processing of Biomass and Vacuum Gas Oil*, Calvin Mukarakate, Kellene Orton, Yeonjoon Kim, Stefano Dell'Orco, Carrie A Farberow, Seonah Kim, Michael J Watson, Robert Baldwin and Kim Magrini, *ACS Sustainable Chem. Eng.*, 8, 7, 2652-2664 (2020)

[45] *Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence-ratio*, Richard A. Messerly, Mohammad J. Rahimi, Peter C. St. John, Jon H. Luecke, Ji-Woong Park, Nabila A. Huq, Thomas D. Foust, Tianfeng Lu, Bradley T. Zigler, Robert L. McCormick, Seonah Kim<sup>†</sup>, *Combustion and Flame*, 214, 103-115 (2020) (<sup>†</sup> denotes corresponding author)

[44] *In-situ hydrogenation of bio-oil/bio-oil phenolic compounds with secondary alcohols over a synthesized mesoporous Ni/CeO<sub>2</sub> catalyst*, Hoda Shafaghat, Yiu Fai Tsang, Jong-Ki Jeon, Ji Man Kim, Yuri Park, Yeonjoon Kim, Seonah Kim, Young-Kwon Park, *Chemical Engineering Journal*, 382, 122912 (2020)

[43] *Theoretical Determination of Size Effects in Zeolite-catalyzed Alcohol Dehydration*, Larissa Y. Kunz, Lintao Bu, Brandon C. Knott, Cong Liu, Mark R. Nimlos, Rajeev S. Assary, Larry A. Curtiss, David J. Robichaud, and Seonah Kim<sup>†</sup>, *Catalysts*, 9, 700 (2019) (<sup>†</sup> denotes corresponding author)

[42] *Development of a data-derived sooting index including oxygen-containing fuel components*, Peter St. John, Seonah Kim, Robert L. McCormick, *Energy & Fuels*, 33, 10, 10290-10296 (2019)

[41] *Performance-Advantaged Ether Diesel Bioblendstock Production by a priori Design*, Nabila A. Huq, Xiangchen Huo, Glenn R. Hafenstine, Stephen M. Tiffitt, Jim Stunkel, Earl D. Christensen, Gina M. Fioroni, Lisa Fouts, Robert L. McCormick, Matthew R. Wiatrowski, Mary J. Bidy, Teresa L. Alleman, Raynella M. Connatser, Michael D. Kass, Patrick A. Cherry, Charles S. McEnally, Lisa D. Pfefferle, Peter St. John, Seonah Kim, Derek R. Vardon, 116 (52) 26421-26430, *PNAS* (2019).

[40] *Tailoring Diesel Bioblendstock from Integrated Catalytic Upgrading of Carboxylic Acids: A "Fuel Property First" Approach*, Xiangchen Huo, Nabila A. Huq, Jim Stunkel, Nicholas S. Cleveland, Anne K. Starace, Amy E. Settle, Allyson M. York, Robert S. Nelson, David G. Brandner, Lisa Fouts, Peter C. St. John, Earl D. Christensen, Jon Luecke, J. Hunter Mack, Charles S. McEnally, Patrick A. Cherry, Lisa D. Pfefferle, Timothy J. Strathmann, Davinia Salvachúa, Seonah Kim, Robert L. McCormick, Gregg T. Beckham, Derek R. Vardon, *Green Chem.* 21, 5813-5827 (2019)

[39] *Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers*, Seonah Kim<sup>†</sup>, Gina M. Fioroni, Ji-Woong Park, David J. Robichaud, Dhruvajyoti D. Das, Peter C. St. John, Tianfeng Lu, Charles S. McEnally, Lisa D. Pfefferle, Robert S. Paton, Thomas D. Foust, Robert L. McCormick<sup>†</sup>, *Proceedings of the Combustion Institute*, 37, 1, 1083-1090 (2019) (<sup>†</sup> denotes corresponding author) (Impact Factor: 5.34)

[38] *Sooting tendencies of co-optima test gasolines and their surrogates*, Charles S. McEnally, Yuan Xuan, Peter C. St. John, Dhruvajyoti D. Das, Abhishek Jain, Seonah Kim, Thomas A. Kwan, Lance K. Tan, Junqing Zhu, Lisa D. Pfefferle, *Proceedings of the Combustion Institute*. 37, 1, 961-968 (2019) (Impact Factor: 5.34)

[37] *Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate*, Ahfaz Ahmed, William J. Pitz, Carlo Cavallotti, Marco Mehl, Nitin Lokachari, Elna J.K. Nilsson, Jui-Yang Wang, Alexander A. Konnov, Scott W. Wagnon, Bingjie Chen, Zhandong Wang, Seonah Kim, Henry J. Curran, Stephen J.

Klippenstein, William L. Roberts, S. Mani Sarathy, *Proceedings of the Combustion Institute*, 37, 1, 419-428 (2019) (Impact Factor: 5.34)

[36] *Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors*, Vivek S. Bharadwaj, Seonah Kim, Michael T. Guarnieri, Michael F. Crowley, *Scientific Reports*, 8, 12826 (2018).

[35] *Sooting tendencies of aromatic hydrocarbons with oxygen- containing side-chains*, Brian P. Beekley, Charles S. McEnally\*, Peter C. St. John, Seonah Kim, Abhishek Jain, Hyunguk Kwon, Yuan Xuan, Lisa D. Pfefferle, ESSCI (Eastern States Section of the Combustion Institute) Spring 2018, *Proceedings of the Combustion Institute*.

[34] *Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5*, Lintao Bu, Mark R. Nimlos, David J. Robichaud, Seonah Kim<sup>†</sup>, *Catalysis Today*, 312, 73-81 (2018) (<sup>†</sup> denotes corresponding author)

[33] *Advancing Catalytic Fast Pyrolysis through Integrated Multiscale Modeling and Experimentation: Challenges, Progress and Perspectives*, Peter N. Ciesielski, M. Brennan Pecha, Vivek S. Bharadwaj, Calvin Mukarakate, G. Jeremy Leong, Branden Kappes, Michael F. Crowley, Seonah Kim, Thomas D. Foust, Mark R. Nimlos, *Wiley Interdisciplinary Reviews: Energy and Environment*, (2018) (DOI: 10.1002/wene.297).

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[31] *Experimental and theoretical study of oxidative stability of alkylated furans used as gasoline blend components*, Earl Christensen<sup>†</sup>, Gina M. Fioroni, Seonah Kim<sup>†</sup>, Lisa Fouts, Erica Gjersing, Robert S. Paton, and Robert L. McCormick, *Fuel*, 576-585(2018). (<sup>†</sup> denotes co-corresponding author)

[30] *Measuring and Predicting Sooting Tendencies of Oxygenates, Alkanes, Alkenes, Cycloalkanes, and Aromatics on a Unified Scale*, Dhruhajyoti D. Das, Peter St. John, Charles S. McEnally, Seonah Kim, Lisa D. Pfefferle, *Combustion and Flame*, 190, 349-364 (2018).

[29] *Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research*, Brandon C. Knott, Claire T. Nimlos, David J. Robichaud, Mark R. Nimlos, Seonah Kim<sup>†</sup>, Rajamani Gounder<sup>†</sup>, *ACS Catal.*, 8, 770-784 (2018). (<sup>†</sup> denotes co-corresponding author)

[28] *Improving Biomass Pyrolysis Economics by Integrating Vapor and Liquid Phase Upgrading*, Kristiina Iisa, Michael J. Watson, Jeroen ten Dam, Abhijit Dutta, Robert M. Baldwin, Calvin Mukarakate, Seonah Kim, David J. Robichaud and Mark R. Nimlos, *Green Chem.* 20, 567 (2018).

[27] *Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules*, Lintao Bu, Peter N. Ciesielski, David J. Robichaud, Seonah Kim, Robert L. McCormick, Thomas D. Foust, and Mark R. Nimlos, *J. Phys. Chem. A*, 127, 121, 5475-5486 (2017).

[26] *A quantitative model for the prediction of sooting tendency from molecular structure*, Peter C. St John, Paul Kairys, Dhruhajyoti D. Das, Charles S. McEnally, Lisa D. Pfefferle, David J. Robichaud, Mark R. Nimlos, Bradley T. Zigler, Robert L. McCormick, Thomas D. Foust, Yannick J. Bomble, and Seonah Kim<sup>†</sup>, *Energy & Fuels*, 31 (9), 9983-9990 (2017). (<sup>†</sup> denotes corresponding author)

[25] *Exploring low-temperature dehydrogenation at ionic Cu sites in beta zeolite to enable alkane recycle in dimethyl ether homologation*, Carrie A. Farberow, Singfoong Cheah, Seonah Kim, Jeffrey T. Miller, James R. Gallagher, Jesse Hensley, Joshua A. Schaidle and Daniel A. Ruddy, *ACS Catal.*, 7(5), 3662-3667 (2017).

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David J. Robichaud, and Seonah Kim<sup>†</sup>, *J. Phys. Chem. C*, 121, 500-510 (2017). (<sup>†</sup> denotes corresponding author) (Selected Special Issue as part of The Journal of Physical Chemistry virtual special issue "Mark S. Gordon Festschrift")

[23] *Through-Space Ultrafast Photoinduced Electron Transfer Dynamics of a C70-Encapsulated Bisporphyrin Covalent Organic Polyhedron in a Low-Dielectric Medium*, Michael Ortiz, Sung Cho, Jens Niklas, Seonah Kim, Oleg G. Poluektov, Wei Zhang, Garry Rumbles, Jaehong Park, *JACS*, 139, 4286-4289 (2017).

[22] *Furan production from glycolaldehyde over HZSM-5*, Seonah Kim<sup>†</sup>, Tabitha J. Evans, Calvin Mukarakate, Lintao Bu, Gregg T. Beckham, Mark R. Nimlos, Robert S. Paton and David J. Robichaud<sup>†</sup>, *ACS Sustainable Chem. Eng.*, 4(5), 2615-2623 (2016). (<sup>†</sup> denotes corresponding author)

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[19] *Structural and electronic snapshots during the transition from a Cu(II) to Cu(I) metal center of a lytic polysaccharide monoxygenase by X-ray photo-reduction*, Mikael Gudmundsson<sup>\*</sup>, Seonah Kim<sup>\*</sup>, Miao Wu<sup>\*</sup>, Takuya Ishida, Majid Hadadd Momeni, Gustav Vaaje-Kolstad, Daniel Lundberg, Antoine Royant, Jerry Ståhlberg, Vincent G.H. Eijsink, Gregg T. Beckham, and Mats Sandgren, *JBC* 289, 18782-18792 (2014) (\* denotes equal author contributions).

[18] *Crystal structure of glycoside hydrolase family 127 β-l-arabinofuranosidase from Bifidobacterium longum*, Tasuku Ito<sup>\*</sup>, Kyo Saikawa<sup>\*</sup>, Seonah Kim<sup>\*</sup>, Kiyotaka Fujita, Akihiro Ishiwata, Sophon Kaeothip, Takatoshi Arakawa, Takyoshi Wakagi, Gregg T. Beckhame, Yukishige Ito, Shinya Fushinobu, *Biochem. Biophys. Res. Commun.* 447, 32-37 (2014) (\* denotes equal author contributions).

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[5] *Theoretical Studies of Short Polyproline Systems: Recalibration of a Molecular Ruler*, Elena Dolgih, Wilfredo Ortiz, Seonah Kim, Brent P. Krueger, Jeffrey L. Krause, and Adrian E. Roitberg, *J. Phys. Chem. A* 113, 4639-4646 (2009).

[4] *Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Synchronization of Molecular Dynamics Trajectories in Biomolecules*, Daniel J. Sindhikara, Seonah Kim, Art Voter, and Adrian E. Roitberg, *J. Chem. Theory Chem.* 5(6), 1624-1631 (2009).

[3] *Crystal Structure Prediction (CSP) of Flexible Molecules using Parallel Genetic Algorithms with a Standard Force Field*, Seonah Kim, Anita M. Orendt, Marta B. Ferraro, and Julio C. Facelli, *J. Comput. Chem.* 30, 1973-1985 (2009).

[2] *Simulation Temperature Jumps for Protein Folding*, Seonah Kim and Adrian Roitberg, *J. Phys. Chem. B* 112, 1525-1532 (2008).

[1] *Crystal Structure Prediction of Flexible Molecules with Genetic Algorithms and Standard Force Field*, Julio C. Facelli, Seonah Kim, Anita M. Orendt, Marta B. Ferraro, Ian Pimienta and Victor Bazterra, *Aca Cryst.*, A64, C226 (2008).

### **Invited Talks**

- 6<sup>th</sup> Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 6), July 11<sup>th</sup>, 2013 (Gyeongju, Korea)
- 36<sup>th</sup> Symposium on Biotechnology for Fuels and Chemicals, May 1<sup>st</sup>, 2014 (Clearwater, FL)
- ACS National Meeting & Exposition, August 16 – 20, 2015 (Boston, MA)
- 2015 Korean Society for Biotechnology and Bioengineering (KSBB) Fall Meeting and International Symposium, Oct. 10-14, 2015 (Incheon, South Korea)
- Tcbiomass 2015, Nov. 2-5, 2015 (Chicago, IL)
- ACS 2016 Spring Meeting, Mar. 13-17, 2016 (San Diego, CA)
- Seoul University, July 28, 2016

- ACS 2016 Fall Meeting, Aug. 21-25, 2016 (Philadelphia, PA)
- Frontiers in Biorefining, Nov. 8 – 11, 2016 (St. Simons Island, GA)
- ACS 2017 Spring Meeting, Apr. 2-6, 2017 (San Francisco, CA)
- NAM25, June 4-9, 2017 (Denver, CO)
- Tailor-Made Fuels From Production to Propulsion 5<sup>th</sup> International Conference, June 20-22, 2017 (Aachen, Germany)
- Industrial Biotechnology Research Training Program (bio-GMP), Kookmin University, July 6-8, 2017 (Seoul, Korea)
- ACS 2018 Spring Meeting, March 18-22, 2018 (New Orleans, LA)
- Reaction Mechanisms Conference 2018, June 10-13, 2018 (Vancouver, BC, Canada)
- 31<sup>st</sup> Meeting of Catalysis Research Discussion, June 21-23, 2018 (Pyeongchang, S. Korea)
- 2018 KMB International Symposium & Annual Meeting, June 27-30, 2018 (Yeosu, S. Korea)
- Industrial Biotechnology Research Training Program (bio-GMP), Kookmin University, July 1-3, 2018 (Seoul, Korea)
- 37<sup>th</sup> International Symposium on Combustion, July 29-Aug. 3, 2018 (Dublin, Ireland)
- ACS 2018 Fall Meeting, August 19-23, 2018 (Boston, MA)
- Colorado School of Mines, Chemistry Department, Oct. 6, 2018 (Golden, CO)
- 11<sup>th</sup> US National Combustion Meeting, March 24-27, 2019 (Pasadena, CA)
- ACS 2019 Spring Meeting, March 31-April 4, 2019 (Orlando, FL)
- 23<sup>rd</sup> Annual Green Chemistry & Engineering Conference, June 11.13, 2019 (Reston, VA)
- ACS 2019 Fall Meeting, August 25-29, 2019 (San Diego, CA)
- Machine Learning and Informatics for Chemistry and Materials workshop, Sep. 30 – Oct. 4, 2019 (Telluride, CO)
- Colorado State University, Chemistry Department, Nov. 14, 2019 (Fort Collins, CO)
- University of Texas, San Antonio, Chemical Engineering Department, Jan. 17, 2020 (San Antonio, TX)
- Syracuse University, Chemistry Department, Jan. 21, 2020 (Syracuse, NY)
- University of Arkansas, Chemical Engineering Department, March 18, 2020 (virtual)
- Korea University, Material Engineering Department, Dec., 2020 (south Korea)
- Chonnam University, Food Science Engineering Department, Dec., 2020 (South Korea) (virtual)
- 38<sup>th</sup> International Symposium on Combustion, Jan. 24-29, 2021 (Adelaide, Australia) (virtual)
- Korean Society for Microbiology and Biotechnology (KMB) 2021, 48<sup>th</sup> Annual Meeting & International Symposium, Recent Advances in Industrial Biotechnology and Metabolic Engineering, June 23-25, 2021. (virtual, Busan, South Korea)
- NSF CHE/DATA workshop, Aug. 2021 (virtual)
- Truman State University, Chemistry Department, Sep. 17, 2021 (virtual)
- California Polytechnic State University Seminar, Chemistry Department, Oct. 1, 2021 (virtual)
- Illinois State University, Chemistry Department, Nov. 12, 2021 (virtual)
- University of Colorado, Denver, Chemistry Department, Dec. 10, 2021
- Yonsei University, Chemical Engineering Department, May 24, 2022
- Seoul City University, Environmental Engineering Department, May 30, 2022
- Hanhwa Faculty Award, June 7, 2022 (virtual)
- Summer Research Experience: Computational Chemistry (includes Community College students), Guest Lecture Series, Northeastern University, June 29, 2022 (virtual)
- WATOC 2020 12<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists, July 3-8, 2022 (Vancouver, Canada)
- Gordon Research Conference, Computational Chemistry, July 17-22, 2022 (Barcelona, Spain)
- Houk Symposium, Aug. 11-12, 2022 (UCLA, Los Angeles, CA)
- ACS 2022 Fall Meeting ('Symposium in honor of the 60<sup>th</sup> Birthday of Prof. Adrian Roitberg') Aug. 22, 2022 (Chicago, IL)
- Aslla Symposium on "Accelerated Chemical Science with AI", Sep. 25-28, 2022 (Ganneung, S. Korea)
- ExxonMobil Seminar (Oct. 2022, New Jersey)



- CiTQ Seminar at Universitat Rovira i Virgili (Tarragona, Spain), Nov. 2022 (virtual)
- 7<sup>th</sup> international symposium of quantum beam science at Ibaraki university, Dec. 1-3, 2022 (Mito, Japan) (virtual)
- Department of Chemistry & Nanoscience, Ewha Womans University, December 2022.
- Department of Chemistry, University of Denver, March 2, 2023
- Korea Research Institute of Chemical Technology (KRICT), April 10, 2023 (Daejeon, S. Korea)
- 2023 KSBB Spring Meeting and International Symposium, April 12-14, 2023 (Jeju, S. Korea)
- University of Michigan, Chemistry Department, May 3, 2023.
- Telluride workshop “Machine Learning and Informatics for Chemistry and Materials”, June 25-29, 2023 (Telluride, CO)
- 2023 “Computational Materials Chemistry” Telluride Workshop, July 17-21, 2023 (Telluride, CO)
- ACS 2023 Fall Meeting (Symposium in honor of the 80th Birthday of Prof. Kendall N. Houk: Pushing Back the Frontiers of Computational Organic Chemistry and Chemical Biology), Aug. 13, 2023 (San Francisco, CA)
- Department of Pharmacy, Ewha Womans University, Sep. 2023 (Seoul, S. Korea)
- Department of Chemical Engineering, Seoul National University, Sep. 2023 (Seoul, S. Korea)
- 2023 Powertrain, Energy and Lubricants International Meeting, Aug. 29 – Sep. 1, 2023 (Kyoto, Japan)
- Department of Environmental and Climate Technology/Energy Materials and Devices of Korea Institute of Energy Technology, Oct. 2023 (Najoo, S. Korea)
- Department of Chemistry, Kyung Hee University, Nov. 2023 (Seoul, S. Korea)
- Department of Applied Chemistry, Kyung Hee University, Nov. 2023 (Suwon, S. Korea)
- Department of Food Science & Technology, Chonnam National University, Dec. 2023 (Gwangju, S. Korea)

### **Professional Summary**

- ACS COMP (Computers in Chemistry) Chair-elect, Chair 2020
- ACS COMP (Computers in Chemistry) Newsletter officer (2016 – present)
- C3E (The Clean Energy Education & Empowerment) Award nominated (2019)
- NSF Proposal Reviewer (2019), Swiss National Science Foundation Reviewer (2018)
- NREL President Award (2016)
- Mentor for graduate students and postdocs (arranged visitor/internship programs in NREL)
- ACS 2019 National Meeting career workshop panel for female and underrepresented group undergraduates
- Journal Reviewers (ACS Omega, Catalysis Today, J. Biotechnology, Angew. Chem. Int. Ed., Chemical Science, J. Phys. Chem., Catalysts, and etc.)
- ACS 2019 Spring National Meeting COMP symposium ‘Probing Reactive Intermediates Through Chemical Computations’ Co-organizer
- ACS 2019 Fall National Meeting COMP symposium ‘Advances in Multiscale Computational Modeling of Biomass Conversion Processes’ Organizer
- ACS 2020 Spring/Fall National Meeting Energy & Fuels Symposium ‘Chemistry of Fuel Properties, Combustion & Fuel-Engine Interactions’ Co-organizer
- ACS 2021 Spring/Fall National Meeting Energy & Fuels Symposium ‘Chemistry of Fuel Properties, Combustion & Fuel-Engine Interactions’ Co-organizer
- NSF CHE/DATA workshop (2021. 8)
- ACS 2022 Spring National Meeting, Energy & Fuels Symposium ‘ACS Henry H. Storch Award Symposium in Honor of Robert McCormick’ Co-organizer
- ACS 2022 Fall National Meeting, COMP ‘Symposium in honor of the 60th Birthday of Prof. Adrian Roitberg’ Organizer
- 7<sup>th</sup> Hanwha Non-Tenured Faculty Award (2022), June 2022
- NSF Review Panel (Dec. 2022)
- Arranged two undergraduate school seminar series (Truman State University, CalPoly)
- Telluride workshop “Machine Learning and Informatics for Chemistry and Materials”, Co-organizer, June 2023
- ACS 2023 Fall National Meeting Energy & Fuels Symposium ‘Properties, Catalysis, Combustion, and

Environmental Impacts of Low-Net Carbon Liquid Fuels: Harnessing the Power of Artificial Intelligence/Machine Learning' Organzier

- ACS 2023 Fall National Meeting, COMP 'Symposium in honor of the 80th Birthday of Prof. Kendall N. Houk: Pushing Back the Frontiers of Computational Organic Chemistry and Chemical Biology' Organizer

### **Computational Resources**

- 2019 ASCR Leadership Computing Challenge Awardees, DOE (Co-PI for "Accelerated Catalyst Discovery from First Principles Simulations and Machine Learning")
- PI for Extreme Science and Engineering Development Environment (XSEDE, currently ACCESS, 2021 – current)
- NREL High Performance Computing, DOE (PI for 3 allocations, 2018 – current)

### **Research Supervision**

- Collin Hansen (Graduate student, 2022.6 – 2022.8, 2022. 11 – present)
- Shaylee Seymour (2022. 11 – 2023.5): Co-advising with Prof. Paton
- Olivia Harman (visiting undergraduate student (REU) from Florida Gulf Coast University, 2022.6 – 2022.8)
- Wonjong Ko (visiting high school student, 2022.6 – 2022.8)
- Jessica Lee (CSU Data Science undergraduate student, 2022.4 – present)
- Hojin Jung (Visiting graduate student from Yonsei University, 2021. 1 – 2021. 7, Graduate student, 2022. 11 – present)
- Chris Stubbs (2022. 5 – present): Co-advising with Prof. Chen
- David Price (Graduate student, 2020.11 – 2022.5)
- Sabari Kumar (Graduate student, 2021. 11 – present)
- Alex Claiborne (Undergraduate student, 2021. 8 – 2021.12)
- Dr. Raul Perez-Soto (Postdoc, 2022. 10 – present)
- Dr. Mohammed Javed (Postdoc, 2021. 11 – 2022.10)
- Dr. Juan Vicente Alegre Requena (Research Scientist, 2021. 3 – 2022. 3)
- Dr. Yeonjoon Kim (Postdoc, 2018. 6 – 2023. 8, Assistant Professor at Pukyong National University (S. Korea))
- Dr. Jaeyoung Cho (Postdoc, 2020. 3 – 2021.3, Assistant Professor at UT El Paso)
- Dr. Richard Messerly (Postdoc, 2019. 2 – 2019. 11, Currently Postdoc at Los Alamos National Laboratory)
- Brian Etz (CSM/NREL graduate student, 2018. 11 – 2020. 12, Currently Postdoc at US Army Corps of Engineers)
- Julian Golzwarden (CSM/NREL graduate student, 2019. 11 – 2020.12)
- Dr. Peter St. John (Postdoc, 2016 – 2018, currently NVIDIA)
- Dr. Longwen Ou (Visiting Postdoc from North Carolina State University, 2017, Currently Postdoc at Argonne National Laboratory)
- Shinyoung Oh (Visiting graduate student from Seoul National University, 2018, Currently Postdoc at KIST, South Korea)

### **Current Research Support**

- 06/2022 – 01/2024: "Gasoline Composition Impact on Gasoline Particle Emissions Investigation via Flow Reactor Experiments and Density-Functional Theory" (ExxonMobil) - \$106,900
- 08/2023 – 07/2026: "Self-evolving solubility databases and neural network predictions for organic and polymer applications in multicomponent solvents" (NSF) - \$449,400
- 09/2023 – 08/2026: CCI Phase I: NSF Center for Sustainable Photoredox Catalysis (SuPRCat) (NSF) - \$1,800,000
- 03/2021 – 06/2023: "Machine learning predictive tool development for process monitoring and predictions task" (NREL Subcontract) - \$180,600
- 03/2020 – 02/2023: "Predicting Fuel Properties and Emissions for Advanced Biofuels for Diesel Engines" (ExxonMobil) - \$100,000

### **Previous Research Support**

- 01/2021 – 06/2022: “Application of Theoretical Chemistry to Low-Carbon Fuel Autoignition and Soot Precursor Formation Mechanism Development” (NREL Subcontract) – \$183,235

#### **At NREL**

- 2015 – 2016 NREL LDRD (Laboratory Directed Research & Development) “Renewable Hydrocarbon Fuel Production from Fatty Acid Decarboxylase Engineering” as PI (\$500,000 for 2 year)
- 2015 – 2019: DOE Consortium for Computational Physics and Chemistry (CCPC) as Task Leader for atomistic modeling task (\$500,000/year)
- 2016 – 2020: DOE Co-OPTIMA “chemical kinetics for combustion and fuel property prediction tool using Machine-learning” as PI for modeling task (DFT+MD+ML) (\$550,000/year)
- 2020 – 2022: DOE Systems Development and Integration (SDI) (“Process Monitoring and Predictions of BioRefinery Performance”) as PI (\$500,000/year)