

## Seonah Kim PhD

Associate Professor  
Department of Chemistry  
Colorado State University  
1301 Center Ave, Fort Collins, CO 80523

Cell: (805) 338-1499  
Email: seonah.kim@colostate.edu

### 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
- Bottom-up Predictions (via Machine Learning)/Design of (Bio)Fuels & Engine Performance

### Professional Appointments

Associate Professor, Colorado State University	2021 – present
Senior Scientist/Staff Scientist, National Renewable Energy Laboratory	2015 – 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 • PhD with Dr. Adrian E. Roitberg	2003 – 2007
Computer Science, University of Houston • MS with Dr. B. Montgomery Pettitt	1999 – 2003

### Publications

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

[55] *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)

[54] *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)

[53] *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)

[52] *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)

[51] *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)

[50] *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.* 2020 (in press). († denotes corresponding author)

[49] *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.* 2020 (in press). († 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) († denotes corresponding author)

[47] *Integrating Experimental and Computational Studies Unravels the Ga Species Responsible for Enhancing Alkene Production during Catalytic Upgrading of Biomass Pyrolysis Vapors over Ga/ZSM-5*, 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) († 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) († 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, Rajeew S. Assary, Larry A. Curtiss, David J. Robichaud, and Seonah Kim<sup>†</sup>, *Catalysts*, 9, 700 (2019) († 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. Tiffit, 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).

[32] *Structural and molecular dynamics studies of a C1-oxidizing lytic polysaccharide monoxygenase from *Heterobasidion irregulare* reveal amino acids important for substrate recognition*, Bing Liu, Abhishek A. Kognole, Miao Wu, Bjørge Westereng, Michael F. Crowley, Seonah Kim, Maria Dimarogona, Christina M. Payne, Mats Sandgren, *The FEBS Journal*, 285, 2225-2242 (2018).

[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*, Dhruvajyoti 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, Dhruvjayoti 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).

[24] *Diffusion of biomass pyrolysis products in H-ZSM-5 by molecular dynamics simulations*, Lintao Bu, Mark R. Nimlos, 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)

[21] *Ethanol Dehydration in HZSM-5 studied by Density Functional Theory: Evidence for Concerted Process*, Seonah Kim<sup>†</sup>, David J. Robichaud, Gregg T. Beckham, Robert S. Paton, and Mark R. Nimlos<sup>†</sup>, *J. Phys. Chem. A* 119 (15), 3604-3614 (2015). (<sup>†</sup> denotes corresponding author)

[20] *Carbocation Stability in H-ZSM-5 at High Temperature*, Glen A. Ferguson, Lei Cheng, Lintao Bu, Seonah Kim, David J. Robichaud, Mark R. Nimlos, Larry A. Curtiss, Gregg T. Beckham, *J. Phys. Chem. A*. 119, 11397-11405 (2015).

[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\*, Seonah Kim\*, Miao Wu\*, 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\*, Kyo Saikawa\*, Seonah Kim\*, 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).

[17] *Quantum Mechanical Calculations suggest that Lytic Polysaccharide Monoxygenases employ a Copper-oxyl, Oxygen-rebound Mechanism*, Seonah Kim, Mats Sandgren, Jerry Ståhlberg, Robert S. Paton, Gregg T. Beckham, *PNAS* 111, 149-154 (2014).

[16] *A Mechanistic Investigation of Acid-Catalyzed Cleavage of Aryl-Ether Linkages: Implications for Lignin Depolymerization in Acidic Environments*, Matthew R. Sturgeon\*, Seonah Kim\*, Kelsey Lawrence, Robert S. Paton, Stephen C. Chmely, Mark Nimlos, Thomas D. Foust, Gregg T. Beckham, *ACS Sustainable Chem. Eng.*, 2, 472-485 (2014) (\* denotes equal author contributions).

[15] *Diels-Alder Reactivities of Strained and Unstrained Cycloalkenes with Normal and Inverse-Electron-Demand Dienes: Activation Barriers and Distortion/Interaction Analysis*, Fang Liu, Robert S. Paton, Seonah Kim, Yong Liang, K. N. Houk, *JACS* 135(41), 156442-15649 (2013).

[14] *Aromatic Claisen Rearrangements of O-Phenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements*, Silvia Osuna, Seonah Kim, Guillaume Bollot, K. N. Houk, *Eur. J. Org. Chem.* 2823-2831 (2013).

[13] *Crystal structure and computational characterization of the lytic polysaccharide monoxygenase GH61D from the basidiomycota fungus Phanerochaete chrysosporium*, Miao Wu, Gregg T. Beckham, Anna M. Larsson, Takuya Ishida, Seonah Kim, Christina M. Payne, Michael E. Himmel, Michael F. Crowley, Svein J. Horn, Bjorge Westereng, Kiyohiko Igarashi, Masahiro Samejima, Jerry Stahlberg, Vincent G. H. Eijsink, Mats Sandgren, *J. Biol. Chem.* 288, 12828-12839 (2013).

[12] *Mechanistic study of a Ru-xantphos catalyst for tandem alcohol dehydrogenation and reductive aryl-ether cleavage*, Stephen C. Chmely\*, Seonah Kim\*, Peter N. Ciesielski, Gonzalo Jimenez-Oses, Robert S. Paton, Gregg T. Beckham, *ACS Catal.* 3, 963-974 (2013) (\* denotes equal author contributions)

[11] *A Synthetic Recursive "+1" Pathway for Carbon Chain Elongation*, Ryan J. Marcheschi, Han Li, Kechun Zhang, Elizabeth L. Noey, Seonah Kim, Asha Chaubey, K. N. Houk, and James C. Liao, *ACS Chem. Biol.* 7, 689-697 (2012).

[10] *Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins*, Seonah Kim, Stephen C. Chmely, Mark R. Nimlos, Yannick J. Bomble, Thomas D. Foust, R. S. Paton, and Gregg T. Beckham, *J. Phys. Chem. Lett.* 2, 2846-2852 (2011).

[9] *Computational Design of New Protein Catalysts*, Gert Kiss, Scott A. Johnson, Geoffrey Nosrati, Nihan Celebi-Olcum, Seonah Kim, Robert S. Paton, K. N. Houk, Book Chapter for Modeling of Molecular Properties, Chapter 16, Wiley-VCH Verlag GmbH & Co. (2011).

[8] *Experimental Diels-Alder Reactivities of Cycloalkenones and Cyclic Dienes Explained through Transition-State Distortion Energies*, R. S. Paton, Seonah Kim, Audrey G. Ross, Samuel J. Danishefsky, and K. N. Houk, *Angew. Chem. Int. Ed.* 50, 10366-10368 (2011).

[7] *Facilitation Scientific Discovery using Scientific Workflows on the Grid*, Jianwu Wang, Prakashan Korambath, Seonah Kim, Scott A. Johnson, Kejian Jin, Daniel Crawl, Ilkay Atintas, Shava Smallen, Bill Labate, and K. N. Houk, Book Chapter for Guide to e-Science: Computer Communications and Networks, Part 4, 353-382 (2011).

[6] *Theoretical Enzyme Design using the Kepler Scientific Workflows on the Grid*, Jianwu Wang, Prakashan Korambath, Seonah Kim, Scott A. Johnson, Kejian Jin, Daniel Crawl, Ilkay Atintas, Shava Smallen, Bill Labate, and K. N. Houk, *Procedia Computer Science*, 1, 1, 1175-1184, ICCS 2010 (2010).

[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 Comput.* 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)

### **Professional Summary**

- ACS COMP (Computers in Chemistry) Chair-elect, Chair 2020
- ACS COMP (Computers in Chemistry) Newsletter officer (2016 – present)
- NSF Proposal Reviewer (2019), Swiss National Science Foundation Reviewer (2018)
- 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

### **Computational Resources**

- 2021 XSEDE Startup (PI for “Computational design and prediction of high-performance (bio)fuels and platform chemicals using quantum mechanics and machine learning”)
- 2019 ASCR Leadership Computing Challenge Awardees, DOE (Co-PI for “Accelerated Catalyst Discovery from First Principles Simulations and Machine Learning”)
- Extreme Science and Engineering Development Environment (XSEDE), NSF (NREL team effort, current)
- NREL High Performance Computing, DOE (PI for 3 allocations, 2018 – current)

### **Research Supervision**

- Dr. Yeonjoon Kim (Postdoc, 2018. 6 – present)
- Dr. Jaeyoung Cho (Postdoc, 2020. 3 – present)
- Dr. Richard Messerly (Postdoc, 2019. 2 – 2019. 11, Currently Postdoc at Los Alamos National Laboratory)
- Dr. Brian Etz (CSM/NREL graduate student, 2018. 11 – 2020.12, Currently Postdoc at US Army Corps of Engineers)
- Dr. Peter St. John (Postdoc, 2016 – 2018, currently NREL senior scientist)
- 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)