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HEATHER J. KULIK

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EDUCATION

2010-2013 Postdoctoral associate, Stanford University, Stanford, CA
Postdoctoral advisor: Todd J. Martínez

2009-2010 Postdoctoral associate, Lawrence Livermore Lab, Livermore, CA
Postdoctoral advisor: Felice C. Lightstone

2009 Ph.D. in Materials Science and Engineering, MIT, Cambridge, MA
Doctoral advisor: Nicola Marzari (now at EPFL)

2004 B.E. in Chemical Engineering, The Cooper Union, New York, NY

ACADEMIC APPOINTMENTS

Department of Chemical Engineering, MIT

7/19- Associate Professor (without Tenure)

11/13-6/19 Assistant Professor

SELECTED HONORS AND AWARDS

2019 *The Journal of Physical Chemistry B* Lectureship (ACS PHYS Division)
National Science Foundation CAREER Award
Saville Lecture, Department of Chemical and Biological Engineering, Princeton Univ.
AAAS Marion Milligan Mason Award

2018 DARPA Young Faculty Award
Office of Naval Research Young Investigator Award
ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry (ACS COMP Division)

2017 ACS *Industrial & Engineering Chemistry Research* "Class of Influential Researchers"

2012 Burroughs Wellcome Fund Career Award at the Scientific Interface

2004 National Science Foundation Graduate Research Fellow

2000 United States Presidential Scholar

OTHER RECOGNITION

2020 *Molecular Systems Design & Engineering* Emerging Investigator

2019 *Inorganic Chemistry* Emerging Investigator
Frontiers In Chemistry Rising Star
Reaction Chemistry & Engineering Emerging Investigator

2018 *Journal of Chemical Theory and Computation* ACS Editors' Choice

2017 *Journal of Chemical Physics* 2016 Editors' Choice

2016 *Journal of Physical Chemistry* ACS Editors' Choice

2011 BIOL ACS Student & postdoc symposium speaker *(1 of 8 from over 200).*

2008 DMSE Research Image contest winner

2006 Award for outstanding paper by a 1st- or 2nd-Year graduate student

2005 LLNL CCMS Summer Institute Graduate Fellow

2004 Robert Spice Fund Prize for Excellence in Analytical Chemistry
William C. and Esther Hoffman Beller Prize for Top Graduating Student in Chemical Engineering

2003 Elmer J. Badin Award for Excellence in Chemistry
Rockefeller University Summer Undergraduate Research Fellow

2002 Elected to New York Iota Chapter of Tau Beta Pi Honors Society

2000 Times Academic All-Star in Mathematics
Association for Women in Science Scholar
Robert Byrd Scholar
Elks National Foundation Most Valuable Student

Last updated: 9/7/19.

PUBLICATIONS (since 11/1/13: corresponding author indicated by *).

68. A. Bajaj and **H. J. Kulik*** "Uncovering New Pathways in Polymer Electrolyte Membrane Fuel Cell Nafion Degradation with First Principles Modeling", *in preparation*.

67. R. Mehmood and **H. J. Kulik*** "The Relative Importance of Configuration and QM Region Size in QM/MM modeling: The Case of DNA Methyltransferase", *in preparation*.

66. F. Liu and **H. J. Kulik*** "Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry", *submitted*. https://doi.org/10.26434/chemrxiv.9765065.v1

65. Q. Zhao and **H. J. Kulik*** "Stable Surfaces that Bind too Tightly: Can Range Separated Hybrids or DFT+U Improve Paradoxical Descriptions of Surface Chemistry?", *The Journal of Physical Chemistry Letters*, **10**, 5090-5098 (2019).

64. A. Nandy, J. Zhu, J. P. Janet, C. Duan, R. B. Getman, and **H. J. Kulik*** "Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metal-Oxo Intermediate Formation", *ACS Catalysis,* **9**, 8243-8255 (2019).

63. J. P. Janet, C. Duan, T. Yang, A. Nandy, and **H. J. Kulik*** "A quantitative uncertainty metric controls error in neural network-driven chemical discovery", *Chemical Science,* **10**, 7913-7922 (2019). http://doi.org/10.1039/C9SC02298H **Selected as HOT article,** Featured in *Chemistry World*: https://www.chemistryworld.com/news/uncertainty-metric-builds-confidence-in-machine-learned-chemistry/3010759.article

62. S. Gugler, J. P. Janet, and **H. J. Kulik*** "Enumeration of *de novo* inorganic complexes for chemical discovery and machine learning", *Molecular Systems Design & Engineering*, **Advance Article**. http://doi.org/10.1039/c9me00069k ***"2020 Emerging Investigators" special issue.***

61. **H. J. Kulik*** "Making machine learning a useful tool in the accelerated discovery of transition metal complexes", *Wiley Interdisciplinary Research: Computational Molecular Science*, just accepted.

60. Z. Yang, F. Liu, A. H. Steeves, and **H. J. Kulik*** "Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases", *The Journal of Physical Chemistry Letters,* **10**, 3779-3787 (2019).

59. S. Faucher, N. Aluru, M. Bazant, D. Blankschtein, A. Brozena, J. Cumings, J. Pedro de Souza, E. Menachem, R. Epsztein, J. Fourkas, R. A. Govind, **H. J. Kulik**, A. Levi, A. Majumdar, C. Martin, M. McEldrew, R. P. Misra, A. Noy, T. A. Pham, M. Reed, E. Schwegler, Z. Siwy, Y. Wang, and M. Strano "Critical Knowledge Gaps in Mass Transport Through Single- Digit Nanopores: A Review and Perspective", *The Journal of Physical Chemistry C*, **123**, 21309-21326 (2019).

58. R. Mehmood, H. W. Qi, A. H. Steeves, and **H. J. Kulik*** "The Protein's Role in Substrate Positioning and Reactivity for Biosynthetic Enzyme Complexes: the Case of SyrB2/SyrB1", *ACS Catalysis*, **9**, 4930-4943 (2019).

57. A. Bajaj, F. Liu, and **H. J. Kulik*** "Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT", *Journal of Chemical Physics*, **150**, 154115 (2019).

56. F. Liu, T. Yang, J. Yang, E. Xu, A. Bajaj, and **H. J. Kulik*** "Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin and Reactivity in Single Atom Catalysis", *Frontiers in Chemistry*, **7**, 219 (2019). ***"Rising Stars" special topic.***

55. H. W. Qi and **H. J. Kulik*** "Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis", *Journal of Chemical Information and Modeling*, **59**, 2199-2211 (2019).

54. C. Duan, J. P. Janet, F. Liu, A. Nandy, and **H. J. Kulik*** "Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models", *Journal of Chemical Theory and Computation*, **15**, 2331-2345 (2019).

53. J. P. Janet, F. Liu, A. Nandy, C. Duan, T. Yang, S. Lin, and **H. J. Kulik*** "Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry", *Inorganic Chemistry*, **58**, 10592-10606 (2019). https://doi.org/10.1021/acs.inorgchem.9b00109 ***Invited Forum Article for Special Issue "Year of the Periodic Table: Emerging Investigators in Inorganic Chemistry"***

52. W. Transue, M. Nava, M. Terban, J. Yang, M. Greenberg, G. Wu, C. Mustoe, P. Kennepohl, J. Owen, S. Billinge, **H. J. Kulik**, and C. Cummins "Anthracene as a Launchpad for a Phosphinidene Sulfide and for Generation of a Phosphorus-Sulfur Material having the Composition P2S, a Vulcanized Red

Phosphorus that is Yellow", *Journal of the American Chemical Society*, **141**, 431-440 (2019).
51. Y.-G. Park, C. H. Sohn, R. Chen, M. McCue, G. Drummond, T. Ku, D. H. Yun, N. Evans, H. Oak, W. Trieu, H. Choi, X. Jin, V. Lilascharoen, J. Wang, M. Truttmann, H. W. Qi, H. Ploegh, T. Golub, S.-C. Chen, M. Frosch, **H. J. Kulik**, B. Lim, and K. Chung "Simultaneous global protection of biomolecules, protein fluorescence, and tissue architecture via polyfunctional crosslinkers", *Nature Biotechnology*, **37**, 73-83 (2019).
50. Z. Yang, R. Mehmood, M. Wang, H. W. Qi, A. H. Steeves, and **H. J. Kulik*** "Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation", *Reaction Chemistry & Engineering*, **4**, 298-315 (2019). ***"2019 Emerging Investigators" special issue.***
49. F. Liu, D. M. Sanchez, **H. J. Kulik**, and T. J. Martínez "Exploiting Graphical Processing Units to Enable Quantum Chemistry Calculation of Large Solvated Molecules with Polarizable Continuum Models", *International Journal of Quantum Chemistry*, **119**, e25760 (2019). ***Special issue on "Advances in Simulating Solvation".***
48. A. Nandy, C. Duan, J. P. Janet, S. Gugler, and **H. J. Kulik*** "Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry", *Industrial & Engineering Chemistry Research,* **57**, 13973-13986 (2018). ***Invited article for Virtual Special Issue "Best Papers of ACS New Orleans 2018".***
47. Q. Zhao and **H. J. Kulik*** "Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots", *Chemistry of Materials,* **30**, 7154-7165 (2018).
46. **H. J. Kulik*** "Large-scale QM/MM free energy simulations of enzyme catalysis reveal the influence of charge transfer", *Physical Chemistry Chemical Physics*, **20**, 20650-20660 (2018).
45. J. Y. Kim and **H. J. Kulik*** "When is Ligand pK_a a Good Descriptor for Catalyst Energetics? In Search of Optimal CO_2 Hydration Catalysts", *The Journal of Physical Chemistry A,* **122**, 4579-4590 (2018).
44. J. P. Janet, L. Chan, and **H. J. Kulik*** "Accelerating Chemical Discovery with Machine Learning: Simulated Evolution of Spin Crossover Complexes with an Artificial Neural Network", *The Journal of Physical Chemistry Letters,* **9**, 1064-1071 (2018). ***Featured in Chemical & Engineering News February 19, 2018, "2018 Year in Chemistry" December 10, 2018, Most read article in JPC Lett in 2018.***
43. Q. Zhao and **H. J. Kulik*** "Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U", *Journal of Chemical Theory and Computation*, **14**, 670-683 (2018). ***ACS Editors' Choice, Most read article in JCTC in 2018.***
42. T. Z. H. Gani and **H. J. Kulik*** "Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane-to-Methanol Conversion by Fe(IV)=O", *ACS Catalysis*, **8**, 975-986 (2018). ***Featured in Comp. Chem. Highlights:*** http://www.compchemhighlights.org/2017/11/understanding-and-breaking-scaling.html.
41. H. W. Qi, M. Karelina, and **H. J. Kulik*** "Quantifying electronic effects in QM and QM/MM biomolecular modeling with the Fukui function", *Acta Physico-Chimica Sinica,* **34**, 81-91 (2018). http://dx.doi.org/10.3866/PKU.WHXB201706303 ***Invited Article for "Concepts in Conceptual Density Functional Theory", ed. Shubin Liu.***
40. A. Bajaj, J. P. Janet, and **H. J. Kulik*** "Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost", *Journal of Chemical Physics*, **147**, 191101 (2017).
39. J. P. Janet and **H. J. Kulik*** "Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure-Property Relationships", *The Journal of Physical Chemistry A,* **121**, 8939-8954 (2017). ***Top 5 most read JPCA in Nov. 2017. Featured in Machine Learning Special Issue.*** http://pubs.acs.org/page/vi/jpc-machine-learning.html
38. T. Z. H. Gani and **H. J. Kulik*** "Unifying Exchange Sensitivity in Transition Metal Spin-State Ordering and Catalysis Through Bond Valence Metrics", *Journal of Chemical Theory and Computation,* **13**, 5443-5457 (2017). ***Top 5 most read JCTC in Nov. 2017.***
37. J. P. Janet and **H. J. Kulik*** "Predicting Electronic Structure Properties of Transition Metal Complexes with Neural Networks", *Chemical Science*, **8**, 5137-5152 (2017).
36. J. P. Janet, T. Z. H. Gani, A. H. Steeves, E. I. Ioannidis, and **H. J. Kulik*** "Leveraging Cheminformatics Strategies for Inorganic Discovery: Applications to Redox Potential Design", *Industrial & Engineering Chemistry Research*, **56**, 4898-4910 (2017). ***Invited Cover Article for "2017 Class of Influential Researchers" Virtual Issue.*** http://pubs.acs.org/page/iecred/vi/influential-researchers-2017

35. J. Y. Kim, A. H. Steeves, and **H. J. Kulik*** "Harnessing Organic Ligand Libraries for First-Principles Inorganic Discovery: Indium Phosphide Quantum Dot Precursor Design Strategies", *Chemistry of Materials*, **29**, 3632-3643 (2017).
34. E. I. Ioannidis and **H. J. Kulik*** "Ligand-Field-Dependent Behavior of meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering", *The Journal of Physical Chemistry A*, **121**, 874-884 (2017).
33. M. Karelina and **H. J. Kulik*** "Systematic Quantum Mechanical Region Determination in QM/MM Simulation", *Journal of Chemical Theory and Computation*, **13**, 563-576 (2017). ***Top 5 most read for JCTC in Feb. 2017***.
32. B. D. Mar and **H. J. Kulik*** "Depolymerization Pathways for Branching Lignin Spirodienone Units Revealed with ab initio Steered Molecular Dynamics", *The Journal of Physical Chemistry A,* **121**, 532-543 (2017).
31. J. P. Janet, Q. Zhao, E. I. Ioannidis, and **H. J. Kulik*** "Density functional theory for modelling large molecular adsorbate-surface interactions: a mini-review and worked example", *Molecular Simulation*, **43**, 327-345 (2017). ***Invited cover article for "Surface Chemistry" special issue.***
30. T. Z. H. Gani and **H. J. Kulik*** "Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U", *Journal of Chemical Theory and Computation,* **12**, 5931-5945 (2016).
29. **H. J. Kulik**, J. Zhang, J. P. Klinman, and T. J. Martínez "How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol O-Methyltransferase" *The Journal of Physical Chemistry B*, **120**, 11381-11394 (2016). ***ACS Editors' Choice, Top 5 most read in 2016 for JPCB.***
28. N. Patra, E. I. Ioannidis, and **H. J. Kulik*** "Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase" *PLOS ONE* **11**, e0161868 (2016).
27. T. Z. H. Gani, E. I. Ioannidis, and **H. J. Kulik*** "Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation" *Chemistry of Materials* **28**, 6207-6218 (2016).
26. Q. Zhao, E. I. Ioannidis, and **H. J. Kulik*** "Global and local curvature in density functional theory" *Journal of Chemical Physics* **145**, 054109 (2016). ***JCP 2016 Editors' Choice.***
25. Q. Zhao, S. S. H. Ng, and **H. J. Kulik*** "Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table" *The Journal of Physical Chemistry C* **120**, 17035-17045 (2016).
24. **H. J. Kulik***, N. Seelam, B. D. Mar, and T. J. Martínez "Adapting DFT+U for the Chemically-Motivated Correction of Minimal Basis Set Incompleteness" *The Journal of Physical Chemistry A* **120**, 5939-5949 (2016).
23. E. I. Ioannidis, T. Z. H. Gani, and **H. J. Kulik*** "molSimplify: a Toolkit for Automating Discovery in Inorganic Chemistry" *Journal of Computational Chemistry* **37**, 2106-2117 (2016).
22. X. Su, **H. J. Kulik**, T. F. Jamison, and T. A. Hatton "Anion-Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces" *Advanced Functional Materials* **26**, 3394-3404 (2016).
21. L. Xie, Q. Zhao, K. F. Jensen, and **H. J. Kulik*** "Direct Observation of Early-Stage Quantum Dot Growth Mechanisms with High-Temperature Ab Initio Molecular Dynamics" *The Journal of Physical Chemistry C* **120**, 2472-2483 (2016).
20. Q. Zhao, L. Xie, and **H. J. Kulik*** "Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature *Ab Initio* Molecular Dynamics" *The Journal of Physical Chemistry C* **119**, 23238–23249 (2015).
19. E. I. Ioannidis and **H. J. Kulik*** "Towards quantifying the role of exact exchange in predictions of transition metal complex properties" *Journal of Chemical Physics* **143**, 034104 (2015).
18. F. Liu, N. Luehr, **H. J. Kulik**, and T. J. Martínez "Quantum Chemistry for Solvated Molecules on Graphical Processing Units (GPUs) Using Polarizable Continuum Models" *Journal of Chemical Theory and Computation* **11**, 3131–3144, (2015).
17. **H. J. Kulik*** "Perspective: Treating electron over-delocalization with the DFT+U method" *Journal of Chemical Physics* **142**, 240901 (2015). ***Invited Cover Perspective***.
16. B. D. Mar, H. W. Qi, F. Liu, and **H. J. Kulik*** "Ab Initio Screening Approach for the Discovery of Lignin Polymer Breaking Pathways." *The Journal of Physical Chemistry A* **119**, 6551-6562 (2015).

15. J. Zhang, **H. J. Kulik**, T. J. Martínez, and J. P. Klinman "Dependence of Active Site Compaction in Catechol-O-Methyltransferase on Residues Both Local and Remote from the Transferred Methyl Group" *Proceedings of the National Academy of Sciences* **112**, 7954–7959 (2015).
14. C.E. Diesendruck, G.I. Peterson, **H.J. Kulik**, J.A. Kaitz, B.D. Mar, P.A. May, S.R. White, T.J. Martínez, A.J. Boydston, and J.S. Moore "Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer" *Nature Chemistry* **6**, 623-628 (2014).
13. **H.J. Kulik**, S.E. Wong, S.E. Baker, C.A. Valdez, J.H. Satcher, Jr., R.D. Aines, and F.C. Lightstone "Developing an approach for first-principles catalyst design: application to carbon capture catalysis" *Acta Crystallographica C* **70**, 123-131 (2014).

PUBLICATIONS PRIOR TO CURRENT APPOINTMENT

12. **H.J. Kulik** and C.L. Drennan "Substrate placement influences reactivity in non-heme Fe(II) halogenases and hydroxylases" *Journal of Biological Chemistry* **288**, 11233-11241 (2013).
11. **H.J. Kulik**, N. Luehr, I.S. Ufimtsev, and T.J. Martínez "*Ab initio* quantum chemistry for protein structures" *The Journal of Physical Chemistry B* **116**, 12501-12509 (2012).
10. **H.J. Kulik**, E. Schwegler, and G. Galli "Probing the structure of salt water under confinement with first-principles molecular dynamics and theoretical X-ray absorption spectroscopy" *The Journal of Physical Chemistry Letters* **3,** 2653-2658 (2012).
9. **H.J. Kulik** and N. Marzari "Accurate potential energy surfaces with a DFT+U(R) approach" *Journal of Chemical Physics* **135***,* 194105 (2011).
8. **H.J. Kulik** and N. Marzari "Transition metal dioxides: a case for the intersite term in Hubbard-model functionals" *Journal of Chemical Physics* **134**, 094103 (2011).
7. U.G.E. Perera, **H.J. Kulik**, V. Iancu, L.G.G.V. Dias da Silva, S.E. Ulloa, N. Marzari, and S.-W. Hla "Charge transfer and spatially extended Kondo resonance in magnetic molecules" *Physical Review Letters* **105**, 106601 (2010).
6. **H.J. Kulik** and N. Marzari "Systematic study of first-row transition metal diatomic molecules: a self-consistent DFT+U approach" *Journal of Chemical Physics* **133**, 114103 (2010).
5. **H.J. Kulik**, N. Marzari, A.A. Correa, D. Prendergast, E. Schwegler and G. Galli "Local effects in the X-ray absorption spectrum of salt water" *The Journal of Physical Chemistry B* **114**, 9594 (2010).
4. **H.J. Kulik**, L.C. Blasiak, N. Marzari, and C.L. Drennan "First-principles study of the non-heme Fe(II) halogenase SyrB2" *Journal of the American Chemical Society* **131**, 14426 (2009).
3. **H.J. Kulik**, A.H. Steeves, and R.W. Field "Ab initio investigation of high multiplicity Σ^+–Σ^+ optical transitions in the spectra of CN and isoelectronic species" *Journal of Molecular Spectroscopy* **258**, 6 (2009).
2. **H.J. Kulik** and N. Marzari "A Self-consistent Hubbard U density-functional theory approach to the addition-elimination reactions of hydrocarbons on bare FeO^+" *Journal of Chemical Physics* **129**, 134314 (2008).
1. **H.J. Kulik**, M. Cococcioni, D.A. Scherlis, and N. Marzari "Density Functional Theory in Transition-Metal Chemistry: A Self-Consistent Hubbard U Approach" *Physical Review Letters* **97**, 103001 (2006).

PROCEEDINGS & BOOK CHAPTERS

5. J. P. Janet and H. J. Kulik "Machine Learning in Chemistry", *ACS In Focus Series*, *submitted*.
4. **H. J. Kulik*** "Modeling mechanochemistry from first principles", *Reviews in Computational Chemistry* **31**, 6 (2018).
3. J.H. Satcher, Jr., S.E. Baker, **H.J. Kulik**, C.A. Valdez, R.L. Krueger, F.C. Lightstone, and R.D. Aines "Modeling, synthesis and characterization of zinc containing carbonic anhydrase active site mimics" *Energy Procedia* **4**, 2090 (2011).
2. S.E. Wong, E.Y. Lau, **H.J. Kulik**, J.H. Satcher, Jr., C.A. Valdez, M. Worsely, F.C. Lightstone, and R.D. Aines "Designing small-molecule catalysts for CO_2 capture" *Energy Procedia* **4**, 817 (2011).
1. **H.J. Kulik** and N. Marzari Chapter entitled "Catalytic activity of transition-metal complexes" in *Fuel Cell Science: Theory, Fundamentals, and Bio-Catalysis*, a Wiley monograph, eds. Jens Norskov and Andrzej Wiezcowski (2010).

INVITED PRESENTATIONS

132. 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada. "TBD". *August 2020.*

131. 2020 Pittsburgh Quantum Institute Annual Symposium, Pitsburgh, PA. "TBD". *April 2020.* **Plenary**

130. Exxon-Mobil, Baytown, Texas. "TBD". *Spring 2020.*

129. South Dakota School of Mines & Technology, Chemical and Biological Engineering, Rapid City, South Dakota. "TBD". *March 2020.*

128. Netherlands' Catalysis and Chemistry Conference (NCCC), Noordwijkerhout, Netherlands. "TBD". *March 2020.* **Keynote**

127. Cornell University, Chemical & Biomolecular Engineering, Ithaca, NY. "TBD". *January 2020.*

126. UC Merced, Chemistry Department, Merced, CA. "TBD". *January 2020.*

125. UC San Diego, Chemistry Department, San Diego, CA. "TBD". *January 2020.*

124. Stanford University, Chemical Engineering, Stanford, CA. "TBD". *January 2020.*

123. Helsinki Winter School on Computational Inorganic Chemistry, Helsinki, Finland. "TBD". (three lectures) *December 2019*.

122. Materials Research Society Fall Meeting, Boston, MA. "Accelerating Discovery in Inorganic Chemistry with Machine Learning". *December 2019*.

121. Clemson University, Chemical & Biomolecular Engineering Department, Clemson, SC. "TBD". *November 2019.*

120. NSF MolSSI workshop "Machine learning and chemistry: challenges on the way forward", University of Maryland, College Park, MD. "TBD". *November 2019.*

119. American Institute of Chemical Engineers National Meeting, Orlando, FL. Area 1A/COMSEF "Spotlights in Thermodynamics and Computational Molecular Science." "Exploiting Electronic Structure and Machine Learning Models for Discovery in Transition Metal Chemistry". *November 2019.*

118. NanoGE Conference, Berlin, Germany. "Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots." *November 2019.*

117. North Dakota State University, Chemistry Department, Fargo, ND. "TBD". *October 2019.*

116. Northwestern University, Catalysis Center, Evanston, IL. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *October 2019.*

115. Northwestern University, Chemical & Biological Engineering Department, Evanston, IL. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *October 2019.*

114. "Interpretable Learning in Physical Sciences" workshop, Institute for Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, CA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *October 2019.*

113. Saville lecture, Princeton University, Chemical and Biological Engineering Department, Princeton, NJ. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools." *October 2019.*

112. Penn State University, Physical Chemistry Seminar, State College, PA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *September 2019.*

111. University of Michigan, Chemical Engineering Department, Ann Arbor, MI. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *September 2019.*

110. University of Pittsburgh, Chemical Engineering Department, Pittsburgh, PA. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *September 2019.*

109. Central Michigan University, Physics Department, Mt. Pleasant, MI. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *September 2019.*

108. 258th American Chemical Society Meeting, San Diego, CA. "AAAS Marion Milligan Mason Awardees" symposium "Predicting properties, learning design rules, and accelerating discovery in inorganic chemistry with computational chemistry" *August 2019.*

107. 258th American Chemical Society Meeting, San Diego, CA. COMP "Elucidating reaction mechanisms with computational and experimental chemistry" symposium "High-throughput first-

principles and machine learning discovery of open-shell transition metal catalyst design rules." *August 2019.*
106. 258th American Chemical Society Meeting, San Diego, CA. BIOL/COMP "Frontiers in interdisciplinary research: new paradigms for integration of theory and experiment" symposium "Understanding the protein's role in substrate positioning and reactivity with simulation: the case of SyrB2/SyrB1" *August 2019.*
105. 258th American Chemical Society Meeting, San Diego, CA. PHYS Division Award Symposium: The Journal of Physical Chemistry Lectureship. "Predicting properties, learning design rules, and accelerating discovery in inorganic chemistry with computational chemistry". *August 2019.*
104. 2019 International Materials Research Society Symposium on AI for Materials, Cancun, Mexico. "Transition metal chemical space exploration: artificial intelligence for first-principles design". *August 2019.*
103. DARPA Accelerated Molecular Discovery PI meeting, Arlington, VA. "Adaptive-focus topological features for machine-learning-driven discovery of 2D coordination polymers." *August 2019.*
102. Energy Frontier Research Center PI meeting, Washington, DC. "Inorganometallic Catalyst Design Center: Theory Driving Next-Generation Catalyst Design." *July 2019.*
101. International Society for Theoretical Chemical Physics X, Tromsø, Norway. "Transition metal catalyst discovery with high-throughput screening and machine learning." *July 2019.*
100. Molecular Kinetics: Sampling, Design and Machine Learning (MolKin2019), Berlin, Germany. "Machine learning models for accelerated discovery in transition metal chemistry." *June 2019*.
99. Eni S.p.A. PI meeting, Milan, Italy. "OFR Calculator." *June 2019.*
98. 102nd Canadian Chemistry Conference and Exhibition, Quebec, Canada. "Designing in the face of uncertainty: exploiting electronic structure and machine learning models for discovery in inorganic chemistry." *June 2019.*
97. Silicon Therapeutics, Boston, MA. "Accelerating discovery with machine learning and high throughput screening." *May 2019.*
96. Emory University, Chemistry Department, Atlanta, GA. "Transition metal chemical space exploration: artificial intelligence for first-principles design." *April 2019.*
95. 257th American Chemical Society Meeting, Orlando, FL. COMP "Machine Learning in Chemistry" "Accelerating discovery in inorganic chemistry with machine learning" *April 2019.*
94. 257th American Chemical Society Meeting, Orlando, FL. COMP "Probing Reactive Intermediates through Chemical Computations" "Discovering and breaking design rules in single-site catalysis with new computational tools" *April 2019*.
93. Washington State University, Chemical Engineering Department, Chemistry Department, and CIRC Joint Colloquium, Pullman, WA. "Designing in the face of uncertainty: exploiting electronic structure and machine learning models for discovery in transition metal chemistry." *March 2019.*
92. MIT Center for Computational Engineering Symposium, Cambridge, MA. "Exploiting electronic structure and machine learning models for discovery in transition metal chemistry." *March 2019.*
91. Hebrew University of Jerusalem, Jerusalem, Israel. "Exploiting electronic structure and machine learning models for discovery in transition metal chemistry." *February 2019.*
90. Tel Aviv University, Tel Aviv, Israel. "Exploiting electronic structure and machine learning models for discovery in transition metal chemistry." *February 2019.*
89. 84th Annual Meeting of the Israel Chemical Society. Tel Aviv, Israel. "Transition metal chemical space exploration: artificial intelligence for first-principles design." *February 2019.* **Keynote**
88. Ben Gurion University of the Negev, Beersheba, Israel. "Designing in the face of uncertainty: exploiting electronic structure and machine learning models for discovery in transition metal chemistry." *February 2019.*
87. Weizmann Institute of Science, Rehovot, Israel. "Recovering exact conditions at semi-local DFT cost to mitigate energy and density errors for transition metal chemistry." *February 2019.*
86. University of Minnesota, Chemistry Department, Minneapolis, MN. "Accelerating discovery in transition metal catalysis with machine learning and computational chemistry." *January 2019.*
85. Exxon-Mobil, Annandale, NJ. "Accelerating Catalyst Discovery with Machine Learning." *January 2019.*

84. AAAS Marion Milligan Mason Award ceremony, Washington D.C. “Chemistry in a computer: a new era for molecular design.” *December 2018.*
83. 1st International Symposium on Chemical Concepts from Theory and Computation (CCTC2018), Changsha City, China. “Systematically improvable QM/MM with concepts from conceptual DFT.” *December 2018.*
82. Special symposium “Interdisciplinary research in the fields of machine learning and computational chemistry” in conjunction with Löwdin lectures, Uppsala University, Sweden. “Advancing inorganic discovery with machine learning.” *November 2018*.
81. Telluride workshop on "Machine Learning and Informatics for Chemistry and Materials", Telluride, CO. “Machine learning in inorganic chemistry.” *October 2018.*
80. "Electronic structure theory in molecular spintronics" workshop, Donostia-San Sebastian, Spain. “Overcoming functional sensitivity in DFT predictions of spin state ordering.” *September 2018.*
79. Resnick Young Investigators Symposium 2018, Caltech, Pasadena, CA. “Accelerating Sustainable Inorganic Design with Machine Learning.” *September 2018.*
78. National Academy of Sciences, Engineering, and Medicine BCST “A Research Agenda for a New Era in Separations Science” Study Meeting. “Accelerating inorganic discovery with machine learning” *August 2018.*
77. 256th American Chemical Society Meeting, Boston, MA. YCC “Artificial Intelligence & The Chemical Enterprise” symposium. “Transition metal chemical space exploration: artificial intelligence for first-principles design” *August 2018*.
76. 256th American Chemical Society Meeting, Boston, MA. COMP “Recent Advances in DFT & TDDFT: Theory & Simulations” symposium. “Recovering exact conditions at semi-local DFT cost to mitigate energy and density errors for transition metal chemistry” *August 2018*.
75. 256th American Chemical Society Meeting, Boston, MA. COMP “Revolutionizing Chemistry with Artificial Intelligence” symposium. “Accelerating inorganic discovery with machine learning and automation” *August 2018.*
74. RIKEN, Tokyo, Japan. “Machine learning and large scale electronic structure for discovery.” *August 2018.*
73. 43rd International Conference on Coordination Chemistry (ICCC2018), Sendai, Japan. “Overcoming functional sensitivity in DFT predictions of spin state ordering.” *August 2018.*
72. Telluride workshop on "Multi-scale quantum mechanical analysis of condensed phase systems: methods and applications", Telluride, CO. “How systematic QM/MM modeling reveals enzymatic rate enhancements.” *July 2018.*
71. IAQMS 16-ICQC Satellite Meeting: Computational Chemistry Meets Artificial Intelligence, EPFL, Lausanne, Switzerland. “Accelerating inorganic discovery with machine learning.” *June 2018.*
70. Eni S.p.A. PI meeting, Milan, Italy. “OFR Calculator.” *June 2018.*
69. Low-scaling and Unconventional Electronic Structure Techniques, Telluride, CO. “Recovering exact conditions of electronic structure theory with semi-local DFT cost.” *June 2018.*
68. ETH Zürich, Theoretical Chemistry Colloquium, Zürich, Switzerland. “Computational strategies for inorganic design.” *May 2018.*
67. DOE CTC/CCS PI meeting, Gaithersburg, MD. “Recovering exact conditions with DFT for transition metal chemistry.” *May 2018.*
66. Pfizer, Cambridge, MA. “New computational tools for inorganic design.” *May 2018.*
65. Universal Display Corporation, Ewing, NJ. “New computational tools for inorganic design.” *April 2018.*
64. University of Washington, Chemistry Department, Seattle, WA. “New computational tools for inorganic molecular design.” *April 2018.*
63. Oklahoma State University, Chemical Engineering Department, Stillwater, OK. “New computational tools for inorganic molecular design.” *March 2018.*
62. 255th American Chemical Society Meeting, New Orleans, LA. “Uncovering the quantum mechanical origins of enzymatic catalysis with systematic QM/MM methods and accelerated, large-scale electronic structure.” *March 2018.*

61. 255th American Chemical Society Meeting, New Orleans, LA. "Choosing the right chemical representation for machine-learning-accelerated discovery and design in transition metal catalysis." *March 2018.*
60. Michigan State University, Chemistry Department, East Lansing, MI. "New computational tools for inorganic molecular and materials design." *February 2018.*
59. University of New Hampshire, Chemistry Department, Durham, NH. "New computational tools for inorganic molecular design." *February 2018.*
58. University of Southern California, Chemical Engineering and Materials Science Department, Los Angeles, CA. "New strategies for inorganic molecular and materials design." *January 2018.*
57. University of California, Irvine, Chemistry Department and CasTL CCI, Irvine, CA. "New strategies for inorganic molecular design with machine learning and automated simulation." *January 2018.*
56. University of Illinois – Urbana-Champaign, Chemical & Biomolecular Engineering Department, Urbana, IL. "New Computational Strategies for Inorganic Catalyst and Materials Design." *December 2017.*
55. Worcester Polytechnic Institute, Chemical Engineering Department, Worcester, MA. "New computational tools for inorganic molecular design." *November 2017.*
54. Boston Regional Inorganic Colloquium at Tufts University, Medford, MA. "New computational tools for inorganic molecular design." *October 2017.*
53. Brown University, Chemistry Department, Providence, RI. "New computational tools for inorganic molecular design." *September 2017.*
52. Corning Incorporated, Corning, NY. "New computational tools for inorganic molecular design." *July 2017.*
51. American Conference on Theoretical Chemistry, Boston, MA. "New computational tools for inorganic molecular design." *July 2017.*
50. MIT School of Engineering Dean's Faculty Lunch, Cambridge, MA. "Designing molecules with quantum mechanics and computation." *May 2017.*
49. MIT Chemical Engineering Visiting Committee, Cambridge, MA. "Computational tools for molecular design." *May 2017.*
48. Robert Bosch LLC, Cambridge, MA. "Predictive computational tools for discovery." *April 2017.*
47. 253rd American Chemical Society Meeting, San Francisco, CA. "New discovery tools for transition metal catalyst design." *April 2017.*
46. 253rd American Chemical Society Meeting, San Francisco, CA. "Understanding and eliminating delocalization error in transition metal chemistry." *April 2017.*
45. IHI Corporation Executive Briefing at MIT ILP, Cambridge, MA. "Computational tools for catalyst discovery." *December 2016.*
44. 4th International Conference on Molecular Simulation, Shanghai, China. "Quantifying electronic effects in enzyme active sites." *October 2016.*
43. EMN Theory Meeting, Las Vegas, NV. "Global and local curvature and delocalization error in DFT." *October 2016.*
42. Materials Theory Division Seminar in Uppsala University, Uppsala, Sweden. "Enabling predictive materials discovery with new computational and theoretical tools." *September 2016.*
41. 252nd American Chemical Society Meeting, Philadelphia, PA. "Automating discovery in inorganic chemistry." *August 2016.*
40. 252nd American Chemical Society Meeting, Philadelphia, PA. "Delocalization error in DFT for computational catalysis." *August 2016.*
39. International Society for Theoretical Chemical Physics IX, Grand Forks, ND. "Quantifying electronic effects in enzyme active sites." *July 2016.*
38. 251st American Chemical Society Meeting, San Diego, CA. "Computational catalysis: functional tuning meets automated discovery." *March 2016.*
37. MITEI Seed Fund Awardees Program Review, Cambridge, MA. "A computational toolbox for catalyst and materials design." *March 2016.*
36. 2015 Psi-k Meeting, San Sebastian, Spain. "Applications of large scale AIMD DFT: growth and structure of quantum dots." *September 2015.*

35. 250th American Chemical Society Meeting, Boston, MA. “Applications and some observations on large-scale DFT.” *August 2015.*
34. MIT Information Systems & Technology All Hands Meeting, Cambridge, MA. “Computational Chemistry Research at MIT.” *May 2015.*
33. AIChE New England Regional Meeting, Cambridge, MA. “Computational modeling, the research universe, and everything.” *March 2015.*
32. ACS Central Eastern Regional Meeting, Pittsburgh, PA. “Efficient DFT-based modeling for catalysis.” *October 2014.*
31. MIT Materials Processing Center Review, Cambridge, MA. “First-principles modeling for catalysis and materials.” *October 2014.*
30. MIT Summer Research Program, Cambridge, MA. “Computational chemistry for biology, catalysis and materials science.” *June 2014.*
29. GTC Express Webinar. “Challenges and advances for DFT on GPUs.” *April 2014.*
28. Center for Nano Materials Colloquium, Argonne National Lab, Argonne, IL. “Efficient and accurate quantum chemistry for biological systems.” *December 2013.*

INVITED PRESENTATIONS PRIOR TO CURRENT APPOINTMENT
27. Cooper Union Colloquium, New York, NY. “Computational chemistry for biology, catalysis, and materials science.” *October 2013.*
26. LLNL CCMS Summer School Colloquia, Livermore, CA. “The Practioner's Guide to Density Functional Theory” and “Life, the Universe and Everything: Efficient and Accurate Quantum Chemistry for Biological Systems.” *June 2013.*
25. CanBIC-4 4th Georgian Bay International Conference on Bioinorganic Chemistry, Parry Sound, Ontario, Canada. “Simulations reveal how substrate placement influences reactivity in non-heme Fe(II) halogenases.” *May 2013.*
24. University of Illinois – Urbana-Champaign, Chemical & Biomolecular Engineering Department, Urbana, IL. “Predictive and fast: new first-principles tools for catalysis.” *March 2013.*
23. Massachusetts Institute of Technology, Chemical Engineering Department, Cambridge, MA. “Predictive and fast: new first-principles tools for catalysis.” *March 2013*.
22. University of Washington, Chemical Engineering Department, Seattle, WA. “Predictive and fast: new first-principles tools for catalysis.” *February 2013.*
21. Columbia University, Chemical Engineering Department, New York, NY. “Predictive and fast: new first-principles tools for catalysis.” *February 2013*.
20. New Jersey Institute of Technology, Chemical, Biological & Pharmaceutical Engineering Department, Newark, NJ. “Predictive and fast: new first-principles tools for materials and catalyst design.” *February 2013*.
19. Yale University, Chemical Biology Institute & Chemical Engineering Department, New Haven, CT. “Predictive and fast: new first-principles tools for biological catalysis.” *February 2013.*
18. Pennsylvania State University, Chemistry Department, University Park, PA. “Predictive and fast: new first-principles tools for biological catalysis.” *February 2013.*
17. Washington University in St. Louis, Mechanical Engineering & Materials Science Department, St. Louis, MO. “Predictive and fast: new first-principles tools for materials and catalyst design.” *February 2013*.
16. University of Minnesota, Chemical Engineering & Materials Science Department, Minneapolis, MN. “Predictive and fast: new first-principles tools for materials and catalyst design.” *February 2013*.
15. Johns Hopkins University, Materials Science & Engineering Department, Baltimore, MD. “Predictive and fast: new first-principles tools for materials and catalyst design.” *January 2013*.
14. Rensselaer Polytechnic Institute, Chemical & Biological Engineering Department, Troy, NY. “Predictive and fast: new first-principles tools for catalysis.” *January 2013*.
13. Carnegie Mellon University, Materials Science & Engineering and Chemical Engineering Departments, Pittsburgh, PA. “Predictive and fast: new first-principles tools for materials and catalyst design.” *January 2013.*
12. University of Delaware, Chemical Engineering Department, Newark, DE. “Predictive and fast: new

first-principles tools for catalysis." *January 2013*.
11. University of California Davis, Chemical Engineering & Materials Science Department, Davis, CA. "Predictive and fast: new first-principles tools for materials and catalyst design." *December 2012.*
10. University of Rochester, Chemical Engineering Department, Rochester NY. "Predictive and fast: new first-principles tools for materials and catalyst design." *December 2012*.
9. Boston University, Chemistry Department, Boston, MA. "Predictive and fast: new first-principles tools for materials and catalyst design." *November 2012*.
8. Theory seminar, University of North Carolina, Chemistry Department, Chapel Hill, NC. "Recent developments in Hubbard-augmented DFT." *October 2012.*
7. Theory seminar, Duke University, Chemistry Department, Durham, NC. "Predictive enzyme catalysis with quantum chemistry on GPUs." *October 2012.*
6. Theory seminar, Wake Forest University, Physics Department, Winston-Salem, NC. "Recent developments in Hubbard-augmented DFT." *October 2012.*
5. University of Illinois – Chicago, Chemical Engineering Department, Chicago, IL. "Predictive and fast: new first-principles tools for transition-metal catalysis." April 2012.
4. University at Buffalo, Chemical Engineering Department, Buffalo, NY. "Predictive and fast: new first-principles tools for transition-metal catalysis." *March 2012*.
3. Theory seminar, University of Pennsylvania, Chemistry Department, Philadelphia, PA. "Recent developments in Hubbard-augmented DFT+U." *February 2012*.
2. Drexel University, Chemical Engineering Department, Philadelphia, PA. "Predictive and fast: new first-principles tools for transition-metal catalysis." *February 2012.*
1. Rutgers University, Chemistry Department, Newark, NJ. "Predictive and fast: new first-principles tools for transition-metal catalysis." *January 2012*.

SELECTED CONTRIBUTED PRESENTATIONS
11. 26th North American Catalysis Society Meeting (NAM), Chicago, IL. "Understanding spin-active-site-activity relationships in open-shell SACs with first principles modeling." *June 2019.*
10. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany. "Recovering the flat plane condition in electronic structure theory at semi-local density functional theory cost." *August 2017.*
9. American Physical Society March Meeting, New Orleans, LA. "New discovery tools for molecular materials design." *March 2017.*
8. American Institute of Chemical Engineers National Meeting, San Francisco, CA. "Global and local curvature in density functional theory and delocalization errors." *November 2016.*
7. American Chemical Society Meeting, Boston, MA. "Substrate positioning in catalysis: catechol *O*-methyltransferase." YI Symposium. *August 2015.*
6. American Institute of Chemical Engineers National Meeting, Atlanta, GA. "+U for small basis sets." *November 2014.*
5. American Institute of Chemical Engineers National Meeting, Atlanta, GA. "Lignin depolymerization dynamics." *November 2014.*
4. American Chemical Society Meeting, San Francisco, CA "Advances and challenges for DFT on GPUs." *March 2014.*
3. American Physical Society March Meeting, Denver, CO "Challenges and advances for DFT on GPUs." *March 2014.*
2. American Institute of Chemical Engineers National Meeting, San Francisco, CA. "Tuning reaction pathways for first-principles catalyst design." *November 2013.*
1. American Institute of Chemical Engineers National Meeting, San Francisco, CA. "Not just a fitting parameter: the untold story of DFT+U." *November 2013.*

GRANTS RECEIVED ($6.01M)
External funding ($5.48M)
Exxon Mobil, 11/1/19-10/31/20 $171,544
Bio-inspired computational catalyst design

National Science Foundation CAREER, 6/1/19-5/31/24 $593,678
CAREER: Revealing spin-state-dependent reactivity in open-shell single atom catalysts with systematically-improvable computational tools
AAAS Marion Milligan Mason Award*, 12/13/18-12/12/20 $50,000
Navigating Transition Metal Chemical Space: Artificial Intelligence for First-Principles Design
Department of Energy, 8/1/18-7/31/22 $440,000
Inorganometallic Catalyst Design Center (ICDC)
(Laura Gagliardi, U. Minnesota PI; Kulik co-PI)
Department of Energy, 9/1/18-8/31/22 $480,000
The Center for Enhanced Nanofluidic Transport (CENT)
(Michael S. Strano, MIT PI; Kulik co-PI)
DARPA Young Faculty Award, 6/30/18-6/30/20 $500,000
Adaptive-focus topological features for machine-learning-driven discovery of 2D coordination polymers
Office of Naval Research Young Investigator Program, 6/1/18-5/31/21 $510,000
Adaptive-Resolution Chemical Discovery Strategies for Precise and Fast Computer-Aided Transition Metal Complex Design
Office of Naval Research, 9/1/17-8/31/20 $450,000
Computer-aided design of functional transition metal complexes
Department of Energy, 9/1/17-8/31/20 $292,725
Simultaneous mitigation of density and energy errors in approximate DFT for transition metal chemistry
National Science Foundation, 8/1/17-7/31/20 $317,245
Enabling high-throughput computational discovery of stable and active single-site oxidation catalysts
Eni S.p.A, 6/1/17-5/31/20 $500,000
OFR calculator
Robert Bosch, LLC, 5/1/17-4/30/19 $250,000
Developing new methods for the accurate ionization potential calculation in polymer electrolyte modeling for energy storage
National Science Foundation, 9/1/14-2/15/19 $433,333
SNM: Knowledge-based continuous and scalable manufacture of quantum dots
(Klavs F Jensen, MIT PI; Kulik co-PI w/ Moungi Bawendi, MIT)
Burroughs Wellcome Fund*, 7/1/12-6/30/21 $500,000
Deciphering the role of the protein scaffold in enzyme catalysis with fast and accurate computation

Internal funding ($529k)

NIH Center for Environmental Health Sciences Pilot Grant 9/1/17-8/31/18 $39,000
Quantum mechanical contributions to methyltransferase inhibition
MIT-RSC NEC Corporation Grant* 9/1/17-8/31/18 $75,000
New computational tools for unveiling electronic contributions to rate enhancements in methyltransferases
MIT Energy Initiative Seed Grant 6/1/17-5/31/19 $150,000
Next generation quantitative structure property relationships for lubricants from machine learning and advanced simulation
(Kulik PI; w/ co-PI: Youssef Marzouk, MIT)
MISTI-Israel Ben Gurion Seed Grant* 1/1/17-8/31/18 $19,525
New Tools for Predictive Computational Catalysis Through Collaboration
(Kulik PI; w/ co-PI: Sebastian Kozuch, Ben Gurion University of the Negev)
Ibn Khaldun Faculty Award* 9/1/16-8/31/17 $20,000
Theoretical prediction of protein-substrate interactions
MIT-RSC Reed Grant* 9/1/14-8/31/15 $75,000
Screening for catalyzable bonds in highly heterogeneous feedstocks

MIT Energy Initiative Seed Grant 4/1/14-9/30/15 $150,000
New computational tools for direct methane-to-methanol catalyst design

*All funds are only portion allocated to Kulik, amount includes indirect costs unless indicated by *, in which case funds are not subject to overhead. Select industrial sponsors are not named out of intellectual property concerns.*

Computing proposals (over 4.4 M CPU/GPU hours)

NSF XSEDE renewal 4/1/19-3/31/20
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
382k SUs SDSC Comet, 15k SUs on Bridges GPU, 72k SUs on Comet GPU (est. value $28,830.39)

NSF XSEDE renewal 10/1/17-3/31/19
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
1.1M SUs SDSC Comet, 100k SUs on XStream (est. value: $51,276.04)

NSF XSEDE renewal 10/1/16-9/30/17
Catalytic Mechanism Discovery with First-Principles Simulation: From Enzymes to Heterogeneous Catalysis
617k SUs SDSC Comet, 200k SUs on Maverick, 68k SUs on XStream (est. value: $25,764.59)

NSF XSEDE renewal 10/1/15-9/30/16
Identifying contributions to the free-energy landscape of enzyme-substrate complex dynamics: the case of Catechol O-Methyltransferase
915k SUs SDSC Comet, 915k SUs Stampede, 100k SUs on Maverick (est. value: $63,874.31)

NSF XSEDE 7/1/14-6/30/15
Probing the structure of early-stage reactive intermediates in the growth of Indium Phosphide Quantum Dots with collisionally-accelerated MD and path-based sampling
250k SUs on Maverick (est. value: $8,587.37)

Argonne CNM 4/29/14-5/28/15
Indium Phosphide Growth at Early Stage from Precursors Molecules: A collisionally-accelerated ab initio Molecular Dynamics Study
170k CPU hours

STUDENTS SUPERVISED

Graduate Students

2018-	Naveen Arunachalam, ChemE	
2018-	Vyshnavi Vennelakanti, Chemistry	
2018-	Daniel Harper, Chemistry	
2018-	Mengyi Wang, DMSE	
2018	Stefan Gugler, ETH Zürich Chemistry	(M.S. ’18; now Ph.D. ETH Zürich)
2017-	Chenru Duan, Chemistry	
2017-	Aditya Nandy, Chemistry	
2016-	Akash Bajaj, DMSE	
2016-	Rimsha Mehmood, Chemistry	
2015-	Terry Z. H. Gani, ChemE	
2015-	Jon Paul Janet, ChemE	
2015-17	Yusu Liu, DMSE	(Ph.D. ’19)
2014-19	Helena W. Qi, Chemistry	(Ph.D. ’19; Senior Scientist, Pfizer)
2014-18	Qing Zhao, MechE	(Ph.D. ’18; PD Carter Group, Princeton)
2014-16	Lisi Xie, ChemE	(Ph.D. ‘16; Lam Research)
2013-16	Efthymios I. Ioannidis, ChemE	(Ph.D. ‘16; MIT MBA ’18, Consultant)
2013-15	Natasha Seelam, ChemE	(Ph.D. student, BE MIT)

Undergraduate, High School Students

2018-	Natalia Haljasz via Harvard	
2018-19	Ava Waggett, MIT 10 UROP	(MIT S.B. ’19)
2018	Eve Xu*, Wellesley exchange	(B.S. Smith, ’20 expected)

2018-9	Sahasrajit Ramesh, Oxford	(Oxford M.S. Thesis, ’19)
2018	Sean Lin*, HS via Troy H.S.	(Troy H.S., ’19, now: UC Berkeley UG)
2017-18	June Yang, MIT 10 UROP	(MIT S.B. ’20)
2018	Demar Edwards, MIT 10 UROP	(MIT S.B. ’21)
2017	Yu Jin, UG via Peking U.	(Peking U. UG ’18)
2017	Lydia Chan*, HS via Troy H.S.	(Troy H.S. ’18, now: Stanford UG)
2016-17	Maria Karelina*, MIT 6-7 UROP	(S.B. ’17, now: Stanford Ph.D.)
2016	Naomi Bright, MIT 10 UROP	(MIT S.B. 10 ‘19)
2015-16	Kristen Eller, MIT 10 UROP	(S.B. ’16, now: CU Boulder Ph.D.)
2015	Shouping Chen, UG via Tsinghua	(UC Berkeley Ph.D.)
2015	Jose Salcedo Perez, MIT-MSRP	(MIT Ph.D.)
2015	Stanley Ng*, Phillips Academy	(Imperial College UG)
2014	Zach Giaccone, UG via Holy Cross	
2014	John La, MIT 10 UROP	(MIT S.B. ‘18)

** indicates author on a published or in preparation Kulik group manuscript*

TEACHING

10.37 “Chemical kinetics & reactor design” undergraduate chemical engineering core course co-instructor (2017-)
2017 evaluations: *6.0/7.0 instructor, 5.7/7.0 course.*

10.637/10.437/5.697/5.698 “Quantum Chemical Simulation”, renamed “Computational Chemistry” in 2017. Course designer for graduate/advanced undergraduate elective with 16 lectures, 8 hands-on labs using XSEDE resources. Enrollment is 30-40 students across engineering and science, crosslisted in chemistry and at Harvard University. (‘14-)
2017 evaluations: *6.4/7.0 instructor, 6.3/7.0 course.*

10.65 “Chemical reactor engineering” graduate chemical engineering core course co-instructor (‘14-16)

BIOS 203 “Introduction to Atomistic Simulation for Biochemical Applications” (Stanford University). Course designer and primary instructor for (2 hr lab / 1 hr lecture) course. Awarded $10k seed grant for course development (2013).

PROFESSIONAL AFFILIATIONS

American Chemical Society (2005-Present)
American Physical Society (2006-Present)
American Institute of Chemical Engineers (2012-Present)
Israel Chemical Society, Honorary lifetime member (2019-Present)

CONSULTING

Universal Display Corporation, Ewing, NJ. 2018-

SERVICE

External

Outreach

Faculty mentor and speaker for MIT Summer Research Program (2015)
Faculty speaker for women in STEM at AIChE Regional meeting (2015)
MIT ACCESS weekend for underrepresented minorities in STEM facilitator (2015-)
Web tutorials: Created monthly web tutorials for quantum chemistry, quantum-ESPRESSO, TeraChem, molSimplify that have been used by researchers (avg. unique visitors per month: 2,000) in over 110 countries worldwide and all 50 states (2011-)
Slideshow instruction: Course materials for MIT 10.637, DFT+U instruction, and GPU-accelerated quantum chemistry have been cumulatively viewed over 30,000 times.

Conference organization

AIChE Annual Meeting session chair
-“Applications of DFT+X in Catalysis” session co-chair (2013)
-“Applications of DFT+X in Catalysis” session co-chair (2014)

-"Applications of DFT+X in Catalysis" session chair (2015)
-"New Developments in Computational Catalysis" session co-chair (2016)
-"New Developments in Computational Catalysis" session chair (2017)
-"Computational Catalysis" session co-chair (2018)
-"Software Engineering in and for the Molecular Sciences"
CoMSEF session co-chair (2018)
-Data Science Topical co-chair (2019)
North American Catalysis Society Meeting abstract review (2017)
American Chemical Society presider CATL (Spring 2018), COMP (Summer 2018), session organizer "Data Science for Catalysis" Spring 2019
"Coding Solvation" NSF-MolSSI-funded workshop in Livorno, Italy co-organizer (2017)
New England Catalysis Society Regional Meeting co-organizer (2018)

Thesis Defense Opponent for Iulia Brumboiu, Uppsala University.

Proposal review for NSF CAREER (2014), NSF DMREF (2014), NSF CBET ad hoc/virtual (2015, 2018), NSF SBIR (2017), NSF CHE ad hoc/virtual (2018), ACS PRF (2015-2017), Kentucky Science and Engineering Foundation (2015, 2016), Brookhaven CFN (computer proposals, 2015-), DOE INCITE (computer proposals, 2016, 2017), Research Corporation Cottrell Scholars (2016), DOE BES (2015-2018), DOE BES CCS (2017, 2018), and the Netherlands Organisation for Scientific Research (2017).

Journal review for the *Journal of the American Chemical Society, Journal of Catalysis, Journal of Chemical Physics*, *The Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Inorganic Chemistry*, *Journal of Theoretical Biology, Molecular Simulation, Chemical Physics Letters, Nature Materials*, *Nano Letters*, *Applied Catalysis B, Chemical Science, Journal of Computational Chemistry, Journal of Chemical Theory and Computation*, *Crystal Growth & Design, Journal of Physical Chemistry Letters, Physical Review B, Industrial & Engineering Chemistry Research*, *Nature Catalysis*, *Journal of Molecular Graphics and Modeling, Molecular Systems Design & Engineering, Reaction Chemistry & Engineering, Physical Review Letters, Physical Review X, Angewandte Chemie, Science Advances, Science, and Journal of Catalysis*.

International Journal of Quantum Chemistry Editorial Board member.

At MIT

Thesis Committees 18 students across Civil Engineering, Chemistry, Chemical Engineering, and Mechanical Engineering (2013-)
ChemE undergraduate academic advisor (2014-)
ChemE graduate admissions (2014-)
ChemE department head search committee (2015)
ChemE graduate academic advisor (2016-)
Computational Science and Engineering Liaison on behalf of ChemE (2016-)
ChemE Seminar series coordinator (2016-)
Institute-wide Center for Computational Engineering working group (2018)
ChemE undergraduate curriculum revitalization (10.37) (2018-)

RECENT PRESS

"Uncertainty metric builds confidence in machine learned-chemistry"
Chemistry World, 7/25/19
https://www.chemistryworld.com/news/uncertainty-metric-builds-confidence-in-machine-learned-chemistry/3010759.article

"Meet the 2019 Recipients of *The Journal of Physical Chemistry* and PHYS Division Lectureship Awards"
ACS Axial, 7/2/19
https://axial.acs.org/2019/07/02/meet-the-2019-recipients-of-the-journal-of-physical-chemistry-and-phys-division-lectureship-awards/

"Finding novel materials for practical devices"
MIT Energy Futures, 5/15/19, *Also featured in MIT News*
http://mitener.gy/CF0K50ulGhF

"Marion Milligan Mason Awards"
Angewandte Chemie, 1/25/19

https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201900118

"Mason awardees display benefits of outsider perspectives"
Science, 1/25/19
http://science.sciencemag.org/content/363/6425/357

"Machine Learning Marched Forward" (part of *C&EN's 2018 Year in Chemistry*)
Chemical & Engineering News, 12/17/18
https://pubs.acs.org/doi/full/10.1021/cen-09649-cover2

"Five Women Chemists Awarded the 2019 Mason Award" American Association for the Advancement of Sciences, 10/26/18
https://www.aaas.org/news/five-women-chemists-awarded-2019-mason-award

"Is machine learning overhyped?" *Chemical & Engineering News*, 8/27/18
https://cen.acs.org/physical-chemistry/computational-chemistry/machine-learning-overhyped/96/i34

"COMP names 2018 winners" *Chemical & Engineering News*, 4/9/18
https://cen.acs.org/people/awards/COMP-names-2018-winners/96/i15

"Best and Brightest: ONR, 2018 Young Investigator Program" Office of Naval Research, 2/21/18
https://www.onr.navy.mil/Media-Center/Press-Releases/2018/ONR-2018-YIP-Awards

"Machine learning identifies potential inorganic complexes for switches and sensors"
Chemical & Engineering News, 2/19/18
https://cen.acs.org/articles/96/i8/Machine-learning-identifies-potential-inorganic.html

"Investing in U.S. Universities: Bosch hosts energy research symposium, awards energy research grants to scholars from top universities" Businesswire.com, 10/23/17
http://www.businesswire.com/news/home/20171023005971/en/Investing-U.S.-Universities

"Viewpoints on the 2017 American Conference on Theoretical Chemistry" *The Journal of Physical Chemistry A,* 10/19/17
http://pubs.acs.org/doi/10.1021/acs.jpca.7b09624

"Announcing the 2017 Class of Influential Researchers" *I & EC Research*, 9/27/17
http://pubs.acs.org/doi/full/10.1021/acs.iecr.7b03758

"Heather Kulik: Innovative modeling for chemical discovery" MIT News, 9/15/17
http://news.mit.edu/2017/heather-kulik-innovative-modeling-for-chemical-discovery-0915

"MIT Energy Initiative awards 10 seed fund grants for early-stage energy research" MIT News, 5/2/17
http://news.mit.edu/2017/mit-energy-initiative-awards-seed-fund-grants-for-early-stage-energy-research-0502
(Also featured in MIT Energy Initiative's *Energy Futures* magazine).

"Understanding Electronic Structure; Making Better Materials" MIT ILP Tech Insider, 8/1/16
http://ilp.mit.edu/newsstory.jsp?id=22124