77 Massachusetts Ave
Room 66-464
Cambridge, MA 02139

HEATHER J. KULIK

ph:(617)-253-4584
e: hjkulik@mit.edu
w: http://hjkgrp.mit.edu

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

07/2021 -	Associate Professor (with Tenure)
07/2019 - 06/2021	Associate Professor
11/2013 - 06/2019	Assistant Professor

Department of Chemistry, MIT

07/2022 -	Associate Professor (with Tenure)

HONORS AND AWARDS

2022	Distinguished Romberg Guest Professorship, University of Heidelberg Kwang-Yu and Lee-Chien Wang Fellowship Lecture, Department of Chemical Engineering, University of Rochester
2021	Alfred P. Sloan Research Fellowship in Chemistry *Molecular Systems Design & Engineering* (2020) Outstanding Early-Career Paper Award
2020	DARPA Director's Fellowship *Molecular Systems Design & Engineering* Emerging Investigator
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 *Inorganic Chemistry* Emerging Investigator *Frontiers In Chemistry* Rising Star Prize *Reaction Chemistry & Engineering* Emerging Investigator
2018	DARPA Young Faculty Award Office of Naval Research Young Investigator Award ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry (ACS COMP Division) Resnick Young Investigator Symposium Speaker *Journal of Chemical Theory and Computation* ACS Editors' Choice
2017	ACS *Industrial & Engineering Chemistry Research* "Class of Influential Researchers" *Journal of Chemical Physics* 2016 Editors' Choice
2016	*Journal of Physical Chemistry* ACS Editors' Choice
2012	Burroughs Wellcome Fund Career Award at the Scientific Interface
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	National Science Foundation Graduate Research Fellow 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 United States Presidential Scholar
Times Academic All-Star in Mathematics
Association for Women in Science Scholar
Robert Byrd Scholar
Elks National Foundation Most Valuable Student

PUBLICATIONS (corresponding author indicated by *).

131. A. Nandy, S. Yue, C. Oh, C. Duan, G. Terrones, Y. G. Chung, and **H. J. Kulik*** "A Database of Ultrastable MOFs Reassembled from Stable Fragments with Machine Learning Models", *in preparation.*

130. Y. Cho, A. Nandy, C. Duan, and **H. J. Kulik*** "DFT-based Multireference Diagnostics in the Solid State: Application to Metal-organic Frameworks", *submitted.* https://doi.org/10.26434/chemrxiv-2022-c129n

129. N. Arunachalam, S. Gugler, M. G. Taylor, C. Duan, A. Nandy, J. P. Janet, R. Meyer, J. Oldenstaedt, D. B. K. Chu, and **H. J. Kulik*** "Ligand additivity relationships enable efficient exploration of transition metal chemical space", *submitted.* https://arxiv.org/abs/2209.05412

128. C. Duan, A. Nandy, G. Terrones, D. W. Kastner, and **H. J. Kulik*** "Active Learning Exploration of Transition Metal Complexes to Discover Method-Insensitive and Synthetically Accessible Chromophores", *submitted.* http://arxiv.org/abs/2208.05444

127. C. Duan, A. Nandy, R. Meyer, N. Arunachalam, and **H. J. Kulik*** "A Transferable Recommender Approach for Selecting the Best Density Functional Approximations in Chemical Discovery", *submitted.* https://arxiv.org/abs/2207.10747

126. C. Y. Kim, A. J. Mitchell, D. W. Kastner, C. E. Albright, M. Gutierrez, C. M. Glinkerman, **H. J. Kulik**, and J-K Weng*, "Emergence of a proton exchange-based isomerization and lactonization mechanism in the plant coumarin synthase COSY", *submitted.* https://www.biorxiv.org/content/10.1101/2022.07.19.500703v1

125. X. He, T. Yang, A. Iliescu, M. Arguilla, T. Chen, **H. J. Kulik**, and M. Dinca* "Reversible O–O Bond Scission and O2 evolution at MOF-supported Tetramanganese Clusters", *submitted.* https://doi.org/10.26434/chemrxiv-2022-14g3n

124. W.-S. Lee, Y. Cho, E. R. Powers, W. Paritmongkol, T. Sakurada, **H. J. Kulik**, and W. A. Tisdale* "Self-Trapped Excitons in 2D Silver Phenylchalcogenolates", *submitted.*

123. S. Lee, I. Kevlishvili, **H. J. Kulik**, H.-T. Kim, Y. G. Chung*, and D.-Y. Koh* "Highly Efficient Bromine Capture and Storage using N-containing Porous Organic Cages", *submitted.*

122. N. Aluru, F. Aydin, M. Z. Bazant, D. Blankschtein, A. H. Brozena, J. Pedro de Souza, M. Elimelech, S. Faucher, J. T. Forkas, V. B. Koman, M. Kuehne, **H. J. Kulik**, H.-K. Li, Z. Li, A. Majumdar, J. Martis, R. P. Misra, A. Noy, T. A. Pham, H. Qu, A. Rayabharam, M. A. Reed, C. L. Ritt, Z. Siwy, M. S. Strano, Y. Wang, C. Zhan, Z. Zhang "Fluids and Electrolytes Under Confinement in Single-Digit Nanopores", *submitted.*

121. A. H. Steeves and **H. J. Kulik*** "Insights into the stability of engineered mini-proteins from their dynamic electronic properties", *Electronic Structure*, **4**, 034005 (2022).

120. N. H. Chan, C. Gomez, V. Vennelakanti, Q. Du, **H. J. Kulik***, and J. C. Lewis* "Non-native Anionic Ligand Binding and Reactivity in Engineered Variants of the Fe(II)- and α-Ketoglutarate-Dependent Oxygenase, SadA", *Inorganic Chemistry,* **61**, 14477-14485 (2022).

119. C. Duan, A. J. Ladera, J. C.-L. Liu, M. G. Taylor, I. R. Ariyarathna, and **H. J. Kulik*** "Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character Across Known Transition Metal Complex Ligands", *Journal of Chemical Theory and Computation*, **18**, 4836-4845 (2022).

118. A. Nandy, H. Adamji, D. W. Kastner, V. Vennelakanti, A. Nazemi, M. Liu, and **H. J. Kulik*** "Using Computational Chemistry to Reveal Nature's Blueprints for Single-Site Catalysis of C–H Activation", *ACS Catalysis,* **12**, 9281-9306 (2022).

117. C. Brown, D. Lundberg, J. Lamb, I. Kevlishvili, D. Kleinschmidt, Y. Alfaraj, **H. J. Kulik**, M. Ottaviani, N. Oldenhuis, and J. Johnson* "Endohedrally Functionalized Metal–Organic Cage-Cross-Linked Polymer Gels as Modular Heterogeneous Catalysts", *Journal of the American Chemical Society*, **144**, 13276-13284 (2022).

116. C. Duan, A. Nandy, H. Adamji, Y. Roman-Leshkov, and **H. J. Kulik*** "Machine learning models predict calculation outcomes with the transferability necessary for computational catalysis", *Journal of Chemical Theory and Computation,* **18**, 4282-4292 (2022).

115. B. Fu, A. Nazemi, B. J. Levin, Z. Yang, **H. J. Kulik**, and E. P. Balskus* "Mechanistic Studies of a Skatole-Forming Glycyl Radical Enzyme Suggest Reaction Initiation via Hydrogen Atom Transfer", *Journal of the American Chemical Society*, **144**, 11110-11119 (2022).

114. Y. Cytter, A. Nandy, A. Bajaj, and **H. J. Kulik*** "Ligand Additivity and Divergent Trends in Two Types of Delocalization Errors from Approximate Density Functional Theory", *The Journal of Physical Chemistry Letters*, **13**, 4549-

4555 (2022).
113. A. Nazemi, A. H. Steeves, D. W. Kastner, and **H. J. Kulik*** "Influence of the Greater Protein Environment on the Electrostatic Potential in Metalloenzyme Active Sites: The Case of Formate Dehydrogenase", *The Journal of Physical Chemistry B*, **126**, 4069-4079 (2022). **Cover article**
112. I. R. Ariyarathna, C. Duan, and **H. J. Kulik*** "Understanding the chemical bonding of ground and excited states of HfO and HfB with correlated wavefunction theory and density functional approximations", *Journal of Chemical Physics*, **156**, 184113 (2022).
111. A. Bajaj, C. Duan, A. Nandy, M. G. Taylor, and **H. J. Kulik*** "Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry", *Journal of Chemical Physics*, **156**, 184112 (2022).
110. A. Nandy, C. Duan, C. Goffinet, and **H. J. Kulik*** "New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts", *JACS Au,* **2**, 1200-1213 (2022).
109. Z. Yang, N. Hajlasz, and **H. J. Kulik*** "Computational Modeling of Conformer Stability in Benenodin-1, A Thermally-Actuated Lasso Peptide Switch", *The Journal of Physical Chemistry B*, **126**, 3398-3406 (2022).
108. V. Vennelakanti, R. Mehmood, and **H. J. Kulik*** "Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis", *ACS Catalysis*, **12**, 5489-5501 (2022).
107. C. Duan, D. B. K. Chu, A. Nandy, and **H. J. Kulik*** "Detection of multi-reference character imbalances enables a transfer learning approach for chemical discovery with coupled cluster accuracy at DFT cost", *Chemical Science,* **13**, 4962-4971 (2022).
106. A. del rio Flores, D. W. Kastner, Y. Du, M. Narayanamoorthy, Y. Shen, W. Cai, V. Vennelakanti, N. A. Zill, L. B. Dell, **H. J. Kulik***, and W. Zhang* "Probing the mechanism of isonitrile formation by a non-heme iron(II)-dependent oxidase/decarboxylase", *Journal of the American Chemical Society*, **144**, 5893-5901 (2022). **Cover article**
105. **H. J. Kulik**, T. Hammerschmidt, J. Schmidt, S. Botti, M. A. L. Marques, M. Boley, M. Scheffler, M. Todorovic, P. Rinke, C. Oses, A. Smolyanyuk, S. Curtarolo, S. Pilati, A. Tkatchenko, A. P. Bartok, S. Manzhos, M. Ihara, T. Carrington, J. Behler, O. Isayev, M. Veit, A. Grisafi, J. Nigam, M. Ceriotti, K. T. Schütt, J. Westermayr, M. Gastegger, R. J. Maurer, B. Kalita, K. Burke, R. Nagai, R. Akashi, O. Sugino, J. Hermann, F. Noe, C. Draxl, M. Kuban, S. Rigamonti, M. Scheidgen, M. Esters, D. Hicks, C. Toher, P. V. Balachandran, I. Tamblyn, S. Whitelam, C. Bellinger, and L. M. Ghiringhelli "Roadmap on Machine Learning in Electronic Structure", *Electronic Structure*, **4**, 023004 (2022). **Roadmap**
104. D. R. Harper[#], A. Nandy[#], N. Arunachalam, C. Duan, J. P. Janet, and **H. J. Kulik*** "Representations and strategies for transferable machine learning improve model performance in chemical discovery", *Journal of Chemical Physics*, **156**, 074101 (2022).
103. A. Nandy[#], G. Terrones[#], N. Arunachalam, C. Duan, D. W. Kastner, and **H. J. Kulik*** "MOFSimplify, machine learning models with extracted stability data of three thousand metal-organic frameworks", *Scientific Data*, **9**, 74 (2022).
102. A. Bajaj and **H. J. Kulik*** "Eliminating Delocalization Error to Improve Heterogeneous Catalysis Predictions with Molecular DFT+U", *Journal of Chemical Theory and Computation,* **18**, 1142-1155 (2022).
101. H. Jia, A. Nandy, M. Liu, and **H. J. Kulik*** "Modeling the roles of rigidity and dopants in single-atom methane-to-methanol catalysts", *Journal of Materials Chemistry A*, **10**, 6193-6203 (2022).
100. D. R. Harper and **H. J. Kulik*** "Computational Scaling Relationships Predict Experimental Activity and Rate Limiting Behavior in Homogenous Water Oxidation", *Inorganic Chemistry*, **61**, 2186-2197 (2022).
99. Y. Zeng, P. Gordiichuk, T. Ichihara, G. Zhang, E. Sandoz-Rosado, E. D. Wetzel, J. Tresback, J. Yang, Z. Yang, D. Kozawa, M. Kuehne, P. Liu, A. T. Liu, J. Yang, **H. J. Kulik**, and M. S. Strano "Irreversible synthesis of an ultrastrong two-dimensional polymeric material ", *Nature*, **602**, 91-95 (2022).
98. C. L. Ritt, M. Liu, T. A. Pham, R. Epsztein, **H. J. Kulik***, and M. Elimelech* "Machine learning reveals key ion selectivity mechanisms in polymeric membranes with sub-nanometer pores", *Science Advances*, **8**, eabl5771 (2022).
97. A. Nandy[#], C. Duan[#], and **H. J. Kulik*** "Audacity of huge: overcoming challenges of data scarcity and data quality for machine learning in computational materials discovery", *Current Opinion in Chemical Engineering*, **36**, 100778 (2022).
96. M. Liu, A. Nazemi, M. G. Taylor, A. Nandy, C. Duan, A. H. Steeves, and **H. J. Kulik*** "Large-scale Screening Reveals Geometric Structure Matters More than Electronic Structure in Bioinspired Catalyst Design of Formate Dehydrogenase Mimics", *ACS Catalysis*, **12**, 383-396 (2022).
95. D. G. A. Smith, A. T. Lolinco, Z. L. Glick, J. Lee, A. Alenaizan, T. A. Barnes, C. H. Borca, R. Di Remigio, D. L. Dotson, S. Ehlert, A. G. Heide, H. Kruse, S. J. R. Lee, J. P. Misiewicz, L. N. Naden, F. Ramezanghorbani, M. Scheurer, J. B. Schriber, A. C. Simmonnett, J. Steinmetzer, J. R. Wagner, L. Ward, M. Welborn, D. Altarawy, J. Anwar, J. D. Chodera, A. Dreuw, **H. J. Kulik**, F. Liu, T. J. Martinez, D. A. Matthews, H. F. Schaefer III, J. Sponer, J. M. Turney, L.-P. Wang, N. De Silva, R. A. King, J. F. Stanton, M. S. Gordon, T. L. Windus, C. D. Scherrill, and L. A. Burns "Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and Interoperability among Computational Chemistry Programs", *Journal of Chemical Physics,* **155**, 204801 (2021).
94. A. Nandy, C. Duan, and **H. J. Kulik*** "Using Machine Learning and Data Mining to Leverage Community

Knowledge for the Engineering of Stable Metal-Organic Frameworks", *Journal of the American Chemical Society*, **143**, 17535–17547 (2021).
93. M. G. Taylor, A. Nandy, C. C. Lu, and **H. J. Kulik*** "Deciphering Cryptic Behavior in Bimetallic Transition Metal Complexes with Machine Learning", *The Journal of Physical Chemistry Letters,* **12**, 9812-9820 (2021).
92. R. Mehmood, V. Vennelakanti, and **H. J. Kulik*** "Spectroscopically Guided Simulations Reveal Distinct Strategies for Positioning Substrates to Achieve Selectivity in Non-heme Fe(II)/αKG-dependent Halogenases", *ACS Catalysis,* **11**, 12394-12408 (2021).
91. C. Duan, S. Chen, M. G. Taylor, F. Liu, and **H. J. Kulik*** "Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles", *Chemical Science,* **12**, 13021-13036 (2021).
90. M. G. Taylor and **H. J. Kulik*** "Mapping the Electronic Structure Origins of Surface- and Chemistry-Dependent Doping Trends in III-V Quantum Dots" *Chemistry of Materials,* **33**, 7713-7723 (2021).
89. V. Vennelakanti, A. Nazemi, R. Mehmood, A. H. Steeves, and **H. J. Kulik*** "Harder, better, faster, stronger: large-scale QM and QM/MM for predictive modeling in enzymes and proteins", *Current Opinion in Structural Biology,* **72**, 9-17 (2022).
88. V. Vennelakanti, A. Nandy, and **H. J. Kulik*** "The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for C–H Activation Catalysts", *Topics in Catalysis* **65**, 296-311 (2022).
87. A. Nandy[#], C. Duan[#], M. G. Taylor, F. Liu, A. H. Steeves, and **H. J. Kulik*** "Computational Discovery of Transition-Metal Complexes: From High-throughput Screening to Machine Learning", *Chemical Reviews,* **121**, 9927–10000 (2021).
86. Z. Yang and **H. J. Kulik*** "Protein Dynamics and Substrate Protonation State Mediate the Catalytic Action of Trans-4-Hydroxy-L-Proline Dehydratase", *The Journal of Physical Chemistry B,* **125**, 7774-7784 (2021).
85. Z. Yang, N. Hajlasz, A. H. Steeves, and **H. J. Kulik*** "Quantifying the long-range coupling of electronic properties in proteins with *ab initio* molecular dynamics", *Chemistry – Methods,* **1**, 362-373 (2021).
84. C. Duan, F. Liu, A. Nandy, and **H. J. Kulik*** "Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery", *The Journal of Physical Chemistry Letters*, **12**, 4628-4637 (2021). ***Featured by ACS on X-Mol.***
83. **H. J. Kulik*** "What's Left for a Computational Chemist To Do in the Age of Machine Learning?", *Israel Journal of Chemistry,* **62**, e202100016 (2022).
82. A. Bajaj and **H. J. Kulik*** "Molecular DFT+U: a Transferable, Low-Cost Approach to Eliminate Delocalization Error", *The Journal of Physical Chemistry Letters*, **12**, 3633-3640 (2021).
81. C. Dawson, S. Irwin, L. Backman, C. Le, J. X. Wang, V. Vennelakanti, Z. Yang, **H. J. Kulik***, C. L. Drennan*, and E. P. Balskus*, "Molecular Basis of C–S Bond Cleavage in the Glycyl Radical Enzyme Isethionate Sulfite-Lyase", *Cell Chemical Biology*, **28**, 1-14 (2021).
80. J. P. Janet, C. Duan, A. Nandy, F. Liu, and **H. J. Kulik*** "Navigating Transition-metal Chemical Space: Artificial Intelligence for First-principles Design", *Accounts of Chemical Research*, **54**, 532-545 (2021). ***Invited Article for Special Issue "Data Science Meets Chemistry"***
79. R. Jonnalagadda, A. del rio Flores, W. Cai, R. Mehmood, M. Narayanamoorthy, C. Ren, J. P. T. Zaragoza, **H. J. Kulik***, W. Zhang*, and C. L. Drennan* "Biochemical and crystallographic investigations into isonitrile formation by a non-heme iron-dependent oxidase/decarboxylase", *Journal of Biological Chemistry*, **296**, 100231 (2021).
78. V. Vennelakanti, H. W. Qi, R. Mehmood, and **H. J. Kulik*** "When are two hydrogen bonds better than one? Accurate first-principles models explain the balance of hydrogen bond donors and acceptors found in proteins", *Chemical Science,* **12**, 1147-1162 (2021).
77. A. Nandy and **H. J. Kulik*** "Why Conventional Design Rules for C–H Activation Fail for Open-Shell Transition-Metal Catalysts", *ACS Catalysis*, **10**, 15033-15047 (2020).
76. C. L. Ritt, J. R. Werber, M. Wang, Z. Yang, Y. Zhao, **H. J. Kulik**, and M. Elimelech* "Ionization behavior of nanoporous polyamide membranes", *Proceedings for the National Academy of Sciences*, **117**, 30191-30200 (2020).
75. F. Liu, C. Duan, and **H. J. Kulik*** "Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening", *The Journal of Physical Chemistry Letters*, **11**, 8067-8076 (2020). ***Featured by ACS on X-Mol.***
74. A. Nandy, D. B. K. Chu, D. R. Harper, C. Duan, N. Arunachalam, Y. Cytter, and **H. J. Kulik*** "Large-scale comparison of 3*d* and 4*d* transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics", *Physical Chemistry Chemical Physics*, **22**, 19326-19341 (2020). ***Invited Article for Special Themed Collection "Quantum Theory: The Challenge of Transition Metal Complexes"***
73. S. M. Moosavi, A. Nandy, K. M. Jablonka, D. Ongari, J. P. Janet, P. G. Boyd, Y. Lee, B. Smit*, and **H. J. Kulik*** "Understanding the diversity of the metal-organic framework ecosystem", *Nature Communications,* **11**, 4068 (2020).
72. C. Duan, F. Liu, A. Nandy, and **H. J. Kulik*** "Semi-Supervised Machine Learning Enables the Robust Detection of

Multireference Character at Low Cost", *The Journal of Physical Chemistry Letters,* **11**, 6640-6648 (2020)**.**
71. C. Duan, F. Liu, A. Nandy, and **H. J. Kulik*** "Data-Driven Approaches Can Overcome the Cost-Accuracy Tradeoff in Multireference Diagnostics", *Journal of Chemical Theory and Computation,* **16**, 4373-4387 (2020).
70. A. Bajaj, F. Liu, and **H. J. Kulik*** "Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling", *The Journal of Physical Chemistry C*, **124**, 15094-15106 (2020).
69. R. Mehmood and **H. J. Kulik*** "Both Configuration and QM Region Size Matter: Zinc Stability in QM/MM Models of DNA Methyltransferase", *Journal of Chemical Theory and Computation*, **16**, 3121-3134 (2020).
68. M. G. Taylor, T. Yang, S. Lin, A. Nandy, J. P. Janet, C. Duan, and **H. J. Kulik*** "Seeing is Believing: Experimental Spin States from Machine Learning Model Structure Predictions", *The Journal of Physical Chemistry A,* **124**, 3286-3299 (2020). ***Invited contribution to JPC virtual special issue "Machine Learning in Physical Chemistry"***
67. J. P. Janet, S. Ramesh, C. Duan, and **H. J. Kulik*** "Accurate multi-objective design in a space of millions of transition metal complexes with neural-network-driven efficient global optimization", *ACS Central Science*, **6**, 513-524 (2020). ***Featured in MIT News, C&E News***
66. F. Liu and **H. J. Kulik*** "Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry", *Journal of Chemical Theory and Computation*, **16**, 264-277 (2020).
65. **H. J. Kulik*** "Making machine learning a useful tool in the accelerated discovery of transition metal complexes", *Wiley Interdisciplinary Research: Computational Molecular Science*, **10**, e1439 (2020).
64. 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*, **5**, 139-152 (2020).
"2020 Emerging Investigators" special issue; Recipient of "MSDE 2020 Outstanding Early-Career Paper Award"
63. 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).
62. 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). ***Featured in ACS Catalysis Virtual Issue "Blurring the Lines Between Catalysis Subdisciplines"***
https://axial.acs.org/2020/08/13/blurring-the-lines-between-catalysis-subdisciplines/
61. 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).
Selected as HOT article, Featured in *Chemistry World*:
https://www.chemistryworld.com/news/uncertainty-metric-builds-confidence-in-machine-learned-chemistry/3010759.article
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. 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).
57. 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).
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; recipient of Rising Stars Prize.***
55. 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).
54. 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).
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). ***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. 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".***
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. 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 "Protection of tissue physicochemical properties using polyfunctional crosslinkers", *Nature Biotechnology*, **37**, 73-83 (2019).
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. 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.***
41. 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.
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. 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.***
33. 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).
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 Using Polarizable Continuum Models" *Journal of Chemical Theory and Computation* **11**, 3131–3144, (2015).
17. J. Zhang, **H. J. Kulik**, T. J. Martínez, and J. P. Klinman "Mediation of donor–acceptor distance in an enzymatic methyl transfer reaction" *Proceedings of the National Academy of Sciences* **112**, 7954–7959 (2015).
16. **H. J. Kulik*** "Perspective: Treating electron over-delocalization with the DFT+U method" *Journal of Chemical Physics* **142**, 240901 (2015). ***Invited Cover Perspective***.
15. 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).
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).
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. **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).

6. 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 "Spatially Extended Kondo State in Magnetic Molecules Induced by Interfacial Charge Transfer" *Physical Review Letters* **105**, 106601 (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**, 9594-9601 (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 $\Sigma^+-\Sigma^+$ optical transitions in the spectra of CN and isoelectronic species" *Journal of Molecular Spectroscopy* **258**, 6-12 (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, BOOKS, BOOK CHAPTERS, CONFERENCE PAPERS, AND EDITORIALS

11. D. H. Ess, K. Jelfs, and **H. J. Kulik*** "Chemical Design by Artificial Intelligence", *Journal of Chemical Physics*, **in press**. **Editorial**
10. C. Duan, A. Nandy, and **H. J. Kulik*** " A Density Functional Recommendation Approach for Accurate Predictions of Vertical Spin Splitting of Transition Metal Complexes", *ICML* (2022). **Conference paper**
9. C. Duan#, A. Nandy#, and **H. J. Kulik*** "Machine Learning for the Discovery, Design, and Engineering of Materials", *Annual Review of Chemical and Biomolecular Engineering*, **13**, 18.1-18.25 (2022). **Review chapter**
8. **H. J. Kulik*** and M. Sigman "Advancing Discovery in Chemistry with Artificial Intelligence: From Reaction Outcomes to New Materials and Catalysts", *Accounts of Chemical Research*, **54**, 2335-2336 (2021). **Editorial**
7. R. Mehmood and **H. J. Kulik*** "Quantum-mechanical/Molecular-mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics", *Enzyme Engineering: Methods and Protocols,* 227-248 (2022). **Book chapter**
6. J. P. Janet and **H. J. Kulik*** "Machine Learning in Chemistry", *ACS InFocus Series* (2020). **Book**
5. L. Frediani, O. Andreussi, and H. J. Kulik "Coding solvation: Challenges and opportunities", *International Journal of Quantum Chemistry* **119**, e25839 (2019). **Editorial**
4. **H. J. Kulik*** "Modeling mechanochemistry from first principles", *Reviews in Computational Chemistry* **31**, 6 (2018). **Book chapter**
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). **Proceedings**
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). **Proceedings**
1. **H.J. Kulik** and N. Marzari Chapter entitled "Electronic Structure and Reactivity of Transition Metal Complexes" in *Fuel Cell Science: Theory, Fundamentals, and Bio-Catalysis*, a Wiley monograph, eds. Jens Norskov and Andrzej Wiezcowski (2010). **Book chapter**

INVITED PRESENTATIONS

Upcoming, confirmed:

210. 13th International Conference on Hydrogenases and Other Redox (Bio)catalysts for Energy Conversion, Walla Walla, WA. "Understanding and overcoming limits in bioinspired catalyst design for small molecule activation". *June 2023. Postponed due to COVID-19.*
209. IPAM: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing, Los Angeles, CA. "TBD". *March 2023.*
208. ETH Zürich, Laboratory of Inorganic Chemistry Colloquium, Zürich, Switzerland. "Designing new materials and catalysts with simulation and machine learning tools". *November 2022.*
207. Co-Design for Materials Discovery, Reliability, & Extreme Environments, Sandia National Laboratories, Sandia, CA. "TBD". *November 2022. Virtual workshop.*
206. "Automation and Digital Chemistry for Catalysis" Workshop at Imperial College, London. "TBD". *November 2022.*
205. ETH Zürich, Laboratory for Physical Chemistry Colloquium, Zürich, Switzerland. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *November 2022.*
204. Korean Institute of Science and Technology (KIST), Seoul, Korea. "TBD" *October 2022.*
203. Boston University Materials Day "Simulation and Modeling of Extended Materials: Connecting Scales for Practical

Applications", Boston University, Boston, MA. "Discovering transition metal catalysts and materials with machine learning" *October 2022*.

Completed:

202. Telluride Workshop "Machine Learning and Informatics for Chemistry and Materials", Telluride, CO. "Overcoming challenges of data scarcity and data quality for machine learning" *October 2022*.
201. Kwang-Yu and Lee-Chien Wang Fellowship Lecture, Department of Chemical Engineering, University of Rochester, Rochester, NY. "TBD" *September 2022*.
200. Rennes Institute of Chemistry 2022, Rennes, France. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *September 2022*.
199. DFT 2022, Brussels, Belgium. "Putting density functional theory to the test in machine-learning accelerated discovery". *August 2022*.
198. Psi-k 2020, Lausanne, Switzerland. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *August 2022. Postponed due to COVID-19*.
197. 33rd IUPAP Conference on Computational Physics , "Recent developments and applications of DFT+U" Symposium, Austin, TX (Virtual). "Recovering exact conditions for both delocalization and fractional spin error in transition-metal chemistry with molecular-orbital projector-based DFT+U and jmDFT". *August 2022*.
196. International Younger Chemists Network Webinar on Machine Learning and Artificial Intelligence. "What problems can machine learning solve in inorganic materials discovery?". *July 2022. Virtual.*
195. Foundations of Molecular Modeling and Simulation 2022, Delavan, WI. "New Strategies for Catalyst Discovery from Machine Learning Exploration". *July 2022.* ***Plenary***.
194. NIST-JARVIS Artificial Intelligence for Materials Science (AIMS) 2022 Workshop, NIST (Virtual). "Revealing molecular design blueprints for open shell transition metal materials and catalysts with machine learning". *July 2022*.
193. 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada. "Putting density functional theory to the test in machine-learning accelerated discovery for transition metal chemistry". *July 2022. Postponed due to COVID-19*.
192. 10th Molecular Quantum Mechanics, Blacksburg, VA. "Putting density functional theory to the test with machine learning". *June 2022.* ***Plenary***.
191. 75th International Symposium on Molecular Spectroscopy, Urbana-Champaign, IL. "Putting density functional theory to the test with machine learning". *June 2022*.
190. Dow (Virtual). "Discovering transition metal catalysts and materials with machine learning". *June 2022*.
189. MolSSI/Tapia Workshop, Rice University, Houston, TX. "Quantum mechanics and quantum chemistry" and "Navigating transition metal chemical space with computational quantum chemistry and machine learning". *June 2022*.
188. Cornell University, Cornell Energy Systems Institute Distinguished Lecturer Series, Ithaca, NY. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *May 2022*.
187. "Machine Learning in Chemical and Materials Sciences" Virtual Symposium, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM. "Audacity of huge: overcoming challenges of data scarcity and data quality for machine learning in computational materials discovery". *May 2022*.
186. Caltech, Chemical Physics Seminar Series, Pasadena, CA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *May 2022*.
185. Virginia Tech, Chemical Engineering Department, Blacksburg, VA. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *April 2022*.
184. George Washington University, Department of Chemistry, Washington, DC. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *April 2022*.
183. Harvard University, Department of Chemistry, Cambridge, MA. "Putting first-principles modeling to the test with machine learning". *March 2022*.
182. American Chemical Society Spring 2022 Meeting, San Diego, CA, PHYS Division. "Using machine learning and data mining to leverage community knowledge for the engineering of materials and catalysts". *March 2022*.
181. American Chemical Society Spring 2022 Meeting, San Diego, CA, CATL Division. "Methods for systematic multi-scale modeling of enzyme catalysis". *March 2022*.
180. American Chemical Society Spring 2022 Meeting, San Diego, CA, Presidential Symposium. "Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning". *March 2022*.
179. Massachusetts Institute of Technology, Department of Chemistry, Cambridge, MA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *March 2022*.
178. Molecular Chemistry Meets Materials Science, MolSSI Virtual Workshop. "Molecular design blueprints: materials

and catalysts from new simulation and machine learning tools". *March 2022.*
177. 61st Sanibel Symposium, Sanibel, FL. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *February 2022.* ***Plenary.***
176. Oregon State University, Department of Chemistry, Corvallis, OR. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *January 2022.*
175. UC Santa Barbara, Graduate Simulation Seminar Series (GS^3), Santa Barbara, CA. "Learning from failure". *January 2022.* ***Keynote.***
174. UC Santa Barbara, Graduate Simulation Seminar Series (GS^3), Santa Barbara, CA. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *January 2022.* ***Keynote.***
173. International Conference on Theoretical and High Performance Computational Chemistry 2021 (ICT-HPCC21), Beijing, China "Putting density functional theory to the test in machine-learning accelerated materials discovery". *December 2021. Virtual.*
172. ELLIS Machine Learning for Molecule Discovery Workshop "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *December 2021. Virtual.*
171. Pacifichem 2020, Honolulu, HI. "Supercharging Computational Chemistry with AI" Symposium. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *December 2021. Virtual due to COVID-19.*
170. Pacifichem 2020, Honolulu, HI. "Chemical Concepts from Theory and Computation" Symposium. "Using conceptual DFT to understand and improve electronic structure method errors for complex systems". *December 2021. Virtual due to COVID-19.*
169. Clarkson University, Department of Chemistry, Potsdam, NY. "What problems can machine learning solve in inorganic materials discovery?". *December 2021. Virtual talk.*
168. Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery (AI3SD), University of Southampton, Southampton, UK. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials". *December 2021. Virtual talk.*
167. International Symposium on Machine Learning in Quantum Chemistry, Xiamen University, China. "Audacity of huge: machine learning for the discovery of transition metal catalysts and materials" *November 2021. Virtual due to COVID-19.*
166. Ohio State University, Department of Biophysics, Columbus, OH. "What can quantum chemistry teach us about protein structure and function?". *October 2021. Virtual due to COVID-19.*
165. SUNCAT Workshop on Challenges and opportunities in data-driven catalysis research. Stanford & SLAC, Stanford, CA. "Audacity of huge: exploring transition metal chemical space with machine learning". *September 2021. Virtual due to COVID-19.*
164. CU Denver, Department of Chemistry, Denver, CO. "Uncovering convergent design principles for C-H activation from nature and machine learning". *September 2021. Virtual due to COVID-19.*
163. Chemical Reviews Thematic Talk Series on Machine Learning. "Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning" *September 2021.*
162. UT Knoxville, Department of Chemistry, Knoxville, TN. "Putting density functional theory to the test in machine-learning accelerated discovery". *August 2021.*
161. American Chemical Society Fall 2021 Meeting, Atlanta, GA. "Finding the needle in the haystack with ML-accelerated multi-objective design". *August 2021.*
160. IUPAC/CCCE World Congress of Chemistry, Montreal, Quebec, Canada. "Frontiers in Chemical Understanding and Prediction: New Descriptors and Concepts for Chemical Phenomena" Symposium. "Putting density functional theory to the test in machine-learning accelerated discovery" *August 2021. Virtual due to COVID-19.*
159. IUPAC/CCCE World Congress of Chemistry, Montreal, Quebec, Canada. "Computational Design of Materials and Systems for Energy Applications" Symposium. "What can machine learning do to accelerate the design of catalysts and materials?" *August 2021. Virtual due to COVID-19.* **Keynote.**
158. International Workshop on High-Performance Computing in Science and Engineering – 2021, IISER TVM, India. "What can machine learning do to accelerate the design of catalysts and materials?" *August 2021. Virtual workshop.* **Keynote**.
157. Virtual Conference on 'Machine Learning/Data Science assisted Synthesis', MPI-Kohlenforschung, Germany. "Audacity of huge: exploring transition metal chemical space with machine learning". *July 2021.*
156. Annual Workshop on Recent Developments in Electronic Structure Methods (ES21), Center for Computational Quantum Physics (CCQ), Flatiron Institute, New York, NY. "Putting density functional theory to the test in machine-learning accelerated discovery." *July 2021. Virtual due to COVID-19.*
155. 35th Anniversary Symposium of The Protein Society, Boston, MA. "What can machine learning and big data teach

us about metalloenzymes?". *July 2021. Virtual due to COVID-19.*
154. Telluride Workshop on Computational Materials Chemistry, Telluride, CO. "Putting DFT to the test in ML-accelerated discovery". *June 2021.*
153. HBCU-MI, ONR Naval Research Lab Summer Internship Program. "Navigating transition metal chemical space with computational chemistry". June 2021.
152. Molecular Systems Design & Engineering Virtual Conference, Royal Society of Chemistry, UK. "What problems can machine learning solve in transition metal complex discovery?". *June 2021.*
151. Catalysis Club of Chicago, Chicago, IL. "What problems can machine learning solve in transition metal complex discovery?". *May 2021. Virtual due to COVID-19.* **Keynote**.
150. "Machine Learning in Chemical and Materials Sciences" Virtual Symposium, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM. "Putting density functional theory to the test in machine-learning accelerated discovery for transition metal chemistry". *May 2021.*
149. New York University, Department of Chemistry, New York, NY. "Putting density functional theory to the test in machine-learning accelerated discovery for transition metal chemistry". *May 2021. Virtual due to COVID-19.*
148. South Dakota School of Mines & Technology, Chemical and Biological Engineering, Rapid City, South Dakota. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *April 2021. Postponed, then virtual due to COVID-19.*
147. American Chemical Society Spring 2021 Meeting. "Putting density functional theory to the test in machine-learning-accelerated discovery". *April 2021. Virtual due to COVID-19.*
146. Computational Chemistry, Theory, and Dynamics theme of the School of Chemistry, University of Bristol, Bristol, UK. "Putting density functional theory to the test in machine-learning-accelerated discovery". *April 2021. Virtual due to COVID-19.*
145. DMAV-T, ETH Zurich, Zurich, Switzerland. "What problems can machine learning solve in transition metal complex discovery?" *April 2021. Virtual due to COVID-19.*
144. Exxon-Mobil, Baytown, TX. "What problems can machine learning solve in transition metal complex discovery?" *March 2021. Virtual due to COVID-19.*
143. American Physical Society March Meeting, Nashville, TN. "Understanding confinement effects on ion permeability with computation: from first-principles to data-driven models". *March 2021. Virtual due to COVID-19.*
142. Boston Regional Inorganic Colloquium at University of New Hampshire, Durham, NH. "What problems can machine learning solve in transition metal complex discovery?" *February 2021.*
141. Virtual Winter School on Computational Chemistry. "Putting density functional theory to the test in machine-learning accelerated discovery for transition metal chemistry". *February 2021.*
140. University of Houston, Department of Chemical Engineering, Houston, TX. "Molecular design blueprints: catalysts and principles from new simulation and machine learning tools". *November 2020. Virtual seminar due to COVID-19.*
139. American Institute of Chemical Engineers National Meeting, San Francisco, CA. Area 20 "Molecular design blueprints: catalysts and principles from new simulation and machine learning tools". *November 2020.*
138. Pennsylvania State University, MRSEC, Department of Materials Science & Engineering, Pittsburgh, PA. "What problems can machine learning solve in inorganic materials discovery?". *October 2020. Virtual seminar due to COVID-19.*
137. Carnegie Mellon University, Chemical Engineering, Pittsburgh, PA. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *October 2020. Virtual seminar due to COVID-19.*
136. University of Massachusetts Amherst, Chemistry Department, Amherst, MA. "Molecular design blueprints: catalysts and principles from new simulation and machine learning tools". *October 2020. Virtual seminar due to COVID-19.*
135. ICTP – East African Institute for Fundamental Research, Kigali, Rwanda. "DFT+U and beyond for recovering exact conditions and improving properties in correlated materials". *September 2020.*
134. Molecular Modeling & Materials Design (M3DC) "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *July 2020. Virtual symposium.*
133. 2020 Pittsburgh Quantum Institute Annual Symposium, Pittsburgh, PA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *July 2020.* **Plenary** *Postponed & made virtual due to COVID-19.*
132. University of Delaware, Chemical Engineering Virtual Seminar Series "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *June 2020.*
131. Low-scaling and Unconventional Electronic Structure Techniques, Telluride, CO. "Diagnosing strong correlation with machine learning". *June 2020. Held virtually due to COVID-19.*
130. ML4Science, Virtual Seminar Series hosted by Stefano Sanvito, Trinity College Dublin. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *May 2020.*
129. Netherlands' Catalysis and Chemistry Conference (NCCC), Noordwijkerhout, Netherlands. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *March 2020.* **Keynote**

128. UC Merced, Chemistry Department, Merced, CA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *January 2020*.
127. UC Berkeley, Chemical & Biomolecular Engineering Department, Berkeley, CA. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *January 2020*.
126. Cornell University, Chemical & Biomolecular Engineering, Ithaca, NY. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *January 2020*.
125. UC San Diego, Chemistry Department, San Diego, CA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *January 2020*.
124. Stanford University, Chemical Engineering, Stanford, CA. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *January 2020*.
123. Helsinki Winter School on Inorganic Chemistry, Helsinki, Finland. "Machine learning for accelerating discovery in inorganic chemistry" and "Approximate density functional theory for transition metal chemistry – Parts 1 and 2". (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. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *November 2019*.
120. 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*.
119. NanoGE Conference, Berlin, Germany. "Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots." *November 2019*.
118. North Dakota State University, Chemistry Department, Fargo, ND. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *October 2019*.
117. Northwestern University, Catalysis Center, Evanston, IL. "Accelerating the computational discovery of catalyst design rules and exceptions with machine learning". *October 2019*.
116. Northwestern University, Chemical & Biological Engineering Department, Evanston, IL. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *October 2019*.
115. "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*.
114. 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*. ***Named lecture***
113. Soft matter seminar, Columbia University, Chemical Engineering Department, New York, NY. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *September 2019*.
112. Pennsylvania 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*.
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 ($11M)

External funding ($10.2M)

Department of Energy, 08/01/22-07/31/26 $787,500
The Center for Enhanced Nanofluidic Transport (CENT)
(Michael S. Strano, MIT PI; Kulik co-PI)

National Science Foundation, 09/01/21-08/31/26 $1,140,000
NSF Center for Molecularly Optimized Networks
(Steve Craig, Duke PI; Kulik co-PI) – only amount to Kulik shown

Department of Energy, 09/01/21-08/31/25 $700,000
Large-scale algorithms and software for modeling chemical reactivity in complex systems
(Martin Head-Gordon, UC Berkeley PI; Kulik co-PI) – only amount to Kulik shown

Sloan Foundation, 09/01/21-08/31/23 $75,000
Alfred Sloan Fellowship in Chemistry

Department of Energy, 09/01/20-8/31/25 $8,550,000
CESMIX: Center for the Exascale Simulation of material Interfaces in Extreme Environments
(Youssef Marzouk, MIT PI; Kulik co-PI) – approx. $855,000 to Kulik

Office of Naval Research, 03/01/20-02/29/24 $800,000
A Database for Functional Transition Metal Complex Discovery

DARPA Young Faculty Award and Director's Fellowship, 6/30/18-6/30/22 $875,000
Adaptive-focus topological features for machine-learning-driven discovery of 2D coordination polymers

Exxon Mobil, 11/01/19-04/30/21 $171,544
Bio-inspired computational catalyst design

National Science Foundation CAREER, 06/1/19-05/31/24 $593,678
CAREER: Revealing spin-state-dependent reactivity in open-shell single atom catalysts with systematically-improvable computational tools

AAAS Marion Milligan Mason Award*, 12/13/18-12/12/21 $50,000
Navigating Transition Metal Chemical Space: Artificial Intelligence for First-Principles Design

Department of Energy, 08/01/18-7/31/22 $440,000
Inorganometallic Catalyst Design Center (ICDC)
(Laura Gagliardi, U. Minnesota PI; Kulik co-PI)

Department of Energy, 08/01/18-7/31/22 $480,000
The Center for Enhanced Nanofluidic Transport (CENT)
(Michael S. Strano, MIT PI; Kulik co-PI)

Office of Naval Research Young Investigator Program, 06/01/18-08/31/22 $510,000
Adaptive-Resolution Chemical Discovery Strategies for Precise and Fast Computer-Aided Transition Metal Complex Design

Office of Naval Research, 09/01/17-10/31/21 $450,000
Computer-aided design of functional transition metal complexes

Department of Energy, 09/01/17-09/30/21 $292,725
Simultaneous mitigation of density and energy errors in approximate DFT for transition metal chemistry

National Science Foundation, 08/01/17-07/31/21 $317,245
Enabling high-throughput computational discovery of stable and active single-site oxidation catalysts

Eni S.p.A, 06/01/17-05/31/20 $500,000
OFR calculator

Robert Bosch, LLC, 05/01/17-04/30/19 $250,000
Developing new methods for the accurate ionization potential calculation in polymer electrolyte modeling for energy storage

National Science Foundation, 09/01/14-02/15/19 $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*, 07/01/12-6/30/22 $500,000
Deciphering the role of the protein scaffold in enzyme catalysis with fast and accurate computation

Internal funding ($0.78M)

MIT-Portugal Program Seed Fund 06/01/22-05/31/23 $100,000
Engineering Metal-Organic Frameworks for Stabiltiy in Gas Storage Applications
2022 Abdul Latif Jameel Water and Food Systems Lab (J-WAFS) Seed Fund 09/01/22-08/31/24 $150,000
In Silico Discovery of Metal–Organic Frameworks for Selective Ion Separation
MIT-Israel Broshy Brain and Cognitive Sciences Fund Grant* 05/01/22-01/31/24 $29,975
Understanding the behavioral decision making behind chemical discoveries
NIH Center for Environmental Health Sciences Pilot Grant 09/01/17-08/31/18 $39,000
Quantum mechanical contributions to methyltransferase inhibition
MIT-RSC NEC Corporation Grant* 09/01/17-08/31/18 $75,000
New computational tools for unveiling electronic contributions to rate enhancements in methyltransferases
MIT Energy Initiative Seed Grant 06/01/17-05/31/19 $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* 01/01/17-08/31/18 $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* 09/01/16-08/31/17 $20,000
Theoretical prediction of protein-substrate interactions
MIT-RSC Reed Grant* 09/01/14-08/31/15 $75,000
Screening for catalyzable bonds in highly heterogeneous feedstocks
MIT Energy Initiative Seed Grant 04/01/14-09/30/15 $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.*

Computing proposals (over 5.5 M CPU/GPU hours)

NSF XSEDE renewal 07/01/22-06/30/23
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
2.96M SUs SDSC Expanse 1k SUs on Comet GPU (est. value $14,109.78)
NSF XSEDE renewal 07/01/21-06/30/22
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
1.05M SUs SDSC Comet, 19k SUs on Bridges GPU, 55k SUs on Comet GPU
NSF XSEDE renewal 07/01/20-06/30/21
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
1.05M SUs SDSC Comet, 19k SUs on Bridges GPU, 55k SUs on Comet GPU
NSF XSEDE renewal 04/01/19-06/30/20
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 10/01/17-03/31/19
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 10/01/16-09/30/17
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 10/01/15-09/30/16
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 07/01/14-06/30/15
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 04/29/14-05/28/15
Indium Phosphide Growth at Early Stage from Precursors Molecules: A collisionally-accelerated ab initio Molecular Dynamics Study
170k CPU hours

STUDENTS SUPERVISED

Graduate Students

2022-	Changhwan Oh, DMSE	
2021-	Xiao Huang, Chemistry	
2021-	Allison Keys, CSBi	
2021-	David Kastner, BE	
2020-	Husain Adamji, ChemE	
2020-	Gianmarco Terrones, ChemE	
2019-	Daniel B. K. Chu, ChemE	
2019-	Hao-Jun Jia, Chemistry	
2018-	Naveen Arunachalam, ChemE	
2018-	Vyshnavi Vennelakanti, Chemistry	
2017-	Aditya Nandy, Chemistry	
2017-22	Chenru Duan, Chemistry	(Ph.D. '22: PD T. and M. Head-Gordon, UC Berkeley)
2016-21	Akash Bajaj, DMSE	(Ph.D. '21; PD Sanvito Group, Trinity College Dublin)
2016-21	Rimsha Mehmood, Chemistry	(Ph.D. '21; Senior Scientist, Merck)
2018-21	Daniel Harper, Chemistry	(S.M. '21; Consultant at Sage Analysis)
2018	Stefan Gugler, ETH Zürich Chemistry	(M.S. '18 ETH Zürich; now Ph.D. ETH Zürich)
2015-18	Terry Z. H. Gani, ChemE	(Ph.D. '20; Research Scientist, National University of Singapore)
2018-20	Mengyi Wang, DMSE	(S.M. '20)
2015-19	Jon Paul Janet, ChemE	(Ph.D. '19; Senior Scientist, Astra-Zeneca)
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; TT Asst. Prof. Northeastern ChemE)
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. '21 Tidor lab; MindsDB)

Undergraduate, High School Students

2022-	Hongqian Zheng, UG via USTC	
2022-	Jelissa Kamguem, MIT MSRP (Lafayette College U.G. thesis '23)	
2022-	Jonas Oldenstaedt*, TUM M.S.	
2022-	Mugyeom Jeon, MIT 5 UROP	
2021-	Freya Edholm, MIT 10 UROP	
2022	Grace Li, MIT 6-3 UROP	
2022	Rafa Chavez, MIT UROP	
2022	Bryan Gough, MIT 20 UROP	
2022	David Gonzalez Narvaez, MIT MSRP-BIO	
2021	Irem Kilic, via Bogazici University	
2021	Adriana Ladera*, MIT MSRP	(UCF B.S. '22, now: MIT M.S.)
2021	Julian Liu*, MIT 8 UROP	(MIT S.B. '22)
2021	Anna Bair, MIT 5 UROP	(MIT S.B. '24 expected)
2020	Dechen Rota, MIT 10 UROP	(MIT S.B. '23 expected)
2020	Shuxin Chen*, MIT 10 UROP	(MIT S.B. '22)
2020	Conrad Goffinet*, MIT 10 UROP	(MIT MSCEP '22)
2018-20	Natalia Haljasz*, Harvard UROP	(B.S. Harvard, '21 expected)
2018-19	Ava Waggett, MIT 10 UROP	(MIT S.B. '19, now: U Washington Ph.D.)
2018	Eve Xu*, Wellesley exchange	(B.S. Smith, '20, now: Princeton Ph.D.)
2018-19	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, now: U Chicago Ph.D.)
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 ('17-)
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-)
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)
Materials Research Society (2004-Present)

CONSULTING

Universal Display Corporation, Ewing, NJ. 2018-19
Silicon Therapeutics/Roivant, Boston, MA. Open Science Fellow 2020-22

SERVICE

External

Advisory Councils and Boards

The Cooper Union Engineering Advisory Council (2020-)
DOE Chemical Sciences, Geosciences, and Biosciences Council Member (2021-)
SIMPLAIX (Heidelberg Institute for Theoretical Studies) Scientific Advisory Board (2022-)

Editorial service

International Journal of Quantum Chemistry Editorial Board member (2018-).
The Journal of Physical Chemistry Editorial Board member (2020-).
Reaction Chemistry and Engineering Advisory Board member (2020-2021).
Reaction Chemistry and Engineering Editorial Board member (2021-).
The Journal of Chemical Physics Editorial Board member (2021-).
Molecular Systems Design & Engineering Advisory Board member (2022-).
Digital Discovery Advisory Board member (2022-).
Guest co-editor for special *Int. J. Quantum. Chem.* issue on "Advances in Simulating Solvation" (with Luca Frediani and Oliviero Andreussi)
Guest co-editor for special *Acc. Chem. Res.* issue on "Data Science Meets Chemistry" (with Matt Sigman)

Guest co-editor for special *J. Chem. Phys*. issue "Chemical Design by Artificial Intelligence" (with Dan Ess and Kim Jelfs)
Guest co-editor for *MRS Bulletin* on Machine Learning (with Pratyush Tiwary)
Guest co-editor for *Electronic Structure* issue on "Electronic Structure in Biology" (with Marc van der Kamp and Amir Karton)
Section editor for "Molecular Interactions and Catalysis" in "Comprehensive Computational Chemistry" (editors-in-chief: M. Yanez and R. Boyd) Major Reference Work (Elsevier Publishers)

Conference organization and professional organization service

Chair for GRC on Computational Materials Science and Engineering with K. Thornton (2024)
Vice-chair for GRC on Computational Materials Science and Engineering with R. Ramprasad and K. Thornton (2022)
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, 2020-)
North American Catalysis Society Meeting abstract review (2017)
American Chemical Society presider CATL (Spring 2018), COMP (Fall 2018), session organizer "Data Science for Catalysis" CATL Spring 2019, session organizer ENFL Fall 2021
"Coding Solvation" NSF-MolSSI-funded workshop in Livorno, Italy co-organizer (2017)
New England Catalysis Society Regional Meeting co-organizer (2018)
AIChE Area 1A/CoMSEF Liaison (2019-)

Thesis Defense Opponent or Examiner

Iulia Brumboiu, Uppsala University, Uppsala, Sweden (2016)
Joshua Brown, University of Newcastle, New South Wales, Australia (2021)
Søren Meldgaard, Aarhus University, Aarhus, Denmark (2021)

Outreach

Faculty mentor and speaker for MIT Summer Research Program (2015, 2021)
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.

Proposal review for NSF CAREER (2014, 2019, 2020, 2021), NSF DMREF (2014), NSF CBET ad hoc/virtual (2015, 2018, 2020), NSF SBIR (2017,2018), NSF CHE ad hoc/virtual (2018, 2019), NSF DMR ad hoc/virtual (2020). 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), the Netherlands Organisation for Scientific Research (2017), NIH NIGMS (2021), ETH Zürich (2021).

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, PNAS, Angewandte Chemie, Science Advances, Science, and Journal of Catalysis*.

At MIT

Thesis committee member for over 20 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 (2016-2019)
Institute-wide Center for Computational Engineering working group (2018)
ChemE undergraduate curriculum revitalization (10.37) (2018-2019)

RECENT PRESS

"Computational modeling guides development of new materials" *MIT News* 03/11/22
https://news.mit.edu/2022/metal-oxide-frameworks-model-0311
"An explorer in the sprawling universe of possible chemical combinations" *MIT News* 02/06/22
https://news.mit.edu/2022/heather-kulik-chemical-materials-0206
"Accounts of Chemical Research: At the Intersection of Data Science and Chemistry" *ACS Axial,* 06/11/21
https://axial.acs.org/2021/06/11/intersection-data-science-chemistry/
"Materials researchers put machine-learning performance to the test" *Chemical & Engineering News*, 04/11/21
https://cen.acs.org/physical-chemistry/computational-chemistry/Materials-researchers-put-machine-learning/99/i13
"Spying on enzymes while they perform chemical reactions could help treat gut ailments" *MIT Biology News,* 03/26/21
https://biology.mit.edu/news/spying-on-enzymes-to-treat-gut-ailments/
"Eight from MIT named 2021 Sloan Research Fellows" *MIT News,* 02/19/21
https://news.mit.edu/2021/eight-from-mit-named-sloan-research-fellows-0219
"MIT researchers use UC San Diego-based Comet to develop breakthrough artificial neural networks" *SDSC/XSEDE Press Release*, 02/8/21
https://www.sdsc.edu/News%20Items/PR20210208_computational_chemistry.html
"Center to advance predictive simulation research established at MIT Schwarzman College of Computing" *MIT News*, 11/24/20
https://news.mit.edu/2020/center-advance-predictive-simulation-research-established-mit-schwarzman-college-computing-1124
"A close look gets answers about water filters" *Yale School of Engineering & Applied Science News,* 11/12/20
https://seas.yale.edu/news-events/news/close-look-gets-answers-about-water-filters
"Silicon Therapeutics Supports Five Researchers Through Open Science Fellows Program" *Silicon Therapeutics,* 10/22/20
https://silicontx.com/news/press-releases/silicon-therapeutics-supports-five-researchers-through-open-science-fellows-program/
"Exploring chemical space: Can AI take us where no human has gone before?" *Chemical & Engineering News*, 04/03/20
https://cen.acs.org/physical-chemistry/computational-chemistry/Exploring-chemical-space-AI-take/98/i13
"Neural networks facilitate optimization in the search for new materials" *MIT News*, 03/26/20
http://news.mit.edu/2020/neural-networks-optimize-materials-search-0326
"Paper Interview - Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models"
Materials and Megabytes podcast, 01/13/20
https://www.buzzsprout.com/190021/2469740-paper-interview-learning-from-failure-predicting-electronic-structure-calculation-outcomes-with-machine-learning-models
"Uncertainty metric builds confidence in machine learned-chemistry"
Chemistry World, 07/25/19
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, 07/02/19
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, 05/15/19, *Also featured in MIT News*
http://mitener.gy/CF0K50ulGhF
"Marion Milligan Mason Awards"
Angewandte Chemie, 01/25/19
https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201900118
"Mason awardees display benefits of outsider perspectives"
Science, 01/25/19
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*, 02/21/18
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*, 02/19/18
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*, 09/27/17
http://pubs.acs.org/doi/full/10.1021/acs.iecr.7b03758

"Heather Kulik: Innovative modeling for chemical discovery" *MIT News*, 09/15/17
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*, 05/02/17
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*, 08/01/16
http://ilp.mit.edu/newsstory.jsp?id=22124