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EDUCATION

2010-2013	Postdoctoral associate, Stanford University, Stanford, CA *Postdoctoral advisor: Todd J. Martínez*
2009-2010	Postdoctoral associate, Lawrence Livermore Lab, Livermore, CA *Postdoctoral advisor: Felice C. Lightstone*
2009	Ph.D. in Materials Science and Engineering, MIT, Cambridge, MA *Doctoral advisor: Nicola Marzari (now at EPFL)*
2004	B.E. in Chemical Engineering, The Cooper Union, New York, NY

ACADEMIC APPOINTMENTS

Department of Chemical Engineering, MIT

07/2024 -	Lammot Du Pont Professor
07/2021 - 06/2024	Associate Professor (with Tenure)
07/2019 - 06/2021	Associate Professor
11/2013 - 06/2019	Assistant Professor

Department of Chemistry, MIT

07/2024 -	Professor
07/2022 - 06/2024	Associate Professor (with Tenure)

HONORS AND AWARDS

2024	Sydney Ross Lecturer 2024, Renssalaer Polytechnic Institute, Department of Chemistry Löwdin Lecturer for 2023 (awarded 2024), Uppsala University, Sweden, Department of Chemistry TCI Hirschfelder Visitor/Lecturer, Department of Chemistry, University of Wisconsin
2023	AIChE CoMSEF Impact Award Hans Fischer Senior Fellowship, Technical University of Munich (2024-2026) *Current Opinion in Structural Biology* Best Paper Award
2022	Distinguished Romberg Guest Professorship, Heidelberg University 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 *).

197. B. I. Z. Ahmad, R. T. Jerozal, S. Meng, C. Oh, Y. Cho, **H. J. Kulik***, T. H. Lambert*, and P. J. Milner* "Defect-Engineered Metal−Organic Frameworks as Bioinspired Heterogeneous Catalysts for Amide Bond Formation", *submitted.*

196. J. W. Toney, R. G. St. Michel, A. G. Garrison, I. Kevlishvili, and **H. J. Kulik*** "Graph neural networks for predicting metal–ligand coordination of transition metal complexes", *submitted.*
https://doi.org/10.26434/chemrxiv-2024-nzk5q

195. C. Violet, M. Parkinson, A. K. Ball, **H. J. Kulik**, J. D. Fortner*, and M. Elimelech* "Tuning Metal-Organic Framework Linker Chemistry for Transition Metal Ion Separations", *submitted.*

194. D. B. K. Chu, D. A. González-Narváez, R. Meyer, A. Nandy, and **H. J. Kulik*** "Ligand Many-Body Expansion as a General Approach for Accelerating Transition Metal Complex Discovery", *submitted.*
https://doi.org/10.26434/chemrxiv-2024-m39d9

193. C. R. Reinhardt, J. Lee, L. Hendricks, T. Green, L. Feng, L. Kunczynski, A. J. Roberts, N. Miller, N. Rafalin, **H. J. Kulik**, C. J. Pollock*, R. N. Austin* "Moving beyond the first structural models of alkane monooxygenase (AlkB): Active site characterization by extended X-ray absorption fine structure (EXAFS) and molecular dynamics (MD) simulations"

192. V. Vennelakanti, M. Jeon, and H. J. Kulik* "A Computational Investigation of the Role of Metal Center Identity in Cytochrome P450 Enzyme Model Reactivity", *submitted.*

191. A. M. Keys, D. W. Kastner, L. L. Kiessling*, and **H. J. Kulik*** "The Energetic Landscape of CH–π Interactions in Protein–Carbohydrate Binding", *submitted.* https://doi.org/10.26434/chemrxiv-2024-k3bw2

190. M. P. Rivera, G. G. Terrones, T. H. Lee, Z. P. Smith, and **H. J. Kulik*** "Data-driven Screening and Discovery of Metal-organic Frameworks as C_2 Adsorbents from Over 900 Experimental Isotherms", *submitted.*

189. M. Aleksich, Y. Cho, D. W. Paley, M. C. Wilson, H. N. Nyiera, P. A. Kotei, V. Oklejas, D. W. Mittan-Moreau, E. A. Schriber, K. Christensen, I. Inoue, S. Owada, K. Tono, M. Sugahara, S. Inaba-Inoue, M. Vaikili, C. J. Milne, F. Dall'Antonia, D. Khakhulin, F. Ardana-Lamas, F. Lima, J. Valerio, H. Han, T. Gallo, H. Yousef, O. Turkot, I. J. Bermudez Macias, T. Kluyver, P. Schmidt, L. Gelisio, A. R. Round, Y. Jiang, D. Vinci, Y. Uemura, M. Kloos, A. P. Mancuso, M. Warren, N. K. Sauter, J. Zhao, T. Smidt, **H. J. Kulik**, S. Sharifzadeh*, A. S. Brewster*, and J. N. Hohman* "Ligand-mediated Quantum Yield Enhancement in 1-Dimensional Silver Organothiolate Metal-Organic Chalcogenolates", *submitted.*

188. I. Kevlishvili, J. Vakil, D. W. Kastner, X. Huang, S. L. Craig, and **H. J. Kulik*** "High-Throughput Discovery of Ferrocene Mechanophores with Enhanced Reactivity and Network Toughening", *submitted.*
https://doi.org/10.26434/chemrxiv-2024-dsj2g

187. H. Wakefield IV, J. Jiang, N. J. Fromel, I. Kevlishvili, Y. Yao, S. L. Craig, **H. J. Kulik**, and R. S. Klausen* "Isomer-Driven Polymerization, Depolymerization, and Reconstruction", *submitted.*

186. A. Herzog-Arbeitman, I. Kevlishvili, D. Sen, J. Lian, J. Chakraverty, S. Wang, B. D. Olsen*, **H. J. Kulik***, S. L. Craig*, and J. A. Johnson* "Toughening polymer networks via chemo- and regioselective junction mechanochemistry", *submitted.*

185. D. W. Kastner, C. R. Reinhardt, H. Adamji, M. T. Manetsch, Y. Román-Leshkov, and **H. J. Kulik*** "Dynamic Charge Distribution as a Key Driver of Catalytic Reactivity in an Artificial Metalloenzyme", *submitted.*
https://doi.org/10.26434/chemrxiv-2024-xhlgh

184. R. Zhu, H. Adamji, Z. J. Berkson, J. Zhu, A. R. Head, **H. J. Kulik**, C. Copéret, and Y. Román-Leshkov, "Insights

into the catalytic promotion of propylene self-metathesis over silica-supported molybdenum oxide using substituted olefins", *submitted.* https://doi.org/10.26434/chemrxiv-2024-f7dh4
183. Y. Du*, C. Duan*, A. M. Bran*, A. Sotnikova, Y. Qu, **H. J. Kulik**, A. Bosselut, J. Xu, and P. Schwaller "Large Language Models are Catalyzing Chemistry Education", *submitted.*
182. C. Duan*, G.-H. Liu, Y. Du, T. Chen, Q. Zhao, H. Jia, C. P. Gomes, E. A. Theodorou, and **H. J. Kulik** "React-OT: Optimal Transport for Generating Transition States in Chemical Reactions", *submitted.* https://doi.org/10.48550/arXiv.2404.13430
181. M. Torrens-Spence, J. O. Matos, T. Li, D. W. Kastner, C. Y. Kim, Z. Wang, C. M. Glinkerman, J. Sherk, **H. J. Kulik**, Y. Wang, and J.-K. Weng* "Mechanistic basis for the emergence of EPS1 as a catalyst in salicylic acid biosynthesis of Brassicaceae", *Nature Communications,* **in press**.
180. C. Oh, A. Nandy, S. Yue, and **H. J. Kulik*** "MOFs with the Stability for Practical Gas Adsorption Applications Require New Design Rules", *ACS Applied Materials & Interfaces,* **in press**. https://doi.org/10.1021/acsami.4c13250
179. A. Del Rio Flores, R. Zhai, D. W. Kastner, K. Seshadri, S. Yang, K. De Matias, Y. Shen, W. Cai, M. Narayanamoorthy, N. B. Do, Z. Xue, D. Al Marzooqi, **H. J. Kulik***, and W. Zhang* "Enzymatic synthesis of azide by a promiscuous N-nitrosylase", *Nature Chemistry,* **in press**. https://doi.org/10.1038/s41557-024-01646-2
178. S. Rajpurohit*, V. Vennelakanti, and **H. J. Kulik** "Improving Predictions of Spin-Crossover Complex Properties through DFT Calculations with a Local Hybrid Functional", *The Journal of Physical Chemistry A*, **in press**. https://doi.org/10.1021/acs.jpca.4c05046
177. Y. Sun*, K. Wang, X. Huang, S. Wei, E. Contreras, P. K. Jain, L. M. Campos, **H.J. Kulik***, and J. S. Moore* "Caged AIEgens: Multi-Color and White Emission Triggered by Mechanical Activation", *Journal of the American Chemical Society,* **146**, 27117-27126 (2024).
176. C. R. Reinhardt, M. T. Manetsch, W.-L. Li, Y. Román-Leshkov, T. Head-Gordon, and **H. J. Kulik*** "Computational Screening of Putative Catalyst Transition Metal Complexes as Guests in a $Ga_4L_6^{-12}$ Nanocage", *Inorganic Chemistry*, **63**, 14609-14622 (2024).
175. R. C. Diehl, R. S. Chorghade, A. M. Keys, M. M. Alam, S. A. Early, A. E. Dugan, M. Krupkin, K. Ribbeck, **H. J. Kulik**, and L. L. Kiessling* "CH-π interactions Are Required for Human Galectin-3 Function", *JACS Au,* **4**, 3028-3037 (2024).
174. I. Kevlishvili, R. G. St. Michel, A. G. Garrison, J. W. Toney, H. Adamji, H. Jia, Y. Román-Leshkov, and **H. J. Kulik*** "Leveraging natural language processing to curate the tmCAT, tmPHOTO, tmBIO, and tmSCO datasets of functional transition metal complexes", *Faraday Discussions*, **in press**. https://doi.org/10.1039/D4FD00087K
173. G. G. Terrones, S.-P. Huang, M. P. Rivera, S. Yue, A. Hernandez, and **H. J. Kulik*** "Metal–Organic Framework Stability in Water and Harsh Environments from Data-Driven Models Trained on the Diverse WS24 Data Set", *Journal of the American Chemical Society,* **146**, 20333–20348 (2024).
172. C. Violet, A. Ball, M. Heiranian, L. F. Villalobos, J. Zhang, B. Uralcan, **H. J. Kulik**, A. Haji-Akbari, and M. Elimelech* "Designing membranes with specific binding sites for selective ion separations", *Nature Water,* **2**, 706-718 (2024).
171. Y. Sun, I. Kevlishvili, T. B. Kouznetsova, Z. P. Burke, S. L. Craig*, **H. J. Kulik***, and J. S. Moore* "The Tension Activated Carbon-Carbon Bond", *Chem*, **in press**. https://doi.org/10.1016/j.chempr.2024.05.012
170. E. R. Wearing, Y-C Yeh, G. G. Terrones, S. G. Parikh, I. Kevlishvili, **H. J. Kulik***, and C. S. Schindler* "Visible-Light-Mediated aza Paternò-Büchi Reaction of Acyclic Oximes and Alkenes for the Synthesis of Monocyclic Azetidines", *Science*, **384**, 1468-1476 (2024).
169. R. Khamlue, T. Sakurada, Y. Cho, W. S. Lee, P. Leangtom, M. G. Taylor, W. Naewtong, P. Sripetch, B. N. Ranong, T. Autila, T. Rungseesumran, T. Sudyodsuk, A. Kopwitthaya, P. Mueller, V. Promarak, **H. J. Kulik**, W. A. Tisdale*, W. Paritmongkol*, "Heterocyclic Modification Leading to Luminescent 0D Metal Organochalcogenide with Stable X-ray Scintillating Properties", *Chemistry of Materials*, **36**, 5238-5249 (2024).
168. V. Zhang, C. Ou, I. Kevlishvili, C. Hemmingsen, J. V. Accardo, **H. J. Kulik**, and J. A. Kalow* "Internal Catalysis in Dynamic Hydrogels with Associative Thioester Cross-links", *ACS Macro Letters,* **13**, 621-626 (2024).
167. H. Roh, D.-H. Kim, Y. Cho, Y.-M. Jo, J. A. del Alamo, **H. J. Kulik***, M. Dinca*, and A. Gumyusenge* "Robust Chemiresistive Behavior in Conductive Polymer/MOF Composites", *Advanced Materials*, **36**, 2312382 (2024).
166. H. Wakefield IV, S. J. Melvin, J. Jiang, I. Kevlishvili, M. A. Siegler, S. L. Craig, **H. J. Kulik**, and R. S. Klausen* "Angle-Strained Sila-Cycloalkynes", *Chemical Communications,* **60**, 4842-4845 (2024).
165. Y. Cho and **H. J. Kulik*** "Improving Gas Adsorption Modeling for MOFs by Local Calibration of Hubbard U Parameters", *Journal of Chemical Physics,* **160**, 154101 (2024).
164. D. J. Lundberg, C. M. Brown, E. O. Bobylev, N. J. Oldenhuis, Y. S. Alfaraj, J. Zhao, I. Kevlishvili, **H. J. Kulik**, and J. A. Johnson* "Nested Non-covalent Interactions Expand the Functions of Supramolecular Polymer Networks", *Nature Communications,* **15**, 39541 (2024).

163. Y. Sun, W. J. Neary, X. Huang, T. B. Kouznetsova, T. Ouchi, I. Kevlishvili, K. Wang, Y. Chen, **H. J. Kulik*,** S. L. Craig*, and J. S. Moore* "A Thermally Stable SO_2 Releasing Mechanophore: Facile Activation, Single-Event Spectroscopy, and Molecular Dynamic Simulations", *Journal of the American Chemical Society*, 146, 10943-10952 (2024).
162. Y. Hu, L. Wang, I. Kevlishvili, S. Wang, C.-Y. Chiou, P. Shieh, Y. Lin*, **H. J. Kulik***, J. A. Johnson*, and S. L. Craig* "Self-Amplified HF Release and Polymer Deconstruction Cascades Triggered by Mechanical Force", *Journal of the American Chemical Society,* **146**, 10115-10123 (2024).
161. T. Kench, A. Rahardjo, G. G. Terrones, A. Bellamkonda, T. E. Maher, M. Storch, **H. J. Kulik**, and R. Vilar* "A semi-automated, high-throughput approach for the synthesis and identification of highly photo-cytotoxic iridium complexes", *Angewandte Chemie*, **63**, e202401808 (2024).
160. V. Vennelakanti, M. Jeon, and **H. J. Kulik*** "How Do Differences in Electronic Structure Affect the Use of Vanadium Intermediates as Mimics in Non-heme Iron Hydroxylases?", *Inorganic Chemistry*, **63**, 4997-5011 (2024).
159. H. Adamji, I. Kevlishvili, A. Nandy, Y. Roman-Leshkov, and **H. J. Kulik*** "Large-scale Comparison of Fe and Ru Polyolefin C–H Activation Catalysts", *Journal of Catalysis,* **431**, 115361 (2024).
158. C. H. Ng, S. L. Kim, I. Kevlishvili, G. G. Terrones, E. R. Wearing, **H. J. Kulik***, and C. S. Schindler* "Visible-Light-Mediated Macrocyclization for the Formation of Azetine-Based Dimers", *ACS Catalysis,* **14**, 4175-4185 (2024).
157. H. Jia, C. Duan, I. Kevlishvili, A. Nandy, M. Liu, and **H. J. Kulik*** "Computational Discovery of Codoped Single-Atom Catalysts for Methane-to-Methanol Conversion", *ACS* Catalysis, **14**, 2992-3005 (2024).
156. T. A. Pitt, H. Jia, T. J. Azbell, M. E. Zick, A. Nandy, **H. J. Kulik**, and P. J. Milner* "Benchmarking Nitrous Oxide Adsorption and Activation in Metal-Organic Frameworks Bearing Coordinatively Unsaturated Metal Centers", *Journal of Materials Chemistry C*, **12**, 3164-3174 (2024).
155. V. Vennelakanti, I. B. Kilic, G. G. Terrones, C. Duan, and **H. J. Kulik*** "Machine Learning Prediction of the Experimental Transition Temperature of Fe(II) Spin-Crossover Complexes", *The Journal of Physical Chemistry A*, **128**, 204-216 (2024).
154. F. Edholm, A. Nandy, C. R. Reinhardt, D. W. Kastner, and **H. J. Kulik*** "Protein3D: Enabling Analysis and Extraction of Metal-Containing Sites from the Protein Data Bank with molSimplify", *Journal of Computational Chemistry,* **45**, 352-361 (2024).
153. I. Kevlishvili, C. Duan, and **H. J. Kulik* "**Classification of Hemilabile Ligands Using Machine Learning", *The Journal of Physical Chemistry Letters*, **14**, 11100-11109 (2023).
152. M. Rasmussen, C. Duan, **H. J. Kulik**, and J. H. Jensen* "Uncertain of uncertainties? A comparison of uncertainty quantification metrics for chemical data sets", *Journal of Cheminformatics,* **15**, 121 (2023).
151. S. Yue, A. Nandy, and **H. J. Kulik*** "Discovering Molecular Coordination Environments for Selective Ion Binding Using Machine Learning", *The Journal of Physical Chemistry B*, **127**, 10592-10600 (2023).
150. V. Vennelakanti, G. Li, and **H. J. Kulik*** "Why non-heme iron halogenases do not fluorinate C-H bonds: a computational investigation", *Inorganic Chemistry*, **62**, 19758-19770 (2023).
149. C. Duan*, Y. Du, H. Jia, and **H. J. Kulik** "Accurate transition state generation with an object-aware equivariant elementary reaction diffusion model", *Nature Computational Science*, **3,** 1045-1055 (2023).
148. I. R. Ariyarathna, Y. Cho, C. Duan, and **H. J. Kulik*** "Gas-Phase and Solid-State Electronic Structure Analysis and DFT Benchmarking of HfCO", *Physical Chemistry Chemical Physics*, **25**, 26632-26639 (2023).
147. P. N. Johnson, Y. Yao, X. Huang, I. Kevlishvili, S. Schrettl, C. Weder, **H. J. Kulik**, and S. L. Craig* "Metal Identity Effects in the Fracture Behavior of Coordinatively Crosslinked Elastomers", *Polymer*, **285**, 126337 (2023).
146. J. Zhao, E. O. Bobylev, D. J. Lundberg, N. J. Oldenhuis,H. Wang, I. Kevlishvili, S. L. Craig, **H. J. Kulik**, X. Li, and J. A. Johnson* "Polymer Networks with Cubic, Mixed Pd(II) and Pt(II) M_6L_{12} Metal–Organic Cage Junctions: Synthesis and Stress Relaxation Behavior", *Journal of the American Chemical Society*, **145**, 21879-21885 (2023).
145. K. E. Wentz, Y. Yao, I. Kevlishvili, T. B. Kouznetsova, B. A. Mediavilla, **H. J. Kulik**, S. L. Craig, and R. S. Klausen* "Systematic Investigation of Silicon Substitution on Single Macromolecule Mechanics", *Macromolecules*, **56**, 6776-6782 (2023).
144. 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", *Journal of the American Chemical Society,* **145**, 16872-16878 (2023).
143. H. Roh, S. Yue, H. Hu, K. Chen, **H. J. Kulik***, and A. Gumyusenge* "Unraveling Polymer–Ion Interactions in Electrochromic Polymers for their Implementation in Organic Electrochemical Synaptic Devices", *Advanced Functional Materials*, 20304893 (2023).
142. V. Vennelakanti, M. G. Taylor, and **H. J. Kulik*** "Assessing the Performance of Approximate Density Functional Theory on 95 Experimentally Characterized Fe(II) Spin Crossover Complexes", *Journal of Chemical Physics*, **159**, 024120 (2023).
141. H. Adamji, A. Nandy, I. Kevlishvili, Y. Román-Leshkov, and **H. J. Kulik*** "Computational Discovery of Stable

Metal-Organic Frameworks for Methane-to-Methanol Catalysis"*, Journal of the American Chemical Society*, **145**, 14365-14378 (2023).
140. A. Nandy, M. G. Taylor, and **H. J. Kulik*** "Identifying Underexplored and Untapped Regions in the Chemical Space of Transition Metal Complexes", *The Journal of Physical Chemistry Letters*, **14**, 5798-5804 (2023).
139. G. G. Terrones, Y. Chen, A. Datar, L-C. Lin, **H. J. Kulik**, and Y. G. Chung* "SESAMI APP: An Accessible Interface for Surface Area Calculation of Materials from Adsorption Isotherms"*, Journal of Open Source Software*, **8**, 5429 (2023).
138. V. Zhang, J. V. Accardo, I. Kevlishvili, E. F. Woods, S. J. Chapman, C. T. Eckdahl, **H. J. Kulik**, J. A. Kalow* "Tailoring Dynamic Hydrogels by Controlling Associative Exchange Rates", *Chem*, **9**, 1-20 (2023).
137. H. Wakefield IV, I. Kevlishvili, K. E. Wentz, Y. Yao, T. B. Kouznetsova, S. J. Melvin, E. G. Ambrosius, A. Herzog-Arbeitman, M. A. Siegler, J. A. Johnson, S. L. Craig, **H. J. Kulik**, and R. S. Klausen* "Synthesis and Ring-opening Metathesis Polymerization of a Strained trans-Silacycloheptene and Single Molecule Mechanics of its Polymer", *Journal of the American Chemical Society*, **145**, 10187-10196 (2023).
136. A. Nandy, S. Yue, C. Oh, C. Duan, G. G. Terrones, Y. G. Chung, and **H. J. Kulik*** "A Database of Ultrastable MOFs Reassembled from Stable Fragments with Machine Learning Models", *Matter*, **6**, 1585-1603 (2023).
135. Y. Cytter, A. Nandy, C. Duan, and **H. J. Kulik*** "Insights into the deviation from piecewise linearity in transition metal complexes from supervised machine learning models", *Physical Chemistry Chemical Physics*, **25**, 8103-8116 (2023). **Invited article**
134. T. Sakurada, Y. Cho, W. Paritmongkol, R. Wan, A. Su, W. S. Lee, W. Shcherbakov-Wu, P. Müller, **H. J. Kulik**, and W. A. Tisdale* "1D hybrid semiconductor silver 2,6-difluorophenylselenolate", *Journal of the American Chemical Society*, **145**, 5183-5190 (2023).
133. D. W. Kastner, A. Nandy, R. Mehmood, and **H. J. Kulik*** "Mechanistic Insights Into Substrate Positioning that Distinguish Non-heme Fe(II)/α-ketoglutarate-dependent Halogenases and Hydroxylases", *ACS Catalysis,* **13**, 2489-2501 (2023). **Cover article**
132. G. G. Terrones, C. Duan, A. Nandy, and **H. J. Kulik*** "Low-cost machine learning prediction of excited state properties of iridium-centered phosphors", *Chemical Science*, **14**, 1419-1433 (2023).
131. 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", *Nature Communications,* **14**, 597 (2023).
130. S. Yue, C. Oh, A. Nandy, G. G. Terrones, and **H. J. Kulik*** "Effects of MOF linker rotation and functionalization on methane uptake and diffusion", *Molecular Systems Design & Engineering*, **8**, 527-537 (2023). **Invited article, HOT article.**
129. 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", *Chemical Reviews*, **123**, 2737-2831 (2023).
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", *JACS Au,* 3, 391-401 (2023). **Cover article**
127. K. E. L. Husted, C. M. Brown, P. Shieh, I. Kevlishvili, S. Kristufek, J. V. Accardo, J. Cooper, H. Zafar, R. S. Klausen, **H. J. Kulik**, J. S. Moore, N. R. Sottos, J. Kalow, and J. A. Johnson* "Remolding and Deconstruction of Industrial Thermosets via Carboxylic Acid-Catalyzed Bifunctional Silyl Ether Exchange", *Journal of the American Chemical Society*, **145**, 1916-1923 (2023).
126. Y. Cho, A. Nandy, C. Duan, and **H. J. Kulik*** "DFT-based Multireference Diagnostics in the Solid State: Application to Metal-organic Frameworks", *Journal of Chemical Theory and Computation*, **19**, 190-197 (2023).
125. 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", *Nature Computational Science* **3**, 38-47 (2023).
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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

15. **H. J. Kulik*** "Reaction: The Challenge of Open-Shell Transition Metal Catalysis in "Systems Chemistry"" *Chem*, 8, 2338-2339 (2024).
14. A. Nandy and **H. J. Kulik*** "Learning Design Rules for Catalysts through Computational Chemistry and Machine Learning", in *Exploring Chemical Concepts through Theory and Computation,* ed. Shubin Liu **(in press) Book chapter**
13. H. J. Kulik* "Molecular Interactions and Catalysis", in *Comprehensive Computational Chemistry*, eds. Manuel Yanez and Russell Boyd (H. J. Kulik section editor) **4**, 449-453 (2024).
12. **H. J. Kulik** and P. Tiwary* "Artificial intelligence in computational materials science", *MRS Bulletin*, **47**, 1 (2022).
11. D. H. Ess, K. Jelfs, and **H. J. Kulik*** "Chemical Design by Artificial Intelligence", *Journal of Chemical Physics*, **157**, 120401 (2022). **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:

280. Pacifichem 2025, Honolulu, HI. "Chemical Concepts from Theory and Computation" Symposium. "TBD" *December 2025*.
279. 7th Quantum Bio-Inorganic Chemistry Conference (QBIC VII), Berlin, Germany. "TBD". *August 2025*.
278. 13th Triennial Congress of the World Association of Theoretical and Computational Chemists, Oslo, Norway. "TBD". *June 2025*. **Plenary**
277. Materials Research Society Spring Meeting, Seattle, WA. "Leveraging experimental literature data to discover novel metal-organic frameworks and mechanophores". *April 2025*.
276. American Chemical Society National Meeting, San Diego, CA. "Accelerating the discovery of transition metal complexes with machine learning". *March 2025*.
275. American Chemical Society National Meeting, San Diego, CA. "High-Throughput Discovery of Ferrocene Mechanophores with Enhanced Reactivity and Network Toughening". *March 2025*.
274. American Chemical Society National Meeting, San Diego, CA. "Leveraging experimental literature data to discover novel metal-organic frameworks". *March 2025*.
273. German Physical Society (DPG), Regensburg, Germany. "TBD". *March 2025*.
272. 2025 ONLINE Molecular Machine Learning symposium, University of Muenster. "TBD". *January 2025*. **Virtual**
271. Löwdin lectures, Uppsala University, Sweden. "TBD". *December 2024*.
270. Materials Research Society Fall Meeting, Boston, MA. "Using experimental data in computationally-guided rational design with machine learning". *December 2024*.
271. 8th International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE 2024), Jeju Island, Korea. "Discovery of Metal-organic Design Rules with Natural Language Processing and Machine Learning". *November 2024*.
270. Busan National University, Busan, Korea. "TBD". *November 2024*.
269. Seoul National University, Seoul, Korea. "TBD". *November 2024*.
268. Sydney Ross Lecture, Department of Chemistry, Renssalaer Polytechnic Institute, Troy, NY. "TBD". *November 2024*.
267. American Institute of Chemical Engineers National Meeting, San Diego, CA. "Using Machine Learning to Overcome Limitations in Electronic Structure Methodology for Chemical Discovery". *October 2024*.
266. American Institute of Chemical Engineers National Meeting, San Diego, CA. "Leveraging experimental data in machine learning models to accelerate the discovery of new materials and catalysts". *October 2024*.

Completed:

265. MIT School of Engineering, Dean's Advisory Committee, Cambridge, MA. "Leveraging experimental data for machine learning accelerated computational materials discovery". *October 2024*.
264. 7th RSC AI in Chemistry Meeting, Cambridge, UK. "Leveraging community knowledge in transition metal complex and metal organic framework discovery". *September 2024*.
263. "Data-driven discovery in the chemical sciences" Faraday Discussions, Oxford, UK. "TBD". *September 2024*.
262. 60th Symposium on Theoretical Chemistry, Braunschweig, Germany. "TBD". *September 2024*.
261. American Chemical Society National Meeting, Denver, CO. "Accelerating the discovery of novel transition metal catalysts through divide and conquer analytical and machine learning strategies". *August 2024*.
260. 45th International Conference on Coordination Chemistry, Fort Collins, CO. "Using computation to unify understanding of metal-oxos from transition metal complexes to metal-organic frameworks and enzymes". *July 2024*.
259. CECAM-Chicago Conference on Computational Reactivity, Chicago, IL. " Discovering reactive intermediates and

catalysts that bypass scaling limitations with high-throughput screening and machine learning". *July 2024.*
258. Gordon Research Conference on Organometallics, Newport, RI. "Machine learning accelerated DFT for homogeneous open-shell transition metal catalyst discovery". *July 2024.*
257. 18th Triennial European Seminar on Computational Methods in Quantum Chemistry (ESCMQC) "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *June 2024.* **Plenary**
256. Gordon Research Conference on Catalysis, New London, NH. "Addressing both activity and stability in computational catalyst discovery with machine learning". *June 2024.*
255. CCSC '24, Heidelberg Germany. "Machine Learning for Open Shell Transition Metal Complex and Metal-Organic Framework Discovery". *May 2024.*
254. University of Wisconsin, Hirschfelder Visitor, Departments of Chemistry and Chemical Engineering, Madison, WI. "Machine Learning for Open Shell Transition Metal Complex and Metal-Organic Framework Discovery". *April 2024.*
253. Brown University, Chemistry Department, Providence, RI. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *April 2024.* **Student-selected speaker**
252. Stanford University, Department of Chemistry, Stanford, CA. "Leveraging experimental data in machine learning models to accelerate the discovery of new materials". *April 2024.* **Student-selected speaker**
251. Asahi x MIT Knowledge Session, MIT ILP, Cambridge MA. "First-principles and machine learning computational strategies for natural and synthetic transition metal catalysts". *April 2024.*
250. Institute for Mathematical and Statistical Innovation "Machine Learning in Electronic-Structure Theory" Workshop, University of Chicago, Chicago, IL. "Addressing electronic structure method uncertainty in machine learning accelerated materials discovery". *March 2024.*
249. American Chemical Society National Meeting, New Orleans, LA. "Discovering catalysts that overcome scaling limitations with high-throughput screening and machine learning". *March 2024.*
248. American Physical Society March Meeting, Minneapolis, MN. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *March 2024.*
247. *R*oyal Society of Chemistry Desktop Seminar "Machine Learning and AI in Chemistry". "What artificial intelligence can do to accelerate chemical discovery". *February 2024.* **Virtual**
246. Tufts University, Department of Chemistry, Medford, MA. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *January 2024.*
245. Gordon Research Conference on Chemical Separations, Galveston, TX. "Discovering Ultrastable Metal-Organic Frameworks for Separations with Machine Learning". *January 2024.*
244. UC Berkeley, Inorganic Chemistry Colloquium, Berkeley, CA. "Machine learning for homogeneous open-shell transition metal catalyst discovery". *January 2024.*
243. Chemical Concepts from Theory and Computation (CCTC3) CECAM Workshop, Lyon, France. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *December 2023.*
242. Materials Research Society Fall Meeting, Boston, MA. "Leveraging community knowledge in machine learning models to accelerate the discovery of new catalysts and materials". *November 2023.*
241. Materials Research Society Fall Meeting, Boston, MA. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *November 2023.*
240. LightChEC Consortium, University of Zurich, Zurich, Switzerland. "Machine learning for discovery in open shell transition metal catalysis". *November 2023.* **Virtual**
239. American Institute of Chemical Engineers National Meeting, Orlando, FL. "Accelerating discovery with computational chemistry in challenging materials spaces". *November 2023.*
238. American Institute of Chemical Engineers National Meeting, Orlando, FL. "Machine learning for homogeneous open-shell transition metal catalyst discovery". *November 2023.*
237. American Institute of Chemical Engineers National Meeting, Orlando, FL. "Discovering single site and single atom catalysts with high-throughput computational screening". *November 2023.*
236. XXII Brazilian Symposium on Theoretical Chemistry (SBQT), Niteroi City, Rio de Janeiro, Brazil "Leveraging community knowledge in machine learning models to accelerate the discovery of new catalysts and materials". *October 2023.* **Plenary**
235. Johns Hopkins University, Department of Chemical & Biological Engineering, Baltimore, MD. "Leveraging community knowledge in machine learning models to accelerate the discovery of new catalysts and materials". *October 2023.*
234. Merck Research Laboratories, Rahway, NJ. "Machine learning accelerated discovery for metal organic frameworks and transition metal catalysts". *September 2023.*
233. 1st Virtual Workshop on Single Atom Catalysis. "Discovering Single Site and Single Atom Catalysts with High-

throughput Computational Screening". *August 2023*. **Virtual**
232. American Chemical Society National Meeting, San Francisco, CA. "Leveraging community knowledge in machine learning models to accelerate the discovery of new catalysts and materials". *August 2023*.
231. American Chemical Society National Meeting, San Francisco, CA. "Machine learning for homogeneous open-shell transition metal catalyst discovery". *August 2023*.
230. American Chemical Society National Meeting, San Francisco, CA. "What artificial intelligence can do to accelerate chemical discovery". *August 2023*. **Plenary**
229. American Chemical Society National Meeting, San Francisco, CA. "Overcoming the limits of approximate electronic structure models in machine learning accelerated materials discovery". *August 2023*.
228. SUNCAT Summer School Workshop, SLAC, Stanford, CA. "Addressing challenges for electronic structure and machine learning in open shell transition metal catalysis". *August 2023*.
227. 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*. **Keynote**
226. North American Catalysis Society Meeting (NAM-28), Providence, RI. "Discovering Stable and Active Catalysts with Machine Learning and Community Knowledge". *June 2023*. **Keynote**
225. Heidelberg University, IWR, Romberg Lecture, Heidelberg, Germany. "Exploring multi-million compound spaces with chemical accuracy using machine learning". *May 2023*. **Named lecture**
224. Technical University of Munich, Joint Theory Seminar, Munich, Germany. "Choosing the right electronic structure method in materials discovery: Autonomous artificial intelligence workflows to the rescue ". *May 2023*.
223. Technical University of Munich, Physical Chemistry Colloquium, Munich, Germany. "Machine learning accelerated discovery for metal organic frameworks and transition metal catalysts ". *May 2023*.
222. Molecular Systems Design & Engineering Symposium, London, UK. "Materials discovery in challenging spaces with machine learning: from transition metal complexes to metal-organic frameworks". *May 2023*.
221. Heidelberg University, IWR Tutorial Lectures, Heidelberg, Germany. "Addressing challenges of machine learning accelerated materials discovery". *May 2023*. **Two 1.5 hr tutorial lectures**
220. Heidelberg University, Department of Chemistry, Lieseberg Colloquium, Heidelberg, Germany. "Using machine learning to tame electronic structure errors in chemical discovery". *May 2023*
219. SIMPLAIX Workshop, Heidelberg, Germany. "Machine learning tools for discovery in open shell transition metal chemistry ". *May 2023*.
218. University of Bonn, Bonn, Germany. "Machine learning tools for discovery in open shell transition metal chemistry". *April 2023*.
217. IPAM, Los Angeles, CA. "Exploring multi-million compound spaces with chemical accuracy using machine learning." *March 2023. Virtual talk*
216. University of Oslo, Oslo, Norway. "Accelerating metal-organic frameworks and transition metal complex design with new simulation and machine learning tools". *March 2023*.
215. Denmark Technical University, Lyngby, Denmark. "Machine learning tools for discovery in open shell transition metal chemistry". *February 2023*.
214. Intellectual Ventures, *Virtual Talk*. "Opportunities for metal-organic frameworks". *February 2023*.
213. University of Copenhagen, Copenhagen, Denmark. "Machine learning tools for discovery in open shell transition metal chemistry". *January 2023*.
212. Distinguished MARVEL Lecture Series, EPFL, Lausanne, Switzerland. "Materials discovery in challenging spaces with machine learning: from transition metal complexes to metal-organic frameworks". *December 2022*.
211. IBM Zürich, Zürich, Switzerland. "Machine learning tools for discovery in open shell transition metal chemistry". *December 2022*.
210. ETH Zürich, Laboratory for Physical Chemistry Colloquium, Zürich, Switzerland. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *December 2022*.
209. Norwegian Chemical Society, Bergen, Norway. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools". *November 2022. Virtual presentation.*
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. "Addressing challenges of data scarcity and quality in machine-learning-accelerated computational materials discovery". *November 2022. Virtual workshop*.
206. "Automation and Digital Chemistry for Catalysis" Workshop at Imperial College, London. "Accelerating open shell transition metal catalyst discovery with machine learning". *November 2022*.

205. Korean Institute of Science and Technology (KIST), Seoul, Korea. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools" *October 2022.*
204. University of Zurich, Special Chemistry Seminar, Zürich, Switzerland. "Accelerating the design of materials and open shell transition metal catalysts with machine learning" *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.*
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. "Molecular design blueprints: materials and catalysts from new simulation and machine learning tools" *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 ($15.4M)

External funding ($14.5M)

National Institutes of Health, 08/01/24-07/31/29 $1,987,000
Revealing Nature's Blueprints for Single-Site Catalysis of C–H Activation with First-principles Modeling and Machine Learning

Murata LLC, 05/01/24-04/30/27 $592,052
Computational Discovery of Metal-Organic Frameworks for Direct Air Capture

Defense Advanced Research Projects Agency, 09/25/23-09/24/24 $127,787
Metal-Free Mechanically Interlocked Junctions through Organic Dative Covalent Bonds (Jeremiah Johnson, MIT PI; Kulik co-PI) – only amount to Kulik shown

Technical University of Munich*, 12/01/23-11/30/26 $120,000
Systematically Improvable Modeling of Electrochemical Processes, Hans Fischer Senior Fellowship

Dow Chemical, 09/01/23-08/31/26 $823,624
Developing a 3D Structure Encoder for Deep Learning Methods to Discover a Sn-free Catalyst

Department of Energy, 08/01/23-07/31/26 $525,000
Multi-scale modeling for time-dependent phenomena in the condensed phase

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 *– only amount to Kulik shown* $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, 09/01/21-08/31/25 $75,000
Alfred Sloan Fellowship in Chemistry

Department of Energy, 09/01/20-8/31/24 $8,550,000
CESMIX: Center for the Exascale Simulation of material Interfaces in Extreme Environments (Youssef Marzouk, MIT PI; Kulik co-PI) – approx. $600,000 to Kulik

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

National Science Foundation CAREER, 06/1/19-05/31/25 $593,678
CAREER: Revealing spin-state-dependent reactivity in open-shell single atom catalysts with systematically-improvable computational tools

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

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 ($0.88M)

ChemE Faculty Research Innovation Fund* 04/01/23-03/31/24 $100,000
Understanding the Human Element in Chemical Discovery
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
MIT-Portugal Program Seed Fund 06/01/22-05/31/23 $100,000
Engineering Metal-Organic Frameworks for Stability in Gas Storage Applications
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 4 M CPU/GPU hours)

NSF ACCESS renewal 10/01/24-09/30/25
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
4.31M CPU core hours + 74.75k GPU hours SDSC Expanse (est. value $68,319.44)
NSF ACCESS renewal 07/01/23-10/02/24
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
5.92M SUs SDSC Expanse (est. value $26,215.80) + 2M SU supplement

NSF ACCESS supplement 12/01/22-06/30/23
Developing Accurate Materials Design Strategies Across Method- and Length-Scales
4.55M SUs SDSC Expanse
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

Current

2024- Aaron Garrison, ChemE
2024- Anh Nguyen, ChemE
2023- Weiliang Luo, Chemistry
2023- Oluremi Akindele, BE
2023- Jacob Toney, ChemE
2023- Melissa Manetsch, ChemE
2023- Akash Ball, ChemE
2022- Roland St. Michel II, DMSE
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

Past

2019-24	Hao-Jun Jia, Chemistry	(Ph.D. '24; Deep Principle, Shenzhen, China)
2018-23	Vyshnavi Vennelakanti, Chemistry	(Ph.D. '23; PD Carter Group, Princeton U. MAE)
2018-23	Naveen Arunachalam, ChemE	(Ph.D. '23; Independent Consultant)
2017-23	Aditya Nandy, Chemistry	(Ph.D. '23; Schmidt AI Futures PD Fellow '23-25, TT Asst. Prof. UCLA '25-onward)
2017-22	Chenru Duan, Chemistry	(Ph.D. '22: Deep Principle, Shenzhen, China)
2016-21	Akash Bajaj, DMSE	(Ph.D. '21; Data Scientist, Dublin, Ireland)
2016-21	Rimsha Mehmood, Chemistry	(Ph.D. '21; Senior Scientist, Merck)
2018-21	Daniel Harper, Chemistry	(S.M. '21; Consultant at Sage Analysis)
2018-20	Mengyi Wang, DMSE	(S.M. '20)
2015-19	Jon Paul Janet, ChemE	(Ph.D. '19; Senior Scientist, Astra-Zeneca)
2014-19	Helena W. Qi, Chemistry	(Ph.D. '19; Principal Scientist, Pfizer)
2015-18	Terry Z. H. Gani, ChemE	(Ph.D. '20; Senior scientist, Cabot Corporation)
2014-18	Qing Zhao, MechE	(Ph.D. '18; TT Asst. Prof. Northeastern ChemE)
2015-17	Yusu Liu, DMSE	(Ph.D. '19 Grossman lab; Quant. Rsrcher., Weiss Asset Mgmt.)
2014-16	Lisi Xie, ChemE	(Ph.D. '16; Lam Research)
2013-16	Efthymios I. Ioannidis, ChemE	(Ph.D. '16; MIT MBA '18, Co-founder Homli)
2013-15	Natasha Seelam, ChemE	(Ph.D. '21 Tidor lab; MindsDB)

Postdoctoral Associates

Current

2024-	Daniel Mukasa	
2022-	Clorice Reinhardt	
2021-	Ilia Kevlishvili	

Past

2022-24	Matt Rivera	(Chief Technical Officer, First Light Solutions, Inc.)
2021-24	Yeongsu Cho	(TT Asst. Prof., Dept. Chemistry, U. Houston, Fall 2024)
2021-24	Ralf Meyer	(Postdoctoral Associate, U. Graz)
2021-23	Shuwen Yue	(TT Asst. Prof., Dept. of Chem. Eng., Cornell University)
2021-22	Isuru Ariyarathna	(Feynman Distinguished Postdoc. Fellow, LANL)
2020-22	Azadeh Nazemi	(Senior Scientist, Pfizer)
2020-22	Mingjie Liu	(TT Asst. Prof., Dept. of Chemistry, University of Florida)
2020-22	Yael Cytter	(Research Scientist in Israel)
2020-21	Yashraj Kulkarni	(Postdoctoral Associate, University of Copenhagen)
2019-21	Michael Taylor	(Staff Scientist, LANL)
2018-20	Jing Yang	(Assoc. Prof., Dept. of Chem. Eng., Sun Yat-sen University)
2018-20	Zhongyue Yang	(TT Asst. Prof., Dept. of Chemistry, Vanderbilt Univ.)
2017-20	Fang Liu	(TT Asst. Prof., Dept. of Chemistry, Emory Univ.)
2018-19	Tzuhsiung Yang	(TT Asst. Prof., Dept. of Chemistry, National Tsing Hua Univ.)
2016-18	Jeong Yun Kim	(Scientist, Samsung, Korea)
2014-15	Niladri Patra	(TT Asst. Prof., Dept. of Chemistry, IIT Dhanbad)

Visiting Faculty

Current

2024	Egil de Brito Sa (UFPI, Brazil)

Past

2022	Yongchul Chung (Pusan National University, Korea)
2016	Alexandre Rocha Reilly (Universidade Estadual Paulista, Brazil)

Visiting M.S., Ph.D. Students, and Postdoctoral Associates

Current

2024	Kwanchanok Kaewkwan (M.S. Boodsarin Sawotlon, Chulalongkorn University, Thailand)

Past

2024	Mohamed El-Safy (Ph.D. David Balcells, UiO, Norway)
2024	Jose Caetano (Ph.D. MIT-Portugal)
2023-4	Jakob Teetz (Kulik lab M.S. ETH Zurich, Switzerland)
2023	Frederik Ørsted Kjeldal (Ph.D. Janus Juul Eriksen, DTU, Denmark)
2023	Sangeeta Rajpurohit (P.D. LBNL)
2023	Hannes Kneiding (Ph.D. David Balcells, UiO, Norway)
2022	Jonas Oldenstaedt (M.S. '22 TUM M.S.; now at TUM)
2019	Seyed Mohamad Moosavi (Ph.D. Berend Smit lab, EPFL, Switzerland, now U. Toronto)
2018-19	Sahasrajit Ramesh (Kulik lab M.S. '19 Oxford)
2018	Stefan Gugler (Kulik lab M.S. '18 ETH Zürich; now P.D. TU Berlin)

Undergraduate, High School Students

Current

2024-	Gabriel Sanchez, MIT UROP, Class of 2027
2024-	Sunwoo Lee, MIT UROP, Class of 2027
2024-	Porter Bowen, MIT 10 UROP, Class of 2025
2024-	Gozel Dovranova, MIT 10-ENG UROP, Class of 2026
2024-	Davut Muhammetgulyyev, MIT 6-3 UROP, Class of 2027
2024-	Sukrith Velmineti, MIT Class of 2027
2023-	Almira Nurlanova, MIT 5 UROP, Class of 2027
2023-	Tigest Aboye, MIT Class of 2027
2023-	Shih-Peng Huang*, MIT 5/6-3 UROP

Past

2024	Terence Oscar-Okpala, MIT MSRP-BIO	
2023-24	Wilson Ho, MIT 6-7 UROP	
2024	Joey Lin, MIT Class of 2027	
2024	Husam Elnager, MIT Class of 2027	
2023	Titus Tsai, MIT 5 UROP	
2023	Shaheer Syed, MIT MSRP-BIO	(B.S. '24, Mount St. Mary's University, Post-Bac NIH)
2023	Alondra Hernandez*, MIT 10-ENG UROP	
2022-23	Maximiliano Martinez, MIT 10-ENG UROP	
2022-23	Mugyeom Jeon*, MIT 5 UROP	
2022-23	Jelissa Kamguem*, MIT MSRP (Lafayette College U.G. thesis '23, now: Cornell Ph.D.)	
2021-23	Freya Edholm*, MIT 10 UROP (S.B. '23, now: CSE M.S. '24 MIT)	
2022	Hongqian Zheng, UG via USTC	(now: Berkeley Ph.D.)
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	(now: Columbia Ph.D.)
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	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

10.10 "Intro to Chemical Engineering" undergraduate chemical engineering core course co-instructor ('24)

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/Psivant, Boston, MA. Open Science Fellow 2020-24

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-)
IDREAM EFRC Scientific Advisory Board (2023-)

Editorial service

International Journal of Quantum Chemistry Editorial Board member (2018-).
Reaction Chemistry and Engineering Editorial Board member (2021-).
Molecular Systems Design & Engineering Advisory Board member (2022-).
Digital Discovery Advisory Board member (2022-).
Chem Advisory Board member (2023-)
Reaction Chemistry and Engineering Advisory Board member (2020-2021).
The Journal of Physical Chemistry Editorial Board member (2020-2022).
The Journal of Chemical Physics Editorial Board member (2021-2023).
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)
Guest co-editor for *Chemical Reviews* issue on "Mechanochemistry" (with Jeff Moore and Kerstin Blank)

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, 2021)
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 (2019-2021)
ACS PHYS Councilor (2023-2025)

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/MIT MSRP-BIO (2015, 2021-2024)
Faculty speaker for women in STEM at AIChE Regional meeting (2015)
MIT ACCESS weekend for underrepresented minorities in STEM facilitator (2015-2022)
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, 2023), 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, Journal of Catalysis, and the Journal of Physical Chemistry Au, ACS Applied Materials & Interfaces, Journal of Chemical Information & Modeling.

At MIT

Thesis committee member for over 30 students across Civil Engineering, Chemistry, Chemical Engineering, and Mechanical Engineering (2013-)
ChemE undergraduate academic advisor (2014-)
ChemE graduate admissions (2014-)
Computational Systems Biology (CSBi) 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)
Freshman advising (2021-2022)
MIT Climate & Sustainability Consortium ChemE departmental representative (2022-)
Faculty Search Committee (2023-)
ChemE department head search committee (2023)
MIT ChemE Rising Stars Co-Chair (w/ K. Dane Wittrup, 2023-)
Chemistry graduate admissions (2022-)

PRESS

"The rules for assembling azetidines" *C&E News* 06/28/24
https://cen.acs.org/synthesis/rules-assembling-azetidines/102/i20
"Scientists use computational modeling to guide a difficult chemical synthesis" *MIT News* 06/27/24
https://news.mit.edu/2024/scientists-use-computational-modeling-for-difficult-chemical-synthesis-0627
"Researchers develop a detector for continuously monitoring toxic gases" *MIT News* 05/17/24
https://news.mit.edu/2024/researchers-develop-continuously-monitoring-toxic-gases-detector-0517
"Computational model captures the elusive transition states of chemical reactions" *MIT News* 12/15/23
https://news.mit.edu/2023/computational-model-captures-elusive-transition-states-1215
"A map of every conceivable molecule could be possible with AI" *New Scientist* 08/23/23
https://www.newscientist.com/article/2388562-a-map-of-every-conceivable-molecule-could-be-possible-with-ai/
"Scientists use computational modeling to design "ultrastable" materials" *MIT News* 04/04/23
https://news.mit.edu/2023/scientists-computational-modeling-design-ultrastable-materials-0404
"Mining the right transition metals in a vast chemical space" *MIT News* 03/13/23
https://news.mit.edu/2023/mining-right-transition-metals-vast-chemical-space-0313
"Scientists Use SDSC's Expanse to Advance Green Chemistry" *SDSC News* 1/27/23
https://www.sdsc.edu/News%20Items/PR20230127_GreenChemistry.html
"Heather J. Kulik to join the Chemistry Faculty" *MIT Chemistry News* 12/22/22
https://chemistry.mit.edu/chemistry-news/heather-j-kulik-to-join-the-chemistry-faculty/
"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*, 02/08/21
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
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