CHAD MICHAEL RISKO

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EDUCATIONAL BACKGROUND

PhD	Georgia Institute of Technology *Thesis Title:* Theoretical Evaluations of Electron-Transfer Processes in Organic Semiconductors	Theoretical/Physical Chemistry	2005
BS *Magna Cum Laude*	Baker University (Kansas)	Chemistry; Environmental Technology and Management	1998

EMPLOYMENT HISTORY

John C. Hubbard Professor of Chemistry	University of Kentucky	2023 – present
Faculty Director, Office of Undergraduate Research	University of Kentucky	2021 – present
Associate Professor of Chemistry	University of Kentucky	2020 – present
Assistant Professor of Chemistry	University of Kentucky	2014 – 2020
Senior Research Scientist	Georgia Institute of Technology	2011 – 2014
Research Scientist II	Georgia Institute of Technology	2009 – 2011
Scientific Officer & Industrial Liaison	Northwestern University, International Institute for Nanotechnology *IIN Director: Chad A. Mirkin*	2008 – 2009
Postdoctoral Fellow	Northwestern University *Advisors: Mark A. Ratner and Tobin J. Marks*	2005 – 2008
Visiting Graduate Researcher	Université de Mons (Belgium) *Funded by the Fonds National de la Recherche Scientifique (Belgium)* *Advisor: Jérôme Cornil*	2004 May-July
Graduate Research Assistant	Georgia Institute of Technology and University of Arizona *Advisor: Jean-Luc Brédas*	2000 – 2005
Polymer Additives Chemist	PATCO Additives, American Ingredients Co. (Kansas City, MO)	1998 – 2000

HONORS, AWARDS, & GRANTS

Honors & Awards

- John C. Hubbard Endowed Professor of Chemistry (2023 – present)
- 2022 University of Kentucky Ken Freedman Outstanding Advisor Award, Nominee
- 2021 University of Kentucky Alumni Association Great Teacher Award
- 2020 University of Kentucky Center for Appalachian Research in Environmental Sciences (UK CARES) Faculty Fellow in Science Communication
- 2019 University of Kentucky College of Arts & Sciences Award for Outstanding Undergraduate Research Mentoring
- 2019 Reviewer Award – Chemistry of Materials (The Top Reviewer; American Chemical Society)
- 2018-2019 Scialog Fellow for Advanced Energy Storage (Research Corporation for Science Advancement, RCSA)
- 2018 Office of Naval Research Young Investigator Program (ONR YIP) Award
- 2018 Cottrell Scholar (Research Corporation for Science Advancement, RCSA)
- Visiting Professor, University of Angers (Angers, France), June 17-23, 2018
- 2018 Reviewer Award – Chemistry of Materials (Top 1%; American Chemical Society)
- 2018 Top Review – *Journal of Chemical Physics* (American Institute Physics)
- 2017 Top Reviewer – *Journal of Chemical Physics* (American Institute of Physics)
- 2017 University of Kentucky Ken Freedman Outstanding Advisor Award, Nominee
- 2016 Reviewer Award, *Chemistry of Materials* (Top 1%; American Chemical Society)
- 2016 Emerging Investigator, *Journal of Materials Chemistry* (Royal Society of Chemistry)
- 2011 Best Poster, ICMR Summer Program on Emerging Materials for Thin Film Solar Cells
- 2001 Outstanding Teaching Assistant, The University of Arizona, Department of Chemistry
- 1998 Graduation with Honors, *Magna Cum Laude*, Baker University
- 1998 University of Kansas Section of the ACS Outstanding Senior Chemistry Student, Baker University
- 1997 Barry M. Goldwater Scholarship Nominee, Baker University
- 1996, 1997 E. J. Cragoe Scholarship Recipient, Chemistry Department Award, Baker University
- 1995, 1996, 1997 National Collegiate Natural Sciences Award, Baker University
- 1995 CRC Freshmen Chemistry Achievement Award, Baker University
- 1995 Phi Eta Sigma National Honors Society, Baker University

Grants Funded (total funding amounts listed)

23. Variable Temperature Studies of Redox-Active Materials for Non-Aqueous Redox Flow Batteries. PI. LG&E and KU Services Company. 10/01/2023 – 01/31/2024. $44,885.

22. Collaborative Research: DMREF: Accelerating the Commercial Readiness of Organic Semiconductor Systems (ACROSS). PI. National Science Foundation (2323422). 10/01/2023 – 09/30/2027. $952,291.

21. Robust Engineered Catalysts for the Conversion of Algae and Waste Oleaginous Biomass Feedstocks to Fuel-like Hydrocarbons via Decarboxylation/Decarbonylation. Co-PI (PI: Eduardo Santillan-Jimenez, UK). Department of Energy (DE-EE0010447). 09/01/2023 – 08/31/2026. $1,384,630.

20. Porous, Lightweight, and Semiconducting Chalcogels as High Energy Density Electrodes for Lithium-ion and Sodium-ion Batteries. Co-PI (PI: Saiful M. Islam, Jackson State University). Department of Energy (DE-SC0023485). 09/01/2022 – 08/31/2025. $224,899 (total to UK).

19. Center for Soft Photo-Electro-Chemical Systems (SPECS). Co-PI (PI: Erin Ratcliff, University of Arizona). Department of Energy, Energy Frontier Research Center (DE-SC0023411). 08/02/2022 – 08/01/2026. $649,985 (total at UK)

18. MRI: Acquisition of the Kentucky Research Informatics Composable Cloud (KyRICC). Co-PI (PI: Jeffrey C. Talbert, UK; co-PI: James N. Griffioen, Hunter M. Mosely, Vernon Bumgardner, UK). National Science Foundation Major Research Instrumentation Program (1626364). 10/01/2022 – 09/30/2023. $1,136,612 ($487,120 cost share).

17. Thermomechanical Stability of Organic Semiconductors. PI. Office of Naval Research (N00014-22-1-2179). 04/01/2022 – 12/31/2024. $284,988.

16. Beckman Scholars Program – Scholars United by Chemistry: Cultivating Excellence through Science Stewardship (SUCCESS). PI. Arnold and Mabel Beckman Foundation. 01/17/2022 – 10/15/2022. $156,000.

15. Scanning Electron Microscope and Ion Beam Milling System for Nanoscale Analysis of Next-Generation Thermionic Cathodes and Novel Nanostructured Materials. co-PI (PI: Thomas J. Balk; co-PI: John Craddock). Office of Naval Research. 08/17/2021 – 08/16/2022. $76,277.

14. EPSCoR: RII Track-2 FEC: Data-enabled Discovery and Design to Transform Liquid-based Energy Storage. PI. National Science Foundation (Cooperative Agreement 2019574). 10/01/2020 – 09/30/2024. $3,979,525.

13. DMREF: Collaborative Research: Achieving Multicomponent Active Materials through Synergistic Combinatorial, Informatics-enabled Materials Discovery. PI. National Science Foundation. 10/01/2019 – 09/30/2024. $295,990.

12. Disentangling Relationships among Dopant Structure, Dopant and Polymer Energetics, Thin-Film Morphology, and the Electrical Properties of Doped Conducting Polymer Films. Co-PI. National Science Foundation (1905734). 08/15/2019 – 08/14/2023. $452,189.

11. EPSCoR: RII Track 1: Kentucky Advanced Manufacturing Partnership for Enhanced Robotics and Structures (KAMPERS). Senior Personnel (PI: Rodney Andrews; co-PI: John Anthony, Czarena Crofcheck, Seth DeBolt, Dan Popa). National Science Foundation (1849213). 07/01/19 – 06/30/24. $20,000,000 (funding received for graduate student research assistant).

10. An DMREF-NIST Collaboration to Design and Build the OSCAR Data Curation Platform (Supplement to DMR 1627428). PI. National Science Foundation; 10/01/2018 – 09/30/2019; $100,000.

9. Decoding Nucleation and Growth in Organic Semiconductor Films. PI. Office of Naval Research (ONR) Young Investigator Program (N00014-18-1-2448); 06/01/2018 – 05/30/2021; $510,000.

8. High Energy Density Metal Oxides for Energy Storage: *in silico* Electrochemistry to Control Interface Chemistry. PI. Research Corporation for Science Advancement (RCSA) Cottrell Scholar Award (24432); 07/01/2018 – 06/30/2021; $100,000.

7. 2018 University of Kentucky Vice President for Research Minor Research Grant. Co-PI. $50,000.

6. DMREF Collaborative Research: Organic Semiconductors by Computationally Accelerated Refinement (OSCAR). Co-PI. National Science Foundation (1627428); 10/15/2016 – 09/30/2024; $539,422.

5. Collaborative Research: Solution Processing of Organic Semiconductors: A Coupled Atomistic-Continuum Framework. PI. National Science Foundation (1563412); 08/15/2016 – 07/31/2019; $208,597.

4. Directing the Thin-Film Morphologies of Organic Semiconductors by Design. PI. Office of Naval Research (N00014-16-1-2985); 08/16/2016 – 08/15/2018; $200,000.

3. A Computational, Shape-Based Approach to Crystal Engineering. PI. University of Kentucky Center for Applied Energy (CAER). 07/15/2015 – 12/31/2015; $15,000.

2. Density Functional Theory Investigations of the Stability and Reactivity of Organic Compounds in Energy Storage Applications. Co-PI. University of Kentucky College of Arts & Sciences Diversity Enhancement Grant. 12/17/2014; $2,000.

1. Functionalization Approaches to High-Mobility Organic Semiconductors. Collaborator. Merck & Company, Incorporated; 11/16/2014 – 11/15/2015; $153,380.

Computational & User Facility Grants Funded

18. Machine-Learning Approaches for π-Conjugated Polymers. Center for Integrated Nanotechnologies (CINT), Department of Energy Office of Science Nanoscale Science Research Center (NSRC). Award No. 2023BC0105. PI. User Access. 01/01/2024 – 06/30/2025.

17. High-Throughput Calculations of Non-covalent Intermolecular Interactions for Organic Semiconductors to Create Machine Learning Models. National Science Foundation Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) DISCOVER Allocation Award (CHE230081). 750,000 ACCESS Credits. PI. 08/15/2023 – 08/14/2024.

16. High-Throughput Computational Data for a Curated Database of Redox-Active Organic Materials. National Science Foundation Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) DISCOVER Allocation Award (PHY220121). 750,000 ACCESS Credits. PI. 10/26/2022 – 10/25/2023.

15. Tools to Enhance the Simulation of Polymer Semiconductors. Center for Integrated Nanotechnologies (CINT), Department of Energy Office of Science Nanoscale Science Research Center (NSRC). Award No. 2022AU0048. PI. User Access. 07/01/2022 – 12/31/2023.

14. FY 2022 Department of Defense High Performance Computing Modernization Program (HPCMP). 720,000 CPU Hours. PI.

13. High-Throughput Computational Data for a Curated Database of Organic Electronic Materials. National Science Foundation Extreme Science and Engineering Discovery Environment (XSEDE) Resource Allocation Award (CHE200119). 67,000 Node Hours. PI. 07/01/2021 – 06/30/2022.

12. High-Throughput Computational Data for a Curated Database of Organic Electronic Materials. National Science Foundation Extreme Science and Engineering Discovery Environment (XSEDE) Resource Allocation Provisional Award. 23,900 Node Hours. PI. 01/01/2021 – 06/30/2021.

11. FY 2021 Department of Defense High Performance Computing Modernization Program (HPCMP). 2,035,000 CPU Hours. PI.

10. Extending Neural Network-based Potentials to π-Conjugated Polymers. Center for Integrated Nanotechnologies (CINT), Department of Energy Office of Science Nanoscale Science Research Center (NSRC). PI. User Access. 07/01/2020 – 12/31/2021.

9. FY 2020 Department of Defense High Performance Computing Modernization Program (HPCMP). 2,200,000 CPU Hours. PI.

8. Thermodynamic Drivers and Kinetic Control for Stable and Optimized Self-Assembled π-Conjugated Microstructures. Center for Integrated Nanotechnologies (CINT), Department of Energy Office of Science Nanoscale Science Research Center (NSRC). PI. User Access. 01/26/2019 – 06/30/2020.

7. FY2019 Naval High Performance Computing Pathfinder Competition; Department of Defense, Office of the Navy. 750,000 CPU Hours. PI.

6. FY2019 Department of Defense High Performance Computing Modernization Program (HPCMP). 6,150,000 CPU Hours. PI.

5. FY2018 Naval High Performance Computing Pathfinder Competition; Department of Defense, Office of the Navy. 1,000,000 CPU Hours. PI.

4. FY2018 Access Grant to Hokule'a System at the Maui High Performance Computing Center (MHPCC). Department of Defense. PI.

3. FY 2018 Department of Defense High Performance Computing Modernization Program (HPCMP). 9,220,000 CPU Hours. PI.

2. FY 2017 Department of Defense High Performance Computing Modernization Program (HPCMP). 2,830,000 CPU Hours. PI.

1. Computational Design of Interfaces for Photovoltaics. Department of Energy Advanced Scientific Computing Research Leadership Computing Challenge (ALCC). Co-PI. February 3, 2015. Computing Time: 1,500,000 MPP units on Edison, 130,000,000 CPU hours on Mira.

RESEARCH AND CREATIVE SCHOLARSHIP

Academic Career: 183 Peer-Reviewed Publications; 2 Digital Research Products; 5 Book Chapters; 1 Invited Article Perspective; 89 Invited Presentations. ISI h-index = 50; 7,700+ citations without self-citation. Google Scholar h-index = 56, 10,100 citations, i-10 index = 131 (as of July 20, 2023). 1 Patent, 4 Provisional Patents, 8 Invention Disclosures.

Risko and Risko laboratory members are highlighted in **bold**: ***italics*** denotes postdoctoral researcher or visiting scientist; **underline** denotes graduate researcher; ***italics+underline*** denotes undergraduate researcher; * denotes corresponding author. Since independent career began in 2014: 29 undergraduate researcher co-authorships; 68 graduate researcher co-authorships; 36 postdoctoral researcher or research professor co-authorships; and, 1 visiting scientist co-authorship.

Digital Research Products

D2. Data-enabled Discovery and Design to Transform Liquid-based Energy Storage (D^3TaLES) Database. https://d3tales.as.uky.edu/

D1. Organic Crystals in Electronic and Light-Oriented Technologies (OCELOT) Database. https://oscar.as.uky.edu/ocelot/

Published Journal Articles

183. Beyond n-dopants for Organic Semiconductors: Use of Bibenzo[d]imidazoles in UV-promoted Dehalogenation Reactions of Organic Halides. K. Tang, **M.R. Brown**, **C. Risko**, M.K. Gish, G. Rumbles, P.H. Pham, O.R. Luca, S. Barlow & S.R. Marder. *Beilstein Journal of Organic Chemistry* (2023), 19, 1912-1922. DOI: 10.3762/bjoc.19.142

182. ExpFlow: A Graphical User Interface for Automated Reproducible Electrochemistry. **R. Duke**, ***S. Mahmoudi***, ***A.P. Kaur***, **V. Bhat**, I.C. Dingle, N.C. Stumme, S.K. Shaw, D. Eaton, A. Vego & **C. Risko***. *Digital Discovery* (2023), online. DOI: 10.1039/D3DD00156C

181. Chain Conformation and Exciton Delocalization in a Push−Pull Conjugated Polymer. Y. Zheng, R. Venkatesh, ***C.P. Callaway***, C. Viersen, **K.H. Fagbohungbe**, A.L. Liu, **C. Risko**, E. Reichmanis & C. Silva-Acuña. *Chemistry of Materials* (2023), online. DOI: 10.1021/acs.chemmater.3c02665

180. Chalcocarbogels as High-Capacity and Cycle-stable Electrode Materials for Lithium and Sodium Ion Batteries. T. Islam, M. Li, A. Blanton, K.A. Pitton, **K.R. Rao**, **S. Bayat**, K.M. Wiaderek, M. Adigo Weret, S.C. Roy, R. Feng, D. Li, R. Alam, J. Nie, O. Oketola, A. Pramanik, B.S. Guiton, **C. Risko**, I. Belharouak, R. Amin & S.M. Islam. *ACS Energy Letters* (2023), online. DOI: 10.1021/acsenergylett.3c02112

179. Multiexciton Quintet State Populations in a Rigid Pyrene-bridged Parallel Tetracene Dimer. L. Liang-Chun, T. Smith, **Q. Ai**, B.K. Rugg, **C. Risko**, J.E. Anthony, N.H. Damrauer & J.C. Johnson. *Chemical Science* (2023), 14, 11554-11565. DOI: 10.1039/D3SC03153E

178. An Atomistic Perspective of the Crystallization of a Naphthodithiophene in Two Hydrocarbon Solvents. **C. Karunasena**, Z. Bjelobrk & **C. Risko***. *Chemistry of Materials* (2023), 35, 17, 6823-6834. DOI: 10.1021/acs.chemmater.3c01120

177. Engineering Ligand Reactivity Enables High-Temperature Operation of Stable Perovskite Solar Cells. S.M. Park, M. Wei, J. Xu, H.R. Atapattu, F.T. Eickemeyer, K. Darabi, L. Grater, Y. Yang, C. Liu, S. Teale, B. Chen, H. Chen, T. Wang, L. Zeng, A. Maxwell, Z. Wang, **K.R. Rao**, Z. Cai, S.M. Zakeeruddin, J.T. Pham, **C. Risko**, A. Amassian, M.G. Kanatzidis, K.R. Graham, M. Grätzel & E.H. Sargent. *Science* (2023), 381, 209-215. DOI: 10.1126/science.adi4107

176. The Impact of Molecular Geometry and Functionalization on Solution Complexation of Coronene-based Buckybowls and Fullerenes. M. Ivancevic, M. Ball, **V. Bhat**, J. Wisch, S. Parkin, **C. Risko**, B. Rand & Y.L. Loo. *Chemistry of Materials* (2023) 35, 5524-5531. DOI: 10.1021/acs.chemmater.3c00903

175. Towards a Comprehensive Data Infrastructure for Redox-Active Organic Molecules Targeting Non-Aqueous Redox Flow Batteries. **R. Duke**, **V. Bhat**, ***P. Sornberger***, S.A. Odom & **C. Risko***. *Digital Discovery* (2023), 2, 1152-1162. DOI: 10.1039/D3DD00081H

174. Thin Film Organic Heteroepitaxy. J.T. Dull, X. He, J. Viereck, **Q. Ai**, R. Ramprasad, M.C. Otani, J. Sorli, J.W. Brandt, B.P. Carrow, A.D. Tinoco, Y.L. Loo, **C. Risko**, S. Rangan, A. Kahn & B.P. Rand. *Advanced Materials* (2023), 2302871. DOI: 10.1002/adma.202302871

173. New Chemical Dopant and Counterion Mechanism for Organic Electrochemical Transistors and Organic Mixed Ionic–Electronic Conductors. V.N. Le, ***J.H. Bombile***, G.S. Rupasinghe, K.N. Baustert, R. Li, I.P. Maria, M. Shahi, P. Alarcon Espejo, I. McCulloch, K.R. Graham, **C. Risko** & A.F. Paterson. *Advanced Science* (2023), 2207694. DOI: 10.1002/advs.202207694

172. Factors Impacting Dihedral Angle Rotation and Classification in π-Conjugated Systems. **R. Duke**, **V. Bhat**, ***A. Smith***, ***S. Goodlett***, S. Tretiak & **C. Risko***. *Macromolecules* (2023), 56, 5259-5267. DOI: 10.1021/acs.macromol.3c00824

171. Carboxylic Acid Decarbonylation on Nickel: The Critical Role of the Acid Binding Geometry. **K.R. Rao**, R.B. Pace, ***H. Suarez***, E. Santillan-Jimenez & **C. Risko***. *ACS Catalysis* (2023), 13, 9102-9112. DOI: 10.1021/acscatal.3c01489

170. Hydrogen-Bonding Trends in a Bithiophene with 3- or 4-Pyridyl Substituents. A.M. Costello, **R. Duke**, S. Sorensen, N.L. Kothalawala, **M. Ogbaje**, N. Sarkar, D.Y. Kim, **C. Risko**, S.A. Parkin & A.J. Huckaba. *ACS Omega* (2023) 8, 24485-24494. DOI: 10.1021/acsomega.3c02423

169. Shear-Aligned Large-Area Organic Semiconductor Crystals through Extended π-π Interaction. S. Zhang, F. Talnack, T. Jousselin-Oba, **V. Bhat**, Y. Wu, Y. Lei, Y. Tomo, H. Gong, L. Michalek, D. Zhong, C. Wu, A. Yassar, S. Mannsfeld, **C. Risko***, M. Frigoli & Z. Bao. *Journal of Materials Chemistry C* (2023) 11, 8992-9001. DOI: 10.1039/d3tc01311a

168. Computational Approaches for Organic Semiconductors: From Chemical and Physical Understanding to Predicting New Materials. **V. Bhat**, ***C.P. Callaway*** & **Chad Risko***. *Chemical Reviews* (2023) 123, 7498-7547. DOI: 10.1021/acs.chemrev.2c00704

167. Resonant X-ray Diffraction Reveals the Location of Counterions in Doped Organic Mixed Ionic Conductors. L.Q. Flagg, J.W. Onorato, C.K. Luscombe, **V. Bhat**, **C. Risko**, B. Levy-Wendt, M.F. Toney, C.R. McNeill, G. Freychet, M. Zhernenkov, R. Li & L.J. Richter. *Chemistry of Materials* (2023) 35, 10, 3960-3967. DOI: 10.1021/acs.chemmater.3c00180

166. Twisted Crystalline Organic Semiconductor Photodetectors. S. Jeong, N. Barbosa, A. Tiwari, E.K. Holland, ***L.Y. Huang***, **V. Bhat**, Y. Yang, Y. Zhang, S.J. Whittaker, M.W. Kim, A. Alaei, P. Sundaram, R. Spencer, J. Brazard, D.M. Kalyon, **C. Risko**, J.E. Anthony, T.B.M. Adachi, A.G. Shtukenberg, B. Kahr & S.S. Lee. *Advanced Functional Materials* (2023), 33, 2212531. DOI: 10.1002/adfm.202212531

165. Probing Redox Properties of Extreme Concentrations Relevant for Nonaqueous Redox-Flow Batteries. N. Stumme, **A.S. Perera**, A. Horvath, **S. Ruhunage**, D.H. Duffy, E.M. Koltonowski, J. Tupper, C. Dzierba, A.D. McEndaffer, C.M. Teague, **C. Risko*** & S.K. Shaw. *ACS Energy Materials* (2023), 6, 2819-2831. DOI: 10.1021/acsaem.2c03712

164. Relating Reorganization Energies, Exciton Diffusion Length and Non-Radiative Recombination to the Room Temperature UV-Vis Absorption Spectra of NF-SMA. S. Kashani, Z. Wang, **C. Risko** & H. Ade. *Materials Horizons* (2023), 10, 443-453. DOI: 10.1039/D2MH01228F

163. Electronic, Redox, and Optical Property Prediction of Organic π-conjugated Molecules through a Hierarchy of Machine Learning Approaches. **V. Bhat**, ***P. Sornberger***, B.S.S. Pokuri, **R. Duke**, B. Ganapathysubramanian & **C. Risko***. *Chemical Science* (2023), 14, 203-213. DOI: 10.1039/D2SC04676H

162. Data Storage Architectures to Accelerate Chemical Discovery: Data Accessibility for Individual Laboratories and the Community. **R. Duke**, **V. Bhat** & **C. Risko***. *Chemical Science* (2022), 13, 13646 -13656. DOI: 10.1039/D2SC05142G

161. Large Variability and Complexity of Isothermal Solubility for a Series of Redox-Active Phenothiazines. **A.S. Perera**, T.M. Suduwella, N.H. Attanayake, R.K. Jha, W.L. Eubanks, I. Shkrob, **C. Risko***, A.P Kaur & S.A. Odom. *Materials Advances* (2022), 3, 8705-8715. DOI: 10.1039/D2MA00598K

160. The Role of Crystal Packing on the Optical Response of Trialkyltetrelethynyl Acenes. ***L.Y. Huang***, **Q. Ai** & **C. Risko***. *Journal of Chemical Physics* (2022), 157, 084703. DOI: 10.1063/5.0097421

159. PARyOpt: A Software for Parallel Asynchronous Remote Bayesian Optimization. Algorithm 1025. B.S.S. Pokuri, A. Lofquist, **C. Risko** & B. Ganapathysubramanian. *ACM Transactions on Mathematical Software* (2022), 48, 24. DOI. 10.1145/3529517

158. Challenges in Information-Mining the Materials Literature: A Case Study and Perspective. ***A. Smith***, **V. Bhat**, **Q. Ai** & **C. Risko***. *Chemistry of Materials* (2022), 34, 4821-4827. DOI: 10.1021/acs.chemmater.2c00445

157. Computational Characterization of Charge Transport Resiliency in Molecular Solids. B.S.S. Pokuri, ***S.M. Ryno***, R. Noruzi, **C. Risko*** & B. Ganapathysubramanian. *Molecular Systems Design & Engineering* (2022), 7, 651-660. DOI: 10.1039/D1ME00163A

156. Unveiling the Structural, Electronic, and Optical Effects of Carbon-doping on Multi-layer Anatase TiO_2 (101) and the Impact on Photocatalysis. N. Umisyuhada Mohd Nor, E. Mazalan, **C. Risko**, M. Crocker & N. Aishah Saidina Amin. *Applied Surface Science* (2022), 586, 152641. DOI: 10.1016/j.apsusc.2022.152641

155. The Solution is the Solution: Data-Driven Elucidation of Solution-to-Device Feature Transfer for π-Conjugated Polymer Semiconductors. ***C.P. Callaway***, A.L. Liu, R. Venkatesh, Y. Zheng, M. Lee, J.C. Meredith, M. Grover, **C. Risko*** & E. Reichmanis. *ACS Applied Materials & Interfaces* (2022), 2022, 14, 3, 3613-3620. DOI: 10.1021/acsami.1c20994

154. Following the Crystal Growth of Anthradithiophenes through Atomistic Molecular Dynamics Simulations and Graph Characterization. ***S.M. Ryno***, R. Noruzi, **C. Karunasena**, B.S.S. Pokuri, **S. Li**, B. Ganapathysubramanian & **C. Risko***. *Molecular Systems Design & Engineering* (2022), 7, 112-122. DOI: 10.1039/D1ME00157D

153. Nanoribbons or Weakly Connected Acenes? The Influence of Pyrene Insertion on Linearly Extended Ring Systems. **Q. Ai**, T. Smith, A.D. Thilanga Liyanage, S.M. Mazza, S.R. Parkin, J.E. Anthony & **C. Risko***. *Journal of Materials Chemistry C* (2021), 9, 16929-16934. DOI: 10.1039/D1TC05193H

152. Reconsidering the Roles of Noncovalent Intramolecular "Locks" in π-Conjugated Molecules. **C. Karunasena**, **S. Li**, ***M.C. Heifner***, ***S.M. Ryno*** & **C. Risko***. *Chemistry of Materials* (2021), 33, 9139-9151. DOI: 10.1021/acs.chemmater.1c02335

151. Biotinylation as a Tool to Enhance the Uptake of Small Molecules in Gram-Negative Bacteria. A. Pandeya, L. Yang, O. Alegun, **C. Karunasena**, **C. Risko**, Z. Li & Y. Wei. *PLoS ONE* (2021), 16, e0260023. DOI: 10.1371/journal.pone.0260023

150. Lowering Electrocatalytic CO_2 Reduction Overpotential Using N-Annulated Perylene Diimide Rhenium Bipyridine Dyads with Variable Tether Length. J.D. B. Koenig, Z.S. Dubrawski, **K.R. Rao**, J. Willkomm, B.S. Gelfand, **C. Risko**, W.E. Piers & G.C. Welch. *Journal of the American Chemical Society* (2021), 143, 16849-16864. DOI: 10.1021/jacs.1c09481

149. Thermomechanical Enhancement of DPP-4T through Purposeful π-Conjugation Disruption. ***C.P. Callaway***, ***J.H. Bombile***, **W. Mask**, ***S.M. Ryno*** & **C. Risko***. *Journal of Polymer Science* (2022), 60, 559. DOI: 10.1002/pol.20210494

148. Evolution of Chain Dynamics and Oxidation States with Increasing Chain Length for a Donor–Acceptor-Conjugated Oligomer Series. S. Chaudhry, Y. Wu, Z. Cao, **S. Li**, ***J.L. Canada***, X. Gu, **C. Risko*** & J. Mei. *Macromolecules* (2021), 54, 8207-8219. DOI: 10.1021/acs.macromol.1c00963

147. Genetic Algorithms and Machine Learning for Predicting Surface Composition, Structure, and Chemistry: A Historical Perspective and Assessment. **J. Roberts**, J.R.S. Bursten & **C. Risko***. *Chemistry of Materials* (2021), 33, 6589-6615. DOI: 10.1021/acs.chemmater.1c00538

146. Synthesis, Structures, and Reactivity of Isomers of $[RuCp^*(1,4\text{-}(Me_2N)_2C_6H_4)]_2$. E. Longhi, **C. Risko**, J. Bacsa, V. Khrustalev, S. Rigin, K. Moudgil, T.V. Timofeeva, S.R. Marder & S. Barlow. *Dalton Transactions* (2021), 50, 13020-13030. DOI: 10.1039/D1DT02155A

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8. Electron Affinities of 1,1-diaryl-2,3,4,5-tetraphenyisiloles: Direct Measurements and Comparison with Experimental and Theoretical Estimates. X.W. Zhan, **C. Risko**, F. Amy, C. Chan, W. Zhao, S. Barlow, A. Kahn, J.L. Brédas & S.R. Marder. *Journal of the American Chemical Society* (2005) 127, 9021-9029. DOI: 10.1021/ja051139i

7. Bis-Aryl Substituted Dioxaborines as Electron-Transport Materials: A Comparative Density Functional Theory Investigation with Oxadiazoles and Siloles. **C. Risko**, E. Zojer, P. Brocorens, S.R. Marder & J.L. Brédas. *Chemical Physics* (2005) 313, 151-157. DOI: 10.1016/j.chemphys.2004.12.020

6. Electronic Coupling in Tetraanisylarylenediamine Mixed-Valence Systems: The Interplay between Bridge Energy and Geometric Factors. C. Lambert, **C. Risko**, V. Coropceanu, J. Schelter, S. Amthor, N.E. Gruhn, J.C. Durivage & J.L. Brédas. *Journal of the American Chemical Society* (2005) 127, 8508-8516. DOI: 10.1021/ja0512172

5. High Charge-Carrier Mobility in an Amorphous Hexaazatrinaphthylene Derivative. B.R. Kaafarani, T. Kondo, J.S. Yu, Q. Zhang, D. Dattilo, **C. Risko**, S.C. Jones, S. Barlow, B. Domercq, F. Amy, A. Kahn, J.L. Brédas, B. Kippelen & S.R. Marder. *Journal of the American Chemical Society* (2005) 127, 16358-16359. DOI: 10.1021/ja0553147

4. A Mixed-Valence Bis(diarylamino) Stilbene: Crystal Structure and Comparison of Electronic Coupling with Biphenyl and Tolane Analogues. S. Barlow, **C. Risko**, V. Coropceanu, N.M. Tucker, S.C. Jones, Z. Levi, V.N. Khrustalev, M.Y. Antipin, T.L. Kinnibrugh, T. Timofeeva, S.R. Marder & J.L. Brédas. *Chemical Communications* (2005), 764-766. DOI: 10.1039/B415018J

3. Intervalence Transitions in the Mixed-Valence Monocations of Bis(triarylamines) Linked with Vinylene and Phenylene-Vinylene Bridges. S. Barlow, **C. Risko**, S.J. Chung, N.M. Tucker, V. Coropceanu, S.C. Jones, Z. Levi, J.L. Brédas & S.R. Marder. *Journal of the American Chemical Society*(2005) 127, 16900-16911. DOI: 10.1021/ja054136e

2. Electronic Properties of Silole-Based Organic Semiconductors. **C. Risko**, G.P. Kushto, Z.H. Kafafi & J.L. Brédas. *Journal of Chemical Physics* (2004) 121, 9031-9038. DOI: 10.1063/1.1804155

1. An Anionic Organic Mixed-Valence System with a Remarkably Well-Resolved Vibrational Structure in Its Intervalence Band. **C. Risko**, S. Barlow, V. Coropceanu, M. Halik, J.L. Brédas & S.R. Marder. *Chemical Communications* (2003), 194-195. DOI: 10.1039/B210429F

Book Chapters

5. Recent Advances in the Computational Characterization of π-Conjugated Systems. J.L. Brédas, X. Chen, T. Körzdörfer, H. Li, **C. Risko**, ***S.M. Ryno*** & T. Wang. In *Handbook of Conducting Polymers*, 4th Edition. Eds. Terje A. Skotheim, Barry C. Thompson & John R. Reynolds. CRC Press, 2019.

4. Non-covalent Interactions in Organic Electronic Materials. M.K. Raava, **C. Risko** & J.L. Brédas. In *Non-Covalent Interactions in Quantum Chemistry and Physics*. Eds. de la Roza, A.O. & DiLabio, G. Elsevier, 2017.

3. Understanding the Relationships Among Molecular Structure, Excited-State Properties, and Polarizabilities of π-Conjugated Chromophores. R.L. Gieseking, **C. Risko**, S.R. Marder & J.L. Brédas. In *WSPC Reference on Organic Electronics*, Eds. Brédas, J.L. and Marder, S.R. World Scientific Publishing Company Pte. Ltd. 2017.

2. Small Optical Gap Molecules and Polymers: Using Theory to Design More Efficient Materials for Organic Photovoltaics. **C. Risko** & J.L. Brédas. In *Topics in Current Chemistry*. Eds. Beljonne, D. and Cornil, J. Springer-Verlag, Berlin. 2013. 1-38.

1. Modeling the Electronic and Optical Processes in Organic Solar Cells: Density Functional Theory and Beyond. J.L. Brédas, V. Coropceanu, C. Doiron, Y.T. Fu, T. Körzdörfer, L. Pandey, **C. Risko**, J.S. Sears, B. Yang, Y. Yi, & C. Zhang. In *Organic Solar Cells: Fundamentals, Devices, and Upscaling*. Eds. Rand, B. and Richter, H. Pan Stanford Publishing. 2013.

Article Reviews

1. **C. Risko*** & J.L. Brédas. News and Views. Organic Semiconductors: Healing Touch. *Nature Materials*, 12, 1084-1085 (2013).

Intellectual Property – Patents

1. 1,9,10-Substituted Phenothiazine Derivatives with Strained Radical Cations and Use Thereof. S.A. Odom, **C. Risko**, M.D. Casselman, C.F. Elliot, N.H. Attanayake, S. Modekrutti. U.S. Patent Number 10,854,911. Publication Date: December 1, 2020.

Intellectual Property – Provisional Patent Applications

4. Vial Elevator and Centering Mechanism. R.A. Duke, D.L. Eaton, A.P. Kaur, S. Mahmoudi, **C. Risko**, A. Vego. Provisional Patent Application 63/522,920.

3. High and Multiple Redox Potential, Stable, and Soluble Bis-diarylamine Derivatives and Uses Thereof. **C. Risko**, H. Hijazi, A.P. Kaur. University of Kentucky. Provisional Patent Application 63/492,818.

2. OCELOT Dimer V1 Dataset. V. Bhat, Q. Ai, **C. Risko**. Provisional Patent Application 63/4888713.

1. 1,9,10-Substituted Phenothiazine Derivatives with Strained Radical Cations and Use Thereof. S.A. Odom, **C. Risko**, M.D. Casselman, C.F. Elliot, N.H. Attanayake, S. Modekrutti. Provisional Patent Application 62/364,060.

Intellectual Property – Invention Disclosures

8. Vial Elevator and Centering Mechanism. R.A. Duke, D.L. Eaton, A.P. Kaur, S. Mahmoudi, **C. Risko**, A. Vego. June 22, 2023.
7. High and Multiple Redox Potential, Stable, and Soluble Bis-diarylamine Derivatives and Uses Thereof. **C. Risko**, H. Hijazi, A.P. Kaur. University of Kentucky. March 15, 2023.
6. OCELOT Dimer V1 Machine Learning Models. V. Bhat, **C. Risko**. University of Kentucky. February 12, 2023.

5. OCELOT Dimer V1 Dataset. V. Bhat, Q. Ai, **C. Risko**. University of Kentucky (Invention Disclosure: 2772). February 12, 2023.
4. ExpFlow: A Workflow for Materials Science Data Management. R. Duke, V. Bhat, **C. Risko**. University of Kentucky (Invention Report 2426). February 3, 2022.
3. D^3TaLES Data Infrastructure for Redox-Active Materials. R. Duke, V. Bhat, **C. Risko**. University of Kentucky (Invention Report 2652). February 3, 2022.
2. Data infrastructure for organic semiconductor materials. Q. Ai, V. Bhat, **C. Risko**. University of Kentucky (Invention Report 2651). February 3, 2022.
1. 1,9,10-Substituted Phenothiazine Derivatives with Strained Radical Cations and Use Thereof. S.A. Odom, **C. Risko**, M.D. Casselman, C.F. Elliot, N.H. Attanayake, S. Modekrutti. University of Kentucky (Invention Report 2125).

Invited Lectures and Conference Presentations (89 total)

89. Universal Display Corporation. Colloquium (Virtual). Ewing, New Jersey. Towards Machine-driven Discovery of Organic Materials. November 17, 2023.

88. University of Iowa, Department of Chemistry. Colloquium. Iowa City, Iowa. Towards Machine-driven Discovery of Organic Materials. November 10, 2023.

87. 7th Annual Commonwealth Computational Summit on AI in Education, Medicine, and Research. Lexington, Kentucky. Developments towards Machine-driven Design & Discovery of Organic Semiconductors. October 16, 2023.

86. Kansas State University, Department of Chemistry. Colloquium. Manhattan, Kansas. Towards Machine-driven Discovery of Organic Materials. October 12, 2023.

85. University of Kansas Department of Chemistry. DyMERS Seminar. Lawrence, Kansas. Towards Machine-driven Discovery of Organic Materials. October 11, 2023.

84. Murray State University, Department of Chemistry. Colloquium. Murray, Kentucky. From Molecules to Organic Semiconductors: At the Convergence of Molecular Design, Processing, and Data-Enabled Discovery. September 25, 2023.

83. SPIE Optics + Photonics 2023. Organic and Hybrid Field-Effect Transistors XXII. San Diego, California. Developing a Data Infrastructure and Tools for Organic Semiconductor Discovery. August 22, 2023.

82. Telluride Science & Innovation Center (TSIC) Workshop: Hierarchical Assembly and Function of Organic and Hybrid Materials. What can We do with Data to Aid in the Design and Discovery of Organic Semiconductors? July 14, 2023.

81. 15th International Symposium on Functional π-Electron Systems (F-π-15). Raleigh, North Carolina. Deconstructing the Genome of Organic Semiconductors: Developments towards in silico Materials Design & Discovery. June 17, 2023.

80. American Chemical Society (ACS) Spring 2023 Meeting. New Directions in the Physical Chemistry of Organic Semiconductors. Indianapolis, Indiana. Deconstructing the Genome of Organic Semiconductors: Developments towards in silico Materials Design. March 28, 2023 (noted March 30, 2023, in online abstract).

79. University of Delaware, National Science Foundation Research Traineeship (NRT) Program Computing and Data Science Training for Materials Innovation, Discovery, and AnalyticS (NRT-MIDAS). Do Organic Semiconductors have a Genome? Materials Discovery and the Need for Any and Better Data and Tools. (Virtual) March 24, 2023.

78. Materials Research Society (MRS) Fall 2022 Meeting. SB.06: Structure-Function Relationships and Optoelectronic Processes in Organic and Organic/Inorganic Hybrid Materials for Flexible Electronics and Photovoltaics. Boston, Massachusetts. Atomistic-Level Considerations of the Multitude of Factors to Engineer Crystalline Organic Semiconductors. November 30, 2022.

77. American Chemical Society (ACS) Fall 2022 Meeting. Next-Generation Synthesis & Structure for π-conjugated Polymers. Chicago, Illinois. Interrogating Structure, Dynamics, and Disorder in Organic Semiconductors. August 22, 2022.

76. American Chemical Society (ACS) Fall 2022 Meeting. Next-Generation Synthesis & Structure for π-conjugated Polymers. Chicago, Illinois. Dopants and Charge Carriers in Polymer-based Organic Semiconductors. August 21, 2022.

75. American Chemical Society (ACS) Fall 2022 Meeting. Advances in Crystal Structure Prediction & Crystal Engineering., Chicago, Illinois. Considering the Multitude of Factors to Engineer Crystalline Organic Semiconductors. August 21, 2022.

74. International Conference on the Science and Technology of Synthetic Metals. Glasgow, Scotland. From Molecules to Organic Semiconductors: The Multi-scale Challenge of Structure from the Perspective of Modeling. July 18, 2022.

73. Collaborative Approaches to Advances in Organic and Hybrid Electronics. Boulder, Colorado. Thinking Big (Data) about Organic Materials. May 24, 2022.

72. Centre College, Student Affiliates of the American Chemical Society, Danville, Kentucky. From Molecules to Organic Semiconductors: At the Convergence of Molecular Design, Processing, and Data-Enabled Discovery. April 13, 2022.

71. University of Oregon, Department of Chemistry & Biochemistry. Eugene, Oregon. Organic/Inorganic/Materials Chemistry Seminar. From Molecules to Organic Semiconductors: At the Convergence of Molecular Design, Processing, and Data-Enabled Discovery. February 25, 2022.

70. Northern Kentucky University, Department of Chemistry. Highland Heights, Kentucky. From Molecules to Organic Semiconductors: Perspectives from the Modeling Point of View. September 22, 2021.

69. SPIE Optics + Photonics 2021. Physical Chemistry of Semiconductor Materials and Interfaces XX. San Diego, California. Virtual Presentation. Dynamics and Disorder in the Building Blocks of Organic Semiconductors. (Hybrid Format; Virtual) August 4, 2021.

68. SPIE Optics + Photonics 2021. Organic and Hybrid Field-Effect Transistors XX. San Diego, California. Virtual Presentation. Towards Data-enabled Discovery and Design of Organic Semiconductors. (Hybrid Format; Virtual) August 2, 2021.

67. Telluride Science Research Center (TSRC) Workshop: Hierarchical Assembly and Function of Organic and Hybrid Materials. Telluride, Colorado. Organic Semiconductors: More than We Know. July 22, 2021.

66. Cambridge Crystallographic Data Centre. Virtual Presentation. From Molecules to Organic Semiconductors: Linking Structure, Processing, Polymorphs, and Response. (Virtual) May 26, 2021.

65. Spring 2021 National Meeting of the American Chemical Society. Molecular Crystal Polymorphism: How, When, & Why Molecules Pack in the Solid State. Virtual Presentation. From Molecules to Organic Semiconductors: The Challenges of Processing and Polymorphs from the Perspective of Modeling. (Virtual) April 6, 2021.

64. 2020 MRS Spring/Fall Meeting & Exhibit. Virtual Presentation. S.EL14: New Materials Design for Organic Semiconductors Through Multimodal Characterization and Computational Techniques.

Developing Models to Determine the Impacts of Synthetic Design and Processing on Organic Semiconductors. (Virtual Format) November 29, 2020.

63. Pacific Northwest National Laboratory Energy Materials Storage Initiative (EMSI) Seminar Series. Introducing D^3TaLES: Materials Chemistry, Machine Learning, and Robotics to Discover and Design Liquid-based Energy-Storage Materials. (Virtual) November 9, 2020.

62. Universiti Teknologi Malaysia. 53rd Distinguished Lecture Series. Skudai, Johor, Malaysia. Virtual Presentation. From Molecules to Organic Semiconductors: The Challenges of Processing and Polymorphs from the Perspective of Modeling. (Virtual) September 22, 2020.

61. University of Kentucky, Department of Physics and Astronomy, Condensed Matter Physics Group. Lexington, Kentucky. From Molecules to Organic Semiconductors: The Challenges of Processing and Polymorphs from the Perspective of Modeling. September 22, 2020.

60. Georgia Institute of Technology, School of Chemistry and Biochemistry. Atlanta, Georgia. Frontiers Seminar. From Molecules to Organic Semiconductors: The Challenges of Processing and Polymorphs from the Perspective of Modeling. November 21, 2019.

59. 2019 International Society for Optical Engineering (SPIE) Annual Meeting. Symposium on Physical Chemistry of Semiconductor Materials and Interfaces XVIII. San Diego, California. Small Changes, Large Impact: Understanding How Molecular Structure and Processing Impact the Assembly and Performance of Organic Semiconductors. August 13, 2019.

58. Telluride Science Research Center (TSRC) Workshop on The Role of Assembly in Dictating the Functionality and Applications of Organic Semiconductors. Telluride, Colorado. From Molecules to Materials: The Challenges of Processing and Polymorphs. July 23, 2019.

57. University of Mons Symposium on Contemplating 20 Years of Organic Electronics. Mons, Belgium. Small Changes, Large Impact: Understanding How Molecular Structure and Processing Impact the Assembly and Performance of Organic Semiconductors. July 12, 2019.

56. 3rd International Symposium on Molecular Design of Optoelectronic Materials. Beijing, China. Developing Models to Connect Molecular Topology, Processing, and the Structure of Organic Semiconductors. May 24, 2019.

55. 3rd International Symposium on Molecular Design of Optoelectronic Materials. Beijing, China. From Molecules to Materials: The Challenges of Processing and Polymorphs. May 23, 2019.

54. University of California, Santa Barbara Institute for Energy Efficiency (IEE). Santa Barbara, California. Small Changes, Large Impact: Understanding How Molecular Structure and Processing Impact the Assembly of Organic Semiconductors. May 9, 2019.

53. 2019 Materials Research Society (MRS) Spring Meeting & Exhibit. Phoenix, Arizona. EP06: Organic Electronics − Materials and Devices. From Molecular Design to Materials Properties: Developing Theoretical Tools to Aid in the Design of Organic Semiconductors. April 24, 2019.

52. American Chemical Society (ACS) Spring 2019 National Meeting. Orlando, Florida. PHYS: Materials & Techniques to Advance Redox Flow Batteries. Exploring Chemical Subtleties to Foster Improved Materials Design for Redox Flow Batteries. March 31, 2019.

51. University of Washington, Department of Chemistry. Seattle, Washington. Physical Chemistry Division Seminar. Small Changes, Large Impact: Understanding How Molecular Structure and Processing Impact the Assembly of Organic Semiconductors. March 6, 2019.

50. North Carolina State University, Department of Chemistry. Raleigh, North Carolina. Small Changes, Large Impact: Understanding How Molecular Structure and Processing Impact the Assembly and Performance of Organic Semiconductors. January 25, 2019.

49. University of Kentucky, Department of Chemical and Materials Engineering. Lexington, Kentucky. Can We Define a Genome for Organic Semiconductors? December 5, 2018.

48. 13th World Congress on Computational Mechanics (WCCM XIII). Multiscale Modeling of Structural, Mechanical and Electrochemical Properties of Materials for Energy Applications. New York, New York. Small Changes with Large Impact: Developing Multiscale Models to Understand How Chemical Structure Impacts the Performance of Organic Semiconductors. July 24, 2018.

47. EXTMOS EU-US Workshop. Princeton University, Princeton, New Jersey. Can We Define a Genome for Organic Semiconductors? July 10, 2018.

46. MOLTECH-Anjou, University of Angers. Angers, France. Deconstructing the Genome of Organic Semiconductors: Developments Towards in silico Materials Design. June 19, 2018.

45. Tampere University of Technology, Department of Chemistry. Tampere, Finland. Deconstructing the Genome of Organic Semiconductors: Developments towards in silico Materials Design. May 24, 2018.

44. International Symposium on Molecular Design of Optoelectronic Materials. Beijing, China. Keynote Lecture. Deconstructing the Genome of Organic Semiconductors: Developments towards *in silico* Materials Design. April 26, 2018.

43. Peking University, Department of Materials Science and Engineering. Beijing, China. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. April 25, 2018.

42. Institute of Chemistry, Chinese Academy of Sciences. Beijing, China. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. April 24, 2018.

41. University of Calgary, Department of Chemistry. Calgary, Alberta, Canada. Deconstructing the Genome of Organic Semiconductors: Developments towards in silico Materials Design. April 6, 2018.

40. University of Missouri, Columbia, Department of Physics. Columbia Missouri. O.M. Stewart Colloquium. Noncovalent Interactions in the Design of Organic Semiconducting Materials – A Theoretical Chemistry Perspective. March 12, 2018.

39. North Carolina State University, Department of Chemistry. Raleigh, North Carolina. Deconstructing the Genome of Organic Semiconductors: Developments towards in silico Materials Design. Department of Chemistry. December 1, 2017.

38. Southeastern Regional Meeting of the American Chemical Society (SERMACS 2017). Symposium on Contemporary Computational Chemistry. Charlotte, North Carolina. Considerations of Noncovalent Interactions in the Design of Organic Semiconducting Materials: A Theoretical Perspective. November 9, 2017.

37. XXV International Materials Research Congress (IMRC 2017). Symposium on Advances in Organic and Organic/ Inorganic Hybrid Materials for Electronics and Photonics. Cancun, Mexico. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. August 22, 2017.

36. 2017 International Society for Optical Engineering (SPIE) Annual Meeting. Symposium on Organic Field-Effect Transistors XVI. San Diego, California. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. August 9, 2017.

35. 100th Canadian Chemistry Conference and Exhibition. Symposium on Noncovalent Interactions in Quantum Chemistry and Physics: Theory and Applications. Toronto, Canada. Noncovalent Interactions in Organic Electronic Materials. May 31, 2017.

34. 100th Canadian Chemistry Conference and Exhibition. Symposium on Dye Chemistry. Toronto, Canada. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. May 29, 2017.

33. Wake Forest University. Departments of Physics and Chemistry. Winston-Salem, North Carolina. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. April 12, 2017.

32. University of North Carolina, Charlotte, Nanoscale Science Seminar. Charlotte, North Carolina. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. March 2, 2017.

31. Eastern Kentucky University, Department of Chemistry. Richmond, Kentucky. Developing Theory-Driven Approaches to Design Organic Semiconducting Materials. February 3, 2017.

30. 2016 Fall MRS Meeting, Boston, Massachusetts. EC1: Redox Activity on the Molecular Level – Fundamental Studies and Applications. Establishing Fundamental Connections between Molecular Redox Events and the Performance of Organic-based Electronic and Energy Storage Devices. November 30, 2016.

29. 2016 University of North Carolina at Chapel Hill Solar Energy Research Center (SERC) Conference. Theory-Driven Approaches to Design π-Conjugated Organic Materials for Electronics and Energy-Storage Applications. October 21, 2016.

28. XXV International Materials Research Congress (IMRC). Material Interfaces in Organic Electronics & Electrochemical Energy Storage: A Theoretical Perspective. August 15, 2016.

27. 2016 International Conference on the Science and Technology of Synthetic Metals, ICSM2016. Building a Theoretical Perspective on How Chemical Structure Determines the Performance of Organic Electronic Devices. June 28, 2016.

26. 2015 Fall MRS Meeting, Boston, Massachusetts. Symposium Z: Molecularly Ordered Organic and Polymer Semiconductors – Fundamentals and Devices. Revealing the Relationships among Chemical Structure, Molecular Packing, and the Performance of Organic Electronic Devices. December 2, 2015.

25. Center for Hierarchal Materials Design (CHiMaD) and National Institute of Standards and Technology (NIST) Workshop on Advances and Challenges in Soft Matter Photovoltaic Research, University of Chicago, Chicago, Illinois. Unraveling the Structure-Processing-Property Paradigm: A Theoretical Perspective. November 13, 2015.

24. Telluride Scientific Research Center (TSRC) Workshop on Multiscale Simulations of Organic Electronic Materials, Telluride, Colorado. Untangling Relationships among Chemical Structure, Molecular Packing, and the Performance of Organic Electronic Devices. July 16, 2015.

23. University of Kentucky, Department of Physics and Astronomy, Condensed Matter Physics Group. Unraveling the Molecular-Structure–Materials-Property Paradigm in Organic Electronics Materials: A Theoretical Perspective. April 14, 2015.

22. 249th ACS Meeting and Exposition, Denver, Colorado. Computational Description of Donor-Acceptor π-Conjugated Materials for Organic Photovoltaics Applications. March 22, 2015.

21. 5th Simpósio de Estrutura Eletrônica e Dinâmica Molecular (V SeedMol), Pirenópolis, GO, Brazil. How Molecular Structure and Solid-State Packing Impact Underlying Electronic Processes in Organic Electronic Devices: Insight from Theoretical Materials Chemistry Approaches. September 17, 2014.

20. Kentucky Organic Electronics Meeting (KOEM), Lexington, Kentucky. Solid-State Molecular Packing and the Fundamental Physical Processes in Organic Electronic Devices: Insight from Theoretical Materials Chemistry Approaches. June 23, 2014.

19. European Materials Research Society (E-MRS) Spring 2014, Lille, France. Symposium on Computational Modeling of Organic Semiconductors: From the Quantum World to actual Devices. Solid-State Molecular Packing and the Fundamental Physical Processes in Organic Electronic Devices: Insight from Quantum-Chemical Approaches. May 26, 2014.

18. University of Kentucky, Department of Chemistry. Solid-State Molecular Packing and the Fundamental Physical Processes in Organic Electronic Devices: Insight from Theoretical Materials Chemistry Approaches. March 31, 2014.

17. University of Kansas, Department of Chemistry. Building a Molecular-Scale Perspective on the Fundamental Physical Processes of Organic Electronic Devices. December 19, 2013.

16. Centre Européen de Calcul Atomique et Moléculaire (CECAM) Workshop on Structure-Property Relationships of Molecular Precursors to Organic Electronics, Lausanne, Switzerland. *Young Talent's Talk:* A Molecular Perspective on the Physical Processes in Organic Solar Cells. October 22, 2013.

15. 12th European Conference on Molecular Electronics (ECME) 2013, London, England. Unravelling the Influence of Molecular Packing on the Properties of Organic Solar Cell Active Layers: A Theoretical Perspective. September 7, 2013.

14. Theory and Applications of Computational Chemistry (TACC) 2012, Pavia, Italy. Resolving the Intricacies of the Organic-Organic Interface in Printed Electronic Devices: A Computational Approach. September 4, 2012.

13. Baylor University, Department of Chemistry and Biochemistry. Waco, Texas. Developing Insight into the Complexity of the Electronic and Optical Processes in Organic Solar Cells. November 28, 2011.

12. Kent State University, Department of Physics. Kent, Ohio. Developing Insight into the Complexity of the Electronic and Optical Processes in Organic Solar Cells. November 14, 2011.

11. Global Organic Photovoltaics Conference (GOPV), Hangzhou, China. Electronic and Optical Processes in Organic Solar Cells: Complexity in Action. October 11, 2011.

10. Innovation Lab Gmbh, Heidelberg, Germany. Building the Foundation of an Integrated, Multiscale Theoretical Understanding of the Electronic and Optical Processes in Organic Solar Cells. April 7, 2011.

9. International Conference on Electroluminescence and Organic Optoelectronics (ICEL 2010), Ann Arbor, Michigan. The Donor-Acceptor Interface in Organic Solar Cells: Complexity in Action. October 18, 2010.

8. University of Mons, Mons, Belgium. Research Activities in Atlanta. May 10, 2010.

7. Solvay NOH, Brussels, Belgium. Theoretical Characterization & Screening of OLED Host Materials. May 3, 2010.

6. Michigan State University, Department of Chemistry. Lansing, Michigan. Assessing Energy Levels and Electrostatic Interactions at Organic-Inorganic Interfaces: Implications for Molecular Electronics. February 12, 2009.

5. Texas Christian University, Department of Chemistry. Fort Worth, Texas. Assessing Energy Levels and Electrostatic Interactions at Organic-Inorganic Interfaces: Implications for Molecular Electronics. November 13, 2007.

4. 2007 INAC/NCN Molecular Conduction and Sensing Workshop. West Lafayette, Indiana. Impact of Charge Injection Barrier on Conduction for Two Molecular Wires. July 18, 2007.

3. University of Southern Mississippi, Department of Chemistry and Biochemistry. Hattiesburg, Mississippi. Functional Organic Electronic and Optical Molecular Systems: A Theoretical Perspective. January 31, 2007.

2. University of California, Santa Barbara, Department of Chemistry and Biochemistry. Santa Barbara, California. Functional Organic Electronic and Optical Molecular Systems: A Theoretical Perspective. January 16, 2007.

1. Pennsylvania State University, Department of Chemistry. State College, Pennsylvania. Functional Organic Electronic and Optical Molecular Systems: A Theoretical Perspective. January 8, 2007.

Public Lectures

1. Telluride Scientific Research Center (TSRC) Town Talk: "New Materials for Solar Energy Capture and Conversion". Collaboration with Natalie Stingelin (Georgia Institute of Technology). July 19, 2017.

Conference Presentations with Proceedings (refereed)

3. Effect of Absorption Coefficient on the Performance of Organic Photovoltaics Based on Vinylene-linked Copolymers. S. Ko, R. Mondal, **C. Risko**, J.K. Lee, S. Hong, M.D. McGehee, J.L Brédas & Z. Bao. PMSE Preprints (2010). Presenter: S. Ko.

2. Influence of the Alkyl Side-chain Length on the Packing of Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) (PBTTT) Studied using Molecular Simulations. E.K. Cho, D. Kim, **C. Risko** & J.L. Brédas. PMSE Preprints (2010). Presenter: E.K. Cho.

1. Substrate and Dipole Effects in Metal-Molecule-Semiconductor Heterostructures. P. Carpenter, A. Scott, S. Lodha, **C. Risko**, M.A. Ratner & D. Janes. IEEE Nano2006 (2006). Presenter: A. Scott.

Conference Presentations without Proceedings

25. 2022 Spring American Chemical Society Meeting, San Diego, California. Photocatalysis and Photoelectrocatalysis: from Synthesis, Characterization, and Theoretical Studies of Advanced Materials to Clean Energy Applications. *Contributed Talk*: Dynamics and Disorder in Organic Semiconductors. March 20, 2022.

24. SPIE Optics + Photonics 2018, Organic Field-Effect Transistors XVII. San Diego, California. *Contributed Talk:* Conformational Disorder and Unusual Contacts in Organic Semiconductors. August 23, 2018.

23. SPIE Optics + Photonics 2018, Physical Chemistry of Semiconductor Materials and Interfaces XVII. San Diego, California. *Contributed Talk:* Living on the Edge: Using Novel Edge Topology to Direct Transport Characteristics in Carbon Nanoribbons. August 22, 2018.

22. 2017 Fall Materials Research Society (MRS) Meeting, Boston, Massachusetts. *Contributed Talk:* Raising the Oxidation Potentials of Phenothiazines to Advance Redox Shuttle Performance. November 30, 2017.

21. 47th Central Regional Meeting of the American Chemical Society (CERMACS), Responsive & Functional Polymers (Nano) Materials. *Contributed Talk*: Building a Theoretical Perspective on

How Chemical Structure Determines the Performance of Polymer-Based Electronic Devices. May 20, 2016.

20. Materials Research Society (MRS) Spring 2016, Phoenix, Arizona. *Contributed Talk*: Revealing the Relationships among Chemical Structure, Molecular Packing, and the Performance of Organic Electronic Devices: A Theoretical Perspective. March 29, 2016.

19. 12th International Symposium on Functional π-Electron Systems (F-π-12), Seattle, Washington. *Contributed Talk*: Unraveling the Molecular-Structure–Materials-Property Paradigm: A Theoretical Perspective. July 23, 2015.

18. 2015 Spring Materials Research Society Meeting, San Francisco, California. *Contributed Talk*: Molecular Structure, Packing, and Exchange Repulsion: Impact on Electronic Coupling. April 7, 2015.

17. International Colloquium on Flexible Electronics and Photovoltaics, Thuwal, Saudi Arabia (KAUST). *Poster Presentation*: The Functional Dependence of the Dynamics, Morphology, and Photovoltaic Performance of Polymer/Acene Bulk-Heterojunctions on Acene Molecular Structure. November 3-5, 2013.

16. Organic Solar Cells: Theory and Experiment, From Description to Prediction, Santa Fe, New Mexico. *Invited Contributed Talk*: Materials-Scale Implications of Solvent and Temperature on [6,6]-Phenyl-C_{61}-Butyric Acid Methyl Ester (PCBM): A Theoretical Perspective. May 6-8, 2013.

15. 2012 Materials Research Society (MRS) Fall Meeting & Exhibit, Boston, Massachusetts. *Contributed Talk*: Developing Computational Models to Unravel the Donor:Acceptor Interface in Small-Molecule Organic Solar Cells. November 25-30, 2012.

14. International Conference on Science and Technology of Synthetic Metals (ICSM) 2012, Atlanta, Georgia. *Poster Presentation*: Charge-Carrier Transport at the Organic-Dielectric Interface: Impact of Molecular Packing. July 8-13, 2012.

13. 10th International Symposium on Functional π-Electron Systems (F-π-10), Beijing, China. *Poster Presentation*: Developing Models to Unravel the Complexity of the Donor-Acceptor Interface in Organic Solar Cells. October 13-17, 2011.

12. ICMR Summer Program on Emerging Materials for Thin Film Solar Cells, Santa Barbara, California. *Poster Presentation*: Building the Foundation of an Integrated, Multiscale Theoretical Understanding of the Electronic and Optical Processes in Organic Solar Cells. August 7-12, 2011. *Poster won one of Best Poster prizes.*

11. Light Harvesting Processes (LHP) 2011, Banz Monastery, Bad Staffelstein, Germany. *Poster Presentation*: Building the Foundation of an Integrated, Multiscale Theoretical Understanding of the Electronic and Optical Processes in Organic Solar Cells. April 10 - 14, 2011.

10. Gordon Research Conference on Electronic Processes in Organic Materials. *Poster Presentation*: Structure-Property Relationships of High-Performance Polymers in Bulk-Heterojunction Solar Cell Applications. July 25-30, 2010.

9. 9th International Symposium on Functional π-Electron Systems (F-π-9), Atlanta, Georgia. *Poster Presentation*: Structure-Property Relationships of High-Performance Polymers in Bulk-Heterojunction Solar Cell Applications. Atlanta, May 23-28, 2010. Poster.

8. International Conference on Molecular Photonics: Interaction of Light with Nanostructured Paterials. *Poster presentation*: Investigations of Organic-Modified Metal and Semiconductor Surfaces. August 29, 2007.

7. American Chemical Society 233rd National Meeting and Exposition. *Contributed Talk*: Extended-Molecule Investigations of Organic-Modified Metal and Semiconductor Surfaces.

6. Gordon Research Conference on Electron Donor-Acceptor Interactions. *Poster Presentation*: Extended Molecule Investigations of Metal-Molecule-Semiconductor Heterostructures. 2006.

5. Gordon Research Conference on Electronic Processes in Organic Materials. *Poster Presentation*: Extended Molecule Investigations of Oligo(phenylene-ethynylene)thiol-Metal Systems to Evaluate Parameters of Importance to Energy Level Alignment. 2006.

4. American Chemical Society 231st National Meeting & Exposition. *Poster Presentation*: Characterization and Comparison of the Singlet-Singlet and Triplet-Triplet Transitions in Neutral and Diprotonated Porphyrins and meso-tetraarylporphyrins. March 29, 2006.

3. 55th Southeast Regional Meeting of the American Chemical Society (SERMACS). *Contributed Talk*: Phenylene-Vinylene-Bridged Bis(triarylamine) Mixed-Valence Compounds: A Joint Experimental and Theoretical Investigation. November 19, 2003.

2. Alvin L. Kwiram Symposium on the Electrical, Optical, and Magnetic Properties of Organic and Hybrid Materials. *Poster Presentation*: Electron Transport Materials: Theoretical Characterization of Silole Derivatives. June 23, 2003.

1. Sixth International Conference on Organic Nonlinear Optics (ICONO). *Poster Presentation*: Electronic Structure of Organic Charge Transport Materials: Dioxaborines & Oxadiazoles. December 17, 2001.

SERVICE

Professional Memberships

- Member. American Chemical Society (ACS), 2001-present.
- Member. Materials Research Society (MRS), 2012-present.
- Associate Member. University of Kentucky Center for Appalachian Research in Environmental Sciences (UK CARES), 2020-2023.

International and National Service

- Member. Editorial Advisory Board. *Journal of Chemical Physics* (American Institute for Physics), 2024 – present.
- Associate Editor. *Chemistry of Materials* (American Chemical Society), 2021 – present.
- Member. Editorial Advisory Board, *ACS Applied Materials and Interfaces* (American Chemical Society), 2021-2022.
- Member. Advisory Board, *Materials Advances* (Royal Society of Chemistry), 2020-present.
- Member. Advisory Board, *Journal of Materials Chemistry C* (Royal Society of Chemistry), 2020-present.
- Member. Editorial Advisory Board, *Chemistry of Materials* (American Chemical Society, 2019-2021.
- Guest Editor. *Chemistry of Materials* Special Collection in Honor of Elsa Reichmanis. 2023.

- Guest Editor. *Chemistry of Materials* Festschrift for Jean-Luc Brédas. 2019.
- Facilitator. American Chemical Society (ACS) New Faculty Workshop
  - Pasadena, California. June 27-29, 2019.
  - Virtual NFW. July 21-24, 2020.
- Co-organizer, 2023 Telluride Science and Innovation Center (TSIC) Workshop on Hierarchical Assembly and Function of Organic and Hybrid Material. Telluride, Colorado. July 11-16, 2023.
- Co-organizer, 2021 Telluride Science Research Center (TSRC) Workshop on Hierarchical Assembly and Function of Organic and Hybrid Material. Telluride, Colorado. July 19-23, 2021.
- Collaborator. Cottrell Scholar Collaborative: Moving the Dial: A Network for Systemic Change. 2020-2022.
- Collaborator. Cottrell Scholar Collaborative: Development of the "Enhancing Science Courses by Integrating Python (ESCIP)" Network. 2019-2020. ESCIP Virtual Workshop, June 19 & 30, 2020.
- Co-organizer and collaborator. Cottrell Scholar Collaborative: Cottrell Scholars Collaborative (CSC) for a Science Communication Enabled Community. 2018-2019. "Workshop on Communicating Ideas," Washington, D.C., October 20 – 22, 2019.
- Collaborator. Cottrell Scholar Collaborative: Partnering with CUREnet and Professional Societies for Dissemination of CURE Curricula. 2018-2019.
- General Member. Telluride Science Research Center (TSRC), 2016-present.
- Co-organizer, 2019 Telluride Science Research Center (TSRC) Workshop on The Role of Assembly in Dictating the Functionality and Applications of Organic Semiconductors. Telluride, Colorado. July 22-26, 2019.
- Telluride Town Talk, Telluride Scientific Research Center (TSRC), Telluride, Colorado. July 18, 2017.
- Co-organizer, 2017 Telluride Science Research Center (TSRC) Workshop on Regulating the Interfacial Physicochemical Processes of Organic Semiconductors by Design. Telluride, Colorado. July 17-21, 2017
- Co-organizer, 2015 Telluride Science Research Center (TSRC) Workshop on Multiscale Simulations of Organic Electronic Materials, Telluride, Colorado. July 13-17, 2015
- Co-organizer, INAC/NCN Molecular Conduction and Sensing Workshop. Purdue University, West Lafayette, Indiana. July 18 – 20, 2007.
- Co-founder and co-director of the Northwestern University Postdocs in Chemistry (NUPC), Northwestern University, Department of Chemistry (2006-2008).

University, College, & Department Service

- Member. University of Kentucky Information Technology Advisory Council. (2023-present)
- Member. University of Kentucky Office of the Vice President for Research Project GATeWAY (Grants Administration Transformation as the WAY forward) – Technology Workgroup. (2023-present)
- Member. University of Kentucky Office of the Provost Transdisciplinary Educational Approaches to Advance Kentucky (TEK) Implementation Advisory Committee – TEK Assessment Sub-Committee (2023-present).

- Member. University of Kentucky Office of the Provost Transdisciplinary Educational Approaches to Advance Kentucky (TEK) Implementation Advisory Committee (2023-present).
- Member. University of Kentucky Office of the Provost Quality Enhancement Plan (QEP) Workgroup (2022).
- Member. University of Kentucky Office of the President LSAMP Workgroup (2022).
- Member. University of Kentucky Department of Chemistry Faculty Search Committee (2021).
- Chair. University of Kentucky Department of Chemistry Diversity and Inclusion Committee (2020-2021).
- Member. University of Kentucky Office of Vice President of Research Strategic Planning Committee Specific to Department of Defense Research (2020-2021).
- Member. University of Kentucky Department of Chemistry Executive Committee (2020-2021).
- Member. University of Kentucky Department of Chemistry Graduate Program Committee (2020-2021).
- Faculty Liaison. University of Kentucky Department of Chemistry Graduate Student Association [GSA] (2020-2021).
- Member. External Review Committee (ERC) for University of Kentucky Research (2019).
- Member. University of Kentucky Center for Applied Energy Research Center Unit Review Committee (2019).
- Member. University of Kentucky College of Arts & Sciences Advisory Committee on Industrial Engagement (2018-2020).
- Member. University of Kentucky Department of Chemistry Full-Time Instructor Search Committee (2018).
- Member. University of Kentucky Department of Chemistry Graduate Recruiting Committee (2018-2020).
- Organizer. 2017 University of Kentucky Department of Chemistry Naff Symposium. Bioelectronics: Where Chemistry, Materials, and Medicine Meet (March 31, 2017).
- Member. University of Kentucky President Appointed Committee on Academic Computing (2017-2019).
- Member. University of Kentucky Department of Chemistry *ad hoc* Committee to Develop Industrial Outreach Program (2017-2018).
- Faculty Advisor. University of Kentucky Student Affiliates of the American Chemical Society, *ChemCats* (2015-2018).
- Mentor. University of Kentucky Center for Applied Energy Research National Science Foundation (NSF) Broadening Participation in Engineering Program (2015-2019).
- Mentor. University of Kentucky College of Arts & Sciences Faculty-Student Mentoring Program (2015-2016).
- Co-Director. University of Kentucky Department of Chemistry Mathematics of Physical Chemistry Boot Camp (2015-2018).
- Organizer. 2015 University of Kentucky Department of Chemistry Undergraduate Research in Chemistry Regional Poster Competition (April 17, 2015).

- Member. University of Kentucky College of Arts & Sciences Advisory Committee on Cyberinfrastructure and Technological Advances in Research and Scholarship (2014-2017).
- Member. University of Kentucky Department of Chemistry Undergraduate Program Committee (2014-2018).
- Member. Northwestern University Task Force on Economic Development (2008-2009).
- Member. The University of Arizona Department of Chemistry Safety Committee (2002-2003).
- Member. The University of Arizona Department of Chemistry Graduate Recruiting/Admissions Committee (2001-2002).

TEACHING/INSTRUCTION/STUDENT DEVELOPMENT

Academic Courses Taught
Courses Taught during Independent Career

Spring 2024	CHE 442G: Thermodynamics and Kinetics University of Kentucky
Spring 2023	CHE 442G: Thermodynamics and Kinetics University of Kentucky
Spring 2022	CHE 442G: Thermodynamics and Kinetics University of Kentucky
Spring 2021	CHE 580 Computing and Data Science in Chemistry University of Kentucky
Spring 2020	CHE 442G: Thermodynamics and Kinetics University of Kentucky
Fall 2019	CHE 536: Organic Materials: Electronic and Photonic Properties University of Kentucky
Spring 2019	CHE 580 Computing and Data Science in Chemistry University of Kentucky
Fall 2018	Fundamental Materials Design and Computational Research in Organic Electronics Tampere University of Technology (Finland)
Fall 2018	CHE 536: Organic Materials: Electronic and Photonic Properties University of Kentucky
Fall 2017	CHE 536: Organic Materials: Electronic and Photonic Properties University of Kentucky
Spring 2017	CHE 442G: Thermodynamics and Kinetics University of Kentucky
Fall 2016	CHE 776: Physical Chemistry Seminar University of Kentucky
Fall 2016	CHE 440G: Introduction to Physical Chemistry University of Kentucky
Spring 2016	CHE 107 General College Chemistry II University of Kentucky

Fall 2015	CHE 440G: Introduction to Physical Chemistry University of Kentucky
Spring 2015	CHE 776: Physical Chemistry Seminar University of Kentucky
Spring 2015	CHE 107 General College Chemistry II University of Kentucky
Fall 2014	CHE 107 General College Chemistry II University of Kentucky
Fall 2013	CHEM 6483 Chemistry of Organic Electronic Materials (Lecturer) Georgia Institute of Technology
Spring 2013	CHEM 2803-HP Bright and Smart: Organic Materials for Electronics and Photonics (Lecturer) Georgia Institute of Technology
Fall 2012	CHEM 6483 Chemistry of Organic Electronic Materials (Lecturer) Georgia Institute of Technology
Fall 2011	CHEM 6483 Chemistry of Organic Electronic Materials (Lecturer) Georgia Institute of Technology
Spring 2011	CHEM 2803-HP Bright and Smart: Organic Materials for Electronics and Photonics (Lecturer) Georgia Institute of Technology
Fall 2000-Spring 2001	CHEM104B Fundamental Techniques of Chemistry (Laboratory Instructor) The University of Arizona
Fall 2000-Spring 2001	CHEM103A/B, Fundamentals of Chemistry (Teaching Assistant) The University of Arizona
Fall 1995-Spring 1998	CH137(138) and CH140, General Chemistry I(II) and Quantitative Analysis (Laboratory Assistant) Baker University

Curriculum and/or Short Course Development

- CHE 580 Computing and Data Science in Chemistry. University of Kentucky.
  This course-based [undergraduate] research experience (CURE) explores the application of scientific computing and data science in chemistry. Topics covered include entry level computer programming, data processing, statistics, and advanced data visualization using the Python platform, all within the context of chemical research. The course culminates in a data-driven, research-based inquiry that enables students to practice the knowledge gained, write research reports, and undertake the peer-review process.
- Fundamental Materials Design and Computational Research in Organic Electronics. Tampere University of Technology (TUT; Finland).
  Course developed and taught online with Dr. Terttu Hukka (TUT) with a focus on the design and development of organic electronic materials and the use of computational chemistry approaches to study these materials. Specifically, I developed and recorded lectures that were made available on the Moodle platform, held weekly, live video sessions with students to address questions related to the recorded lectures, and developed and refined computational chemistry laboratories that were taught locally by Dr. Hukka and her colleagues.
- CHE 536 Organic Materials: Electronic and Photonic Properties. University of Kentucky.
  As part of the Materials Chemistry emphasis Bachelor of Science degree in Chemistry, this course provides a foundational quantum-chemical description of the relationships among molecular structure and the solid-state

arrangements of molecules and/or polymers with the electronic and optical properties of organic semiconducting materials. The materials characteristics that are described are then related to their use and performance across several technologies, including displays, lighting, transistors, energy conversion / storage applications, and non-linear optics.

- Mathematics of Physical Chemistry Bootcamp. University of Kentucky.
  Developed in collaboration with Dr. Peter Kekenes-Huskey, this two-morning bootcamp provides undergraduate and graduate students an introduction or refresher to a few key mathematical and numerical approaches encountered in courses and research related to physical chemistry. Each session, which is comprised of two lectures and hands-on tutorials, is motivated by an application in physical chemistry, with a review of the mathematical modeling and solutions necessary to explore the problems. The bootcamp has been presented in mid-August from 2015 to present.
- CHEM 2803-HP Bright & Smart: Organic Materials for Electronics and Photonics. Georgia Institute of Technology.
  Developed in collaboration with Dr. Jean-Luc Brédas, Dr. John S. Sears, and Dr. Massimo Malagoli, this course combines lectures on organic electronic materials with computational chemistry laboratory sessions. I developed two of four laboratory sessions during the initial course, and modified all four laboratories with Dr. Paul Winget during the second iteration of the course.

Teaching Development and Certificates

- Attendee. 2015 Cottrell Scholars Collaborative (CSC) and American Chemical Society (ACS) New Faculty Workshop.
- Certificate. 2005-2006 Northwestern University Preparing Future Faculty (PFF) Program.

Individual Research Guidance & Development

High School Students Supervised (5 total)
Ally Watrous (2019-2020); Franklin Marrs (2019-2021); Tenzin Nangsel (2021, i-STEM program); Sophia Mancini (2022); Vijaykumar Karthikeyan (2023-present).

Undergraduate Students Supervised (22 total)
Corrine F. Elliot (2014-2017; co-advised with S.A. Odom); Tristan Finn (2015-2016); Maxwell Duff (2016); Kristen Brooks (2016-2017); Nicholas Telesz (2017-2019); Michael Heifner (2017-2018); Brandyn Thompson (2017-2018); Asare Nkansah (2017-2018); William Smith (2017-2018); Kate E. Fraser (2018); Camron De'vine (2018-2019; 2020-2021); Stephen Goodlett (2018-2020); Mitchell Stokan (2019); Jodie Canada (2019-2020); Hanna Suarez (2019-2021); Parker Sornberger (2020-2023); Andrew Smith (2020-2022); Eesh Kulshrestha (2021); Corey Roberts (2021); Kyle Eldridge (2023); Shasanka Lamichhane (2023-present); Khamil A. Allen Thomas (2023); Lucy Rosys (2023-present).

Graduate Students Supervised (16 total)
Shi Li (2015-2020; PhD); Qianxiang [Alex] Ai (2015-2021; PhD); Edward Kirkbride Loya (2016-2019; MS-track); Chamikara Karunasena (2017-2022; PhD); Walker Mask (2017-2019; MSc thesis); Josiah Roberts (2018-2021; PhD); Vinayak Bhat (2018-present); Keerthan Rao (2018-present); Uswaththa Liyanage Anton Perera (2018-present; co-advised with S.A. Odom); John C. Quinn (2019-2020; co-advised with E. Santillan-Jimenez); Rebekah Duke (2020-present); Kehinde Fagbohungbe (2021-present); Moses Ogbaje (2021-present); Sashen A. Ruhunage (2021-present); Jordan Chelle (2021-present); Megan Brown (2022-present); Sahar Bayat (2022-present); Zachary Gardner (2023-present); Nolan Lok (2023-present); Emmanual Adejumo (2023-present).

Postdoctoral Fellows Supervised (10 total)
Adam Rigby (2015-2017); Karol Jarolimek (2015-2017); Karl J. Thorley (2016-2017; co-advised with J.E. Anthony); Sean M. Ryno (2016-2018); Uma Shantini Ramasamy (2018); Ling-Yi Huang (2019-2022); Joel

Bombile (2020-present); Connor Callaway (2020-present); Siamak Mahmoudi (2021-present; co-advised with D. Eaton); Hussein Hijazi (2021-2022); Keerthan Rao (2024-present).

Graduate Degrees

Keerthan Rao, PhD (2023)
Vinayak Bhat, PhD (2023)
Chamikara Karunasena, PhD (2022)
Josiah Roberts, PhD (2021)
Qianxiang [Alex] Ai, PhD (2020)
Shi Li, PhD (2020)
Walker Mask, MSc Thesis (2019)

Member on Graduate Student Committees

Chemistry: Anthony Petty II (October 2018; PhD); Emma Holland (January 2017-July 2021; PhD); Samuel Mazza (January 2016-January 2018); Harsha Attanayake (May 2016-September 2020; PhD); Thilini Suduwella (January 2018-July 2020; MSc); Garrett Fregoso (April 2018-May 2022; MSc); Tuo Liu (April 2018-November 2022; PhD); Charles Adeniran (May 2018-April 2023; PhD); Nasir Uddin (January 2019-November 2021; PhD); Manisha De Alwis Goonatilleke (January 2019-present); Dallas Bell (May 2019-September 2020; MSc); Harindi Atapattu (May 2019-present); Zachary Lawson; Tanner Smith (October 2019-September 2023; PhD); Dean Windemuller (October 2019-present); Sharique Khan (October 2019-present); Rahul Jha (May 2020-August 2021); Michael Moore (January 2020-present); Alison Costello (January 2020-present); Kyle Baustert (September 2020-present); Chukwudalu Great Umenweke (May 2021-present); Michael Wells (May 2021-present); Yutong Wan (September 2021-present); Michael Okeke (October 2021; MSc); Keemia Abad (November 2021-present); Reagan Patton (November 2021-present); Kevin Pedersen (April 2022-present); Eve Aldridge (July 2022-present); Barron Cox (August 2022-present); Shuvo Deb Nath (October 2022-present); Piligal Gedara Nipun Chandrasiri (April 2023-present)

Chemical Engineering: Manh Tien Nguyen (August 2019-June 2023; PhD)

Physics: Nisheeta Desai (November 2016-April 2020; PhD); Barry Farmer (July 2020; PhD); Ashkan Abtahi (October 2020; PhD); Da Bi (November 2017-May 2022; PhD); Austin Nelsen (August 2021-present); Julianne Goddard (June 2022-present)

Materials Science and Engineering: Evan Hyde (March 2017-May 2020; PhD); Xiaowen Zhan (August 2016-October 2018; PhD); Aaron Liu (January 2020-April 2023; PhD; student at Georgia Institute of Technology); Sarah O'Brien (January 2022-present)

Mechanical Engineering: Raghava Sai Chaitany Davuluri (April 2018-April 2023; PhD); Siamak Mahmoudi (April 2018-March 2021; PhD); Simon Schmitt (January 2019-October 2020; PhD); Tyler Stoffel (April 2021-present)

Mining Engineering: Alind Chandra (November 2017-December 2019; PhD)

Music: Wing Heng Victor Yuen (January 2023-present)

STEM Education: Tracy Gastineau-Stevens (May 2022-June 2023; PhD)