

ZHOU ALICE LIN

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<https://scholar.google.com/citations?user=FqemY3IAAAAJ&hl=en>

RESEARCH INTERESTS

Quantum Mechanical Modeling of Chemical Reactions in Complex and Exotic Systems.

EDUCATION

The Ohio State University Columbus, OH

2009–2015 Ph.D. in Chemical Physics Advisors: Prof. Anne B. McCoy and Prof. Eric Herbst
Thesis: Theoretical Studies on the Spectroscopy of Astrochemically Significant Species and the Mechanisms of Relevant Reactions.

University of Science and Technology of China Hefei, Anhui, China

2005–2009 B.S. in Chemical Physics Advisor: Prof. Quanxin Li
Thesis: Sol–Gel Synthesis of $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3 \cdot X^-$ Nanoparticles and Investigation of Their Antibacterial Properties.

EMPLOYMENT

University of Massachusetts at Amherst Amherst, MA

2020–2026 Assistant Professor in Computational Materials Chemistry (**Expected**)

University of California, Berkeley and Lawrence Berkeley National Laboratory Berkeley, CA

2018–2020 Postdoctoral Scholar Advisors: Prof. Martin P. Head-Gordon and Prof. Alexis T. Bell
Research: Quantum Mechanical Modeling of Copper-Catalyzed Artificial Photosynthesis.

Massachusetts Institute of Technology Cambridge, MA

2015–2018 Postdoctoral Associate Advisor: Prof. Troy A. Van Voorhis
Research: “Black Box” Density Functional Theory for Molecular Photoelectronics.

GRANTS & AWARDS

University of California, Berkeley and Lawrence Berkeley National Laboratory Berkeley, CA

2019 American Chemical Society Physical Chemistry Young Investigator Award San Diego, CA

2019 Berkeley Postdoctoral Association Professional Development Award

Massachusetts Institute of Technology Cambridge, MA

2017 Massachusetts Institute of Technology Polymer Day Symposium Best Poster Award

2016 Massachusetts Institute of Technology Women in Chemistry Professional Development Grant

The Ohio State University Columbus, OH

2015 Gordon Research Conference Selected Hot Topic Talk Galveston, TX

2014 Presidential Fellowship

2013 Midwest Theoretical Chemistry Conference Poster Award Urbana–Champaign, IL

University of Science and Technology of China Hefei, Anhui, China

- 2009 Excellent Undergraduate Graduation Award
- 2009 Outstanding Bachelor's Thesis Award
- 2008 Outstanding Undergraduate Research Award
- 2008 Excellent Undergraduate Scholarship (Silver and Bronze Awards)
- 2007 Undergraduate Research Contest in Experimental Physics (2nd Place)

RESEARCH EXPERIENCE

University of California, Berkeley and Lawrence Berkeley National Laboratory Berkeley, CA

With Prof. Martin P. Head-Gordon and Prof. Alexis T. Bell Joint Center for Artificial Photosynthesis

- 2018–2020 • Developed multi-scale simulation methods for electrocatalyzed CO₂ reduction reactions.
- Designed copper-based electrocatalysts for the CO₂ reduction reactions.
- Deciphered synthetic mechanisms of C₃ products from CO₂ reduction reactions.

Massachusetts Institute of Technology Cambridge, MA

With Prof. Troy A. Van Voorhis Eni–MIT Solar Frontier Center & MIT–Harvard Center for Excitonics

- 2015–2018 • Developed non-empirical density functionals for improved accuracy of excited states.
- Designed the inexpensive data-driven algorithm for accurate predictions of quantum yields.
- Predicted electronic structures and dynamics for inter- and intra-molecular singlet fissions.
- Designed organic semiconductors with desired photochemical or electrochemical properties.

The Ohio State University Columbus, OH

With Prof. Anne B. McCoy (Now at **University of Washington**)

- 2011–2015 • Calculated rovibrational spectra and proton transfer dynamics of H₅⁺.
- Decoded the effects of large amplitude motions of H₅⁺ in spectroscopy and dynamics.
- Developed diffusion Monte Carlo approaches for rovibrational excited states.
- Derived complete nuclear permutation-inversion symmetry for H₅⁺.

With Prof. Eric Herbst (Now at **University of Virginia**) Center for Chemistry of the Universe

- 2010–2011 • Proposed gas-phase mechanisms for interstellar propene.

University of Science and Technology of China Hefei, Anhui, China

With Prof. Quanxin Li Anhui Province Key Laboratory of Biomass Clean Energy

- 2007–2009 • Developed sol–gel synthesis of polycrystalline 12 CaO · 7 Al₂O₃ · X[−] nanoparticles.
- Evaluated antibacterial properties of 12 CaO · 7 Al₂O₃ · X[−] nanoparticles.

PUBLICATIONS

*As First or Co-First Author †As Corresponding Author

20 Published

- [1] **Zhou Lin***, Alexander W. Kohn, and Troy Van Voorhis. Toward Prediction of Nonradiative Decay Pathways in Organic Compounds II: Two Internal Conversion Channels in BODIPYs. *J. Phys. Chem. C* 124(7):3925–3938, 2020
- [2] Alexander W. Kohn, **Zhou Lin***, and Troy Van Voorhis. Toward Prediction of Nonradiative Decay Pathways in Organic Compounds I: The Case of Naphthalene Quantum Yields. *J. Phys. Chem. C* 123(25):15394–15402, 2019

- [3] Ezra L. Clark, Jonathan Wong, Alejandro J. Garza, **Zhou Lin**, Martin Head-Gordon, Alexis T. Bell. Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. *J. Am. Chem. Soc.* 141(10):4191–4193, 2019
- [4] **Zhou Lin*** and Troy Van Voorhis. Triplet Tuning: A Novel Family of Non-Empirical Exchange–Correlation Functionals. *J. Chem. Theor. Comp.* 15(2):1226–1241, 2019
- [5] Yoonseob Kim, **Zhou Lin**, Intak Jeon, Troy Van Voorhis, and Timothy M. Swager. Polyaniline Nanofiber Electrodes for Reversible Capture and Release of Mercury(II) from Water. *J. Am. Chem. Soc.* 140(43):14413–14420, 2018
- [6] Pan Wang, Sibio Lin, **Zhou Lin**, Martin D. Peeks, Troy Van Voorhis, and Timothy M. Swager. A Semiconducting Conjugated Radical Polymer: Ambipolar Redox Activity and Faraday Effect. *J. Am. Chem. Soc.* 140(34):10881–10889, 2018
- [7] Yinying Ren, **Zhou Lin**, Xianwen Mao, Wenda Tian, Troy Van Voorhis and T. Alan Hatton. Superhydrophobic, Surfactant-Doped, Conducting Polymers for Electrochemically Reversible Adsorption of Organic Contaminants. *Adv. Funct. Mater.* 28(32):1801466, 2018
- [8] Pan Wang, Intak Jeon, **Zhou Lin**, Martin D. Peeks, Suchol Savagatrup, Steven E. Kooi, Troy Van Voorhis, and Timothy M. Swager. Insights into Magneto-Optics of Helical Conjugated Polymers. *J. Am. Chem. Soc.* 140(20):6501–6508, 2018
- [9] Yunfei Zhang, Lev Bromberg, **Zhou Lin**, Paul Brown, Troy Van Voorhis, and T. Alan Hatton. Polydiacetylene Functionalized with Charged Termini for Device-Free Colorimetric Detection of Malathion. *J. Colloid Interface Sci.* 528(1):27–35, 2018
- [10] Tiecheng Zhou, Joshua J. Goings, and **Zhou Lin**[†]. Viewpoints on the 2016 Theory and Applications of Computational Chemistry Conference (**Invited**). *J. Phys. Chem. A* 120(43):8485–8487, 2016
- [11] **Zhou Lin***[†]. Group Theoretical Analysis of the $\text{H}_3^+ + \text{H}_2 \longleftrightarrow \text{H}_5^+$ Reaction. *J. Molec. Spect.* 324(1):36–47, 2016
- [12] **Zhou Lin*** and Anne B. McCoy. Probing the Relationship between Large-Amplitude Motions in H_5^+ and Proton Exchange between H_3^+ and H_2 . *J. Phys. Chem. A* 119(50):12109–12118, 2015
- [13] Melanie L. Marlett, **Zhou Lin**, and Anne B. McCoy. Rotation/Torsion Coupling in H_5^+ , D_5^+ , H_4D^+ and HD_4^+ Using Diffusion Monte Carlo. *J. Phys. Chem. A* 119(35):9405–9413, 2015
- [14] János Sarka, Csaba Fábri, Tamás Szidarovszky, Attila G. Császár, **Zhou Lin**, and Anne B. McCoy. Modelling Rotations, Vibrations, and Rovibrational Couplings in Astructural Molecules – A Case Study Based on the H_5^+ Molecular Ion (**Invited**). *Mol. Phys.* 113(13–14):1873–1883, 2015
- [15] **Zhou Lin*** and Anne B. McCoy. The Role of Large-Amplitude Motions in the Spectroscopy and Dynamics of H_5^+ . *J. Chem. Phys.* 140(11):114305, 2014
- [16] **Zhou Lin*** and Anne B. McCoy. Investigation of the Structure and Spectroscopy of H_5^+ Using Diffusion Monte Carlo. *J. Phys. Chem. A* 117(46):11725–11736, 2013
- [17] **Zhou Lin***, Dahbia Talbi, Evelyne Roueff, Eric Herbst, Nadine Wehres, Callie A. Cole, Zhibo Yang, Theodore P. Snow, and Veronica M. Bierbaum. Can Interstellar Propene (CH_3CHCH_2) be Formed via Gas-Phase Reactions? *Astrophys. J.* 765(2):80, 2013
- [18] **Zhou Lin*** and Anne B. McCoy. Signatures of Large-Amplitude Vibrations in the Spectra of H_5^+ and D_5^+ . *J. Phys. Chem. Lett.* 3(24):3690–3696, 2012
- [19] Jian-Qiu Sun, Lu Gong, Jing Shen, **Zhou Lin**, and Quan-Xin Li. Sol–Gel Preparation of Porous $\text{C}_{12}\text{A}_7 \cdot \text{Cl}^-$ Crystals. *Acta Phys.-Chim. Sin.* 26(3):795–798, 2010
- [20] Lu Gong, **Zhou Lin**, Shen Ning, Jianqiu Sun, Jing Shen, Youshifumi Torimoto, and Quanxin Li.

Synthesis and Characteristics of the $C_{12}A_7 \cdot O^-$ Nanoparticles by Citric Acid Sol–Gel Combustion Method. *Mater. Lett.* 64(11):1322–1324, 2010

1 Under Review

- [21] S.R. Alfarano, S. Pezzotti, F. Sebastiani, C.J. Stein, **Z. Lin**, S. Funke, C. Hoberg, I. Kolling, C.Y. Ma, K. Mauelshagen, T. Ockelmann, G. Schwaab, L. Fu, J.-B. Brubach, P. Roy, M. Head-Gordon, K. Tschulik, M.-P. Gaigeot, and M. Havenith. Double Layer at an Electrified Interface: Water Matters. *Submitted to Science*

PRESENTATIONS

43 Oral Presentations

- [1] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *University of Georgia, Faculty Candidate Seminar*, Athens, GA, 03/2020
- [2] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *Queens College, City University of New York, Faculty Candidate Seminar*, Flushing, NY, 02/2020
- [3] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *University of California, Riverside, Faculty Candidate Seminar*, Riverside, CA, 02/2020
- [4] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *University of Massachusetts Amherst, Faculty Candidate Seminar*, Amherst, MA, 01/2020
- [5] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *Montana State University, Faculty Candidate Seminar*, Bozeman, MT, 12/2019
- [6] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *The University of Texas at Dallas, Faculty Candidate Seminar*, Richardson, TX, 12/2019
- [7] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *The Pennsylvania State University, Faculty Candidate Seminar*, University Park, PA, 12/2019
- [8] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *Emory University, Faculty Candidate Seminar*, Atlanta, GA, 11/2019
- [9] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *Tufts University, Faculty Candidate Seminar*, Medford, MA, 11/2019
- [10] Two-Dimensional Composites as Carbon Dioxide Reduction Catalysts: A Computational Design. *American Institute of Chemical Engineers Annual Meeting*, Orlando, FL, 11/2019
- [11] Formation of C_2 and C_3 Molecules in CO_2 Reduction Reaction: A Computational Exploration. *American Institute of Chemical Engineers Annual Meeting*, Orlando, FL, 11/2019
- [12] Quantum Chemistry for Complex and Exotic Systems (**Invited**). *Mississippi State University, Faculty Candidate Seminar*, Mississippi State, MS, 11/2019
- [13] CO_2 Reduction Reactions in Artificial Photosynthesis: A Computational Exploration (**Invited**). *Haverford College, Faculty Candidate Seminar*, Haverford, PA, 10/2019
- [14] Computationally Aided Design of Copper-Based Two-Dimensional Composites as Alternative, Active Carbon Dioxide Reduction Catalysts (**Physical Chemistry Young Investigator Award**). *American Chemical Society National Meeting & Exposition*, San Diego, CA, 08/2019
- [15] Formation Pathways to Three-Carbon Products from Carbon Dioxide Reduction Reactions Electrochemically Catalyzed by Metallic Copper Surfaces. *American Chemical Society National*

- Meeting & Exposition*, San Diego, CA, 08/2019
- [16] New Directions for Theoretical Models of CO₂RR – New Materials, New Mechanisms, and New Methods *Joint Center for Artificial Photosynthesis Theory Workshop*, Stanford, CA 12/2018
- [17] Understanding Quantum Yields in Naphthalenes and Boron-Dipyrromethenes: Towards a Prediction of Non-Radiative Decay Pathways in Organic Optoelectronic Materials. *American Chemical Society National Meeting & Exposition*, Boston, MA 08/2018
- [18] Theoretical Molecular Spectroscopy for Astrochemical Species and Organic Semiconductors (**Invited**). *Boston University, Special Physical Chemistry Seminar*, Boston, MA, 06/2018
- [19] Triplet-Tuning: A Novel Non-Empirical Construction Scheme of Exchange Functionals (**Selected Contributed Talk**). *Midwest Theoretical Chemistry Conference*, Chicago, IL, 06/2018
- [20] Energetics and Couplings in Oligoacene-Based Singlet Fission: Efficient and Accurate Density Functional Theory Tells the Story. *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2018
- [21] Understanding Quantum Yields in Naphthalenes and Boron-Dipyrromethenes: Towards a Prediction of Non-Radiative Decay Pathways in Organic Optoelectronic Materials. *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2018
- [22] Theoretical Molecular Spectroscopy for Astrochemical Species and Organic Semiconductors (**Invited**). *University of California, Merced, Special Theory Seminar*, Merced, CA, 06/2018
- [23] Intramolecular Singlet Fission Dynamics. *MIT–Harvard Center for Excitonics All Hands Meeting*, Cambridge, MA, 01/2018
- [24] Theoretical Molecular Spectroscopy for Astrochemical Species and Organic Semiconductors (**Invited**). *University of Missouri, Faculty Candidate Seminar*, Columbia, MO, 01/2018
- [25] Theoretical Molecular Spectroscopy for Astrochemical Species and Organic Semiconductors (**Invited**). *Wayne State University, Faculty Candidate Seminar*, Detroit, MI, 12/2017
- [26] Photochemical Dynamics for Intramolecular Singlet Fission in Covalently-Bound Pentacene Dimers (**Invited**). *Materials Day Symposium 2017 Poster Preview Session*, Cambridge, MA, 10/2017
- [27] Photochemical Dynamics for Intramolecular Singlet Fission in Covalently-Bound Pentacene Dimers. *American Chemical Society National Meeting & Exposition*, Washington D.C., 08/2017
- [28] Photochemical Dynamics for Intramolecular Singlet Fission I: Energy Levels and Non-Adiabatic Couplings (**Invited**). *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2017
- [29] Triplet Tuning – “Black-Box” Scheme for Constructing Density Functionals. *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2017
- [30] Optimally-Tuned Hybrid Functionals for Excitonic Energies in Organic Semiconductors. *MIT–Harvard Center for Excitonics All Hands Meeting*, Cambridge, MA, 01/2017
- [31] “Black-Box” Theory for Photophysics and Photochemistry in Organic Electronics (**Invited**). *The Ohio State University, Physical Chemistry Student Lecture Series*, Columbus, OH, 11/2016
- [32] Group Theoretical Analysis for Energetically Feasible Permutation of Protons in the H₃⁺ + H₂ ↔ H₅⁺ Reaction (**Invited**). *60 Years of Molecules, Motion and Matrix Elements*, Gaithersburg, MD, 06/2016
- [33] Can We Predict Quantum Yields for Fluorescent Dyes Using Excited State Density Functional Theory? *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2016
- [34] Energetically Feasible Proton Permutations in the Photodissociation of H₅⁺ (**Invited**). *International*

Symposium on Molecular Spectroscopy, Urbana–Champaign, IL, 06/2016

- [35] Prediction of Quantum Yields for Fluorescent Dyes Using DFT-Based Approach. *Eni–MIT Solar Frontier Center All Hands Meeting*, Cambridge, MA, 03/2016
- [36] Theoretical Studies of Singlet Fission in Polyacenes. *Eni–MIT Solar Frontier Center All Hands Meeting*, Cambridge, MA, 09/2015
- [37] Large Amplitude Motions and Feasible Proton Permutations in the Spectroscopy and Dynamics of H_5^+ . *American Chemical Society National Meeting & Exposition*, Boston, MA, 08/2015
- [38] The Role of Large Amplitude Motions in the Rotation/Torsion Coupling in H_5^+ (**Selected Hot Topic Talk**). *Gordon Research Conference on Gaseous Ions*, Galveston, TX, 02/2015
- [39] Roles of Large Amplitude Motions in the Proton Transfer Reaction $\text{H}_2 + \text{H}_3^+ \longleftrightarrow \text{H}_5^+ \longleftrightarrow \text{H}_3^+ + \text{H}_2$. *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2014
- [40] Investigation of Large-Amplitude Motions of H_5^+ in the Proton Transfer Reaction between H_3^+ and H_2 . *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2013
- [41] A Story of the Spectroscopy of H_5^+ (**Invited**). *The Ohio State University, Physical Chemistry Student Lecture Series*, Columbus, OH, 02/2013
- [42] Diffusion Monte Carlo Studies of the Ground-State Energetics and Structures of H_5^+ and Its Deuterated Isotopologues. *International Symposium on Molecular Spectroscopy*, Urbana–Champaign, IL, 06/2012
- [43] Chemistry of Gas Phase in the Universe and Formation of Interstellar Propylene ($\text{CH}_3\text{CH}=\text{CH}_2$) (**Invited**). *The Ohio State University, Physical Chemistry Student Lecture Series*, Columbus, OH, 10/2011

19 Poster Presentations

- [44] Triplet Tuning: A Novel Family of Non-Empirical Exchange–Correlation Functionals. *American Chemical Society National Meeting & Exposition*, San Diego, CA, 08/2019
- [45] Formation Mechanism of C_2 and C_3 Products – Oxygen Incorporation, C_3 Formation, and Composite Catalysts. *Joint Center for Artificial Photosynthesis All Hands Meeting*, Oxnard, CA, 02/2019
- [46] Photochemical Dynamics for Intramolecular Singlet Fission in Covalently-Bound Pentacene Dimers. *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, 10/2017
- [47] Quantum Models for Spectroscopy and Dynamics on Multiple Potential Surfaces. *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, 10/2017
- [48] Photochemical Dynamics for Intramolecular Singlet Fission in Covalently-Bound Pentacene Dimers. *Materials Day Symposium 2017 Poster Session*, Cambridge, MA, 10/2017
- [49] Photochemical Dynamics for Intramolecular Singlet Fission in Covalently-Bound Pentacene Dimers. *American Chemical Society National Meeting & Exposition*, Washington D.C., 08/2017
- [50] Non-Empirical Triplet Tuning – A Novel Construction Scheme of Optimally-Tuned Density Functionals for Organic Semiconductors. *American Conference on Theoretical Chemistry*, Boston, MA, 07/2017
- [51] A New Magneto–Optic Material with Giant Faraday Rotation (**Best Poster Award**). *MIT Polymer Day Symposium*, Cambridge, MA, 04/2017
- [52] Can We Decipher the Mechanism for Singlet Fission in Polyacene Aggregates Using Density Functional Theory (DFT) Based Approaches? *Merck–MIT Meet-up for Women Scientists and Engineers*, Cambridge, MA, 09/2016

- [53] Can We Decipher the Mechanism for Singlet Fission in Polyacene Aggregates Using Density Functional Theory (DFT) Based Approaches? *Theory and Application of Computational Chemistry*, Seattle, WA, 08/2016
- [54] Can We Decipher the Mechanism for Singlet Fission in Polyacene Aggregates Using Density Functional Theory (DFT) Based Approaches? *Putting the Theory Back in Density Functional Theory Summer School*, Los Angeles, CA, 08/2016
- [55] Large Amplitude Motions and Feasible Proton Permutations in the Spectroscopy and Dynamics of H_5^+ . *Gordon Research Conference on Gaseous Ions*, Galveston, TX, 02/2015
- [56] The Role of Large Amplitude Motions in the $\text{H}_2 + \text{H}_3^+ \longleftrightarrow \text{H}_5^+ \longleftrightarrow \text{H}_3^+ + \text{H}_2$ Reaction. *American Conference on Theoretical Chemistry*, Telluride, CO, 07/2014
- [57] Investigation of the Dynamics of the Proton Transfer Reaction between H_3^+ and H_2 through H_5^+ as the Intermediate. *William Lloyd Evans Lecture Poster Session*, Columbus, OH, 09/2013
- [58] Investigation of Large-Amplitude Motions in the Spectroscopy of H_5^+ and the Dynamics of the Proton Transfer Reaction between H_3^+ and H_2 (**Poster Award**). *Midwest Theoretical Chemistry Conference*, Urbana-Champaign, IL, 05/2013
- [59] Diffusion Monte Carlo Studies of Energetics and Structures of H_5^+ Deuterated Isotopologues. *William Lloyd Evans Lecture Poster Session*, Columbus, OH, 09/2012
- [60] Diffusion Monte Carlo Studies of Structure and Energetics of H_5^+ and Its Deuterated Isotopologues. *Midwest Theoretical Chemistry Conference*, Madison, WI, 05/2012
- [61] Diffusion Monte Carlo Studies of the Ground-state Structure and Energetics of H_5^+ . *Gordon Research Conference on Molecular & Ionic Clusters*, Ventura, CA, 01/2012
- [62] Formation of Interstellar Propylene (CH_3CHCH_2). *Center for Chemistry of the Universe Site Review*, Irvine, CA, 04/2011

PATENTS

- [1] Quanxin Li, Lu Gong, **Zhou Lin**, Lixia Yuan, and Youshifumi Torimoto. Preparation Method of Polycrystal Nano Calcium Aluminum Oxide. *China*, CN101532176, 09/2009
- [2] Quanxin Li, Lu Gong, **Zhou Lin**, Lixia Yuan, and Youshifumi Torimoto. Antibacterial Application of Polycrystalline Nanometer Calcium-Aluminum Oxide. *China*, CN101518259, 09/2009

PROFESSIONAL MEMBERSHIPS

2017–Present	Member	American Institute of Chemical Engineers
2015–Present	Member	American Association for the Advancement of Science
2012–Present	Member	American Chemical Society

PROFESSIONAL TRAINING

2020	American Chemical Society New Faculty Workshop (Pending)	Washington, DC
2018	Joint Center for Artificial Photosynthesis Theory Workshop	Stanford, CA
2018	COACh Launch and Acceleration Workshop	Boston, MA
2017	American Chemical Society Postdoc to Faculty Workshop	Washington, DC
2017	New England Future Faculty Workshop for Women in STEM Fields	Boston, MA
2016	Putting the Theory Back in Density Functional Theory Summer School	Los Angeles, CA
2013	Telluride School on Theoretical Chemistry	Telluride, CO

PROFESSIONAL ACTIVITIES

2019	Committee	<i>Joint Center for Artificial Photosynthesis Final Science Meeting: 2020</i>
2019	Presider	Symposium: Nanoscale & Molecular Assemblies: Designing Matter to Control Energy Transport <i>American Chemical Society National Meeting & Exposition</i>
2017	Presider	Mini-Symposium: Multiple Potential Energy Surfaces <i>International Symposium on Molecular Spectroscopy</i>
2019–Present	Judge	Physical Chemistry Outstanding Student Poster Award <i>American Chemical Society National Meeting & Exposition</i>
2016–Present	Judge	Rao Prize <i>International Symposium on Molecular Spectroscopy</i>
2017–Present	Developer	Q-Chem Package
2019–Present	Reviewer	<i>The Journal of Applied Physics</i>
2019–Present	Reviewer	<i>Molecular Physics</i>
2018–Present	Reviewer	<i>Molecular Crystals and Liquid Crystals</i>
2016–Present	Reviewer	<i>Journal of Molecular Spectroscopy</i>
2016–Present	Reviewer	<i>Physical Chemistry Chemical Physics</i>
2016–Present	Reviewer	<i>Physics Letters A</i>
2016–Present	Reviewer	<i>Journal of Materials Science</i>
2015–Present	Reviewer	<i>The Journal of Physical Chemistry A</i>

TEACHING & MENTORING EXPERIENCE

2018–Present	Research Mentor	Jiashu Liang (Graduate)
2018–Present	Research Mentor	Jonathan Wong (Graduate)
2017–2018	Research Mentor	Changhae A. Kim (Graduate)
2017–2018	Research Mentor	Hikari Iwasaki (Undergraduate)
2015–2018	Research Mentor	Alexander W. Kohn (Graduate)
2013–2015	Research Mentor	Melanie L. Aprahamian (née Marlett) (Graduate)
2011	Teaching Associate	Quantum Chemistry Recitation (Graduate)
2010	Teaching Associate	General Chemistry Lab (Undergraduate)
2009	Grader	Physical Chemistry (Undergraduate)
2005	Home Tutor	High School Mathematics and Physics