Fang Liu

Curriculum Vitae

Emory University, Dept. of Chemistry
1515 Dickey Drive
Atlanta, GA 30322
✆ *+1 (404) 727 6731*
✉ *fang.liu@emory.edu*

Academic Appointments

Aug 2020 -	**Assistant Professor,** *Department of Chemistry, Emory University*
2017 - 2020	**Postdoctoral Fellow,** *Department of Chemical Engineering, MIT*
	Advisor: Heather J. Kulik

Education

2011 - 2017	**Ph.D. in Chemistry,** *Stanford University*
	Advisor: Todd J. Martínez
	Dissertation: *Quantum Chemistry for Solvated Molecules and Electronic Excited States on Graphical Processing Units (GPUs)*
2007 - 2011	**B.S. in Chemical Physics,** *University of Science and Technology of China*

Honors and Awards

2024	**Cottrell Scholar Award,**	RCSA
2023	**Scialog Fellow: Automating Chemical Laboratories,**	RCSA
2023	**JCP-DCP Future of Chemical Physics Lectureship,**	The Journal of Chemical Physics
2022	**ACS PRF Doctorate New Investigator,**	ACS Petroleum Research Foundation
2022	**Scialog Fellow: Signatures of Life in the Universe,**	RCSA
2020	**APS DCOMP Travel Award,**	American Physics Society
2019	**MolSSI Investment Fellowship,**	National Science Foundation
2019	**MolSSI Seed Fellowship,**	National Science Foundation
2018	**NVIDIA GPU Award,**	American Chemical Society
2016	**Evelyn Laing McBain Fellowship,**	Stanford University
2011	**Guo Moruo Scholarship,**	University of Science and Technology of China

Grants

RCSA *Cottrell Scholar Award* **(PI)** 7/1/2024 - 6/30/2027 $120K

Honda Research Institute USA *Demonstrating Quantum Advantage in Material Simulation based on Case Study* **(co-PI)** 9/1/2023 - 8/31/2025 $220K

ACS *PRF Doctorate New Investigator (DNI) Grant* **(PI)** 9/1/2022 - 8/31/2024 $110K

RCSA *Scialog SLU Award* "Computational and Experimental Investigations of Martian Brines as Prebiotic Environments" **(PI)** 10/1/2022 - 9/30/2023 $55K

RCSA *Scialog SLU Award* "Assessing false positive biosignatures and prebiotic synthesis generated by two candidate autocatalytic reaction sets of aqueous sulfur" **(PI)** 10/1/2022 - 9/30/2023 $55K

Publications

Preprints

43.* <u>Xu Chen</u>, Yuanjie Sun, <u>Eugen Hruska</u>,^{PD} Vivek Dixit, Jinming Yang, Yu He,* Yao Wang,* **Fang Liu**,* Explainable Machine Learning Identification of Superconductivity from Single-Particle Spectral Functions *Preprint* arXiv: 2406.04445 (2024)

42.* <u>R. S. K. Gadde</u>,^{R} S. Devaguptam, <u>F. Ren</u>, R. Mittal, <u>L. Dong</u>, Yao Wang, **F. Liu**,* Chatbot-Assisted Quantum Chemistry for Explicitly Solvated Molecules. *ChemRxiv Preprint* DOI: 10.26434/chemrxiv-2024-35f9j (2024)

41.* <u>S. Xun</u>, **F. Liu**,* Comparison of Machine-Learning and Classical Force Fields in Simulating the Solvation of Small Organic Molecules in Acetonitrile *ChemRxiv Preprint* DOI: 10.26434/chemrxiv-2023-sd4b2-v2 (2023)

40.* <u>E. Hruska</u>,^{P} L. Zhao, **F. Liu**,* Ground truth explanation dataset for chemical property prediction on molecular graphs *ChemRxiv Preprint* DOI: 10.26434/chemrxiv-2022-96slq (2022)

Peer-reviewed publications after joining Emory

39.* <u>F. Ren</u>, **F. Liu**,* Data-Driven Insights into the Fluorescence of Asphaltene Aggregates Using Extended Frenkel Exciton Model *Chem. Phys. Rev.* 4, 041401 (2023)

38.* <u>X. Chen</u>, <u>P. Li</u>, <u>E. Hruska</u>,^{P} **F. Liu**,* Δ-Machine Learning for Quantum Chemistry Prediction of Solution-phase Molecular Properties at the Ground and Excited States *Phys. Chem. Chem. Phys.* 25, 13417 (2023)

37.* <u>F. Ren</u>, **F. Liu**,* Impacts of Polarizable Continuum Models on the SCF Convergence and DFT Delocalization Error of Large Molecules *J. Chem. Phys.* 57, 184106 (2022)

36.* <u>E. Hruska</u>,^{P} <u>A. Gale</u>, <u>X. Huang</u>,^{U} **F. Liu**,* AutoSolvate: A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules, *J. Chem. Phys.* 156, 12801 (2022)

35.* <u>E. Hruska</u>,^{P} **F. Liu,*** Machine Learning: An Overview In Pavlo Dral (Eds.), *Quantum Chemistry in the Age of Machine Learning*, Elsevier, (2022)

34.* <u>E. Hruska</u>,^{P} <u>A. Gale</u>, **F. Liu**,* Bridging the experiment-calculation divide: machine learning corrections to redox potential calculations in implicit and explicit solvent models, *J. Chem. Theory Comput.* 18, 1096 (2022)

33. B. Aguado, L. J. Bray, S. Caneva, J.-P. Correa-Baena, G. Di Martino, C. Fang, Y. Fang, P. Gehring, G. Grosso, X. Gu, P. Guo, Y. He, T. J. Kempa, M. Kutys, J. Li, T. Li, B. Liao, **F. Liu**, F. Molina-Lopez, A. Pickel, A. M. Porras, R. Raman, E. M. Sletten, Q. Smith, C. Tan, H. Wang, H. Wang, S. Wang, Z. Wang, G. Wehmeyer, L. Wei, Y. Yang, L. D. Zarzar, M. Zhao, Y. Zheng, S. Cranford, 35 challenges in materials science being tackled by PIs under 35(ish) in 2021, *Matter*, 4, 3804–3810 (2021)

32. D. G. A. Smith, A. T. Lolinco, Z. L. Glick, J. Lee, A. Alenaizan, T. A. Barnes, C. H. Borca, R. Di Remigio, D. L. Dotson, S. Ehlert, A. G. Heide, M. F. Herbst, J. Hermann, C. B. Hicks, J. T. Horton, A. G. Hurtado, P. Kraus, H. Kruse, S. J. R. Lee, J. P. Misiewicz, L. N. Naden, F. Ramezanghorbani, M. Scheurer, J. B. Schriber, A. C. Simmonett, J. Steinmetzer, J. R. Wagner, L. Ward, M. Welborn, D. Altarawy, J. Anwar, J. D. Chodera, A. Dreuw, H. J. Kulik, **F. Liu**, T. J. Mart ınez, D. A. Matthews, H. F. Schaefer, J. ˇSponer, J. M. Turney, L.-P. Wang, N. De Silva, R. A. King, J. F. Stanton, M.

S. Gordon, T. L. Windus, C. D. Sherrill, and L. A. Burns, Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and Interoperability among Computational Chemistry Programs, *J. Chem. Phys.*, 155, 204801 (2021)

31.* A. Gale, E. Hruska,[P] and **F. Liu**,* Quantum Chemistry for Molecules at Extreme Pressure on Graphical Processing Units: Implementation of Extreme Pressure Polarizable Continuum Model, *J. Chem. Phys.* 154, 244103 (2021)

30. C. Duan, S. Chen, M.G. Taylor, **F. Liu**, H.J. Kulik, Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles, *Chem. Sci.*, 12, 13021-13036 (2021)

29. A. Nandy, C. Duan, M. Taylor, **F. Liu**, A. Steeves, and H.J. Kulik, Computational Discovery of Transition-Metal Complexes: From High-throughput Screening to Machine Learning *Chem. Rev.* 54, 532–545 (2021)

28. C. Duan, **F. Liu**, A. Nandy, and H.J. Kulik, Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery, *J. Phys. Chem. Lett.* 12, 4628–4637 (2021)

27. R. Liang, J. Yu, J. Meisner, F. Liu, and T. J. Martínez. Electrostatic Control of Photoisomerization in Channelrhodopsin 2. *J. Am. Chem. Soc.* 143, 5425, (2021)

26.* **F. Liu***, M. Filatov, and T. J. Martínez, Analytical Derivatives of the Individual State Energies in Ensemble Density Functional Theory Method II: Implementation on Graphical Processing Units (GPUs), *J. Chem. Phys.*, 154, 104108 (2021)

25. J. P. Janet, C. Duan, A. Nandy, **F. Liu**, and H. J. Kulik, Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design, *Acc. Chem. Res.*, 54, 532-545, (2021)

24. **F. Liu**, C. Duan, A. Nandy and H. Kulik, Rapid Detection of Strong Correlation with Machine Learning for Transition Metal Complex High-Throughput Screening , *J. Phys. Chem. Lett.* 11, 8067 (2020)

Peer-reviewed publications before joining Emory in Aug 2020

23. C. Duan, **F. Liu**, A. Nandy and H. Kulik, Semi-Supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost, *J. Phys. Chem. Lett.* 11, 6640 (2020)

22. A. Bajaj, **F. Liu**, and H. J. Kulik, Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling, *J. Phys. Chem. C* 124, 15094 (2020)

21. C. Duan, **F. Liu**, A. Nandy and H. Kulik, Data-Driven Approaches Can Overcome Limitations in Multireference Diagnostics, *J. Chem. Theory Comput.* 16, 4373. (2020)

20. S. Seritan, C. Bannwarth, B. S. Fales, E. G. Hohenstein, C. M. Isborn, S. I. L. K. kokkila-Schumacher, X. Li, **F. Liu**, N. Luer, J. Snyder Jr., C. Song, A. Titov, I. Ufimtsev, L.-P. Wang, and T. J. Martínez, TeraChem: A Graphical Processing Units-accelerated electronic structure package for large-scale ab initio molecular dynamics, *Wiley Interdiscip. Rev. Comput. Mol. Sci., e1494* (2020)

19. **F. Liu**, H. J. Kulik, Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry, *J. Chem. Theory Comput.* 16, 264 (2020)

18. Y. Wang, J. P. Dehollain, **F. Liu**, U. Mukhopadhyay, M. S. Rudner, L. M. K. Vandersypen, E. Demler, Ab Initio Exact Diagonalization Simulation of the Nagaoka Transition in Quantum Dots, *Phys. Rev. B* 100, 155133 (2019)

17. J. K. Yu, R. Liang, **F. Liu**, T. J. Martinez, Characterization of the Elusive I Fluorescent State and the Ultrafast Photoisomerization of Retinal Protonated Schiff Base in Bacteriorhodopsin by Nonadiabatic Dynamics Simulation, *J. Am. Chem. Soc.* 141, 18193, (2019)

16. Z. Yang, **F. Liu**, A. H. Steeves, and H. J. Kulik , A Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases, *J. Phys. Chem. Lett.*, 10, 3779 (2019)

15. R. Liang, **F. Liu**, and T. J. Martínez, Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2, *J. Phys. Chem. Lett.* 10, 2862, (2019)

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

13. A. Bajaj, **F. Liu**, and H. J. Kulik, Non-empirical, Low-cost Recovery of Exact Conditions with Model-Hamiltonian Inspired Expressions in jmDFT, *J. Chem. Phys.* 150, 154115 (2019)

12. C. Duan, J. P. Janet, **F. Liu**, A. Nandy, and H. J. Kulik, Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models, *J. Chem. Theory Comput.* 15, 2331-2345 (2019)

11. J. P. Janet, **F. Liu**, A. Nandy, C. Duan, T. Yang, S. Lin, and H. J. Kulik, Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry, *Inorganic Chemistry* 58, 10592 (2019)

10. **F. Liu**, D. Sanchez, H. Kulik, and T. J. Martínez, Exploiting Graphical Processing Units to Enable Quantum Chemistry Calculation of Large Molecules in Polarizable Continuum Models, *Int. J. Quantum Chem.* 119, e25760 (2019)(**Cover for special issue "Advances in Simulating Solvation"**)

9. M. Pinney, A. Natarajan; F. Yabukarski, D. Sanchez, **F. Liu**, R. Liang, T. Doukov, J. Schwans, T. J. Martínez, and D. Herschlag, Structural Coupling Throughout the Active Site Hydrogen Bond Networks of Ketosteroid Isomerase and Photoactive Yellow Protein, *J. Am. Chem. Soc.* 140, 9862 (2018)

8. S. Banerjee,[§] **F. Liu**,[§] T. J. Martínez, and R. N. Zare, Pomeranz-Fritsch Synthesis of Isoquinoline: Gas-Phase Collisional Activation Opens Additional Reaction Pathways, *J. Am. Chem. Soc.* 139, 14352 (2017) [[§]**These two authors contributed equally**]

7. X. Li, R. M. Parrish, **F. Liu**, S. I. L. K. Schumacher, and T. J. Martínez, An *ab initio* Exciton Model Including Charge-Transfer Excited States , *J. Chem. Theory Comput.* 13, 3493 (2017)

6. M. Filatov, **F. Liu**, K. S. Kim, T. J. Martínez, Analytical Derivatives of the Individual State Energies in Ensemble Density Functional Theory Method. I. General formalism , *J. Chem. Phys.* 147, 034113 (2017)

5. M. Filatov, **F. Liu**, K. S. Kim, and T. J. Martínez, Self-Consistent Implementation of Ensemble Density Functional Theory Method for Multiple Strongly Correlated Electron Pairs , *J. Chem. Phys.* 145, 244104 (2016)

4. R. M. Parrish, **F. Liu**, and T. J. Martínez, Communication: A Difference Density Picture for the Self-Consistent Field Ansatz., *J. Chem. Phys.* 144, 131101 (2016)

3. **F. Liu**, N. Luehr, H. J. Kulik, and T. J. Martínez, Quantum Chemistry for Solvated Molecules on Graphical Processing Units (GPUs) using Polarizable Continuum Models, *J. Chem. Theory Comput.* 11, 3131 (2015)

2. B. D. Mar, H. W. Qi, **F. Liu**, and H. J. Kulik, Ab Initio Screening Approach for the Discovery of Lignin Polymer Breaking Pathways, *J. Phys. Chem. A* 119, 6551 (2015)

1. L-P. Wang, A. Titov, R. McGibbon, **F. Liu**, V. S. Pande, and T. J. Martínez, Discovering Chemistry with an *ab initio* Nanoreactor, *Nat. Chem.* 6, 1044 (2014)

Presentations

Invited Talks

46. *TBD*
    The Molecular Interactions and Dynamics Gordon Research Conference, Easton, MA (July 2024)

45. *Towards a big-data ecosystem for quantum chemistry research of solvated molecular systems*
    Physical Chemistry Seminar, Westlake University, Hangzhou, China (July 2024)

44. *Machine Learning Aided Quantum Chemistry Discovery in the Solution Phase*
    2024 International Symposium on Computational Molecular Science and Machine Learning, Shanghai, China (June 2024)

43. *Computational Discovery of Photoredox catalysts with high-throughput simulation and explainable machine learning*
    28th Annual Green Chemistry Engineering Conference, Atlanta, GA (June 2024)

42. *Machine Learning Aided Quantum Chemistry Discovery in the Solution Phase*
    Physical Chemistry Seminar, Georgia Institute of Technology, Atlanta, GA (April 2024)

41. *Towards a big-data ecosystem for quantum chemistry research of solvated molecular systems*
    Chemistry Department Seminar, Georgia State University, Atlanta, GA (March 2024)

40. *Towards a big-data ecosystem for quantum chemistry research of solvated molecular systems*
    American Physics Society March Meeting, Minneapolis, MN (March 2024)

39. *Computational Discovery of Photoredox catalysts with high-throughput simulation and explainable machine learning*
    Inaugural Workshop of the Initiative for Computational Catalysis, Flatiron Institute, New York, NY (Feb 2024)

38. *GPU Accelerated Implementation of 1-electron Integrals for Large Molecules*
    CECAM Workshop: Advancing the Modular Paradigm, Lausanne, Switzerland, presented online due to schedule conflicts (Feb 2024)

37. *Machine Learning Aided Quantum Chemistry Discovery in the Solution Phase*
    2nd International SMLQC Conference, Uppsala, Sweden, presented online due to schedule conflicts (Nov 2023)

36. *Machine learning aided quantum chemical discovery in the solution phase*
    Machine Learning and Informatics for Chemistry and Materials Workshop, Telluride, CO (June 2023)

35. *Solution phase chemical discovery with machine learning*
    SMLQC (Seminars on Machine Learning in Quantum Chemistry and Quantum Computing for Quantum Chemistry), online (May 2023)

34. *Machine learning aided quantum chemical discovery in the solution phase*
    Lennard-Jones Centre Discussion Group, Cambridge, UK, online (March 2023)

33. *Fast and accurate simulation of molecular spectroscopy in complex environments aided by GPU acceleration and machine learning*
    Department of Physics, University of Delaware, DE (Jan 2023)

32. *Quantum Chemistry Discovery Powered by GPU acceleration and Machine Learning*
    Department of Chemistry, University of North Carolina, Chapel Hill, NC (Jan 2023)

31. *Machine learning aided quantum chemical discovery in the solution phase*
    Department of Chemistry, Stony Brook University, NY (Jan 2023)

30. *Solution phase chemical discovery with GPU accelerated quantum chemistry and machine learning*
    Georgia Tech CSE seminar, School of Computational Science and Engineering, Georgia Institute of Technology, (Nov 2022)

29. *Machine learning aided quantum chemical discovery in the solution phase*
    Virtual Theoretical and Computational Seminar, Purdue University, online (Nov 2022)

28. *New computational tools for automated discovery of prebiotic reactions*
    NASA PCE3 workshop, online (Oct 2022)

27. *Fast and accurate quantum chemistry for solvated molecules*
    ACS National Meeting, Chicago, IL (August 2022)

26. *Machine learning aided quantum chemical discovery in the solution phase*
    Molecular Quantum Mechanics Conference, Blacksburg, VA (June 2022)

25. *Exploiting graphical processing units (GPUs) to enable large-scale quantum chemistry of molecules in realistic environments*
    Canadian Chemistry Conference and Exhibition, Calgary, AB, Canada (June 2022)

24. *Machine learning aided quantum chemical discovery in the solution phase*
    Canadian Chemistry Conference and Exhibition, Calgary, AB, Canada (June 2022)

23. *Fast and accurate chemical discovery with GPU accelerated quantum chemistry and machine learning*
    Seminar, Microsoft Research Asia (MSRA), Beijing, China, online due to COVID-19 (May 2022)

22. *Machine learning aided quantum chemistry discovery in complex environment*
    Department Seminar, University of New Haven, New Haven, CT (March 2022)

21. *Machine learning aided quantum chemistry discovery in complex environment*
    Department Seminar, New York University, New York, NY (Jan 2022)

20. *Reducing uncertainty in quantum chemistry discovery with machine learning*
    Department Seminar, Queens College, City University of New York, New York, NY (Dec 2021)

19. *Reducing uncertainty in quantum chemistry discovery with machine learning*
    International Symposium on Machine Learning in Quantum Chemistry (SMLQC), Xiamen, China, online due to COVID-19 (Nov 2021)

18. *Exploiting graphical processing units (GPUs) to enable large-scale quantum chemistry of molecules in realistic environments*
ACS Southeastern Regional Meeting (SERMACS), Birmingham, AL (Nov 2021)

17. *Reducing uncertainty in quantum chemistry discovery with machine learning*
ACS Southeastern Regional Meeting (SERMACS), Birmingham, AL (Nov 2021)

16. *Fast and accurate chemistry discovery with high-performance computing and machine learning*
Atlanta mini symposium on theoretical and computational chemistry, Georgia State University, Atlanta, GA (Oct 2021)

15. *Quantum chemistry for molecules at extreme pressure on graphical processing units*
261st ACS National Meeting ,Atlanta, GA (Aug 2021)

14. *Machine learning guided method selection for simulation of transition metal complexes*
AI workshop for simulation of materials at the 2021 Joint Nanoscience and Neutron Scattering User Meeting , Oak Ridge National Laboratory, online due to COVID-19 (Aug 2021)

13. *New Tools for Detecting Multireference Character in Transition Metal Chemical Space*
EPFL/ETH Summer School "Big Data and Machine Learning in Chemistry", Lausanne, Switzerland, online due to COVID-19 (June 2021)

12. *Fast and Accurate Quantum Chemistry Simulation for molecular design and discovery*
Department of Chemistry and Biochemistry, California State University, Long Beach, CA, online due to COVID-19 (Feb 2021)

11. *Quantum Chemistry Discovery Powered by GPU acceleration and Machine Learning*
Department of Mathematics, Emory University, online due to COVID-19 (Feb 2021)

10. *Fast and Accurate Quantum Chemistry Simulation for molecular design and discovery*
Department of Chemistry, Clemson University, online due to COVID-19 (Jan 2021)

9. *New tools for detecting strong correlation in automated transition metal chemical space*
Virtual Conference on Theoretical Chemistry, online due to COVID-19 (July 2020)

8. *New tools for detecting strong correlation in automated transition metal complex screening*,
APS National Meeting, Denver, CO, USA (March. 6, 2020, canceled due to COVID-19)

7. *Automated control in computational chemical discovery*,
Sanibel Symposium, St Simons Island, GA, USA (Feb. 20, 2020)

6. *Fast and Accurate Quantum Chemistry Simulation in Realistic Environment with High Performance Computing*, Emory University, Atlanta, GA, USA (Dec. 4, 2019)

5. *Implementation of Polarizable Contiuum Model and Restricted Ensemble-Averaged Kohn Sham Methods in TeraChem*, TeraChem/FMS Developer Meeting, Stanford, CA, USA (Mar. 29, 2018)

4. *Quantum Chemistry for Solvated Molecules and Electronic Excited States on Graphical Processing Units (GPUs)*, Massachusetts Institute of Technology, Cambridge, MA, USA (Jul. 2017)

3. *Introduction to TeraChem: Efficient Implementation of Quantum Chemistry On Graphical Processing Units*, PRACE Winter School, Bratislava, Slovakia (Jan. 2016)

2. *Polarizable Continuum Model on Graphical Processing Units*
   Hefei National Laboratory for Physical Sciences at the Microscale, Hefei, China (Sep. 2015)

1. *Polarizable Continuum Model on Graphical Processing Units and and Functional Auto Generation Stuffs*
   Massachusetts Institute of Technology, Cambridge, MA, USA (Sep. 2014)

<div align="center">Contributed Talks</div>

7. *AutoNEB: a Toolkit for Automating Reaction Network Calculation*
   F. Liu, et al. *AIChE National Meeting*, Orlando, FL, USA (Nov. 2019)

6. *Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis*
   F. Liu, et al. *AIChE National Meeting*, Orlando, FL, USA (Nov. 2019)

5. *MultirefPredict: an Automated Workflow for Method Selection of First Principles Calculations on Transition Metal Chemistry*
   F. Liu, C. Duan, H. J. Kulik *AIChE National Meeting* ,Orlando, FL, USA (Nov. 2019)

4. *In-situ Automated Analysis and Control of Transition Metal Chemistry Simulation*
   F. Liu, C. Duan, H. J. Kulik *258th ACS National Meeting*, San Diego, CA, USA (Aug. 2019)

3. *Understanding and Correcting DFT Errors in Transition Metal Chemistry*
   F. Liu, H. J. Kulik *258th ACS National Meeting*, San Diego, CA, USA (Aug. 2019)

2. *Understanding and Correcting DFT Errors in Ground and Excited Electronic States*
   F. Liu, T. J. Martínez, H. J. Kulik *256th ACS National Meeting*, Boston, MA, USA (Aug. 2018)

1. *Exploiting Graphical Processing Units to Enable Accurate Excited State Potential Energy Surface Calculation for Large Molecules*
   F. Liu, T. J. Martínez, *255th ACS National Meeting*, New Orleans, LA, USA (Mar. 2018)

▬▬ Teaching

Instructor (Emory): CHEM 370 Quantum Mechanics, CHEM 531 Intro to Molecular Quantum Mechanics
Teaching Assistant (Stanford 2011-2013): General Chemistry Lab (CHEM 34XN), Organic Chemistry Lab (CHEM 130), Physical Chemistry for pre-meds (CHEM 135) and for chemistry majors (CHEM 171)
Course Designing (Stanford 2013): Atomistic Simulations (BIOS 203)

▬▬ Mentoring

Postdoctoral Scholar

2023 –	Mohammed Pabel Kabir, Emory	
2020–2022	Eugen Hruska, Emory	(now: PI, Charles University, Czechia)

Graduate Student

2020–	Ariel Gale, Emory
2021–	Xu Chen, Emory
2021–	Patrick Li, Emory
2021–	Fangning Ren, Emory

Undergraduate, High School Student

2023–	Kenneth Wingate Jr., Emory U.G.	(B.S. '24 expected)
2023–2023	Ian Su, Peking University U.G.	(B.S. '24 expected)
2023–2023	Qihao Cheng, Peking University U.G.	(B.S. '24 expected)
2022–	Yingrong Chen, Emory U.G.	(B.S. '23 expected)
2022–2023	Jessica Frosstrom, Emory U.G.	(B.S. Emory '23, now: U Penn grad)
2022–2023	Jiechao Feng, Peking University U.G.	(B.S. PKU '23, now: UC Berkeley grad)
2020–2022	Anjanay Nangia, Emory U.G.	(B.S. '23 expected)
2020–2021	Xiao Huang, Emory U.G.,	(B.S. Emory '21, now: Duke grad)
2019	Xingyue Guan, NJU-MIT exchange	(B.S. NJU '20)
2018	Eve Xu, Wellesley-MIT exchange	(B.S. Smith, '20, now: Princeton grad)
2018	Sean Lin, HS via Troy H.S.	(Troy H.S., '19, now: UC Berkeley UG)

Visiting Scholar

2022–	Sangni Xun, Emory	
2022–2022	Matthew Shammani, Emory	(now: UCLA grad)

Awards, Honors, and Special Recognition Received by Group Members

2023	Kenneth Wingate Jr. (undergraduate)	William Jones scholarship (Emory)
2023	Yingrong Chen (undergraduate)	Barry Goldwater Scholar
2023	Fangning Ren (graduate)	Quayle Excellence in Research Award (Emory)
2023	Ariel Gale (graduate)	Quayle Excellence in Research Award (Emory)
2022	Ariel Gale (graduate)	NSF Graduate Research Fellowship
2022	Ariel Gale (graduate)	AFOSR Scholar for ACTC 2022
2022	Eugen Hruska (postdoc)	AFOSR Scholar for ACTC 2022
2021	Ariel Gale (graduate)	ARCS Award
2021	Xiao Huang (undergraduate)	URP research grant (Emory)

Service & Professional Activities

Committee Operation Committee, Department of Chemistry, Emory University (summer 2022 - present), LTS search Committee, Department of Chemistry, Emory University (summer 2022 - present), Graduate Committee, Department of Chemistry, Emory University (fall 2020 - spring 2022)

Journal Referee *Nat. Chem.*, *Chem. Sci.*, *J. Chem. Theory Comput.*, *J. Chem. Phys.*, *Phys. Rev. Lett.*, *Phys. Rev. A.*, *Phys. Rev. Research*, *Phys. Chem. Chem. Phys.*, *J. Chem. Inf. Model.*, *ChemPhysChem*, *Mol. Simulat.*, *Int. J. Quantum Chem.*, *Chem. Mater.*, *ACS Phys. Chem. Au*, *Top. Catal.*

Grant Reviewer ACS Petroleum Research Fund (2021,2022, 2023), NSF panelist (2021), DOE (2021, 2023), DOE Office of Science Graduate Student Research Program (2021), CNM Proposal Evaluation Board at ANL (2020, 2021), DOE ALCC (2020), LLNL Institutional Computing Grand Challenge program (2018-2020)

Conference organizer for ACS PHYS Symposium: Data-Driven Design of Energy Materials (Aug. 2023)

Atlanta Theoretical Chemistry Mini Symposium (Oct. 2022)

Session Presider for *ACS National Meeting* (Aug. 2022, Aug. 2021, Aug. 2018)

K-12 Outreach Volunteer for *ACS Science Coaches program* to help K-12 science teachers with chemistry education (2022-2023), *NetPals* to introduce STEM to underrepresented 7th grade students (2019)

Computation Consultant for Edison Pharmaceuticals Inc. (Summer 2016)