Fang Liu

Curriculum Vitae

Emory University, Dept. of Chemistry
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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
2007 - 2011 **B.S. in Chemical Physics,** *University of Science and Technology of China*

Honors and Awards

2025 **OpenEye Cadence Outstanding Junior Faculty Award**, ACS COMP division
2024 **DOE Early Career Award**, Department of Energy
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
2019 **MolSSI Fellowship**, The Molecular Science Software Institution (NSF funded)
2018 **NVIDIA GPU Award**, ACS COMP division
2016 **Evelyn Laing McBain Fellowship**, Stanford University
2011 **Guo Moruo Scholarship**, University of Science and Technology of China

Grants

DOE *Early Career Award* "Reveal the Structure-Dynamics Relationship in Solution-Phase Photoredox Catalysis with Explainable Machine Learning" **(PI)** 7/1/2024 - 6/30/2029 $875K

RCSA *Cottrell Scholar Award* "Machine Learning Aided Quantum Chemistry Discovery in the Solution Phase" **(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 - 2/28/2026 $220K

ACS *PRF Doctorate New Investigator (DNI) Grant* "Quantum Chemistry Investigation of the Structure-Fluorescence Relationship for Asphaltene Aggregates" **(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 (h-index: 27, citation:2718)

* corresponding author(s), graduate student, postdoc[P], undergraduate student[U], research specialist[R]
Journal Impact Factor denoted by [I.F.]

Preprints

50.* S. Xun, **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)

49.* E. Hruska,[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)

Independent Publications (not associated with prior mentors)

48.* F. Ren,[§], P. Li,[§], Xu Chen, Lechen Dong, **F. Liu**,* Data-Driven Recommendation of Optimal Tuning Scheme for Range-Separated Hybrid Functionals in Solution Phase Absorption Energy Prediction, *J. Chem. Theory Comput.* 21, 11106–11125 (2025) [[§]These two authors contribute equally.]

47.* L. Dong, **F. Liu**,* Streamlining Coding Assignments and Grading on the Cloud: A Preconfigured JupyterHub Image for Chemistry Education, *J. Chem. Educ.*, 102, 4130–4138, (2025) [I.F. 2.9]

46.* X. Chen,[§] F. Ren,[§] D. Yu, L. Dong, **F. Liu**,* AutoSolvate-Agent: An Autonomous Agent for GPU-accelerated Solution-phase Quantum Chemistry *KDD'25 SciSoc LLM Workshop, Large Language Models for Scientific and Societal Advances* (2025) [Peer reviewed conference proceeding] [§]These two authors contribute equally.]

45.* X. Chen, D. Yu, L. Zhao, **F. Liu**,* ACES-GNN: Can Graph Neural Network Learn to Explain Activity Cliffs? *Digit. Discov.* 4, 2062-2074 (2025) [I.F. 5.6]
Emerging Investigators collection.

44.* X. Chen, Y. Sun, E. Hruska,[P] V. Dixit, J. Yang, Y. He,* Y. Wang,* **F. Liu**,* Detecting thermodynamic phase transition via explainable machine learning of photoemission spectroscopy *Newton* 1, 100066 (2025) [I.F. not available yet as a new journal]
Newton is a Cell Press journal newly launched in 2025. Newton publishes the most influential research across all areas of fundamental and applied physics, as well as interdisciplinary fields.
Front cover art featured in volume 1, issue 3.
Appeared in Emory News: *New AI tool set to speed quest for advanced superconductors, 04/09/2025*.

43.* S. Datta, M. P. Kabir,[PD] S. Maliha, **F. Liu***, J. Xu* Stimulus-Driven Tuning of Multi-Pathway Emission in 9-Fluorenone Derivatives: Elucidating Charge Transfer Dynamics in Higher Excited Singlet and Triplet States *ACS Appl. Energy Mater.,* 8, 3973–3983 (2025) [I.F. 5.5]

42.* F. Ren, X. Chen, **F. Liu**,* Size-transferable prediction of excited state properties for molecular assemblies with machine-learned exciton model *J. Phys. Chem. Lett.* 16, 2541–2552 (2025) [I.F. 4.9]
Supplementary front cover art featured in volume 16, issue 10.

41.* R.S.K. Gadde,[R] S. Devaguptam, F. Ren, R. Mittal, L. Dong, Yao Wang, **F. Liu**,* Chatbot-Assisted Quantum Chemistry for Explicitly Solvated Molecules. *Chem. Sci.* 16, 3852-3864 (2025) [I.F. 7.6]
Front cover art featured in volume 16 issue 9.
Appeared in Emory News: *Chatbot opens computational chemistry to nonexperts, 03/26/2025*

40. H. Tang, B. Xiao, W. He, P. Subasic, A. R Harutyunyan, Y. Wang, **F. Liu**, H. Xu, J. Li Approaching coupled-cluster accuracy for molecular electronic structures with multi-task learning *Nat. Comput. Sci.* 5, 144–154 (2024) [I.F. 12.0]

39.* F. Ren, **F. Liu**,* Data-Driven Insights into the Fluorescence of Asphaltene Aggregates Using Extended Frenkel Exciton Model *Chem. Phys. Rev.* 4, 041401 (2023) [I.F. 6.1]

38.* X. Chen, P. Li, E. Hruska,[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) [I.F. 3.67]

37.* F. Ren, **F. Liu**,* Impacts of Polarizable Continuum Models on the SCF Convergence and DFT Delocalization Error of Large Molecules *J. Chem. Phys.* 57, 184106 (2022) [I.F. 3.6]

36.* E. Hruska,[P] A. Gale, X. Huang,[U] **F. Liu**,* AutoSolvate: A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules, *J. Chem. Phys.* 156, 12801 (2022) [I.F. 3.6]
Appeared in Emory News: *New chemistry toolkit speeds analyses of molecules in solution, 11/28/2022*

35.* E. Hruska,[P] **F. Liu,*** Machine Learning: An Overview In Pavlo Dral (Eds.), *Quantum Chemistry in the Age of Machine Learning*, Elsevier, (2022) [book chapter]

34.* E. Hruska,[P] A. Gale, **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) [I.F. 5.7]

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) [I.F. 19.967]

32.* 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) [I.F. 3.6]

Publications associated with prior mentors

31. 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. Martınez, D. A. Matthews, H. F. Schaefer, J. Sponer, J. M. Turney, L.-P. Wang, N. De Silva, R. A. King, J. F. Stanton, M. S. Gordon, T. L. Windus, C. D. 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)

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. 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* (2021)

23. **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)

22. 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)

21. 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)

20. 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)

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

64. *Synergizing GPU-Accelerated Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase*
Department Seminar, Department of Chemistry, University of Massachusetts Ahmerst, Ahmerst, MA (Oct 2025)

63. *Synergizing GPU-Accelerated Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase*
Department Seminar, Department of Computer Science, Emory University, Atlanta, GA (Sep 2025)

62. *Machine learning prediction and explanation of molecular properties and interactions in photoredox catalysis*
Emerson Center Symposium, Emory University, Atlanta, GA (Sep 2025)

61. *Synergizing GPU-Accelerated Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase*
Seminar-Physical Chemistry, University of Calorado, Denver (Sep 2025)

60. *Size-Transferable Prediction of Excited State Properties for Molecular Assemblies with a Machine Learning Exciton Model*
ACS National Meeting, Washington, DC (Aug 2025)

59. *Detecting thermodynamic phase transition via explainable machine learning of photoemission spectroscopy*
Accelerate Conference 2025, Toronto, Canada (Aug 2025)

58. *Machine learning prediction and explanation of molecular properties and interactions in photoredox catalysis*
TSRC workshop: Accelerating Reaction Discovery, Telluride, CO (July 2025)

57. *Machine Learning Aided Quantum Chemistry Study of Condensed-phase Molecular Systems*
MERCURY 2025 Conference, Pittsburgh, PA (July 2025)

56. *Size-Transferable Prediction of Excited State Properties for Molecular Assemblies with a Machine Learning Exciton Model*
Machine Learning in Chemical and Materials Sciences 2025, Santa Fe, MN (May 2025)

55. *Synergizing GPU-Accelerated Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase*
Seminar-Physical Chemistry, University of California San Diego, San Diego, CA (March 2025)

54. *Machine learning prediction and explanation of molecular properties and interactions in photoredox catalysis*
ACS National Meeting, San Diego, CA (March 2025)

53. *Towards a big-data ecosystem for computational discovery of solvated molecules*
ACS National Meeting, San Diego, CA (March 2025)

52. *Size-transferable prediction of excited state properties for molecular assemblies with machine-learned exciton model*
CECAM flagship workshop: Density Functional Theory and Artificial Intelligence learning from each other, Laussane, Switzerland (March 2025)

51. *Synergizing GPU-Accelerated Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase*
Greater Boston Area Theoretical Chemistry Seminar, MIT, Cambridge, MA (Feb 2025)

50. *Towards a big-data ecosystem for quantum chemistry research of solvated molecular systems*
ACS Southeastern Regional Meeting (SERMACS), Atlanta, GA (Oct 2024)

49. *AutoSolvateWeb: An open-source chatbot-assisted toolkit for quantum chemistry of explicitly solvated molecules*
American Chemical Society National Meeting, Denver, CO (Aug 2024)

48. *Introduction to AutoSolvate*
Hands-on Workshop & Panel on FAIR Workflows in Materials Science, Purdue University, online (Aug 2024)

47. *A big-data compatible chemistry education plan*
Cottrell Scholar Conference, Tucson, AZ (July 2024)

46. *Applications and Impact of Machine Learning*
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)

Contributed Talks

10. *Detecting thermodynamic phase transition via explainable machine learning of photoemission spectroscopy*
ACS National Meeting, Washington, DC (Aug 2025)

9. *Size-Transferable Prediction of Excited State Properties for Molecular Assemblies with a Machine Learning Exciton Model*
APS National Meeting, Anaheim, CA (March 2025)

8. *Size-transferable prediction of excited state properties for molecular assemblies with machine-learned exciton model*
F. Liu, *APS March meeting*, Anaheim, CA, USA (March 2025)

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)

In the News

5. *Emory News*, 04/09/2025, "New AI tool set to speed quest for advanced superconductors". (Also published in *EurekAlert! by AAAS, Yale News*)

4. *Interesting Engineering*, 03/31/2025, "Chatbot can help you run quantum chemical simulations like a theoretical chemist"

3. *Emory News*, 03/26/2025, "Chatbot opens computational chemistry to nonexperts" (Also published in *Phys.org, EurekAlert! by AAAS, Science Daily, ChemEurope.com*)

2. *Emory News*, 10/22/2024, "DOE funds Emory chemist's goal to optimize light-driven electron transfer"

1. *Emory News*, 11/28/2022, "New chemistry toolkit speeds analyses of molecules in solution"

Teaching

Instructor (Emory):

SP 2024-	CHEM 470 Machine Learning in Chemistry
FA 2021-	CHEM 531 Intro to Molecular Quantum Mechanics
SP 2021-2023	CHEM 370 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)

Mentoring

Postdoctoral Scholar

2024 –	Bushra Alam, Emory	
2024 –	Sangni Xun, Emory	
2023 – 2025	Mohammed Pabel Kabir, Emory	
2020 – 2022	Eugen Hruska, Emory	(now: PI, Charles University, Czech Republic)

Graduate Student

2023 –	Leo Dong, Emory	
2021 –	Xu Chen, Emory	
2021 –	Fangning Ren, Emory	
2020 – 2025	Ariel Gale, Emory	(Ph.D. disseratation defended in April, 2025)
2021 – 2025	Patrick Li, Emory	(M.S. graduated in May, 2025)

Research Specialist

2023 – 2024	Rohit Sai Kiran Gadde, Emory	(now: Caterpillar, Inc.)

Undergraduate, High School Student

2024 –	Ndioba Thiam, Emory U.G.	(B.S. '26 expected)
2024 – 2024	Darion Lian, HS via Johns Creek H.S.	(Johns Creek H.S. '25, now: U Penn UG)
2023 – 2023	Kenneth Wingate Jr., Emory U.G.	(B.S. '24)
2023 – 2023	Ian Su, Peking University U.G.	(B.S. '24)

2023 – 2023	Qihao Cheng, Peking University U.G.	(B.S. '24)
2022 – 2023	Yingrong Chen, Emory U.G.	(B.S. '23)
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 – 2019	Xingyue Guan, NJU-MIT exchange	(B.S. NJU '20)
2018 – 2018	Eve Xu, Wellesley-MIT exchange	(B.S. Smith, '20, now: Princeton grad)
2018 – 2018	Sean Lin, HS via Troy H.S.	(Troy H.S., '19, now: UC Berkeley UG)

Visiting Scholar

2022 – 2023	Sangni Xun, Emory	(now: Emory postdoc fellow)
2022 – 2022	Matthew Shammani, Emory	(now: UCLA grad)

Undergraduate Academic Advisement (19)
Rayna Kremer, Angel Hailemariam, Jackson Maximilian Jacobi, Brianna Goodloe, Evan Huang, Sophie Dobber, Jordan Mandel, Kevin Qi, Irene Jang, Aracell Manuel, Devyn Olivia Wong, Eric Kent, Ashley Hu, Abena Tanoh, Annabelle Phan, Kaiyang Zhu, Olivia Marie DeLucia, Nayan Mallubhotla, Rishikesh Krishnan

Undergraduate Thesis Committee (6)
Charles Qi, Jessica Forsstrom, Sam Lee, Joe Ambarian, Ashley Kim, Evan Myers.

Ph.D. Milestone/Dissertation Committee (12)
Fangning Ren, Patrick Li, Xu Chen, Luona Zhang, Kevin Marin, Shuhang Li, Quynh Giao Vu, Andrew Tran, Qingqing Lei, Reem Nsouli, Brian Zhao, Charli Chen

Awards, Honors, and Special Recognition Received by Group Members

2024	Yingrong Chen (U.G.)	NSF GRFP honorable mention
2023	Kenneth Wingate Jr. (U.G.)	100 Senior Honorary (Emory)
2023	Kenneth Wingate Jr. (U.G.)	William Jones scholarship (Emory)
2023	Yingrong Chen (U.G.)	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 (U.G.)	URP research grant (Emory)

Service & Professional Activities

Committee:

Collective Excellence Committee, Department of Chemistry, Emory University (2025 - present),
Operation Committee, Department of Chemistry, Emory University (2022 - 2025),
LTS search Committee, Department of Chemistry, Emory University (2022 - 2023),
Graduate Committee, Department of Chemistry, Emory University (2020 - 2022)

Editorial Advisory Board APL Computational Physics (2025 - present)

Early Career Editorial Advisory Board Journal of Chemical Physics (2024 - present)

Guest Editor *Artificial Intelligence Chemistry* (2023 - 2024)

Journal Referee:

Nat., *Nat. Chem.*, *Nat. Comp. Sci.*, *J. Am. Chem. Soc.*, *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:

Research Corportation of Science Advancement (2025-present),
ACS Petroleum Research Fund (2021-present),
NSF panelist (2021),
DOE (2021, 2023-present),
AFOSR (2025),
DOE Office of Science Graduate Student Research Program (2021),
CNM Proposal Evaluation Board at Argonne National Lab (2020, 2021),
DOE ASCR Leadership Computing Challenge (ALCC) (2020),
LLNL Institutional Computing Grand Challenge program (2018-2020),
INCITE allocation program (2024)

Conference Organizer:

ACS PHYS Symposium: Machine learning meets electronic structure theory (Aug. 2026)
ACS PHYS Symposium: Data-Driven Design of Energy Materials (Aug. 2023)
Atlanta Theoretical Chemistry Mini Symposium (Oct. 2022)

Conference Session Presider:

ACS National Meeting (Aug. 2024, Aug. 2022, Aug. 2021, Aug. 2018)
The Molecular Interactions and Dynamics Gordon Research Conferenc (July. 2024)

K-12 Outreach Volunteer:

Wilson Creek Elementary School Science Force Lead (2023-present)
ACS Science Coaches program (2022-2023),
NetPals to introduce STEM to underrepresented 7th grade students (2019)

Computation Consultant for Edison Pharmaceuticals Inc. (Summer 2016)