Fang Liu

Curriculum Vitae

MIT, Dept. of Chemical Engineering
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Current Position

2017 - Now **Postdoctoral Fellow,** *Department of Chemical Engineering, MIT*
Advisor: Heather J. Kulik

Education

2011 - 2017 **Ph.D.: Chemistry,** *Stanford University*, GPA *4.0/4.0*
Advisor: Todd J. Martínez
Thesis: *Quantum Chemistry for Solvated Molecules and Electronic Excited States on Graphical Processing Units (GPUs)*

2007 - 2011 **B.S.: Chemical Physics,** *University of Science and Technology of China*, GPA *4.0/4.3*
Advisor: Yi Luo
Thesis: *Density Functional Theory Studies on Catalytic Mechanisms of CO Dissociation on Ir(111) Surface*

Research Interest

Methodology: GPU accelerated electronic structure methods, solvent models, multi-reference methods, DFT/TDDFT theory and implementation, machine learning

Computation: automated workflow for reaction network, ab initio molecular dynamics, QM/MM

Applications: transition metal complexes, single-atom catalyst, redox potential, absorption spectrum, mass spectrometry fragmentation reactions, photochemistry, hydrogen bond

Honors and Awards

2019 **MolSSI Investment Fellowship**, National Science Foundation
18-month fellowship supporting molecular science software development in the MolSSI community

2019 **MolSSI Seed Fellowship**, National Science Foundation
Six-month fellowship supporting molecular science software development in the MolSSI community

2018 **NVIDIA GPU Award**, American Chemical Society
For outstanding research in Computational Chemistry, one awardee for each ACS national meeting

2016 **Evelyn Laing McBain Fellowship**, Stanford University
Awarded to outstanding female graduate students majored in chemistry

2011 **Excellent Undergraduate Thesis**, University of Science and Technology of China
Awarded to top 3% undergraduate students in USTC based on the performance of thesis.

2011 **Guo Moruo Scholarship**, University of Science and Technology of China
Top scholarship in USTC awarded to top 20-30 senior students each year across the university

2009 **National Scholarship of China**, Ministry of Education of China

Research Experiences

Massachusetts Institute of Technology (MIT) 2017 - Now Advisor: Heather Kulik

- Investigated the effects of density delocalization error on structural properties of inorganic molecules
- Built an workflow for in-situ control and analysis of quantum chemistry simulation (MolSSI project)
- Modeled the absorption pattern of organic fraction reducers on iron oxide surface
- Studied the degradation mechanism of nafion membrane in fuel cell
- Proposed a protocol for accurate and efficient ionization potential calculation of polymer electrolytes

Stanford University 2012 - 2017 Advisor: Todd Martínez

- Developed a highly efficient GPU-based algorithm for Polarizable Continuum Model
- Implemented the analytical gradient of a novel excited-state ensemble Kohn-Sham method on GPUs
- Developed a workflow for reaction pathway calculation on mass spectrometry fragmentation reactions
- Modeled structural coupling in hydrogen bond network in proteins with QM/MM
- Proposed a protocol for calculating the redox potential of quinones in solution phase
- Implemented new functionals of TDDFT in the GPU based quantum chemistry package, TeraChem
- Simulated the absorption spectral of proteorhodopsin using QM/MM and TDDFT

University of Science and Technology of China (USTC) 2010 - 2011 Advisor: Yi Luo

- Studied catalytic mechanisms of CO Dissociation on Ir(111) Surface with first principal methods

University of California, Los Angeles (UCLA) 2010 Advisor: Clifton Shen

- Developed a protocol for high-throughput screening of melanoma specific ^{18}F-Labeled PET Probes

Teaching & Mentoring Experiences

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)

Student Mentoring (Stanford 2015-2017 & MIT 2018-2019):

Xingyue Guan (Undergraduate student) – "DFT study of inorganic complexes" (Spring 2019)
Eve Xu (Undergraduate UROP student) – "DFT study of single atom catalysts" (Fall 2018)
Sean Lin (High school intern student) – "Structure database meets machine learning" (Summer 2018)
David Sanchez (Graduate student, Martínez group) – "Absorption spectrum calculation" (2015 - 2017)

Grant Proposal Writing Experiences

Funded Proposal for MolSSI Seed and Investiment Fellowship on "Automated Workflow for Inorganic Molecular Systems" for 2019-2020 (6 months and 18 months) - Total: $100,000
Co-PI of XSEDE Research Allocation proposal for 2019 - 2020 – Total: 97K GPU hours, 381K CPU hours
Alternative PI of DoD HPC Allocation proposal for 2018 - 2020 – Total: 5.3M CPU hours

Service & Professional Activities

Journal Referee for *J. Chem. Theory Comput.* & *Mol. Simulat.*
Grant Reviewer for the proposals of 13th & 14th annual Lawrence Livermore National Laboratory Institutional Computing Grand Challenge program (2018 & 2019)
Session Chair for *256th ACS National Meeting* (Aug. 2018)
Outreach Volunteer for NetPals to introduce STEM to underrepresented 7th grade students (2019)
Computation Consultant for Edison Pharmaceuticals Inc. (Summer 2016)

Publications

Preprints & Manuscript under Review

20. **F. Liu**, H. J. Kulik, Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry, *submitted* (2019)

19. **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), *Preprint* chemrxiv.79856 (2019)

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, *arXiv preprint* arXiv:1907.01658 (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, *submitted* (2019)

Journal Articles

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 contribute 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

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

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

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

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

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

Contributed Talks

- *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)

- *Understanding and correcting DFT errors in transition metal chemistry*
  F. Liu, H. J. Kulik *258th ACS National Meeting*, San Diego, CA, USA (Aug. 2019)

- *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)

- *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)

Posters

- *Improving the Theoretical Prediction of Electronic Properties in Transition Metal Chemistry*
  F. Liu, A. Bajaj, H. J. Kulik, *MIT Stephen A. Schwarzman College of Computing Launch Poster Session*, Cambridge, MA, USA (Feb. 2019)

- *Exploiting Graphical Processing Units (GPUs) to Enable Large-Scale Quantum Chemistry of Solvated Molecules with Polarizable Continuum Models*
  F. Liu, T. J. Martínez, H. J. Kulik *256th ACS National Meeting*, New Orleans, LA, USA (Aug. 2018)

- *Understanding and Correcting Density Delocalization Errors in Approximate DFT for Transition Metal Chemistry*
  F. Liu, A. Bajaj, H. J. Kulik, *Foundations of Molecular Modeling and Simulation (FOMMS) 2018*, Delevan, WI, USA (Jul. 2018)

- *Understanding and Correcting Density Delocalization Errors in Approximate DFT for Transition Metal Chemistry*
  F. Liu, A. Bajaj, H. J. Kulik, *Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST) 2018*, Telluride, CO, USA (Jun. 2018)

- *Accurate Excited State Potential Energy Surface Calculation for Large Molecules*
  F. Liu, T. J. Martínez, *West Coast Theoretical Chemistry Symposium*, Stanford, CA, USA (Mar. 2018)

- *Derivation and Implementation of Analytical Derivatives of the Individual State Energies in the SA-REKS Method*
  F. Liu, T. J. Martínez, *ACTC*, Boston, MA, USA (Jul. 2017)

- *Polarizable Continuum Model on Graphical Processing Units*
  F. Liu, T. J. Martínez, *ACTC*, Telluride, CO, USA (Jul. 2014)

- *High-Throughput Screening of Melanoma Specific ^{18}F-Labeled PET Probes*
  F. Liu, C. K.-F. Shen, *UCLA CSST Summer Research Seminar*, Los Angeles, CA, USA (Sep. 2010)

Computer Skills

Programming Languages:	Proficient in C/C++, CUDA, Python, Linux Shell Scripting, LaTeX; Familiar with Matlab, Mathematica, MPI/OpenMP; Exposure to OpenGL
Algorithms:	*Large-Scale Computational Algebra*, including diagonalization and linear solver *Large-Scale Optimizations*, including least square, simplex, constrained optimization
Developer:	*MultirefPredict, TeraChem, MolSimplify*
Computational Packages:	*Electronic Structure*: Q-Chem, Molcas, Molpro, ORCA, Quantum-ESPRESSO, Gaussian *Molecular Dynamics*: Amber, OpenMM