# **Curriculum Vitae**

Jesse McDaniel, School of Chemistry and Biochemistry, Georgia Institute of Technology

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### Jesse G. McDaniel Assistant Professor School of Chemistry and Biochemistry Georgia Institute of Technology

### I. Earned Degrees

Ph.D.: Theoretical Chemistry, University of Wisconsin-Madison	2014
Advisor: Prof. J.R. Schmidt	
B.A.: Chemistry, Washington University in St. Louis,	2008
(summa cum laude)	

# II. Employment History

Assistant Professor, Department of Chemistry and Biochemistry,	2017-present	
Georgia Institute of Technology		
Postdoctoral Research Associate, University of Wisconsin-Madison	2015-2017	
Advisor: Prof. Arun Yethiraj		

# III. Honors and Awards

National Science Foundation CAREER Award	2023
The Charles and Martha Casey Award, University of Wisconsin-Madison	2014
Hypercube Scholar Award, Washington University in St. Louis	2008

# IV. Research, Scholarship, and Creative Activities

Group Website: <a href="https://mcdaniel.chemistry.gatech.edu">https://mcdaniel.chemistry.gatech.edu</a> Citations: Google Scholar: 1618 and h-index=23 Authorship: \* indicates Georgia Tech Research; **Boldface** indicates grad students `**G**', or undergrads `**UG**' supervised by McDaniel. Superscript `**PD**' indicates postdocs supervised by McDaniel

# A. Published Books, Book Chapters, and Edited Volumes

A1. Books No data

A2. Refereed Book Chapters No data

A3. Edited Volumes No data

# B. Refereed Publications and Submitted Articles

### B1. Published and Accepted Journal Articles (49 total; \*23 from Georgia Tech)

- \*49. **Hymel J**.<sup>G</sup>, Khan S.<sup>PD</sup>, **Pederson J**.<sup>G</sup>, McDaniel J., A Computational Electrosynthesis Study of Anodic Intramolecular Olefin Coupling: Elucidating the Role of the Electrical Double Layer, *Journal of Physical Chemistry C*, **2023**, 127, 19489-19508.
- \*48. **Stoppelman J.P**.<sup>G</sup>, Wilkinson A.P., McDaniel J., Equation of State Predictions for ScF3 and CaZrF6 with Neural Network-Driven Molecular Dynamics, *Journal of Chemical Physics*, **2023**, 159, 084707.
- \*47. **Stoppelman J.P**.<sup>G</sup>, McDaniel J., N-Heterocyclic Carbene Formation in the Ionic liquid [EMIM+][OAc-]: Elucidating Solvation Effects with Reactive Molecular Dynamics Simulations, *Journal of Physical Chemistry B*, **2023**, 127, 5317-5333.
- \*46. Tu Y.-J., Wu S.-C., McDaniel J., Importance of Anion-Anion Pairing for Capacitance of Carbon/Ionic Liquid Interfaces, *Journal of Physical Chemistry C*, **2022**, 126, 20213-20225.
- \*45. **Stoppelman J.P.**<sup>G</sup>, McDaniel J., Cicerone M., Excitations Follow (or Lead?) Density Scaling in Propylene Carbonate, *Journal of Chemical Physics*, **2022**, 157, 204506.
- \*44. Park S.<sup>G</sup>, McDaniel J., Helmholtz Capacitance of Aqueous NaCl Solutions at the Au(100) Electrode from Polarizable and Nonpolarizable Molecular Dynamics Simulations, *Journal of Physical Chemistry C*, 2022, 126, 16461-16476.
- \*43. Philippi F., Rauber D., Palumbo O., Goloviznina K., McDaniel J., Pugh D., Suarez S., Fraenza C., Padua A., Kay C.W.M., Welton T., Flexibility is the Key to Tuning the Transport Properties of Fluorinated Imidebased Ionic Liquids, *Chemical Science*, **2022**.
- \*42. **Pederson J.P.**<sup>UG</sup>, McDaniel J., DFT-based QM/MM with Particle-Mesh Ewald for Direct, Long-Range Electrostatic Embedding, *Journal of Chemical Physics*, **2022**, 156, 174105.
- \*41. McDaniel J., Capacitance of Carbon Nanotube/Graphene Composite Electrodes with [BMIM<sup>+</sup>][BF<sub>4</sub><sup>-</sup>]/Acetonitrile: Fixed Voltage Molecular Dynamics Simulations, *Journal of Physical Chemistry C*, 2022, 126, 5822-5837.
- \*40. Stoppelman, J.P.<sup>G</sup>, McDaniel J., Physics-Based, Neural Network Force Fields for Reactive Molecular Dynamics: Investigation of Carbene Formation from [EMIM<sup>+</sup>][OAc<sup>-</sup>], *Journal of Chemical Physics*, 2021, 155, 104112.
- \*39. Tu Y.-J.<sup>PD</sup>, McDaniel J., Structure-Capacitance Relationships of Graphene/Ionic Liquid Electrolyte Double Layers, *Journal of Physical Chemistry C*, **2021**, 125, 20204-20218.
- 38. Jeong, K.J., McDaniel J., Yethiraj, A. Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field, *Journal of Physical Chemistry B*, **2021**, 125, 7177-7186.
- \*37. McDaniel J., Josowicz M., Janata J.. Quantized Electrodes: Atomic Palladium and Gold in Polyaniline, *ChemElectroChem*, **2021**, 8, 1766-1774.
- 36. Jeong, K.J., McDaniel J., Yethiraj, A. A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions, *Journal of Physical Chemistry B*, **2020**, 124, 7475-7483.
- \*35. **Stoppelman, J.P.**<sup>G</sup>, McDaniel J., Proton Transport in [BMIM<sup>+</sup>][BF<sub>4</sub><sup>-</sup>] / Water Mixtures Near the Percolation Threshold, *Journal of Physical Chemistry B*, **2020**, 124, 5957-5970.
- \*34. **Delmerico S.**<sup>UG</sup>, McDaniel J., Free Energy Barriers for TMEA+, TMA+, and BF4- Ion Diffusion through Nanoporous Carbon Electrodes, *Carbon*, **2020**, 161, 550-561.

- \*33. Tu Y.-J.<sup>PD</sup>, **Delmerico S.<sup>UG</sup>**, McDaniel J. Inner Layer Capacitance of Organic Electrolytes from Constant Voltage Molecular Dynamics, *Journal of Physical Chemistry C*, **2020**, 124, 2907-2922.
- \*32. **Park S.**<sup>G</sup>, McDaniel J. Interference of Electrical Double Layers: Confinement Effects on Structure, Dynamics, and Screening of Ionic Liquids, *Journal of Chemical Physics*, **2020**, 123, 5343-5356.
- \*31. Sun Z.<sup>G</sup>, Fu W., Liu M., Lu P., Zhao E. Magasinski A., Liu M., Luo S., McDaniel J., Yushin G. A Nanoconfined Iron(III) Fluoride Cathode in a NaDFOB Electrolyte: Towards High-Performance Sodium-Ion Batteries, *Journal of Materials Chemistry A*, 2020, 8, 4091.
- \*30. Verma A.<sup>ug</sup>, Stoppelman J.<sup>G</sup>, McDaniel J. Tuning Water Networks via Ionic Liquid/Water Mixtures, International Journal of Molecular Sciences, 2020, 21, 403.
- 29. Son C.-Y., McDaniel J., Cui Q., Yethiraj A. Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-Nose-Hoover Thermostat, *Journal of Physical Chemistry Letters*, **2019**, 10, 7523-7530.
- \*28. McDaniel J., **Verma A**.<sup>ug</sup> On the Miscibility and Immiscibility of Ionic Liquids and Water, *Journal of Physical Chemistry B*, **2019**, 123, 5343-5356.
- \*27. McDaniel J., Yethiraj A. Understanding the Properties of Ionic Liquids: Electrostatics, Structure Factors, and Their Sum Rules, *Journal of Physical Chemistry B*, **2019**, 123, 3499-3512.
- \*26. McDaniel J., Yethiraj A. Influence of Electronic Polarization on the Structure of Ionic Liquids, *Journal of Physical Chemistry Letters*, **2018**, 9, 4765-4770.
- 25. Son C.Y., McDaniel J., Cui Q., Yethiraj A. Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM<sup>+</sup>BF4<sup>-</sup>: A Microsecond Computer Simulation Study Using ab Initio Force Fields, *Macromolecules*, **2018**, 51, 5336-5345.
- \*24. McDaniel J., Son C.Y., Ion Correlation and Collective Dynamics in BMIM/BF<sub>4</sub> Based Organic Electrolytes: From Dilute Solutions to the Ionic Liquid Limit, *Journal of Physical Chemistry B*, **2018**, 122, 7154-7169.
- \*23. McDaniel J. Polarization Effects in Binary [BMIM<sup>+</sup>][BF<sub>4</sub><sup>-</sup>]/1,2-Dichloroethane, Acetone, Acetonitrile, and Water Electrolytes, *Journal of Physical Chemistry B*, **2018**, 122, 4345-4355.
- 22. McDaniel J, Son C.Y., Yethiraj A. Ab Initio Force Fields for Organic Anions: Properties of [BMIM][TFSI], [BMIM][FSI], and [BMIM][OTf] Ionic Liquids, **2018**, *Journal of Physical Chemistry B*, 122, 4101-4114.
- 21. McDaniel J, Yethiraj A. Grotthuss Transport of Iodide in EMIM/I<sub>3</sub> Ionic Crystals. *Journal of Physical Chemistry B*, **2018**, 122, 250-257.
- 20. McDaniel J, Yethiraj A. Proton Diffusion through Bilayer Pores. *Journal of Physical Chemistry B*, **2017**, 121, 9247-9259.
- 19. McDaniel J, Yethiraj A. Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. *Journal of Physical Chemistry B*, **2017**, 121, 5048-5057.
- 18. McDaniel J, Mantha S, Perroni D, Mahanthappa M., Yethiraj A. Electrostatic Interactions Govern "Odd-Even" Effects in Water-Induced Gemini Surfactant Self-Assembly. *Journal of Physical Chemistry B.* **2017**, 121, 565-576.
- 17. McDaniel J, Mantha S, Yethiraj A. Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. *Journal of Physical Chemistry B*, **2016**, 120, 10860-10868.
- 16. McDaniel J, Choi E., Son CY, Schmidt JR, Yethiraj A. Ab Initio Force Fields for Imidazolium Based Ionic Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 7024-7036/
- 15. McDaniel J, Schmidt JR. Next-Generation Force Fields from Symmetry-Adapted Perturbation Theory. *Annual Reviews of Physical Chemistry*, **2016**, 67, 467.

- 14. Son CY, McDaniel J, Schmidt JR, Cui Q, Yethiraj A. First Principles United Atom Force Field for the Ionic Liquid [BMIM][BF4]: An Alternative to Charge Scaling, *Journal of Physical Chemistry B*, **2016**, 120, 3560.
- 13. McDaniel J, Yethiraj A. Comment on "Isolating the Non-Polar Contributions to the Intermolecular Potential for Water-Alkane Interactions [J. Chem. Phys. 141, 064905 (2014)]", *Journal of Chemical Physics*, **2016**, 144, 137101.
- 12. McDaniel J, Yethiraj A. Importance of Hydrophobic Traps for Proton Diffusion in Lyotropic Liquid Crystals, *Journal of Chemical Physics*, **2016**, 144, 094705.
- 11. McDaniel J, Choi E., Son CY, Schmidt JR, Yethiraj A. Conformational and Dynamic Properties of Poly(ethylene oxide) in an Ionic Liquid: Development and Implementation of a First-Principles Force Field, *Journal of Physical Chemistry B.*, **2016**, 120, 231-243.
- McDaniel J, Li S, Tylianakis, E, Snurr R, Schmidt JR. Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metal-Organic Frameworks, *Journal of Physical Chemistry C.*, 2015, 119, 3143-3152.
- 9. Schmidt JR, Yu K, McDaniel J. Transferable Next-Generation Force Fields from Simple Liquids to Complex Materials, *Accounts of Chemical Research*, **2015**, 48, 548-556.
- 8. McDaniel J, Choi E, Schmidt JR, Yethiraj A. A First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF<sub>4</sub>], *Journal of Physical Chemistry Letters*, **2014**, 5, 2670-2674.
- 7. McDaniel J, Schmidt JR. First-Principles Many-Body Force Fields from the Gas-Phase to the Liquid: A "Universal" Approach. *Journal of Physical Chemistry B.* **2014**, 118, 8042-8053.
- 6. McDaniel J, Yu K, Schmidt JR. Microscopic Origins of Enhanced Gas Adsorption and Selectivity in Mixed-Linker Metal-Organic Frameworks. *Journal of Physical Chemistry C.* **2013**, 117, 17131-17142.
- 5. McDaniel J, Schmidt JR. Physically-Motivated Force Fields from Symmetry-Adapted Perturbation Theory. *Journal of Physical Chemistry A.* **2013**, 117, 2053-2066.
- 4. Yu K, McDaniel J, Schmidt JR. An Efficient Multi-Scale Lattice Model Approach to Screening Nano-Porous Adsorbents. *Journal of Chemical Physics*. **2012**, 137, 244102.
- 3. McDaniel J, Schmidt JR. Robust, Transferable, and Physically-Motivated Force Fields for Gas Adsorption in Functionalized Zeolitic Imidazolate Frameworks. *Journal of Physical Chemistry C.* **2012**, 116, 14031-14039.
- 2. McDaniel J, Schmidt JR. Ab Initio, Physically Motivated Force Fields for CO<sub>2</sub> Adsorption in Zeolitic Imidazolate Frameworks. *Journal of Physical Chemistry C.* **2011**, 116, 1892-1903.
- 1. Yu K, McDaniel J, Schmidt JR. Physically-Motivated, Robust, Ab Initio Force Fields for CO<sub>2</sub> and N<sub>2</sub>. *Journal of Physical Chemistry B*. **2011**, 115, 10054-10063.

#### **B2.** Conference Presentation with Proceedings (Refereed)

No data

#### **B3. Other Refereed Material**

No data

### **B4. Submitted Journal Articles (1 total)**

\*1. Cicerone M.T., Zahn J., **Stoppelman J.P.**<sup>G</sup>, McDaniel J, Badilla-Nunez K.,. Excitation Populations Provide a Thermodynamic Order Parameter for Liquids. *Physical Review Letters, Submitted (March 13, 2023)* 

### C. Other Publications and Creative Products

J. McDaniel ""Development and Application of Physically-Motivated, First-Principles Force Fields for Complex Chemical Systems", PhD Dissertation, University of Wisconsin-Madison, Nov. 2014.

### D. Presentations

### **D1. Invited Presentations**

- \*24 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", University of South Carolina, Departmental Seminar, Columbia, SC, December 1<sup>st</sup>, 2023.
- \*23 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", Georgia State University, Departmental Seminar, Atlanta, GA, September 15<sup>th</sup>, 2023.
- \*22 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", Georgia Tech, Departmental Seminar, Atlanta, GA, September 7<sup>th</sup>, 2023.
- \*21 "Electrical Double Layer Modulation of Organic Reactions at Electrode Interfaces", AFOSR Program Review, Arlington, VA, May 16<sup>th</sup>, 2023.
- \*20 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", University of Pittsburgh, Departmental Seminar, Pittsburgh, PA, March 22<sup>nd</sup>, 2023.
- \*19 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", University of California-San Diego, Departmental Seminar, San Diego, CA, February 28<sup>th</sup>, 2023.
- \*18 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", University of Southern California, Departmental Seminar, Los Angeles, CA, February 27<sup>th</sup>, 2023.
- \*17 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", Auburn University, Departmental Seminar, Auburn, AL, February 23<sup>rd</sup>, 2023.
- \*16 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", Boston University, Departmental Seminar, Boston, MA, February 2<sup>nd</sup>, 2023.
- \*15 "Electrochemical Interfaces: Chemical Reactions and Physical Properties", Tufts University, Departmental Seminar, Boston, MA, February 1<sup>st</sup>, 2023.
- \*14 "Dielectric Properties of Ionic Liquids and Implications for Miscibility, Solvation, and Capacitance", Electrochemical Society Meeting (ECS), "Molten Salts and Ionic Liquids" symposium, Atlanta, GA, October 11<sup>th</sup>, 2022.
- \*13 "Ionic Liquids at Electrified Interfaces: Inner Layer Capacitance and the Solvophobic Effect", Gordon Research Conference on Ionic Liquids, Newry, ME, August 9<sup>th</sup>, 2022.
- \*12 "Physics Based, Neural Network Force Fields for Reactive Molecular Dynamics", AutoCheMo International Reactive Force Field Workshop, Ghent, Belgium, December 9<sup>th</sup>, 2021.
- \*11 "Electrochemical Interfaces: Contrasting Ionic Liquids and Aqueous Electrolytes", Kansas University, Departmental Seminar, November 8<sup>th</sup>, 2021.
- \*10. "Aqueous vs Ionic Liquid Double Layers: Incorporating Electric Fields in Computational Electrochemistry", AFRL MURI Seminar, Emory University, August 10<sup>th</sup>, 2021.
- \*9. "Ionic Liquids and Electrochemical Interfaces", Air Force Research Lab (AFRL) Seminar, April 21<sup>th</sup>, 2021
- \*8. "Electrochemical Interfaces and Ionic Media", University of South Carolina, Departmental Seminar, March 29<sup>th</sup>, 2021
- \*7. "First Principles Modeling of Electrochemical Interfaces", Southeastern Theoretical Chemistry Association Meeting, University of Tennessee, May 18<sup>th</sup>, 2019

October 23<sup>rd</sup>, 2023

- \*6. "What Happened to Like-Dissolves-Like? The Miscibility of Ionic Liquids with Low-Dielectric Solvents", Atlanta Mini Symposium on Theoretical and Computational Chemistry, Emory University, September 8<sup>th</sup>, 2018
- \*5. "Collective Processes in Organic Electrolytes: From Dilute Solutions to the Ionic Liquid Limit", Gordon Research Conference: Ionic Liquids, Newry, ME, August 16<sup>th</sup>, 2018
- 4. "Accurate and Transferable Ab Initio Force Fields", D. E. Shaw Research, New York, May 6<sup>th</sup>, 2016
- "Physically-motivated first-principles force fields for molecular simulation: Theory and applications", American Chemical Society, COMP 309, March 24<sup>th</sup>, 2015
- "Development and Application of ab initio Force Fields for Organic and Ionic Liquids", Interdisciplinary Computational Group Seminar, University of Wisconsin-Madison, MRSEC, February 2<sup>nd</sup>, 2015
- 1. "Evaluation of Force Field Performance for High Throughput Screening of Gas Uptake in MOFs.", Nanoporous Materials Genome Center Conference, University of Minnesota, October 18<sup>th</sup>, 2014.

### **D2. Contributed Presentations**

- \*7 "N1888/TFSI Ionic Liquid: Structure, Neutron Scattering, and Validation of Macroscopic Electrostatics", AFOSR Ionic Liquids Working Group, October 18<sup>th</sup>, 2023.
- \*6 "Ionic Liquids: Electrostatic Screening and Water Miscibility", AFOSR Ionic Liquids Working Group, July 20<sup>th</sup>, 2022.
- \*5. "Physics Based, Neural Network Force Fields for Reactive Molecular Dynamics", American Chemical Society (ACS)-Fall Meeting, PHYS-Division, Atlanta, GA, Aug 23<sup>rd</sup>, 2021.
- \*4. "Influence of Electronic Polarization on the Structure of Ionic Liquids", American Chemical Society (ACS)-Fall Meeting, PHYS-Division, San Francisco, CA, Aug 18<sup>th</sup>, 2020.
- \*3. "Hydrophobic Interactions in Organic Electrolyte Double Layers", American Chemical Society (ACS) -Fall Meeting, PHYS-Division, San Francisco, CA, Aug 17<sup>th</sup>, 2020.
- \*2. "Influence of Electronic Polarization on the Structure of Ionic Liquids", American Chemical Society (ACS) -Fall Meeting, Division of Computers in Chemistry, San Diego, CA, Aug 28<sup>th</sup>, 2019.
- \*1. "Inner Layer Capacitance and Structure of Electrochemical Interfaces", American Chemical Society (ACS)-Fall Meeting, Division of Energy and Fuels, San Diego, CA, Aug 26<sup>th</sup>, 2019.

### E. Grants and Contracts

#### E1. As Principal Investigator

**Currently Funded** 

 6. "Solvation Effects at the Solid/Liquid Interface in Heterogeneous Catalysis" Agency: American Chemical Society, Petroleum Research Fund Total: \$110,000 (Direct Costs: \$110,000) Role: PI Collaborators: None Period of Contract: 9/01/2023 – 8/31/2025 Share: 100%

- 5. "CAREER: Accelerated Chemical Reactions in Unique Solvation Environments" Agency: National Science Foundation, Division of Chemistry, Chemical Theory, Models, and Computational Methods Total: \$650,000 (Direct Costs: \$471,805) Role: PI Collaborators: None Period of Contract: 1/01/2023 – 12/31/2027 Share: 100%
- 4. "Electrocatalytic Self-Healing Mechanisms in Energy Storage Materials" Agency: Air Force Office of Scientific Research, Molecular Dynamics and Theoretical Chemistry Total: \$450,000 (Direct Costs: \$325,135) Role: PI Collaborators: None Period of Contract: 11/01/2021 – 10/31/2024 Share: 100%

#### **Previously Funded**

3. "Theoretical Characterization of Correlated Redox Activity and Nanostructure in Hybrid Supercapacitors"

Agency: Department of Energy, Basic Energy Sciences, Computational and Theoretical Chemistry Total: \$390,000 (Direct Costs: \$267,804) Role: PI Collaborators: None Period of Contract: 9/01/2019 – 8/31/2022 Share: 100%

2. "Simulating Crystal Structures"

Agency: Microsoft Azure Cloud Computing Credits Total: \$18,523 (CPU credits) Role: PI Collaborators: None Period of Contract: 12/01/2021 – 6/30/2022 Share: 100%

1. "Energetics of Hydration-mediated Defects in Rare Earth Oxides"

Agency: XSEDE Computing Credits Total: \$2,000 (CPU credits) Role: PI Collaborators: None Period of Contract: 9/01/2017 – 8/31/2018 Share: 100%

#### E2. As Co-Principal Investigator

No data

**E3. As Senior Personnel or Contributor** No data

E4. Pending Proposals

No data

#### E5. Proposals Submitted but Not Funded (Last Two Years)

2. "Electrochemical Kinetics at Ionic Liquid/Electrode Interfaces Investigated by First-Principles, Multiscale Modeling"

Agency: Department of Energy, Basic Energy Sciences, Computational and Theoretical Chemistry Total: \$485,796 Role: PI Collaborators: None Period of Contract: 9/01/2022 – 8/31/2025 Share: 100%

1. "A General, Quantitative Model of Dynamics and Transport in Liquids-Combined Experiment and Theory"

Agency: National Science Foundation, Division of Chemistry, CSDM-A Total: \$929,782 Role: co-PI Collaborators: Marc Cicerone (Georgia Tech) Period of Contract: 6/01/2022 – 5/31/2025 Share: 50%

#### F. Other Scholarly and Creative Accomplishments

No Data

#### G. Societal and Policy Impacts

No Data

#### H. Other Professional Activities

No Data

### V. Education

#### A. Courses Taught

Fall 2022	CHEM-6481	Statistical Mechanics	12 Students
Spring 2022	CHEM-3411	Physical Chemistry I	25 Students
Fall 2021	CHEM-6481	Statistical Mechanics	9 Students
Spring 2021	CHEM-3411	Physical Chemistry I	44 Students
Fall 2020	CHEM-6481	Statistical Mechanics	7 Students
Fall 2019	CHEM-6481	Statistical Mechanics	8 Students
Spring 2019	CHEM-3411	Physical Chemistry I	49 Students
Fall 2018	CHEM-6481	Statistical Mechanics	9 Students
Fall 2017	CHEM-6481	Statistical Mechanics	2 Students

#### B. Individual Student Guidance

#### B1. Ph.D. Students (7 Total)

- 7. John Pederson. GT Chemistry Graduate Student 01/2023-Current Project: "Quantum Mechanics/Molecular Mechanics Method Development" Awards: NSF-GRF Honorable Mention
- Shehan Parmar. GT Chemistry Graduate Student 01/2023-Current Project: "Properties of Room Temperature Ionic Liquids" Awards: DOE-CSGF Graduate Fellowship
- Chloe Renfro. GT Chemistry Graduate Student 01/2022-Current Candidacy Exam passed April, 2023 Project: "Computational Studies of Heterogeneous Electron Transfer"
- John Hymel. GT Chemistry Graduate Student 01/2021-Current Candidacy Exam passed May, 2022 Project: "Computational Electrosynthesis" Awards: Fellowship to 2023 Telluride Summer School on Theoretical Chemistry (TSTC)
- Zifei Sun. GT Chemistry Graduate Student 01/2019-05/2021 Co-advised with Gleb Yushin, MSE PhD defense, 05/2021 Dissertation: "Improving Electrochemical Performance of Iron Trifluoride (FeF3) in Sodium-Ion Batteries"
- Sue Park. GT Chemistry Graduate Student 01/2019-Current Candidacy Exam passed May, 2020 PhD expected, July 2023 Project: "Theory/Modeling of Electrical Double Layers" Awards: 1<sup>st</sup> place talk/presentation at 2023 Chemistry Departmental Research Symposium
- 1. John Stoppelman. GT Chemistry Graduate Student 01/2019-Current

Candidacy Exam passed May, 2020 PhD expected, July 2023 Project: "Physics-Based, Neural Network Reactive Force Fields" Awards: NSF-GRF Honorable Mention

### **B2. M.S. Students (Indicate Thesis Option for Each Student)** No Data

#### **B3. Undergraduate Students (9 Total)**

- 9. John Pederson. GT ChBE Undergraduate Student 01/2019-12/2021 President's Undergraduate Research Award (PURA), Summer 2020 Subsequently: Graduate Student in Chemistry at Georgia Tech
- 8. Devin Hernandez. REU program, UC-Irvine Undergraduate Student 05/2021-07/2021 Subsequently: Graduate Student in Chemistry at UC-Berkeley
- 7. Noah Osman REU program, University of Tennessee Undergraduate Student 05/2021-07/2021
- Archana Verma Stanford Undergraduate Student Summer 2018, Summer 2019 NSF-GRF Fellowship, 2021 Subsequently: Graduate Student in Chemical Engineering at University of Illinois
- Sam Delmerico. GT Chemistry Undergraduate Student 01/2018-05/2020 GT Sigma Xi Best Undergraduate Research Award, 2020 President's Undergraduate Research Award (PURA), Summer 2018 Subsequently: Google (Atlanta, GA)
- 4. Sam Wiley. GT Physics Undergraduate Student 08/2019-12/2019
- Daniel Profili. GT Chemistry Undergraduate Student 01/2018-05/2020 President's Undergraduate Research Award (PURA), Summer 2019 Subsequently: Graduate Student in Mathematics at NC State University
- 2. Aja Nicely. GT Chemistry Undergraduate Student 01/2018-05/2018
- 1. Yong Shan Lee. GT Chemistry Undergraduate Student 01/2018-05/2018

#### B4. Service on Thesis or Dissertation Committees (39 Total)

39.	Qijia Huang	GT Chemistry Candidacy 2023	Advisor Dong Qin
38.	Caroline Sargent	GT Chemistry Candidacy 2023	Advisor David Sherrill
37.	Jordan Hale	GT Chemistry Candidacy 2023	Advisor Josh Kretchmer
36.	Zhihao Feng	GT ChBE. Thesis Proposal 2023	Advisor Thomas Gartner
35.	Kunal Dani.	GT ChBE. Thesis Proposal 2022	Advisor Mark Prausnitz

34.	Jia Yuan Chng.	GT ChBE. Thesis Proposal 2022	Advisor David Sholl
33.	Yuhan Yang.	GT ChBE PhD 2022	Advisor David Sholl
32.	Abby Advincula	GT Chemistry PhD 2022	Advisor John Reynolds
31.	Dariia Yehorova	GT Chemistry Candidacy 2022	Advisor Josh Kretchmer
30.	Philip Nelson	GT Chemistry Candidacy 2022	Advisor David Sherrill
29.	Zach Glick	GT Chemistry PhD 2022	Advisor David Sherrill
28.	Derek Metcalf	GT Chemistry PhD 2022	Advisor David Sherrill
27.	Yi Xie	GT Chemistry PhD 2022	Advisor David Sherrill
26.	Ojuolape Oghenete	ga GT ChBE. Thesis Proposal 202	2 Advisor Krista Walton
25.	Kelly Badilla-Nunez	GT ChBE. Thesis Proposal 2021	Advisor Marc Cicerone
24.	Veronica Pawlik	GT Chemistry Candidacy 2021	Advisor Younan Xia
23.	Elizabeth Gutierrez-	Meza GT Chemistry PhD 2021	Advisor Carlos Silva
22.	Christina Buffo	GT Chemistry Candidacy 2021	Advisor Thom Orlando
21.	Monica Perez Cueva	as GT ChBE. PhD 2021	Advisor Mark Prausnitz
20.	Chao-Wen Chang	GT ChBE. Thesis Proposal 2021	Advisor David Sholl
19.	Xuqing Cai.	GT ChBE. Thesis Proposal 2021	Advisor David Sholl
18.	Sushree Sahoo	GT ChBE. Thesis Proposal 2021	Advisor AJ Medford
17.	Chaoyi Chang	GT ChBE. PhD 2021	Advisor AJ Medford
16.	Xiangyun (Ray) Lei	GT ChBE. PhD 2021	Advisor AJ Medford
15.	Linda Nhon	GT Chemistry PhD 2021	Advisor John Reynolds
14.	Ziying Cao	GT Chemistry Candidacy 2021	Advisor Josh Kretchmer
13.	Asim Alenaizan	GT Chemistry PhD 2021	Advisor David Sherrill
12.	Tania Evans	GT ChBE. Thesis Proposal 2020.	Advisor Krista Walton
11.	Anthony Lloyd II	GT Chemistry PhD 2020	Advisor Angus Wilkinson
10.	Paul Balding.	GT Chemistry PhD 2020	Advisor Paul Russo
9.	Yulong Zheng G	T Chemistry Candidacy 2020	Advisor Carlos Silva
8.	Yuge (Nicole) Hu.	GT ChBE. Thesis Proposal 2020	Advisor AJ Medford
7.	Dominic Sirianni	GT Chemistry PhD 2020	Advisor David Sherrill
6.	Joseph O'Brien	GT CS&E. M.S. 2020	Advisor David Sherrill
5.	Katie Kuo.	GT Chemistry Candidacy 2019	Advisor JC Gumbart
4.	Brandon Bakr	GT Chemistry PhD 2018	Advisor David Sherrill
3.	Curtis Balusek	GT Physics PhD 2018	Advisor JC Gumbart
2.	Nikhil Aravindakshan	University of Regina, PhD 2018	Advisor Allan East
1.	Matthew Schieber	GT CS&E. M.S. 2018	Advisor David Sherrill

# B5. Mentorship of Postdoctoral Fellows or Visiting Scholars (2 Total)

2.	Shahriar Khan.	Postdoctoral Research Associate	01/2022-Current
1.	Yi-Jung Tu.	Postdoctoral Research Associate.	07/2018-02/2020
	Currently: As	ssistant Professor, National Chi Nan	University, Taiwan

### C. Educational Innovations and Other Contributions

- 1. Co-led summer 2021 School of Chemistry REU program. This was entirely virtual (covid) with theoretical/computational research focus. Developed and presented lectures, led/attended work sessions, and social events.
- 2. Served as mentor for Georgia Tech women+ in computational biology mentoring program (2023, Carla Kumbale)

### VI. Service

### A. Professional Contributions

#### A1. Meeting Organization

2022 Session Chair, Electrochemical Society Meeting Fall 2022, Atlanta (GA)

2022. Co-organizer, 2022 Southeastern Theoretical Chemistry Association Meeting, Atlanta GA.

2020 Symposium Organizer (PHYS), Fall American Chemical Society Meeting, San Francisco (virtual)

2019. Organizer, Atlanta Mini-Symposium on Theoretical and Computational Chemistry, Atlanta GA

#### A2. Peer Review

2023 Reviewer, Mathematical and Physical Sciences, LEAPS, National Science Foundation
2023 Reviewer, MSN Program, Division of Chemistry, National Science Foundation
2020-2022 Reviewer, Computational and Theoretical Chemistry, Basic Energy Sciences, DOE
2021-Current Reviewer, Molecular Dynamics and Theoretical Chemistry, AFOSR
2020-Current Reviewer, American Chemical Society-Petroleum Research Fund
2017-Current. Referee, Journal of Physical Chemistry, Journal of Chemical Physics, Chemistry of

Materials, Royal Society Open Science, Electrochemistry Communications, Physical Chemistry Chemical Physics, Journal of the American Chemical Society, Journal of Molecular Liquids

#### A3. Advisory Roles

2020 Guest Editor for Special Issue of International Journal of Molecular Sciences

#### A4. Membership to Professional and Honor Societies

American Chemical Society Electrochemical Society

### B. Public and Community Service

No data

#### **B.** Institute Contributions

#### **C1. School of Chemistry related service**

2023-Current Member, Executive Committee (elected)

2023-Current	Member, Graduate Recruiting Committee
2022-2023	Member, School strategic plan task force
2018-2022	Member, Graduate Admissions Committee
2018-Current	Member, Communications Committee

#### **C2.** Institute related service

2018-2020 Member of Advisory Board for Partnership for Advanced Computing Environment (PACE), Georgia Tech