Dr. Alex Albaugh

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Education

University of California, Berkeley	Ph.D.	Chemical Engineering	Berkeley, CA	2012-2018
University of Michigan	B.S.E.	Chemical Engineering	Ann Arbor, MI	2008-2012

Professional Experience

Postdoctoral Fellow	Todd Gingrich Group	Northwestern University	2018-Present
Quantitative Researcher	Property Options Group	Freelance	2019-Present
Quantitative Researcher	Partial *f*	Freelance	2018-2019
Graduate Student Researcher	Teresa Head-Gordon Group	UC Berkeley	2012-2018
Graduate Student Instructor	Chemical Engineering Dept.	UC Berkeley	2012-2017
Undergraduate Research Assistant	Ronald Larson Group	University of Michigan	2011-2012

Teaching Experience

Transport Processes	UC Berkeley	2017 (GSI)
Process Dynamics and Control	UC Berkeley	2015 (GSI)
Chemical Kinetics and Reactor Design	UC Berkeley	2013 (GSI)
Introduction to Chemical Engineering	UC Berkeley	2012 (GSI)

Selected Coursework

Computer Science: Machine learning, parallel computing
Mathematics: Numerical differential equations
Physical science: Statistical mechanics, quantum mechanics, fluid mechanics, heat transfer, petroleum geology
Engineering: Process design, process control, reactor engineering, separation processes, biomolecular engineering

Computer Proficiencies

Environments: Mac, Linux, Windows
Applications: MATLAB, Aspen, Mathematica, COMSOL, Microsoft Office, Git, LaTeX, TensorFlow
Languages: Fortran, Python, C++, C, Bash, OpenMP/MPI

Honors and Awards

Outstanding Graduate Student Instructor, UC Berkeley, 2017
Summa cum laude, University of Michigan, 2012
Julius F. Bartus Memorial Scholarship, University of Michigan, 2011-2012
James B. Angell Scholar, University of Michigan, 2011-2012
Award of Excellence Scholarship, University of Michigan, 2008-2012
Dean's List and University Honors, University of Michigan, 2008-2012

Publications

1. **A. Albaugh**, T. Gingrich (2020). Simulating a Chemically-Fueled Molecular Motor with Nonequilibrium Molecular Dynamics. *(in review, arXiv:2102.06298)*
2. **A. Albaugh**, T. Gingrich (2020). Estimating Reciprocal Partition Functions to Enable Design Space Sampling. *Journal of Chemical Physics, 153,* 204102.
3. **A. Albaugh,** M. Tuckerman, T. Head-Gordon (2019). Combining Iteration-Free Polarization with Large Time Step Stochastic-Isokinetic Integration. *Journal of Chemical Theory and Computation, 15,* 2195.
4. **A. Albaugh** (2018). Improved Methods for Polarizable Classical Molecular Dynamics Simulations. *UC Berkeley Dissertation published by ProQuest.*

5. **A. Albaugh**, T. Head-Gordon, A. Niklasson (2018). Higher-order Extended Lagrangian Born-Oppenheimer Molecular Dynamics for Classical Polarizable Models. *Journal of Chemical Theory and Computation, 14*, 499.
6. **A. Albaugh**, T. Head-Gordon (2017). A New Method for Treating Drude Polarization in Classical Molecular Simulation. *Journal of Chemical Theory and Computation, 13,* 5207.
7. **A. Albaugh**, A. Niklasson, T. Head-Gordon (2017). Accurate Classical Polarization Solution with No Self-Consistent Field Iterations. *Journal of Physical Chemistry Letters, 8,* 1714.
8. V. Vitale, J. Dziedzic, **A. Albaugh**, A. Niklasson, T. Head-Gordon, C.-K. Skylaris (2017). Performance of Extended Lagrangian Schemes for Molecular Dynamics Simulations with Classical Polarizable Force Fields and Density Functional Theory. *Journal of Chemical Physics, 146,* 124115.
9. **A. Albaugh**, H. Boateng, R. Bradshaw, O. Demerdash, J. Dziedzic, Y. Mao, D. Margul, J. Swails, Q. Zeng, D. Case, P. Eastman, L.-P. Wang, J. Essex, M. Head-Gordon, V. Pande, J. Ponder, Y. Shao, C.-K. Skylaris, I. Todorov, M. Tuckerman, T. Head-Gordon (2016). Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B, 120,* 9811.
10. **A. Albaugh**, O. Demerdash, T. Head-Gordon (2015). An Efficient and Stable Hybrid Extended Lagrangian/Self-Consistent Field Scheme for Solving Classical Mutual Induction. *Journal of Chemical Physics, 143,* 174104.
11. I.S. Dalal, C.-C. Hsieh, **A. Albaugh**, R.G. Larson (2014). Effects of Volume and Hydrodynamic Interactions on the Behavior of Isolated Bead-Rod Polymer Chains in Shearing Flow. *AIChE Journal, 60,* 1400.
12. I.S. Dalal, **A. Albaugh**, N. Hoda, R.G. Larson (2012). Tumbling and Deformation of Isolated Polymer Chains in Shearing Flow. *Macromolecules, 45,* 9493.

Presentations

1. *Complete Dynamics of a Molecular Motor from Nonequilibrium Simulation.* Statistical Thermodynamics and Molecular Simulations Virtual Seminar Series, December 17, 2021.
2. *Simulating Chemically Fueled Molecular Motors*. American Institute of Chemical Engineers Annual Meeting in Boston, MA November 8, 2021.
3. *Applications of Nonequilibrium Thermodynamics & Simulation* (poster). American Institute of Chemical Engineers Annual Meeting in Boston, MA November 7, 2021.
4. *Estimating Reciprocal Partition Functions to Enable Design Space Sampling* (poster). Berkeley Statistical Mechanics Meeting in Berkeley, CA January 10, 2020.
5. *Sampling Designs by Estimating Reciprocal Partition Functions.* Northwestern University Department of Chemistry Theory Seminar in Evanston, IL November 25, 2019.
6. *Improved Methods for Polarizable Classical Molecular Dynamics Simulations.* Northwestern University Department of Chemistry Theory Seminar in Evanston, IL December 3, 2018.
7. *Improved Methods for Polarizable Classical Molecular Dynamics Simulations.* Argonne National Laboratory Institute for Molecular Engineering Seminar in Lemont, IL May 8, 2018.
8. *Novel Methods for Classical Polarizable Molecular Dynamics Simulations.* UC Berkeley Chemical Engineering Department Colloquium in Berkeley, CA March 1, 2017.
9. *Novel Methods for Polarizable Classical Molecular Dynamics Simulations* (poster). Berkeley Statistical Mechanics Meeting in Berkeley, CA January 13, 2017.
10. *Efficient Solutions of Classical Polarization Using Hybrid Extended Lagrangian/Self-Consistent Field Methods.* American Chemical Society National Meeting in Philadelphia, PA August 21, 2016.
11. *A Hybrid Extended Lagrangian/Self-Consistent Field Scheme for Solving Classical Polarization.* National Institutes of Health Laboratory of Computational Biology Weekly Seminar in Rockville, MD January 7, 2016.
12. *Novel Methods and Models for AMOEBA Polarization*. Telluride Science Research Center Advanced Potential Energy Surfaces Workshop in Telluride, CO June 16, 2015.
13. *Increasing the Efficiency of the AMOEBA Force Field Using Drude Oscillators* (poster). American Chemical Society Annual Meeting in San Francisco, CA August 12, 2014.
14. *A Drude Polarization Model for the AMOEBA Force Field*. Telluride Science Research Center Many-Body Interaction Workshop in Telluride, CO June 18, 2014.

15. *Non-monotonic Stretch of Isolated Semi-Flexible Polymer Chains* (poster). Macromolecular Science and Engineering Symposium in Ann Arbor, MI October 27, 2011.

16. *Non-monotonic Stretch of Isolated Semi-Flexible Polymer Chains* (poster). Society of Rheology Annual Meeting in Cleveland, OH October 12, 2011.