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Carl Simon Adorf

Education

2014–2019 (expected) **Doctor of Philosophy**, *University of Michigan*, Ann Arbor, MI
Chemical Engineering
Thesis: "The Inverse Design of Simple Models for the Self-Assembly of Complex Materials"
Advisor: Prof. Sharon C. Glotzer, member of the National Academy of Sciences (NAS)

2016 **Master of Engineering**, *University of Michigan*, Ann Arbor, MI
Chemical Engineering

2008–2013 **Bachelor of Science in Engineering**, *RWTH Aachen University*, Aachen, Germany
Mechanical Engineering
Thesis: "Learning Monte-Carlo algorithm for the reconstruction of coarse-grained molecular configurations"
Advisors: Prof. Ahmed E. Ismail, Dr. Christopher R. Iacovella

Experience

2014–present **Graduate Student Researcher under Prof. Sharon C. Glotzer**, *University of Michigan*, Ann Arbor, MI
Developed algorithms for the inverse design of models for kinetic self-assembly pathways of complex structures. Contributed to scientific open- and closed-source applications and led the development of an open-source framework for scientific data and workflow management called signac.

2017–2018 **Graduate Student Instructor**, *University of Michigan*, Ann Arbor, MI
Led discussion sections, office hours, developed lesson plans, created homework and exam problems and solutions, and supervised graders.

2016–2018 **XSEDE Student Campus Champion**, *University of Michigan*, Ann Arbor, MI
Conducted outreach for XSEDE resources and held workshops on high-performance computing applications on campus.

2011–2014 **Undergraduate/Graduate Research Assistant under Prof. Ahmed E. Ismail**, *RWTH Aachen University*, Aachen, Germany
Developed an algorithm for the inverse mapping of coarse-grained to fine-grained atomistic models of polymers and presented the work at international conferences.

2012 **Engineering Intern**, *Linde AG Engineering Division*, Pullach, Germany
Performed basic and detailed engineering of Liquid Nitrogen Liquefaction (LNG) receiving terminals, including the development of piping and instrumentation diagrams and participated in a HAZOP safety study with client contact.

2009–2011 **Undergraduate Research Assistant**, *Institute for Information Management in Mechanical Engineering*, RWTH Aachen University, Aachen, Germany

2008 **Intern**, *Daimler AG*, Stuttgart, Germany

Software Development

signac *Lead-developer* https://signac.io

- Open-source framework for the management of data and file-based workflows implemented in Python.
- Led initial and continuing conceptualization and development, guiding internal and external contributors.
- Conducted surveys and feedback sessions to obtain user input to guide development and improve documentation.
- Implemented continuous integration for unit and integration tests and deployment.

HOOMD-blue *Contributor* http://glotzerlab.engin.umich.edu/hoomd-blue

- Open-source application for the simulation of particle systems implemented in C++, CUDA and Python.
- Implemented features for the automated capture of metadata, the installation of analyzer callbacks, and a hook for the integration of external tools to enable advanced sampling techniques.

freud *Contributor* http://glotzerlab.engin.umich.edu/freud

- Open-source application for the analysis of particle simulation trajectories.
- Implemented the box-module.

Professional Skills

Coding Proficiency: Python (Expert), C++ (Advanced), CUDA (Intermediate), MATLAB (Intermediate)
Continuous integration (CI): TravisCI, CircleCI, and Bitbucket pipelines
git, MPI, bash scripting, LaTeX
Python packages: NumPy, SciPy, TensorFlow, Keras
Supercomputing: Parallel computing on national supercomputers: OLCF Titan, SDSC Comet, PSC Bridges
Languages: German (Native), English (Fluent)
Other Skills: Machine Learning, Adobe Creative Suite, Microsoft Office

Teaching

2017–2018 **CHE 330 Chemical & Engineering Thermodynamics**, *University of Michigan*
2013–2014 **Introduction to Materials Science**, *RWTH Aachen University*, (*German*: Material- und Stoffkunde)
2009–2011 **Computer Science for Mechanical Engineers**, *RWTH Aachen University*

Mentorship

2017–present **Yannah Melle**, *B.Sc. Chemical Engineering (class of 2021)*, University of Michigan
As part of the Undergraduate Research Opportunity Program (UROP) from 2017–2018.
2016 **Kyle Pettibone**, *B.Sc. Chemical Engineering (class of 2017)*, University of Michigan
As part of the Summer Undergraduate Research Experience (SURE).
2015 **Markus Höhnerbach**, *M.Sc. Simulation Science (class of 2015)*, RWTH Aachen University

Professional Activities, Awards and Scholarships

2014–present **MICDE Fellowship**, *Michigan Institute for Computational Discovery & Engineering (MICDE)*
2016 **Ad-hoc reviewer**, *ACS Nano*, (ISSN 1936-0851)
2016 **Member of search and hiring committee**, *for Research IT Specialist*
2016 **Charles G. Overberger Conference Travel Award**, *Macromolecular Science and Engineering Program*
2016 **SDSC Summer Institute Room and Board Scholarship**, *National Science Foundation (NSF)*
2012 **RWTH UROP Abroad**, *Vanderbilt University*, Nashville, TN

Publications

5. Allen LaCour, **Carl S. Adorf**, Sharon C. Glotzer, "*The Influence of Softness on Binary Sphere Crystals,*" *In preparation.*

4. **Carl S. Adorf**, Vyas Ramasubramani, Joshua A. Anderson, Sharon C. Glotzer, "*How to professionally develop reusable scientific software — and when not to,*" *Computing in Science & Engineering* (*accepted*).

3. **Carl S. Adorf**, James Antonaglia, Julia Dshemuchadse, Sharon C. Glotzer, "*Inverse Design of Simple Pair Potentials for the Self-Assembly of Complex Structures,*" *J. Chem. Phys.*, vol. 149 (20), p. 204102, 2018. DOI:10.1063/1.5063802

2. Vyas Ramasubramani, **Carl S. Adorf**, Paul M. Dodd, Bradley D. Dice, Sharon C. Glotzer, "*signac: A Python framework for data and workflow management,*" Proc. 17th Python Sci. Conf., pp. 91-98, 2018. DOI:10.25080/Majora-4af1f417-016.

1. **Carl S. Adorf**, Paul M. Dodd, Vyas Ramasubramani, Sharon C. Glotzer, "*Simple Data and Workflow Management with the signac Framework,*" *Comput. Mater. Sci.*, vol. 146, pp. 220-229, 2018. DOI:10.1016/j.commatsci.2018.01.035. **Editor's choice.**

Colloquia and Conference Presentations

Oral Presentations

12. **Carl S. Adorf**, **Vyas Ramasubramani**, **Joshua A. Anderson**, Sharon C. Glotzer, "*Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud,*" **invited workshop** at the American Institute of Chemical Engineers (AIChE) Annual Meeting 2018, Pittsburgh, PA, November 2018.

11. **Carl S. Adorf**, Paul M. Dodd, Vyas Ramasubramani, Bradley Dice, Sharon C. Glotzer, "*Reproducible Computational Workflows with signac,*" contributed talk at the AIChE Annual Meeting 2018, Pittsburgh, PA, November 2018.

10. **Carl S. Adorf**, James Antonaglia, Julia Dshemuchadse, Sharon C. Glotzer, "*Optimization of Smooth Isotropic Pair Potentials for the Self Assembly of Complex Structures,*" contributed talk at the AIChE Annual Meeting 2018, Pittsburgh, PA, November 2018.

9. **Carl S. Adorf**, James Antonaglia, Julia Dshemuchadse, Sharon C. Glotzer, "*Optimization of Smooth Isotropic Pair Potentials for the Self-Assembly of Complex Structures,*" contributed talk at the American Physical Society (APS) March Meeting 2018, Los Angeles, CA, March 2018.

8. **Carl S. Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Highly scalable metadata management with signac,*" contributed talk at the MICDE Symposium of the Center for Network and Storage Enabled Collaborative Computational Science, Ann Arbor, MI, May 2017.

7. **Carl Simon Adorf**, **Joshua A. Anderson**, Eric S. Harper, Sharon C. Glotzer, "*Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud,*" **invited workshop** at the AIChE Annual Meeting 2017, Minneapolis, MN, October 2017.

6. **Carl Simon Adorf**, Paul Dodd, Sharon C. Glotzer, "*Materials Data Management with signac,*" contributed talk at the Materials Research Society (MRS) Spring Meeting 2017, Phoenix, AZ, April 2017.

5. **Carl Simon Adorf**, "*Getting a PhD in the US,*" **invited talk** at the MSE Konferenz, Darmstadt, Germany, September 2016.

4. **Carl Simon Adorf**, "*Database aided Simulation Data Management,*" **invited talk** at the Kinetic Networks Workshop, Santa Fe, NM, September 2015.

3. **Carl Simon Adorf**, Pablo F. Damasceno, Sharon C. Glotzer, "*Relating crystal structure and shape with simple self-assembly models,*" **invited** talk at the Gordon Research Conference on Crystal Growth & Assembly, Biddeford, ME, June 2015.

2. **Carl Simon Adorf**, Animesh Agarwal, Christopher R. Iacovella, Ahmed E. Ismail, "*Multiresolution Modeling of Polymers: Wavelet-Based Reconstruction,*" contributed talk at the AIChE Annual Meeting 2014, Atlanta, GA, November 2014.

1. **Carl Simon Adorf**, Animesh Agarwal, Christopher R. Iacovella, Ahmed E. Ismail, "*Multiresolution Modeling of Polymers,*" contributed talk at the 27th European Symposium on Applied Thermodynamics, Eindhoven, The Netherlands, July 2014.

Poster Presentations

15. **Carl S. Adorf**, Vyas Ramasubramani, Bradley D. Dice, Sharon C. Glotzer, "*Highly flexible and fully reproducible computational workflows with signac,*" The Midwest Integrated Center for Computational Materials (MICCoM) Scientific Advisory Board (SAB) Meeting 2018, Argonne National Laboratory, IL, September 2018.

14. **Carl S. Adorf**, Paul M. Dodd, Vyas Ramasubramani, Bradley Dice, Sharon C. Glotzer, "*Simple Data and Workflow Management with the signac Framework,*" Foundations of Molecular Modeling and Simulation (FOMMS) 2018, Delavan, WI, July 2018.

13. **Carl S. Adorf**, James Antonaglia, Julia Dshemuchadse, Sharon C. Glotzer, "*Optimization of Smooth Isotropic Pair Potentials for the Self Assembly of Complex Structures,*" 12th Annual Engineering Graduate Symposium, Ann Arbor, MI, November 2017.

12. **Carl S. Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Materials Data Management with signac,*" Macromolecular Science and Engineering 41st Annual Symposium, Emergent Polymer Science & Engineering, Ann Arbor, MI, October 2017.

11. **Carl S. Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Materials Data Management with signac,*" Materials at Michigan Symposium 2017, Ann Arbor, MI, October 2017.

10. **Carl S. Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Materials Data Management with signac,*" MIDAS Symposium 2017, Ann Arbor, MI, October 2017.

9. **Carl S. Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Materials Data Management with signac,*" MICCoM SAB Meeting, Chicago, IL, September 2017.

8. **Carl S. Adorf**, Julia Dshemuchadse, Sharon C. Glotzer, "*Optimization of isotropic pair potentials for the self assembly of complex structures,*" Chemical Engineering Graduate Symposium 2017, Ann Arbor, MI, May 2017.

7. **Carl S. Adorf**, Paul Dodd, Sharon C. Glotzer, "*Scalable Provenance and Metadata Management with signac,*" MICDE Symposium 2017, Ann Arbor, MI, April 2017.

6. **Carl Simon Adorf**, Paul M. Dodd, Sharon C. Glotzer, "*Scalable Provenance and Metadata Management with signac,*" MICCoM All-Hands Meeting, Argonne National Laboratory, IL, October 2016.

5. **Carl Simon Adorf**, Pablo F. Damasceno, Sharon C. Glotzer, "*Isotropic self-assembly models for anisotropic convex shapes,*" Engineering Graduate Symposium, Ann Arbor, MI, October 2016.

4. **Carl S. Adorf**, Paul Dodd, Sharon C. Glotzer, "*signac – A simple Data Management Framework,*" XSEDE Conference 2016, Miami, FL, July 2016.

3. **Carl S. Adorf**, Paul Dodd, Sharon C. Glotzer, "*signac – A simple Data Management Framework,*" MICDE Annual Symposium 2016, Ann Arbor, MI, April 2016.

2. **Carl Simon Adorf**, Pablo F. Damasceno, Sharon C. Glotzer, "*Isotropic self-assembly models for anisotropic shapes,*" Engineering Graduate Symposium 2015, Ann Arbor, MI, October 2015.

1. **Carl Simon Adorf**, Pablo F. Damasceno, Sharon C. Glotzer, "*Relating crystal structure and shape with simple self-assembly models,*" contributed poster at the Gordon Research Conference on Crystal Growth & Assembly, Biddeford, ME, June 2015.

Professional Affiliations

since 2014 **American Institute of Chemical Engineers (AIChE)**

since 2015 **American Physical Society (APS)**, *Units: DCOMP, FGSA, FPS, GSOFT, SOH*

since 2017 **Materials Research Society (MRS)**

since 2015 **Association for Computing Machinery (ACM)**, *Units: SIGHPC*

2013–2015 **Linde AG CONTINUE Program**