

# Carl Simon Adorf

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## Education

- 2014–2019 **Doctor of Philosophy**, *University of Michigan*, Ann Arbor, MI  
(expected) 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.* (accepted), vol. 149 (20), 2018. arXiv:1711.04153 [cond-mat.soft].
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, GSOF, SOH*
- since 2017 **Materials Research Society (MRS)**
- since 2015 **Association for Computing Machinery (ACM)**, *Units: SIGHPC*
- 2013–2015 **Linde AG CONTINUE Program**