*January 7, 2023*

# Cory M. Hargus


**Contact Information**

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**Education**

**University of California, Berkeley** — August 2018 – December 2022
Doctor of Philosophy, Chemical and Biomolecular Engineering (GPA 3.97/4.0)
*Thesis: Odd transport phenomena in active matter*

**Brown University** — August 2009 – May 2014
Bachelor of Science *cum honoribus*, Chemical engineering (GPA 3.87/4.0)
*Thesis: Computational design of catalyst materials for biomass conversion*

**Professional Experience**

**D. E. Shaw Research**, New York, NY. United States. — August 2014 – March 2018
Scientific Associate
*High-accuracy interaction potentials for simulating dynamics of biological macromolecules*

**Technical Skills**

**Software development and Numerical Simulation**: Python (Numpy vectorization, Scipy, Jupyter, etc.), C++, MPI, Bash, MATLAB, Mathematica

**Awards and Fellowships**

**Best Poster**, Berkeley Statistical Mechanics Meeting – January 2022

**Graduate Student Research Fellowship**, National Science Foundation – August 2018–*present*

**Joseph Kestin Award of Excellence in Thermodynamics**, Brown University – May 2014

**Member**, Sigma Xi Scientific Research Society – May 2014

**Member**, Tau Beta Pi Engineering Honors Society – Dec 2013

**Selected Publications**

C. Hargus, J. M. Epstein, K. K. Mandadapu. "Odd Diffusivity of Chiral Random Motion." *Physical Review Letters*, **127**(17), 178001 (2021). [Editors' Suggestion]

A. G. Donchev, A. G. Taube, E. Decolvenaere, C. Hargus, *et al.* "Quantum chemical benchmark databases of gold-standard dimer interaction energies." *Scientific Data*, **8**(1), 1-9, (2021).

V. Jamali, C. Hargus, A. Ben-Moshe, A. Aghazadeh, H. D. Ha, K. K. Mandadapu, A. P. Alivisatos. "Anomalous nanoparticle surface diffusion in LCTEM is revealed by deep learning-assisted analysis." *Proceedings of the National Academy of Sciences*, **118**(10) e2017616118 (2021).

C. Hargus, K. Klymko, J. M. Epstein, K. K. Mandadapu (2020). "Time reversal symmetry breaking and odd viscosity in active fluids: Green-Kubo and NEMD results." *The Journal of Chemical Physics*, **152**(20), 201102 (2020). [Cover Feature, Editors' Pick]

R. McGibbon, A. Taube, A. G. Donchev, K. Siva, F. Hernndez, C. Hargus, K. Law, J. L. Klepeis, D. E. Shaw, "Improving the accuracy of Møller-Plesset perturbation theory with neural networks." *The Journal of Chemical Physics*, **147**(16), 161725 (2017).

A.H. Larsen, *et al.* "The Atomic Simulation Environment A Python library for working with atoms." *Journal of Physics: Condensed Matter*, **29**, 273002 (2017).