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Cory M. Hargus

CONTACT INFORMATION

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EDUCATION

University of California, Berkeley
Ph.D. in Chemical and Biomolecular Engineering
August 2018 – December 2022

Brown University
Sc.B. *cum honoribus* in Chemical Engineering
Sept. 2009 – May 2014

RESEARCH AND EMPLOYMENT

Postdoctoral researcher, Université Paris Cité — January 2023 – present
Mechanical ratchets and universal equations of state in chiral active fluids — Paris, France
Supervisors: Julien Tailleur (MIT & U. Paris Cité), Frédéric van Wijland

Ph.D., University of California, Berkeley — Sept 2018 – Dec 2022
Odd transport phenomena in active matter — Berkeley, CA
Supervisor: Kranthi K. Mandadapu

Scientific Associate, D. E. Shaw Research — July 2014 – May 2018
Ab initio force field development for computational drug discovery — New York, NY
Supervisors: Alexander Donchev and John Klepeis

DiMase Fellow, Catalyst Design Lab, Brown University — June 2012 – June 2014
Activity trends in bio-oil deoxygenation from theory and experiment — Providence, RI
Supervisor: Andrew A. Peterson

Summer Intern, Institute for Systems Biology — May 2010 – Sept 2010
MicroRNA biomarkers in PTSD spectrum profile — Seattle, WA
Supervisor: David Galas

Undergraduate Researcher, Jason Sello Lab, Brown University — Dec 2009 – May 2010
Wax ester synthesis in Streptomyces *bacteria* — Providence, RI
Supervisor: Jason Sello

Research Assistant, University of Washington Medicine — June 2008 – Sept 2009
Endothelial nitric oxide signaling and vascular inflammation — Seattle, WA
Supervisor: Francis Kim

PUBLICATIONS

C. Hargus, A. Deshpande, A. K. Omar, K. K. Mandadapu, "The Flux Hypothesis for Odd Transport Phenomena." *arXiv:2405.08798* (2024).

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, R. T. Mcgibbon, K. Law, B. Gregersen,

J. Li, K. Palmo, K. Siva, M. Bergdorf, J. L. Klepeis, D. E. Shaw. "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 and Editor's Pick]

R. McGibbon, A. Taube, A. G. Donchev, K. Siva, F. Hernández, 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, J.J. Mortensen, J. Blomqvist, I.E. Castelli, R. Christensen, M. Dułak, J. Friis, M.N. Groves, B. Hammer, C. Hargus, E.D. Hermes, P.C. Jennings, P.B. Jensen, J. Kermode, J.R. Kitchin, E.L. Kolsbjerg, J. Kubal, S. Lysgaard, J.B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, A.A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, K.W. Jacobsen, "The Atomic Simulation Environment — A Python library for working with atoms." *Journal of Physics: Condensed Matter*, **29**, 273002 (2017).

A.A. Peterson, C. Hargus, R. Michalsky, "Solar-enriched biofuels via looped oxide catalysis." U.S. Patent 9,834,490 B1 (2017).

R. Michalsky, V. Botu, C. Hargus, A.A. Peterson, A. Steinfeld, "Design Principles for Metal Oxide Redox Materials for Solar-Driven Isothermal Fuel Production." *Adv. Energy Mater.*, **5**, 1401082 (2015).

C. Hargus, R. Michalsky, A.A. Peterson, "Looped-oxide catalysis: a solar thermal approach to bio-oil deoxygenation." *Energy and Environmental Science*, **7**(10), 3122–3134 (2014).

Teaching Experience

Graduate Student Instructor, UC Berkeley — Aug 2021 – Dec 2021
CBE 140 – *"Introduction to Chemical Processes"* — Berkeley, CA
Named Outstanding Graduate Student Instructor

Substitute Teacher, The Wheeler School — Jan 2012 – May 2014
Upper School Math Substitute, Assistant Teacher, and After-School Librarian — Providence, RI

Teaching Assistant, Brown University — Aug 2013 – Dec 2013
BIOL 0400 – *"Biological Design: The Structural Architecture of Organisms"* — Providence, RI

Grants and Fellowships

U.S. Department of Energy, Office of Advanced Scientific Computing **Research Grant**, award DE-SC0023273 (*contributing author*, 2022)

National Science Foundation CBET Nanoscale Interactions **Research Grant**, award 2039624 (*contributing author*, 2020)

Graduate Student Research Fellowship, National Science Foundation (2018 – 2021)

American Public Power Association **DEED Student Research Grant** (2009)

Brown University **Undergraduate Teaching and Research Award** (2009)

Vincent and Ruby DiMase Research Fellowship, Brown University (2013)

Institute for Molecular and Nanoscale Innovation **Research Grant** (2012)

Awards and Honors

Finalist, Emerging Soft Matter Excellence Award, APS DSOFT (2023)

Reviewer of the month, Nature Communications Physics (2023)

Outstanding Graduate Student Instructor Award, UC Berkeley (2022)

Best Poster Award, Berkeley Statistical Mechanics Meeting (2022)

Joseph Kestin Award of Excellence, Brown University (2014)

Member, Sigma Xi Scientific Research Society (2014)

Member, Tau Beta Pi Engineering Honors Society (2013)

American Institute of Chemical Engineers 2013 Annual Meeting, **3rd Prize Poster** (2013)

New England Catalysis Society Spring Symposium **1st Prize Poster** (2013)

HCURA National Collegiate Research Conference **Award of Excellence** (2013)

Association of Energy Engineers New England **Academic Scholarship** (2010 – 2013)

Talks and Seminars

"Microscopic origins of odd transport phenomena in chiral active matter," *Université Paris Cité*, **Invited seminar**, MSC theory seminar, Host: Ada Altieri, Paris, France (2023)

"Microscopic origins of odd transport phenomena in chiral active matter," *Sorbonne University*, **Invited seminar**, LPTMC theory seminar, Host: Alexandre Solon, Paris, France (2023)

"Non-equilibrium statistical mechanics of odd transport phenomena," *Journées de Physique Statistique*, Paris, France (2023)

"Odd transport in active matter," *AIChE Annual Meeting*, Phoenix, AZ, USA (2022)

"Odd diffusivity of chiral active matter" (poster), *Berkeley Statistical Mechanics Meeting*, Berkeley, USA (2022)

"Broken symmetries and odd transport phenomena," *APS March Meeting*, Chicago, USA (2022)

"Odd transport in active fluids," *APS March Meeting*, [virtual] (2021)

"Microscopic origins of active fluid transport properties," *AIChE Annual Meeting*, [virtual] (2020)

"Active matter, time reversal symmetry breaking, and Green-Kubo calculations" (poster), *Berkeley Statistical Mechanics Meeting* (2020)

"Applying modern methods for global optimization to fitting high-accuracy electrostatic models," *Many-Body Interactions: From Quantum Mechanics to Force Fields*, Telluride, USA (2016)

"Designing ab initio force fields: From dimer energies to condensed phase properties," *Technical University of Denmark*, **Invited seminar**, Host: Tejs Vegge, Lyngby, Denmark (2016)

"From silicon to medicine: Rational drug design with molecular dynamics," *oSTEM Annual Conference*, Pittsburgh, USA (2015)

"Webinar #26: Computational Science at D. E. Shaw Research," *MOSTEC, MIT*, Cambridge, USA

(2015)

"The theory, practice and philosophy of *ab initio* force field development," *Brown University*, **Invited seminar**, Host: Andrew Peterson, Providence, USA (2015)

"A solar thermal approach to bio-oil deoxygenation," *New England Catalysis Society Spring Symposium*, Worcester, USA (2014)

"Looped oxide catalysis: the prospect of bio-oil deoxygenation over reduced metal oxides" (poster), *AIChE Annual Meeting*, San Francisco (2013)

"Utilizing bulk-reduced metal oxides as bifunctional catalysts and energy carriers in bio-oil deoxygenation" (poster), *New England Catalysis Society Spring Symposium*, Worcester, USA (2013)

"Solar enriched biofuels via oxidizable metal catalysts" (poster), *Harvard College Undergraduate Research Society: National Collegiate Research Conference*, Cambridge, USA (2013)

Community Involvement

Coordinator (2022) and Facilitator (2019-2021), Respect is a Part of Research, Berkeley, CA

Student-Invited Speaker Chair, CBE GSAC, Berkeley, CA (2019-2022)

Tutor and mentor, Underground Scholars Initiative and NavCal, Berkeley, CA (2018-2022)

Tutor, Petey Greene Program, Rikers Island, New York, NY (2017-2018)

Languages

English, Spanish (conversational), French (conversational)