Contact   **Dr. Lester Hedges**
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Computational physicist with research interests in soft matter,
materials science, algorithm development, and data visualization.

Education

9/2004–12/2007	*University of Nottingham, UK*

PhD in Physics. Thesis: "Aspects of Dynamic Heterogeneity in Models of Super-cooled Liquids"

9/2000–7/2004   *University of Nottingham, UK*
MSci in Physics. First-class honors. Salmon prize for undergraduate research.

Experience

1/2010–present   *Molecular Foundry, Lawrence Berkeley National Laboratory with Dr. Steve Whitelam*
Postdoctoral researcher.
- Developed simple model systems and adapted advanced sampling algorithms to study nucleation and self-assembly.
- Collaborated with experimentalists and theorists as part of the Center for Nanoscale Control of Geologic CO_2 (DOE EFRC).
- Ran large-scale Monte Carlo simulations on high-performance computing clusters.
- Defined project goals for and mentored 2 summer interns.

1/2008–12/2009   *College of Chemistry, UC Berkeley with Prof. David Chandler*
Postdoctoral researcher.
- Developed fast, robust, and versatile molecular dynamics software for model super-cooled liquids (faster than a standard physics library for specialized uses).
- Implemented novel algorithms to selectively access rare jammed configurations.
- Created smoothed animations of particle motions to aid spatial reasoning.

9/2004–5/2007   *School of Physics and Astronomy, University of Nottingham, UK*
Programming instructor.
- Supervised 3 hrs/wk of introductory MATLAB workshops for classes of ∼40 first-year Physics undergraduates.
- Provided individual assistance with debugging and programming fundamentals.

Languages and Tools

code/HPC	C/C++, bash/zsh, awk, git, SGE/PBS, MPI, CMake, Doxygen, screen/tmux, MATLAB/Octave, Python
viz/animation	MEncoder, FFMpeg, POV-Ray, ImageMagick, gnuplot, Grace, VMD, PostScript, OpenGL, Keynote, LaTeX
physics/modeling	Metropolis Monte Carlo, molecular dynamics, rare event sampling, phase diagrams, structural analysis, rejection-free Monte Carlo, coarse-grained modeling
web	HTML, CSS

Journal Publications

13. *Microscopic Evidence for Liquid-liquid Separation in Supersaturated CaC0$_3$ Solutions*
    A.F. Wallace, L.O. Hedges, A.J. Fernandez-Martinez, P. Raiteri, S, Whitelam,
    G.A. Waychunas, J.D Gale, J.F. Banfield, and J.J DeYoreo
    Science, **341** 885 (2013)

12. *Selective nucleation in porous media*
    L.O. Hedges and S. Whitelam
    Soft Matter, doi:10.1039/c3sm51946e (2013)

11. *Uncovering the intrinsic size dependence of hydriding phase transformations in nanocrystals*
    R. Bardhan, L.O. Hedges, C.L. Pint, A. Javey, S. Whitelam, and J.J Urban
    Nature Materials, doi:10.1038/nmat3716 (2013)

10. *Self-assembly of multicomponent structures in and out of equilibrium*
    S. Whitelam, R. Schulman, and L.O. Hedges
    Phys. Rev. Lett. **109**, 265506 (2012)

9. *Patterning a surface so as to speed nucleation from solution*
    L.O. Hedges and S. Whitelam
    Soft Matter, **8**, 8624 (2012)

8. *Preparation and relaxation of very stable glassy states of a simulated liquid*
    R.L. Jack, L.O. Hedges, J.P. Garrahan, and D. Chandler
    Phys. Rev. Lett. **107**, 275702 (2011)

7. *Excitations are localized and relaxation is hierarchical in glass-forming liquids*
    A.S. Keys, L.O. Hedges, R.L. Jack, J.P. Garrahan, S.C. Glotzer, and D. Chandler
    Phys. Rev. X. **1**, 021013 (2011)

6. *Limit of validity of Ostwald's rule of stages in a statistical mechanical model of crystallization*
    L.O. Hedges and S. Whitelam
    J. Chem. Phys. **135**, 164902 (2011)

5. *Dynamic order-disorder in atomistic models of structural glass formers*
    L.O. Hedges, R.L. Jack, J.P. Garrahan, and D. Chandler
    Science, **323** 1309 (2009)

4. *Dynamic facilitation explains democratic particle motion of metabasin transitions*
    L.O. Hedges and J.P. Garrahan
    J. Phys. A **41** 3244006 (2008)

3. *De-coupling of exchange and persistence times in atomistic models of glass formers*
    L.O. Hedges, L. Maibaum, J.P. Garrahan, and D. Chandler
    J. Chem. Phys. **127**, 211101 (2007)

2. *Dynamic propensity in a kinetically constrained lattice gas*
    L.O. Hedges and J.P. Garrahan
    J. Phys.: Condens. Matter **19** 3244006 (2007)

1. *Fast simulation of facilitated spin models*
    D.J. Ashton, L.O. Hedges, and J.P. Garrahan
    J. Stat. Mech. P12010 (2005)

Open Source Projects

TaskFarmer   A tool for running serial jobs with mpirun on HPC clusters. [sole developer]

LaTuXiT   A command-line tool for producing cropped LaTeX equations for use in figures and presentations. [sole developer]

rectify/flux   Monte Carlo generative art from the command-line. [sole developer]

Scientific Artwork

- Cover art, *PNAS, 2009; 106 (36)*

- Using *PostScript* for scientific visualization

Selected Presentations

- *Size-scaling behavior of hydriding phase transformations in nanocrystals*
  APS March Meeting (2012)

- *Understanding the microscopic origins of multi-stage nucleation*
  Computational Molecular Biology Group: Free University, Berlin (2011)

- *Limit of validity of Ostwald's rule of stages in a model of solution crystallization*
  APS March Meeting (2011)

- *Homogeneous and heterogeneous nucleation in the Ising model* [†]
  Berkeley Mini Stat-Mech Meeting (2011)

- *Non-classical assembly pathways of anisotropic particles* [†]
  Crystallization: from colloids to pharmaceuticals. CECAM, Lausanne (2010)

- *Structure and relaxation of ideal glass states* [†]
  Berkeley Mini Stat-Mech Meeting (2010)

[†] denotes poster presentation.

Links to visualizations, personal projects, and tutorials here.

September 5, 2013