

## Contact

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Computational physicist with research interests in soft matter, materials science, algorithm development, and data visualization.

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## 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 award 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<sub>2</sub> (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, L<sup>A</sup>T<sub>E</sub>X

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  $\text{CaCO}_3$  Solutions*  
A.F. Wallace, L.O. Hedges, A.J. Fernandez-Martinez, P. Raiteri, S. Whitlam,  
G.A. Waychunas, J.D. Gale, J.F. Banfield, and J.J. DeYoreo  
Science, **341** 6148 (2013)
12. *Selective nucleation in porous media*  
L.O. Hedges and S. Whitlam  
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. Whitlam, and J.J. Urban  
Nature Materials, doi:10.1038/nmat3716 (2013)
10. *Self-assembly of multicomponent structures in and out of equilibrium*  
S. Whitlam, 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. Whitlam  
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. Whitlam  
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** 5919 (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

|                              |  |
|------------------------------|--|
| <a href="#">TaskFarmer</a>   | A tool for running serial jobs with mpirun on HPC clusters. [sole developer]   |
| <a href="#">LaTeXiT</a>      | A command-line tool for producing cropped $\text{\LaTeX}$ equations for use in figures and presentations. [sole developer] |
| <a href="#">rectify/flux</a> | 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* <sup>†</sup>  
Berkeley Mini Stat-Mech Meeting (2011)
- *Non-classical assembly pathways of anisotropic particles* <sup>†</sup>  
Crystallization: from colloids to pharmaceuticals. CECAM, Lausanne (2010)
- *Structure and relaxation of ideal glass states* <sup>†</sup>  
Berkeley Mini Stat-Mech Meeting (2010)

<sup>†</sup> denotes poster presentation.

Links to visualizations, personal projects, and tutorials [here](#).

September 2, 2013