Dr Nicholas Hine

I am a Winton Advanced Research Fellowship at the Cavendish Laboratory, University of Cambridge. My research applies electronic structure methods to problems in materials physics, focussing recently on properties of nanostructures, including polar semiconductor nanorods and carbon nanotubes, and the properties of defects in metal oxides. I have experience with a range of methods including Quantum Monte Carlo, Density Functional Theory, DFT+U, DMFT, empirical potentials, and for several years I have worked on methodological development of Linear-Scaling DFT with the ONETEP code, of which I am an Author. I have an extensive record of well-cited publications, invited conference talks on a wide range of topics, ongoing international collaborations, and take part in numerous outreach activities.

Qualifications:

- **2008: PhD in Physics, CMTH Group, Imperial College London. Supervisor:** Prof Matthew Foulkes. Thesis on "*New Applications of Quantum Monte Carlo*"
- **2004: MPhys in Physics**, Merton College, Oxford. 1st Class Honours (4^{th}/120 in year in finals).
- **2000: A-Levels**: 5 grade A's; **AS**/**AO-Levels**: 2A's; **1998: GCSEs**: 11 grade A*'s.

Employment:

- **2013-2018: Winton Advanced Research Fellowship,** Cavendish Laboratory, University of Cambridge, researching Nanomaterials for Solar Energy.
- **2012-2013: Leverhulme Early Career Fellowship**, Department of Materials, Imperial College London: "Computational Design and Optimisation of Nanomaterials for Solar Energy"
- **2009-2012: Research Associate**, Thomas Young Centre, Department of Materials, Imperial College London, "High Performance Computing Software Development" project adding wide-ranging functionality to the ONETEP code: PAW, NGWFs for excited states, van der Waals interactions, DFT+U, and applications to semiconductor nanorods and crystalline defects. Responsibilities also included supervision of PhD students & MSc course lecturing.
- **2009: Research Associate**, TCM Group, Cavendish Laboratory, Cambridge. Implementation of strongly correlated methods (DFT+U and dynamical mean-field theory), and flexible sparse matrix algebra systems and integral engines for massive parallelisation in ONETEP.
- **2007-2008: Research Associate**, Department of Materials, Imperial College London. Development of ONETEP, including parallel scaling, Cutoff Coulomb interactions, nonlinear-core corrections, and simulation of semiconductor nanorods and defects in Al_2O_3.
- **2004-2007: PhD Research**, Application of QMC to three new areas: i) polarisation and localisation calculations in model systems, ii) the surface energy of the electron gas, a vital benchmark system for the construction of density functionals, and iii) calculation of defect formation energies in technologically important metal oxide systems. Also contributed new code and methods to simulation packages ABINIT, CASINO, and self-written 2D DFT code 'DOTDFT'.
- **Summer 2004: Placement with High Power Laser Group**, Dept. Physics, Oxford University, turning code from MPhys Project into standalone application.
- **Summers 2001, 2002: Assistant (then Lead) Programmer,** Rebellion (software company)

Grants and Awards:

- Volker Heine Young Investigator Award Finalist (2013).
- Winton Advanced Research Fellowship (2013-2018), project entitled "Computational Optimisation of Nanomaterials for Photovoltaics and Photocatalysis".
- Primary Investigator on Hartree Centre Early Access Grant for BlueJoule BG/Q Machine, 320000 hours CPU time, for project "Porting and Benchmarking ONETEP on BG/Q"
- Leverhulme Early Career Fellowship (2012-2015), project entitled " Computational Design and Optimisation of Nanomaterials for Solar Energy".

- Named Researcher on EPSRC-funded Platform Grant: “A platform for future development and application of the ONETEP software”, £1.5M five-year grant (from Mar 2012).
- EPSRC Resource Allocation Panel: £13,710 CPU time on HECToR, "Large-Scale Parallelisation of Linear Scaling DFT Calculations with ONETEP" (Mar 2010), R Co-I with P.D. Haynes (PI).
- Marie-Curie Psi-K Training grant of £6,710 towards running "ONETEP Spring School 2010", jointly with P.D. Haynes, A.A. Mostofi, C.-K. Skylaris and M.C. Payne.
- KAUST Supercomputing Laboratory grant of 1m hours CPU time for “Porting and scalability testing ONETEP", May 2011, jointly with A.A. Mostofi.
- MPhys Project with High Power Laser Group on PIC Code Simulation of Laser/Plasma interactions won Oxford Lasers Prize for best ALP project, (Jul 2004).
- Distinction in Preliminary Examinations, Jun 2001. Promoted to Exhibitioner (Scholar), Sept 2001. Promoted to Postmaster (Upgraded Scholar), Jan 2003.

Publications:

[1] **N. D. M. Hine**, *Linear-Scaling Plane-Wave Density Functional Theory using the Projector Augmented Wave Method: Application to Anatase TiO_2 Nanocrystals*, in preparation (2013).

[2] S. Murphy, **N. D. M. Hine**, *Supercell size convergence of formation energies for charged defects in complex materials, s*ubmitted (2012).

[3] A. H. Heuer, T. Nakagawa, D. B. Hovis, J. L. Smialek, B. Gleeson, **N. D. M. Hine**, H. Guhl, H-S. Lee, P. Tangney, W. M. C. Foulkes, and M. W. Finnis, *On the Growth of Al2O3 Scales*, submitted (2012).

[4] N. Todorova, A. J. Makarucha, **N. D. M. Hine**, A. Mostofi, I. Yarovsky, *Interactions of carbon nanomaterials with amyloidogenic peptides: insights from multiscale theoretical simulations*, submitted (2012).

[5] J. Beaudin, J. Laflamme Janssen, **N.D.M. Hine**, P. D. Haynes and M. Cote, *Bromophenyl functionalization of carbon nanotubes: an ab initio study,* submitted (2012).

[6] G. Lever, D. J. Cole, **N. D. M. Hine**, P. D. Haynes, and M. C. Payne *Electrostatic considerations affecting the calculated HOMO-LUMO gap in protein molecules*, J. Phys. Cond. Mat. (Fast Track Communication) (2013).

[7] C. Weber, D. D. O'Regan, **N. D. M. Hine**, P. B. Littlewood, G. Kotliar, and M. C. Payne, Importance of many-body effects in the kernel of *haemoglobin for ligand binding*, Phys. Rev. Lett. 110, xxxxxx, (2013).

[8] C. Weber, D.D. O'Regan, **N.D.M. Hine**, M.C. Payne, G. Kotliar, and P.B. Littlewood, Vanadium dioxide: A Peierls-Mott insulator stable against disorder, Phys. Rev. Lett. 108, 256402, (2012).

[9] A. Ruiz-Serrano, **N.D.M. Hine** and C.-K. Skylaris, *Pulay forces from localized orbitals optimized in situ using a psinc basis set,* J. Chem. Phys. 136, 234101 (2012).

[10] **N.D.M. Hine**, P.W. Avraam, P.T. Tangney and P.D. Haynes, *Linear-Scaling Density Functional Theory Simulations of Polar Semiconductor Nanorods*, J. Phys. Conf. Ser. 367, 012002 (2012).

[11] P.W. Avraam, **N.D.M. Hine**, P.T. Tangney and P.D. Haynes, Fermi-level pinning can determine polarity in semiconductor nanorods, Phys. Rev. B 85, 115404 (2012).

[12] D.D. O'Regan, **N.D.M. Hine,** M.C. Payne and A.A. Mostofi, *Linear-scaling DFT+U including orbital optimization,* Phys. Rev. B 85 085107 (2012).

[13] **N.D.M. Hine**, J. Dziedzic, C.-K. Skylaris and P.D. Haynes, *Electrostatic Interactions in Finite Systems treated with Periodic Boundary Conditions: Application to Linear-Scaling Density Functional Theory*, J. Chem. Phys, 135, 204101 (2011).

[14] L.E. Ratcliff, **N.D.M. Hine** and P.D. Haynes, *Calculating Optical Absorption Spectra for Large Systems using Linear-Scaling Density-Functional Theory,* Phys. Rev. B 84 165131 (2011).

[15] L. Andrinopoulos, **N.D.M. Hine** and A.A. Mostofi, *Dispersion Interactions with Maximally Localised Wannier Functions*, J. Chem. Phys. 135, 154105 (2011).

[16] M. Barbagallo, H. Kroha, T. Stollenwerk, J.F.K. Cooper, **N.D.M. Hine**, N.-J. Steinke, C.H.W. Barnes, K. Ziebeck, A. Ionescu, and P.M.S. Monteiro, *Thickness-dependent magnetic properties of oxygen-deficient EuO*, Phys. Rev. B. 84, 075219 (2011).

[17] P.W. Avraam, **N.D.M. Hine**, P.T. Tangney and P.D. Haynes, *Factors Influencing the Distribution of Charge in Polar Nanocrystals,* Phys. Rev. B. Rapid Commun. 83, 241402(R) (2011).

[18] **N.D.M. Hine**, M. Robinson, P.D. Haynes, C.-K. Skylaris, M.C. Payne and A.A. Mostofi, *Accurate ionic forces and geometry optimisation in linear scaling density-functional theory with local orbitals,* Phys. Rev. B. 83, 195102 (2011).

[19] **N.D.M. Hine**, P.D. Haynes, A.A. Mostofi, and M.C. Payne, *Linear-Scaling Density-Functional Simulations of Charged Point Defects in Al_2O_3 using Hierarchical Sparse Matrix Algebra,* J. Chem. Phys. 133, 114111 (2010).

[20] D.D. O'Regan, **N.D.M. Hine**, A.A. Mostofi and M.C. Payne, *Projector self-consistent DFT+U using non-orthogonal generalized Wannier functions*, Phys. Rev. B. Rapid Commun. 82, 081102(R) (2010). Chosen as an “Editor's Suggestion” Article by the editors of PRB.

[21] M. Barbagallo, **N.D.M. Hine**, J.F.K. Cooper, N.-J. Steinke, A. Ionescu, C.H.W. Barnes, C. Kinane, R. Dalgliesh, T. Charlton, S. Langridge, *Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO*, Phys. Rev. B. 81, 235216 (2010).

[22] **N.D.M. Hine**, K. Frensch, W.M.C. Foulkes, M.W. Finnis, *Supercell Size Scaling of Formation Energies of Charged Defects*, Phys. Rev. B. 79, 024112 (2009).

[23] **N.D.M. Hine**, P.D. Haynes, C.-K. Skylaris, A.A. Mostofi, M.C. Payne, *Linear-Scaling Density-Functional Theory with Tens of Thousands of Atoms: Expanding the Scope and Scale of Calculations with ONETEP,* Comput. Phys. Commun. 180, 1041 (2008).

[24] **N.D.M. Hine**, W.M.C, Foulkes, *Localization Lengths over Metal to Band Insulator transitions,* J. Phys.: Condens. Matter 19, 506212 (2007).

[25] B. Wood, **N.D.M. Hine**, and W.M.C. Foulkes, P. García-González, *Quantum Monte Carlo calculations of the surface energy of an electron gas,* Phys. Rev. B 76, 035403 (2007). Selected for APS Virtual Journal of Nanoscale Physics and Technology, July 2007.

[26] A. Sorouri, W.M.C. Foulkes, and **N.D.M. Hine**, *Accurate and efficient method for the treatment of exchange in a plane-wave basis,* J. Chem. Phys. 124, 064105 (2006).

Invited Conference Talks

- Invited Speaker, Collaborative Conference on Materials Research (CCMR) 2013, Jeju Island, South Korea, June 2013: *“Charge Distributions in Polar Semiconductor Nanorods explored with Linear-Scaling DFT Calculations”.*
- Invited Speaker, Deutsche Physikalische Gesellschaft (DPG) Spring Meeting, special session of the symposium "Frontiers of Electronic Structure Theory" for award of the Volker Heine Young Investigator Award 2013, Regensburg, Germany, March 2013: *“Semiconductor and Metal-Oxide Nanocrystal Simulations with Linear-Scaling PAW DFT”.*
- Invited Speaker, IDC HPC User Forum, London, July 2012: *"ONETEP: Quantum-Mechanical Simulations at the Nanoscale”*
- Invited Speaker, CECAM Workshop on Local Orbital Methods, Cambridge, July 2012: *“Linear Scaling DFT with in-situ-optimised Local Orbitals using the Projector Augmented Wave Formalism”*
- Invited Speaker & Member of UK Delegation, “Scientific Impacts and Opportunities in High Performance Computing, Young Investigator's Symposium”, Oak Ridge National Laboratory, Tennessee, Oct 2008: “*Linear-Scaling Density-Functional Theory with Tens of Thousands of Atoms: Expanding the Scope and Scale of Calculations with ONETEP”.*
- Invited Speaker, Thomas Young Centre Meeting, Point Defect Electrostatics, UCL, Nov 2007.
- Invited Speaker, CECAM Workshop on “Advances in continuum quantum Monte Carlo methods”, Lyon, Aug 2007. “*Quantum Monte Carlo Investigations of Point Defects in Alumina”.*

- Invited Speaker, “Quantum Monte Carlo in the Apuan Alps” III, Vallico Sotto, Tuscany, July 2007. “*Quantum Monte Carlo Investigations of Point Defects in Alumina”.*
- Invited Speaker, QMCAA II: July 2006. Talked on “*The Surface Energy of the Electron Gas: Resolving a Long-Standing Contradiction*”.
- Invited Speaker, QMCAA I: July 2005. Talked on *“Localization Tensor Calculations on Quantum Dots in DFT and VMC”.*

Other Selected Conferences and Workshops

- APS March Meeting 2012, Boston, MA, talked on *“Charge Distributions in Polar Semiconductor Nanorods explored with Linear-Scaling DFT Calculations”*
- Speaker at “Theory, Modelling and Computational Methods for Semiconductors”, IoP Conference, University of Leeds, Jan 2012, “Fermi-Level Pinning in Polar Semiconductor Nanorods explored with Linear-Scaling DFT Calculations”.
- CECAM Workshop,*”Reducing Empiricism and Speeding Up Progress in Density-Functional Theory”*, University College Dublin, June 2011.
- Conference co-organiser, “ONETEP Developers' Meeting” Nov 2011, several talks.
- “Psi-K 2010” Berlin, Sept 2010, poster presentation *“Linear-Scaling Density Functional Theory with the ONETEP code: Parallel Algorithms for Calculations with Tens of Thousands of Atoms*”.
- APS March Meeting 2010, Portland, OR, talks on “*Linear-Scaling Density-Functional Theory with Tens of Thousands of Atoms*” and on “*Point Defects and Diffusion in Al_2O_3*”.
- Conference co-organiser, “ONETEP Developers' Meeting” Nov 2009, several talks.
- “14th Workshop on Computational Physics and Material Science: Total Energy and Force Methods”, Poster presentation on Parallel Algorithms in ONETEP, ICTP, Trieste, Jan 2009.

Research Collaborations:

- Member of the ONETEP Developers Group (ODG), consisting of P.D. Haynes (Imperial), A.A. Mostofi (Imperial), C.K. Skylaris (Southampton) and M.C. Payne (Cambridge), and myself. The ODG is a close-knit group of academics who oversee the ONETEP project. Recently awarded an EPSRC Platform Grant of £1.2M to support ongoing development of ONETEP.
- Ongoing work with other members of the ODG on: DFT+U methods (A. Mostofi and D.D. O'Regan, EPFL), optimisation of localised orbitals to describe excited states and core-level spectroscopy (P. Haynes and L. Ratcliff), and inclusion of van der Waals interactions in LS-DFT (A. Mostofi and L. Andrinopoulos), Time-Dependent DFT (P. Haynes and T. Zuehlsdorff) and Dynamical Mean Field Theory (C. Weber, D. O'Regan, P. Littlewood, M. Payne and G. Kotliar)
- Collaboration with G. Teobaldi, University of Liverpool, on “In-silico development of doped metal-oxide nanotubes as novel photo-catalysts for energy applications”.
- Collaboration with C.H.W. Barnes and M. Barbagallo, Cavendish Laboratory, Cambridge, on influence of oxygen vacancies on magnetic moment of EuO thin films.
- Close involvement in Leverhulme Trust project “Quantum mechanics of dislocations and grain boundaries in Alumina”, with M. Foulkes, M. Finnis, H. Guhl, P. Tangney and A. Heuer (CWRU).
- Collaboration with J. Beaudin, J. Laflamme Janssen and M. Coté, University of Montreal, on ab initio calculations of the reactivity of carbon nanotubes and graphene.
- Collaboration with S. Pyrlin and M. Ramos, University of Minho, Portugal, on properties of CNT-filled polymer composites, part of Marie-Curie Initial Training Network “CONTACT”.

Teaching:

- Lecturer, Royal Institution Short Course on Quantum Mechanics, Royal Institution of Great Britain, London (scheduled for March 2013).
- Tutor, Co-Organiser and Lecturer, ONETEP Masterclasses, (Cavendish Laboratory, July 2011 and August 2012).
- Lecturer, Centre for Doctoral Training on Theory and Simulation of Materials, Imperial College

London MSc Course. Lecture Series “Introduction to Quantum Mechanics” (2010, 2011, 2012). Designed and taught course as part of the CDT to give students from a non-physics a knowledge of Quantum Mechanics suitable for the electronic structure course.

- Tutor, CDT/TYC Summer School, “Transport of Matter over length and time scales” Imperial College London, July 2010.
- Co-Organise & Lecturer, ONETEP Spring School (Cavendish, Apr 2010).
- Lecturer, CDT TSM Electronic Structure Guest Lecture (2009); Assessor, Mathematics for Theory of Materials (2009).
- Lecturer, Postgraduate Lecture Course on Density Functional Theory, Condensed Matter Theory Group, Imperial College London, (Nov 2008).
- Co-Organiser & Lecturer, ONETEP Summer School (Cavendish, Jul 2008).
- Tutor, 2nd Year Computing practicals (ICL Physics, 2005-2007).
- Tutor, 1st Year Mathematics classwork (ICL Physics, 2004-2005).

Students (Co-)Supervised:

- Lampros Andrinopoulos (PhD, 2009-present), on vdW interactions in nanostructures and molecular systems, with A.A. Mostofi.
- Niccolo Corsini (CDT PhD, 2011-present), on phase transformations in semiconductor nanoparticles, with P.D. Haynes and C. Molteni.
- Philip Avraam (PhD, 2007-11), on polar semiconductor nanorods with P. Haynes and P. Tangney.
- David Schnoerr (BSc, 2010), on the use of Random Structure Search.
- Lukas Medisauskas (MSc, 2011), on the Phase Diagram of Gallium.

Other Activities

- Full member of the Institute of Physics.
- Referee for many international journals including: Physical Review Letters, Physical Review B, Journal of Physics: Condensed Matter, Chemical Physics Letters, Computer Physics Communications, Modelling and Simulation in Materials Science and Engineering, Geochemica and Cosmochemica Acta.
- Participated in Outreach programs and events including the Cavendish Laboratory's “Physics at Work” day for secondary school pupils
- Hosted Outreach Visit by a group of secondary school pupils to the Department of Materials at Imperial, Sept 2011, giving an introductory talk and organising experimental demonstrations.
- Scheduled to give a short lecture course on quantum mechanics at the Royal Institution in March 2013 (see above).

Website:

http://www.tcm.phy.cam.ac.uk/~ndmh3/