Peter David Haynes

I am Professor of Theory & Simulation of Materials and Head of the Department of Materials at Imperial College London. My research focuses on the development of new linear-scaling methods for performing large-scale quantum-mechanical simulations and their application to materials science, nanotechnology and biological systems. I was awarded the 2010 Maxwell Medal and Prize by the Institute of Physics.

Employment

1 Jul 2015 –	Department of Materials, Imperial College London *Head of Department*
1 Aug 2012 –	Departments of Materials and Physics, Imperial College London *Professor of Theory and Simulation of Materials*
1 Jun 2007 – 31 Jul 2012	Departments of Materials and Physics, Imperial College London *Reader in Materials and Physics*
1 Jun 2007 – 30 Sep 2013	Departments of Materials and Physics, Imperial College London *Royal Society University Research Fellow*
1 Oct 2005 – 31 May 2007	Cavendish Laboratory, University of Cambridge *Royal Society University Research Fellow in Physics*
1 Oct 2002 – 30 Sep 2005	Sidney Sussex College, Cambridge *Ramon Jenkins Senior Research Fellow in Physics*
1 Oct 1999 – 30 Sep 2002	Magdalene College, Cambridge *Thomas Nevile Research Fellow in Physics*
1 Oct 1998 – 30 Sep 1999	Cavendish Laboratory, University of Cambridge *Post-doctoral Research Associate in the Theory of Condensed Matter*

Education

1 Oct 1995 – 30 Sep 1998	Cavendish Laboratory, University of Cambridge *PhD research degree* under the supervision of Prof. M. C. Payne FRS in the Theory of Condensed Matter group in the Department of Physics entitled: *Linear-scaling methods in ab initio quantum-mechanical calculations*
Awards	Bachelor Scholarship from Christ's College, Cambridge (1995–98) PhD degree conferred: 14 November 1998
1 Oct 1992– 30 Jun 1995	Christ's College, University of Cambridge *BA (Hons) in Physical Natural Sciences Tripos*: First Class Part II (First Class) in Theoretical Physics (91% overall mark, rank 1=) Part IB (First Class) in Advanced Physics (85%) and Mathematics (95%) Part IA (First Class) in Chemistry (81%), Crystalline Materials (85%), Physics (88%) and Mathematics (95%), rank 1 for Part IA overall
Awards	University Smith System Engineering Prize for Physics (1993) College Scholarship (1993–95) College Darwin Prize for Part II Natural Sciences (1995) College S. W. Greig Prizes for Part I Natural Sciences (1993 & 94) College Fay Prize for Part IA Natural Sciences (1993) BA degree conferred: 30 June 1995; MA degree conferred: 20 March 1999

Honours and Awards

- Maxwell Medal and Prize for Theoretical Physics, Institute of Physics (2010)
- Gold Medal, Theory Prize and overall winner of the British Physics Olympiad (1992)
- Silver Medal at the International Physics Olympiad, Helsinki (1992)

Professional Bodies

- Fellow, Institute of Physics (2010)
- Chartered Physicist, Institute of Physics (2009).
- Committee member, Theory of Condensed Matter group, Institute of Physics (2009–12).

Publications

Refereed papers

1. T. J. Zuehlsdorff, **P. D. Haynes**, F. Hanke, M. C. Payne and N. D. M. Hine, "Solvent effects on electronic excitations of an organic chromophore", to appear in *J. Chem. Theory Comput.* (2016).
2. E. Poli, J. D. Elliott, L. E. Ratcliff, L. Andrinopoulos, J. Dziedzic, N. D. M. Hine, A. A. Mostofi, C.-K. Skylaris, **P. D. Haynes** and G. Teobaldi, "The potential of imogolite nanotubes as (co-) photocatalysts: a linear-scaling density functional theory study", *J. Phys.: Condens. Matter* **28**, 074003 (2016).
3. T. J. Zuehlsdorff, N. D. M. Hine, M. C. Payne and **P. D. Haynes**, "Linear-scaling time-dependent density-functional theory beyond the Tamm-Dancoff approximation: obtaining efficiency and accuracy with *in situ* optimised local orbitals", *J. Chem. Phys.* **143**, 204107 (2015).
4. N. R. C. Corsini, Y. Zhang, W. R. Little, A. Karatutlu, O. Ersoy, **P.D. Haynes**, C. Molteni, N. D. M. Hine, I. Hernandez, J. Gonzalez, F. Rodriguez, V. V. Brazhkin and A. Sapelkin, "Pressure-induced amorphization and a new high density amorphous metallic phase in matrix-free Ge nanoparticles", *Nano Lett.* **15**, 7334–40 (2015)
5. M. Abdulla, K. Refson, R. H. Friend and **P. D. Haynes**, "A first-principles study of the vibrational properties of crystalline tetracene under pressure", *J. Phys.: Condens. Matter* **27**, 375402 (2015).
6. A. E. Goode, N. D. M. Hine, S. Chen, S. D. Bergin, M. S. P. Shaffer, M. P. Ryan, **P. D. Haynes**, A. E. Porter and D. W. McComb, "Mapping functional groups on oxidised multi-walled carbon nanotubes at the nanometre scale", *Chem. Commun.* **50**, 6744–7 (2014).
7. D. J. Cole, A. W. Chin, N. D. M. Hine, **P. D. Haynes** and M. C. Payne, "Toward *ab initio* optical spectroscopy of the Fenna–Matthews–Olson complex", *J. Phys. Chem. Lett.* **4**, 4206–12 (2013).
8. P. K. Silas, **P. D. Haynes** and J. R. Yates, "Evolution of the Fermi surface of arsenic through the rhombohedral to simple-cubic phase transition: A Wannier interpolation study", *Phys. Rev. B* **88**, 134103 (2013).
9. N. R. C. Corsini, A. Greco, N. D. M. Hine, C. Molteni and **P. D. Haynes**, "Simulations of nanocrystals under pressure: Combining electronic enthalpy and linear-scaling density-functional theory", *J. Chem. Phys.* **139**, 084117 (2013).
10. T. J. Zuehlsdorff, N. D. M. Hine, J. S. Spencer, N. M. Harrison, D. J. Riley and **P. D. Haynes**, "Linear-scaling time-dependent density-functional theory in the linear response formalism", *J. Chem. Phys.* **139**, 064104 (2013).

11. L. E. Ratcliff and **P. D. Haynes**, "*Ab initio* calculations of the optical absorption spectra of C_{60}-conjugated polymer hybrids", *Phys. Chem. Chem. Phys.* **15**, 13024–31 (2013).
12. J. Laflamme Janssen, J. Beaudin, N. D. M. Hine, **P. D. Haynes** and M. Côté, "Bromophenyl functionalization of carbon nanotubes: an *ab initio* study", *Nanotechnology* **24**, 375702 (2013).
13. 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.: Condens. Matter* 25, 152101 (2013) [highlighted by IOPscience].
14. P. W. Avraam, N. D. M. Hine, P. Tangney and **P. D. Haynes**, "Fermi level pinning can determine polarity in semiconductor nanorods", *Phys. Rev. B* **85**, 115404 (2012)
15. N. D. M. Hine, J. Dziedzic, **P. D. Haynes** and C.-K. Skylaris, "Electrostatic interactions in finite systems treated with periodic boundary conditions: application to linear-scaling density functional theory", *J. Chem. Phys.* **135**, 204103 (2011).
16. 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).
17. K. T. Al-Jamal, H. Nerl, K. H. Müller, H. Ali-Boucetta, S. Li, **P. D. Haynes**, J. R. Jinschek, M. Prato, A. Bianco, K. Kostarelos and A. E. Porter, "Cellular uptake mechanisms of functionalised multi-walled carbon nanotubes by 3D electron tomography imaging", *Nanoscale* **3**, 2627–35 (2011).
18. P. W. Avraam, N. D. M. Hine, P. Tangney and **P. D. Haynes**, "Factors influencing the distribution of charge in polar nanocrystals", *Phys. Rev. B* **83**, 241402(R) (2011).
19. 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* **82**, 195102 (2011).
20. B. Monserrat and **P. D. Haynes**, "Truncated spherical-wave basis set for first-principles pseudopotential calculations", *J. Phys. A: Math. Theor.* **43**, 465205 (2010).
21. 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).
22. M. Robinson and **P. D. Haynes**, "Dynamical effects in *ab initio* NMR calculations: classical force fields fitted to quantum forces", *J. Chem. Phys.* **133**, 084109 (2010).
23. A. Badinski, **P. D. Haynes**, J. R. Trail & R. J. Needs, "Methods for calculating forces within quantum Monte Carlo", *J. Phys.: Condens. Matter* **22**, 074202 (2010).
24. M. Robinson and **P. D. Haynes**, "Linear-scaling first-principles study of a quasicrystalline molecular material", *Chem. Phys. Lett.* **476**, 73–7 (2009).
25. N. D. M. Hine, **P. D. Haynes**, A. A. Mostofi, C.-K. Skylaris and 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**, 1041–53 (2009).
26. G. J. Conduit and **P. D. Haynes**, "Diffusion Monte Carlo study of a valley-degenerate electron gas and application to quantum dots", *Phys. Rev. B* **78**, 195310 (2008).
27. P. Silas, J. R. Yates and **P. D. Haynes**, "Density-functional investigation of the rhombohedral to simple-cubic phase transition of arsenic", *Phys. Rev. B* **78**, 174101 (2008).
28. **P. D. Haynes**, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, "Density kernel optimisation in the ONETEP code", *J. Phys.: Condens. Matter* **20**, 294207 (2008).

29. A. Badinski, **P. D. Haynes** and R. J. Needs, "Nodal Pulay terms for accurate diffusion quantum Monte Carlo forces", *Phys. Rev. B* **77**, 085111 (2008).
30. C.-K. Skylaris, **P. D. Haynes**, A. A. Mostofi and M. C. Payne, "Recent progress in linear-scaling density functional calculations with plane waves and pseudopotentials: the ONETEP code", *J. Phys.: Condens.Matter* **20**, 064209 (2008).
31. C.-K. Skylaris and **P. D. Haynes**, "Achieving plane wave accuracy in linear-scaling density functional theory applied to periodic systems: A case study on crystalline silicon", *J. Chem. Phys.* **127**, 164712 (2007).
32. A. A. Mostofi, **P. D. Haynes**, C.-K. Skylaris and M. C. Payne, "ONETEP: linear-scaling density-functional theory with plane-waves", *Mol. Simulat.* **33**, 551–5 (2007).
33. **P. D. Haynes**, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, "Elimination of basis set superposition error in linear-scaling density-functional calculations with local orbitals optimised *in situ"*, *Chem. Phys. Lett.* **422**, 345–9 (2006).
34. **P. D. Haynes**, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, "ONETEP: linear-scaling density-functional theory with local orbitals and plane waves", *Phys. Status Solidi B* **243**, 2489–99 (2006).
35. S. von Alfthan, **P. D. Haynes**, K. Kaski and A. P. Sutton, "Are the structures of twist grain boundaries in silicon ordered at 0 K?" *Phys. Rev. Lett.* **96**, 055505 (2006).
36. C.-K. Skylaris, **P. D. Haynes**, A. A. Mostofi and M. C. Payne, "Implementation of linear-scaling plane wave density functional theory on parallel computers", *Phys. Status Solidi B* **243**, 973–88 (2006).
37. C.-K. Skylaris, **P. D. Haynes**, A. A. Mostofi and M. C. Payne, "Using ONETEP for accurate and efficient $O(N)$ density functional calculations", *J. Phys.: Condens. Matter* **17**, 5757–69 (2005).
38. C.-K. Skylaris, **P. D. Haynes**, A. A. Mostofi and M. C. Payne, "Introducing ONETEP: Linear-scaling density functional simulations on parallel computers", *J. Chem. Phys.* **122**, 084119 (2005).
39. E. Artacho, M. Rohlfing, M. Côté, **P. D. Haynes**, R. J. Needs and C. Molteni, "Structural relaxations in electronically excited poly(*para*-phenylene)", *Phys. Rev. Lett.* **93**, 116401 (2004).
40. A. A. Mostofi, **P. D. Haynes**, C.-K. Skylaris and M. C. Payne, "Preconditioned iterative minimisation for linear-scaling electronic structure calculations", *J. Chem. Phys.* **119**, 8842–8 (2003).
41. M. Côté, **P. D. Haynes** and C. Molteni, "Material design from first principles: the case of boron nitride polymers", *J. Phys.: Condens. Matter* **14**, 9997–10009 (2002).
42. C.-K. Skylaris, O. Diéguez, **P. D. Haynes** and M. C. Payne, "Comparison of variational real-space representations of the kinetic energy operator", *Phys. Rev. B* **66**, 073103 (2002).
43. C.-K. Skylaris, A. A. Mostofi, **P. D. Haynes**, O. Diéguez and M. C. Payne, "Nonorthogonal generalized Wannier function pseudopotential plane-wave method", *Phys. Rev. B* **66**, 035119 (2002).
44. A. A. Mostofi, C.-K. Skylaris, **P. D. Haynes** and M. C. Payne, "Total-energy calculations on a real space grid with localized functions and a plane-wave basis", *Comput. Phys. Commun.* **147**, 788–802 (2002).
45. C.-K. Skylaris, A. A. Mostofi, **P. D. Haynes**, C. J. Pickard and M. C. Payne, "Accurate kinetic energy evaluation in electronic structure calculations with localized functions on real space grids", *Comput. Phys. Commun.* **140**, 315–22 (2001).

46. C. K. Gan, **P. D. Haynes** and M. C. Payne, "First-principles density-functional calculations using localized spherical-wave basis sets", *Phys. Rev. B* **63**, 205109 (2001).
47. M. Côté, **P. D. Haynes** and C. Molteni, "Boron nitride polymers: Building blocks for organic electronic devices", *Phys. Rev. B* **63**, 125207 (2001).
48. C. K. Gan, **P. D. Haynes** and M. C. Payne, "Preconditioned conjugate gradient method for the sparse generalized eigenvalue problem in electronic structure calculations", *Comput. Phys. Commun.* **134**, 33–40 (2001).
49. **P. D. Haynes** and M. Côté, "Parallel fast Fourier transforms for electronic structure calculations", *Comput. Phys. Commun.* **130**, 130–6 (2000).
50. **P. D. Haynes** and M. C. Payne, "An *ab initio* linear-scaling scheme", *Mol. Simulat.* **25**, 257–64 (2000).
51. **P. D. Haynes** and M. C. Payne, "Corrected penalty-functional method for linear-scaling calculations in density-functional theory", *Phys. Rev. B* **59**, 12173–6 (1999).
52. **P. D. Haynes** and M. C. Payne, "Failure of density-matrix minimization methods for linear-scaling density-functional theory using the Kohn penalty-functional", *Solid State Commun.* **108**, 737–41 (1998).
53. **P. D. Haynes** and M. C. Payne, "Localised spherical-wave basis set for $O(N)$ total-energy pseudopotential calculations", *Comput. Phys. Commun.* **102**, 17–27 (1997).

Conference proceedings

54. N. D. M. Hine, P. W. Avraam, P. Tangney and **P. D. Haynes**, "Linear-scaling density functional theory simulations of polar semiconductor nanorods", *J. Phys.: Conf. Ser.* **367**, 012002 (2012)
55. D. R.Bowler, J.-L. Fattebert, M. J. Gillan, **P. D. Haynes** and C.-K. Skylaris, "Introductory remarks: Linear scaling methods", *J. Phys.: Condens. Matter* **20**, 290301 (2008).
56. **P. D. Haynes**, A. A. Mostofi, C.-K. Skylaris and M. C. Payne, "ONETEP: linear-scaling density-functional theory with plane-waves", *J. Phys.: Conf. Ser.* **26**, 143–148 (2006).
57. **P. D. Haynes**, A. A. Mostofi, C.-K. Skylaris and M. C. Payne, "ONETEP: linear-scaling density-functional theory with plane waves", *Psi-k Newsletter* **72**, 78–91 (2005).
58. **P. D. Haynes**, D. R. Bowler and E. Artacho, "Report on the CECAM/ESF STRUC-Psi-k Workshop on 'Local orbitals and linear-scaling ab initio calculations'", *Psi-k Newsletter* **48**, 36–66 (2001).

Abstracts and non-refereed papers

59. **P. Haynes**, P. Avraam, N. Hine and P. Tangney, "Understanding polarity in semiconductor nanorods with linear-scaling density-functional theory simulations", *Bull. Am. Phys. Soc.* MAR.L44.10 (2014).
60. **P. Haynes**, L. Ratcliff, G. Conduit, P. Avraam and M. Robinson, "Optimised local orbitals from linear-scaling density-functional theory calculations", *Bull. Am. Phys. Soc.* MAR.A23.2 (2010).
61. **P. D. Haynes**, "Linear-scaling density-functional simulations with local orbitals and plane waves", *Oberwolfach Reports* **5**, 1083–84 (2008).
62. **P. D. Haynes**, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, "ONETEP: linear-scaling density-functional theory with plane waves", *Bull. Am. Phys. Soc.* MAR.B32.3 (2006).
63. **P. D. Haynes**, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, "Linear-scaling density-functional theory with plane-waves", *Bull. Am. Phys. Soc.* MAR.J38.9 (2004).

64. **P. D. Haynes**, C. K. Gan and M. C. Payne, "Density-matrix minimization techniques for linear-scaling DFT calculations using non-orthogonal localized basis sets", *Abs. Pap. Am. Chem. Soc.* **221**, U407-U408 (2001).
65. **P. D. Haynes** and M. C. Payne, "Improved penalty-functional method for $O(N)$ density-functional theory", *Bull. Am. Phys. Soc.* MAR.EC11.7 (1999).
66. **P. D. Haynes** and M. C. Payne, "Linear-scaling method for total energy pseudopotential calculations within density-functional theory", *Bull. Am. Phys. Soc.* MAR.A25.4 (1998).

Presentations

Invited international talks

- European Training Network "TheLink" Project Meeting, Fraunhofer ICT, Karlsruhe, Germany (October 2015)
- CECAM Workshop on "Next generation quantum based molecular dynamics: challenges and perspectives", Bremen, Germany (July 2015)
- Computational Materials Design Department Seminar, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany (May 2015)
- US-UK Materials Theory and Modeling Workshop, Argonne National Laboratory, USA (January 2015)
- 2nd China-UK Workshop on the Chemistry and Physics of Functional Materials, Beijing (September 2014)
- Lecture at the Hands-on Tutorial Workshop "Density functional theory and beyond: Computational materials science for real materials", Trieste, Italy (August 2013)
- CECAM Workshop on "Modelling realistic inorganic nanostructures: bridging the gap between theory and experiment", Zaragoza, Spain (September 2012)
- Conference on Computational Physics, Gatlinburg TN, USA (November 2011)
- Center for Computational Sciences Seminar, University of Basel (May 2011)
- Psi-k Conference, Berlin (September 2010)
- International Symposium of Electronic Structure Calculations, Tokyo (December 2009)
- Opening talk at the Workshop on "Atomistic Models of Materials" at the Mathematical Research Institute of Oberwolfach, Germany (May 2008)
- Accelrys Nanotechnology Consortium Meeting, Trinity College Dublin (September 2007)
- CECAM Workshop on "New developments for first principles molecular dynamics simulations in condensed matter and molecular physics", Lyons (May 2006)
- CECAM Workshop on "State-of-the-art, developments and perspectives of real-space electronic structure techniques in condensed matter and molecular physics", Lyons (June 2005)
- Accelrys Nanotechnology Consortium Meeting, Boston MA (May 2005)
- ES04: the 16th annual workshop on "Recent Developments in Electronic Structure Methods", Rutgers NJ (May 2004)
- Workshop on "Linear Scaling Electronic Structure Methods", Institute for Pure and Applied Mathematics, University of California, Los Angeles (April 2002)
- Symposium on "Methods for Addressing Time and Length Scale Problems in Molecular Simulation", American Chemical Society National Meeting, San Diego (April 2001)

- CECAM Workshop on "Local orbital methods for large scale atomistic simulations", Lyons (July 1998)

Invited UK talks

- Symposium on Recent Advances in Materials Physics: "Pressure-induced structural transformations in germanium nanoparticles" Cumberland Lodge, Windsor Great Park (December 2015)
- Theory of Condensed Matter seminar: "What's the point of linear-scaling electronic structure methods?" Department of Physics, Cambridge (February 2014)
- Plenary talk: "Big Data and Cloud Computing in HPC: Encouraging New Customer Uptake using CORE" High Performance Computing & Big Data Conference, London (February 2014)
- CECAM Distinguished Lecture: "Linear-scaling time-dependent density-functional theory" Theory, Modelling and Computational Methods for Semiconductors, Salford (January 2014)
- Opening address: "CORE: e-Infrastructure solutions" International Data Corporation High Performance Computing User Forum, London (July 2012)
- Thomas Young Centre Soirée on Linear-Scaling Density-Functional Theory, London (November 2011)
- Psi-k/CECAM/CCP9 Biennial Graduate School on Electronic Structure Methods, Oxford (July 2011)
- Theoretical Chemistry Group meeting, Royal Society of Chemistry, Nottingham (June 2011)
- Materials Modelling Laboratory seminar, Department of Materials, Oxford (June 2011)
- Theoretical Physics Group seminar, Department of Physics, Birmingham (January 2011)
- Computational Materials Science Group Annual Meeting, Daresbury Laboratory (November 2009)
- Workshop on "Density Functional Methods for Experimental Spectroscopy", Oxford (August 2009)
- International Data Corporation High Performance Computing User Forum, London (October 2008)
- Hartree Centre meeting on "Materials Simulation on Petascale Systems", London (July 2008)
- First conference of the EPSRC network "Mathematical challenges of Molecular Dynamics" in Warwick (July 2008)
- Materials Modelling Laboratory seminar, Department of Materials, Oxford (May 2008)
- Theory of Condensed Matter seminar, Department of Physics, Cambridge (May 2008)
- Theoretical Chemistry seminar, Physical and Theoretical Chemistry Laboratory, Oxford (January 2008)
- Accelrys Science Forum, Cambridge (November 2007)
- Condensed Matter Theory seminar, Department of Physics, Imperial College London (October 2007)
- Atomistic Simulation Group seminar, Department of Materials, Cambridge (May 2007)
- Accelrys Nanotechnology Consortium Workshop, Cambridge (June 2006)
- Accelrys Nanotechnology Consortium Meeting, Cambridge (October 2005)
- Institute of Physics EMAG-NANO conference, Leeds (September 2005)

- Theory of Condensed Matter / Solid State Theory 50th Anniversary Symposium, Cambridge (July 2005)
- Theoretical Chemistry Colloquium, Department of Chemistry, Cambridge (November 2003)

Grants and Funding

- Principal Investigator, "TheLink – European Training Network to Accelerate the Development Chain of Nanostructured Polymers", Horizon2020 grant 642890, €755k (2014–18)
- Co-Investigator, "Novel excited electron devices: a computational investigation", Leverhulme Trust research grant RPG-2014-125, £147k (2014–17)
- Principal Investigator, "EPSRC Centre for Doctoral Training in Theory and Simulation of Materials", EPSRC grant EP/L015579/1, £4.4M (2014–22)
- Co-Investigator, "Room Temperature, Earth's Field MASER", EPSRC grant EP/K011804/1, £1.2M (2013–15)
- Principal Investigator, "Cambridge-Imperial HPC Centre", EPSRC Promoting Efficiency – Enhancing Equipment Sharing scheme, £130k (2012–13)
- Principal Investigator, "A platform for future development and application of the ONETEP software", EPSRC grant EP/J015059/1, £1.0M (2012–17)
- Co-Investigator, "Bridging the gaps in computational science and engineering", EPSRC Bridging the gaps scheme, £36k (2011–12)
- Principal Investigator, "Large-scale and excited state quantum-mechanical calculations", Royal Society University Research Fellowship renewal, £325k (2010–13)
- Co-Investigator, "Development of wide-ranging functionality in ONETEP", EPSRC grant EP/G05567X/1, £400k (2009–13)
- Principal Investigator (Co-applicant and member of interview team, at time of application), "A centre for doctoral training on the theory and simulation of materials", EPSRC grant EP/G036888/1, £6.4M (2009–17)
- Principal Investigator, "Expanding the scope and scale of first-principles quantum-mechanical simulations with the ONETEP linear-scaling method on high performance computers", EPSRC grant EP/F010974/1, £170k (2007–09)
- Principal Investigator, "Large-scale and excited state quantum-mechanical calculations", Royal Society University Research Fellowship, £300k (pre-FEC) (2005–10)

Teaching Activities

- First year lectures (8) for MSE101: Calculus in the Department of Materials (2015–)
- Postgraduate lectures (16) on Transformations of Materials for the MSc in Theory and Simulation of Materials (2014–)
- Course Director, MSc in Theory and Simulation of Materials (2011–15)
- Developer of the Group Programming Project for the MSc in Theory and Simulation of Materials (2010–15)
- Developer of the 15-week Numerical Methods course for the MSc in Theory and Simulation of Materials (2009–14)
- Co-developer of new mathematics courses for the Department of Materials, including:
  - First year course coordinator (2009–15)
  - First year lectures (12) on Calculus (2007–10)

- First year lectures (6) on Vector Calculus (2008–15)
- Second year lectures (12) on Vector Calculus (2008–15)

- Postgraduate lectures (5) on Computational Physics for the Condensed Matter Theory group and MSc in Physics in the Department of Physics (2007–08)
- Third year lectures (6) on Computational Physics for Part II Experimental and Theoretical Physics in the Natural Sciences Tripos at Cambridge (2001 and 2005)
- Head of Class for the Examples Classes and assessed exercise in Computational Physics, Part II Experimental and Theoretical Physics at Cambridge (2001–06)
- Postgraduate lectures (8) on Solid State Theory for the Theory of Condensed Matter group at the Cavendish Laboratory, Cambridge (2002–03)
- Director of Studies in Natural Sciences, Sidney Sussex College, Cambridge (2005–07)

Research Supervision

PhD Students

1. Robert Charlton (Imperial College PhD Scholar and EPSRC CDT), "Computational Excitonics of Doped Organic Molecular Crystals for a Room-Temperature Maser" (2015–)
2. Jacek Golebiowski ("TheLink" ETN and EPSRC CDT), "Self-diagnosing polymeric CNT composites–first-principles atomistic simulation of the effects of CNT functionalization" (2015–)
3. Hikmatyar Hasan (EPSRC CDT), "Designing next generation high-temperature Co-Al-W based superalloys" (co-supervisor 2015–)
4. Gleb Siroki (EPSRC CDT), "Optical properties of topological insulator nanoparticles" (co-supervisor 2015–)
5. Vadim Nemytov (EPSRC CDT and Materials Design, Inc.), "Nanocrystals by design: combining the power of atomistic force fields and linear-scaling density-functional theory" (co-supervisor 2014–)
6. Adam Ready (EPSRC CDT and Rolls-Royce), "Why is Ti6242 susceptible to cold dwell fatigue, but Ti6246 is not?" (co-supervisor 2013–)
7. Max Boleininger (EPSRC CDT and US Air Force), "Ultrafast laser interactions with thin polymer films" (co-supervisor 2012–)
8. Matthias Kahk (EPSRC Prize Studentship), "Solar water splitting" (co-supervisor 2012–15)
9. Niccolo Corsini (EPSRC CDT), "Pressure-induced transformations in nanomaterials" (2011–15)
10. Tom Poole (EPSRC CDT), "Force fields for carbon nanostructures via algorithmic differentiation" (co-supervisor 2011–15)
11. Tim Zuehlsdorff (EPSRC CDT), "Theory and simulation of metal/semiconductor nanoparticle interfaces for solar energy storage" (2011–14)
12. Lampros Andrinopoulos (EPSRC Project), "Dispersion interactions with linear-scaling density-functional theory" (co-supervisor 2009–13)
13. Hannah Nerl (EPSRC DTA), "Cellular uptake and biostability of carbon nanotubes" (2008–12)

14. Laura Ratcliff (EPSRC DTA), "Calculation of experimental spectra using linear-scaling density-functional theory" (2008–11)
15. Philip Avraam (EPSRC DTA), "Linear-scaling first-principles simulations of entire semiconducting nanorods" (2007–11)
16. Mark Robinson (EPSRC DTA), "Accessing large length and time scales with density functional theory" (2006–10, Cambridge), currently working for MathWorks
17. Gareth Conduit (EPSRC DTA), "Collective phenomena in correlated semiconductors, degenerate Fermi gases, and ferroelectrics" (co-supervisor 2006–09), currently Research Fellow , Gonville & Caius College, Cambridge
18. Patricia Silas (self-funded), "First-principles simulations of structural phase transitions in arsenic" (2003–2010), currently teaching at the University of Cambridge
19. Chee-Kwan Gan (self-funded), "First-principles calculations using localised spherical-wave basis sets" (co-supervisor 1997–2001), currently Senior Scientist A*STAR Insitute of High Performance Computing, Singapore

Post-doctoral Research Associates

1. Niccolo Corsini (EPSRC EP/J015059/1), "A platform for future development and application of the ONETEP software" (2016)
2. Fabiano Corsetti (EPSRC EP/J015059/1), "A platform for future development and application of the ONETEP software" (2015–)
3. Stuart Bogatko (Leverhulme Trust research grant RPG-2014-125), "Novel excited electron devices: a computational investigation" (2014–)
4. Laura Ratcliff (EPSRC EP/D063329/1), "Electron energy-loss spectroscopy with linear-scaling density-functional theory" (2011), currently Postdoctoral Appointee at the Argonne Leadership Computing Facility, USA.
5. Nicholas Hine (EPSRC EP/F010974/1), "Expanding the scope and scale of first-principles quantum-mechanical simulations with the ONETEP linear-scaling method on high performance computers" (2007–09) and (EPSRC EP/G05567X/1), "Development of wide-ranging functionality in ONETEP" (2009–13), currently Assistant Professor at the University of Warwick.
6. Shang-Peng Gao (EPSRC GR/S61263/01), "Core-level spectroscopy within linear-scaling density-functional theory" (2005–06), currently Assistant Professor, Department of Materials Science, Fudan University, Shanghai.

Other Responsibilities

External

- Member, Executive Board, London Centre for Nanotechnology (2015–)
- Member, Organising Committee for the Psi-k Conference, San Sebastian (September 2015)
- External PhD examiner, UCL (October 2014)
- Member, Science and Engineering South e-Infrastructure Board (2013–)
- External examiner, Department of Materials, University of Oxford (2013–14)
- Organiser, Psi-k/CECAM Workshop on "Efficient localised orbitals for large systems, strong correlations and excitations", Cambridge (July 2012)
- Organiser, EPSRC ONETEP Master Class, Cambridge (July 2011)

- External PhD examiner, University of Southampton (February 2011)
- Member and Spokesperson for *N*-scaling, Scientific Advisory Committee of the Psi-k Network (2010–)
- Organiser, EU Marie Curie/Psi-k ONETEP Spring School, Cambridge (April 2010)
- Organiser, EPSRC ONETEP Summer School, Cambridge (July 2008)
- External PhD examiner, University of Cambridge (February 2008)
- Organiser, CCP9/Psi-k/CECAM Workshop on "Linear-scaling *ab initio* calculations: applications and future directions", Lyons (September 2007)
- Member, Working Group for CCP9: the Collaborative Computational Project for the Study of the Electronic Structure of Condensed Matter (2007–)
- Member, Council, Sidney Sussex College, Cambridge (2006–07)
- Consultant, Accelrys Nanotechnology Consortium (2004–07)
- Member, ONETEP Developers' Group, an academic code licensed to BIOVIA (a brand of Dassault Systèmes) for commercial distribution from October 2007 via Cambridge Enterprise Ltd., with total revenue to date in excess of $4.5M
- Organiser, Psi-k/CECAM Workshop on "Local Orbitals and Linear-scaling *ab initio* Calculations", Lyons (September 2001)
- Reviewer, EPSRC, L'Oréal Women in Physics Fellowships and Archimedes III (Greece)
- Referee, journals including Europhysics Letters, Physical Review, Journal of Physics and Journal of Chemical Physics

Internal

- Chair, High Performance Computing Board (2015–)
- Chair, Panel for the President's Award for Excellence in Research Support (2015–)
- Member, Advisory Board for the EPSRC Centre for Doctoral Training on Maths for Planet Earth (2014–)
- College Champion for High Performance Computing (2013–)
- Academic advisor to the Vice Provost (Research) for High Performance Computing and Research Data Management (2013–16)
- Chair, High Performance Computing Advisory Panel (2013–15)
- Director, CORE e-Infrastructure consortium (2012–)
- Director, EPSRC Centre for Doctoral Training on Theory and Simulation of Materials (2011–16)
- Chair, Research Stream Board (ICT Business Systems) (2011–15)
- Member, Management and Information Systems Advisory Board (ICT) (2011–15)
- Deputy Director and Admissions Tutor, EPSRC Centre for Doctoral Training on Theory and Simulation of Materials (2009–11)
- Postgraduate Admissions Tutor, Department of Materials (2008–15)
- Chair, Departmental Users' Committee (ICT) (2008–13)
- Member, Information Technology and Services Strategy Group (ICT) (2008–15)
- Member, High Performance Computing Advisory Panel (ICT) (2008–13)

- Careers Adviser, Department of Materials and Member, Careers Advisers' Committee (2007–09)
- Work placements coordinator, Department of Materials (2008–09)

Contact details

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