

# Peter David Haynes

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Date of birth: 26 February 1974  
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## Summary

I am a computational physicist and holder of a Royal Society University Research Fellowship in the Theory of Condensed Matter group at the Cavendish Laboratory in the University of Cambridge. My research is focussed on the development of new linear-scaling methods for performing large-scale first-principles quantum-mechanical simulations, and their application to biological systems, materials science and nanotechnology. I have a broad range of teaching experience including lecturing and supervising both undergraduates and graduates.

## Employment

- Oct 2005– **Cavendish Laboratory, University of Cambridge**  
Royal Society University Research Fellow in Physics.
- Oct 2002– **Sidney Sussex College, Cambridge**  
Sep 2005 Ramon Jenkins Senior Research Fellow in Physics.
- Oct 1999– **Magdalene College, Cambridge**  
Sep 2002 Thomas Nevile Research Fellow in Physics.
- Oct 1998– **Cavendish Laboratory, University of Cambridge**  
Sep 1999 Post-doctoral Research Associate in the Theory of Condensed Matter.
- Jul–Aug **Chemistry Department, University College London**  
1995 Theoretical research into the dynamic response of gas sensors (under Prof. D. E. Williams).
- Jul–Sep **Physics Department, University of California at Santa Barbara**  
1994 Experimental research into light-emitting conjugated polymers (under Prof. A. J. Heeger, winner of the Nobel Prize in Chemistry, 2000).
- Jul–Aug **Capteur Sensors and Analysers, Milton, Oxon**  
1993 Testing gas sensors and characterising new materials.
- Jul–Aug **Harwell Laboratory, AEA Technology, Oxon**  
1992 Research into the use of sols in ink-jet printers and diesel exhaust catalysis.
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## Education

### 1995–98 Cavendish Laboratory, University of Cambridge

Ph.D. research degree under the supervision of Prof. M. C. Payne in the Theory of Condensed Matter group at the Cavendish Laboratory (Department of Physics in the University of Cambridge). Dissertation entitled:

*Linear-scaling methods in ab initio quantum-mechanical calculations.*

**Awards** Bachelor Scholarship from Christ's College, Cambridge (1995–98).  
Ph.D. degree conferred: 14 November 1998.

### 1992–95 Christ's College, University of Cambridge

1995 B.A. (Hons.) in Physical Natural Sciences Tripos.  
Part II (First Class) in Experimental & Theoretical Physics (91% overall mark).  
1994 Part IB (First Class) in Advanced Physics (85%) and Mathematics (95%).  
1993 Part IA (First Class) in Chemistry (81%), Crystalline Materials (85%),  
Physics (88%) and Mathematics (95%).  
Highest overall mark in the University for Part IA Natural Sciences.

**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 Prize for Part I Natural Sciences (1993 & 94).  
College Fay Prize for Part IA Natural Sciences (1993).  
B.A. degree conferred: 30 June 1995.  
M.A. degree conferred: 20 March 1999.

### 1985–92 Abingdon School, Oxfordshire

1992 'A'- and 'S'-level Physics (A1) and Chemistry (A1).  
'A'-level Further Mathematics (A) and 'AS'-level German (A).  
1991 'A'- and 'S'-level Mathematics (A1).  
1990 Additional (formerly 'A/O') level Mathematics (A).  
G.C.S.E. English (A1), English Literature (A), Latin (A), German (A), Religious  
Studies (A), Physics (A), Chemistry (A), Biology (A) and Geography (A).  
1989 G.C.S.E. French (A) and Mathematics (A).

**Awards** Foundation Scholarship (1987–92).  
Gold medal, Theory Prize and overall winner of the British Physics Olympiad – a  
competition supported by the Royal Society and Institute of Physics (1992).  
Silver medal at the International Physics Olympiad in Helsinki (1992).  
St. Catherine's College (Oxford) Prize for Intellectual Initiative (1992).  
Bennett Prize for Academic Achievement (1991).  
Ingham Prize for Physics (1991 & 92).  
Birnbirg Prize for German and Mathematics Prize (1992).  
Music Exhibition for trombone (1989–92).  
Middle School House Prize (1988) and Lower School Prize (1986).

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## Selected Publications

1. Elimination of basis set superposition error in linear-scaling density-functional calculations with local orbitals optimised *in situ*  
P. D. Haynes, C.-K. Skylaris, A. A. Mostofi & M. C. Payne, *Chem. Phys. Lett.* in press (2006).  
DOI: 10.1016/j.cplett.2006.02.086
  2. ONETEP: linear-scaling density-functional theory with local orbitals and plane waves  
P. D. Haynes, C.-K. Skylaris, A. A. Mostofi & M. C. Payne, *phys. stat. sol. (b)* in press (2006).  
DOI: 10.1002/pssb.200541457
  3. Are the structures of twist grain boundaries in silicon ordered at 0 K?  
S. von Alffhan, P. D. Haynes, K. Kaski & A. P. Sutton, *Phys. Rev. Lett.* **96**, 055505 (2006).
  4. ONETEP: linear-scaling density-functional theory with plane-waves  
P. D. Haynes, A. A. Mostofi, C.-K. Skylaris & M. C. Payne, *J. Phys.: Conf. Ser.* **26**, 143–8 (2006).
  5. Using ONETEP for accurate and efficient  $O(N)$  density functional calculations  
C.-K. Skylaris, P. D. Haynes, A. A. Mostofi & M. C. Payne, *J. Phys.: Condens. Matter* **17**, 5757–69 (2005).
  6. Introducing ONETEP: Linear-scaling density functional simulations on parallel computers  
C.-K. Skylaris, P. D. Haynes, A. A. Mostofi & M. C. Payne, *J. Chem. Phys.* **122**, 084119 (2005).
  7. Structural relaxations in electronically excited poly(*para*-phenylene)  
E. Artacho, M. Rohlfing, M. Côté, P. D. Haynes, R. J. Needs & C. Molteni, *Phys. Rev. Lett.* **93**, 116401 (2004).
  8. Preconditioned iterative minimisation for linear-scaling electronic structure calculations  
A. A. Mostofi, P. D. Haynes, C.-K. Skylaris & M. C. Payne, *J. Chem. Phys.* **119**, 8842–8 (2003).
  9. Material design from first principles: the case of boron nitride polymers  
M. Côté, P. D. Haynes & C. Molteni, *J. Phys. Condens. Matter* **14**, 9997–10009 (2002).
  10. Comparison of variational real-space representations of the kinetic energy operator  
C.-K. Skylaris, O. Diéguez, P. D. Haynes & M. C. Payne, *Phys. Rev. B* **66**, 073103 (2002).
  11. Nonorthogonal generalized Wannier function pseudopotential plane-wave method  
C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Diéguez & M. C. Payne, *Phys. Rev. B* **66**, 035119 (2002).
  12. Total-energy calculations on a real space grid with localized functions and a plane-wave basis  
A. A. Mostofi, C.-K. Skylaris, P. D. Haynes & M. C. Payne, *Comput. Phys. Commun.* **147**, 788–802 (2002).
  13. First-principles density-functional calculations using localized spherical-wave basis sets  
C. K. Gan, P. D. Haynes & M. C. Payne, *Phys. Rev. B* **63**, 205109 (2001).
  14. Boron Nitride Polymers: new building blocks for organic electronic devices  
M. Côté, P. D. Haynes & C. Molteni, *Phys. Rev. B* **63**, 125207 (2001).
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## Selected Publications continued

15. Preconditioned conjugate gradient method for the sparse generalized eigenvalue problem in electronic structure calculations  
C. K. Gan, P. D. Haynes & M. C. Payne, *Comput. Phys. Commun.* **134**, 33–40 (2001).
16. Parallel fast Fourier transforms for electronic structure calculations  
P. D. Haynes & M. Côté, *Comput. Phys. Commun.* **130**, 130–6 (2000).
17. An *ab initio* linear-scaling scheme  
P. D. Haynes & M. C. Payne, *Molecular Simulation* **25** 257–64 (2000).
18. Corrected penalty-functional method for linear-scaling calculations in density-functional theory  
P. D. Haynes & M. C. Payne, *Phys. Rev. B* **59**, 12173–6 (1999).
19. Failure of density-matrix minimization methods for linear-scaling density-functional theory using the Kohn penalty-functional  
P. D. Haynes & M. C. Payne, *Solid State Commun.* **108**, 737–41 (1998).
20. Localised spherical-wave basis set for  $O(N)$  total-energy pseudopotential calculations  
P. D. Haynes & M. C. Payne, *Comput. Phys. Commun.* **102**, 17–27 (1997).

## Meetings

- Principal organiser of a workshop on “Local Orbitals and Linear-scaling *ab initio* Calculations” sponsored by the European Science Foundation and the European Centre for Atomic and Molecular Computations, held in Lyons, September 2001.  
See: Report on the CECAM/ESF STRUC- $\Psi_k$  Workshop on “Local Orbitals and Linear-scaling *ab initio* Calculations”  
P. D. Haynes, D. R. Bowler and E. Artacho,  $\Psi_k$  Newsletter **48**, 36–66 (December 2001).
  - Invited speaker at the workshop on “State-of-the-art, developments and perspectives of real-space electronic structure techniques in condensed matter and molecular physics” in Lyons, June 2005.
  - Invited to speak at the 12th “Workshop on Computational Physics and Materials Science: Total Energy and Force Methods” in Trieste, January 2005.
  - Invited speaker at ES04: the 16th annual workshop on “Recent Developments in Electronic Structure Methods” at Rutgers, New Jersey, May 2004.
  - Invited speaker at a workshop on “Linear Scaling Electronic Structure Methods” at the Institute for Pure and Applied Mathematics, University of California, Los Angeles, April 2002.
  - Invited speaker at a symposium on “Methods for Addressing Time and Length Scale Problems in Molecular Simulation” at the American Chemical Society’s National Meeting in San Diego, April 2001.
  - Invited speaker at a workshop on “Local orbital methods for large scale atomistic simulations” in Lyons, July 1998.
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## Grants & Funding

- Joint Principal Investigator on a pending application to EPSRC entitled “Understanding the dopant effect on dislocation mobility in semiconductors with new linear-scaling methods for large-scale first-principles simulations”.
- Nuffield Foundation Undergraduate Research Bursary to support a summer student (G. J. Conduit) for six weeks (2005).
- Royal Society University Research Fellowship (2005-2010).
- Royal Society Research Grant of £10k for computing equipment (2002).
- Ramon Jenkins Senior Research Fellowship at Sidney Sussex College, Cambridge (2002-2005).
- Thomas Nevile Research Fellowship at Magdalene College, Cambridge (1999-2002).

## Teaching Experience

- Six lectures on Computational Physics for Part II Experimental & Theoretical Physics in the Natural Sciences Tripos (2001 & 2005).
- Head of Class for the Examples Classes and assessed exercise in Computational Physics, Part II Experimental & Theoretical Physics (2001–06).
- Eight lectures on Solid State Theory for graduate students at the Cavendish Laboratory (2002 & 2003)
- Demonstrator at Examples Classes for Part IB Mathematical Physics, Part II Theoretical Physics and Part II Solid State Physics (1995–98).
- Supervisions in Part IA Physics and Part IB Advanced Physics and Mathematics for Sidney Sussex, Magdalene, Christ’s and Corpus Christi Colleges (1995–2006).

## Administrative and Other Responsibilities

- Member of the ONETEP Developers’ Group, an academic partner in the Accelrys Nanotechnology Consortium and author of the ONETEP code licensed to Accelrys Inc. for commercial distribution from October 2007 under an agreement made through Cambridge University Technical Services.
  - Member of the Management Committee, Departmental Representative and Webmaster for the Cambridge-Cranfield High Performance Computing Facility.
  - Graduate Mentor, member of the College Council, and Director of Studies for Part III Natural Sciences at Sidney Sussex College.
  - Member of the EPSRC College (2003–05) and referee for several journals including the *Physical Review*.
  - Undergraduate admissions interviews for Natural Sciences, Mathematics and Computer Science.
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