# JAMES ARTHUR ELLIOTT

## PERSONAL DETAILS


| | | |
|---|---|---|
| Work address | : | Department of Materials Science & Metallurgy,<br>University of Cambridge, Cambridge, CB2 3QZ.<br>Telephone (01223) 335 987<br>Facsimile (01223) 334 567<br>Mobile (07813) 881 282 |
| College address | : | Fitzwilliam College, Cambridge, CB3 0DG<br>Messages only (01223) 332 000 |
| Electronic addresses | : | E-mail : jae1001@cam.ac.uk<br>WWW: http://www.elliotts.org.uk |
| Nationality | : | British |
| Year of Birth | : | 1973 |


## ACADEMIC AND PROFESSIONAL QUALIFICATIONS

2004 **Institute of Physics** : CSci
Chartered Scientist

2000 **Institute of Physics** : CPhys MInstPhys
Chartered Physicist and full Membership of the Institute of Physics

1999 **University of Cambridge** : MA (Cantab)
Honorary Masters degree

1995–98 **University of Bristol** : PhD in Polymer Physics
*"X-ray diffraction and computer modelling of perfluorinated ionomers"*
supervised by Dr Simon Hanna, Polymer Physics Group

1992–95 **University of Cambridge** : MA Honours in Physical Natural Sciences
Part II : Physics & Theoretical Physics [Upper Second Class]

## ACADEMIC APPOINTMENTS HELD

2002-date **Fitzwilliam College**, University of Cambridge
Elected as Fellow, Director of Studies and College Lecturer in Materials Science

2001-date **Department of Materials Science**, University of Cambridge
University Lecturer in *Materials Modelling*

1998–2001 **Polymer Group**, Department of Materials Science, University of Cambridge
EPSRC-funded postdoctoral position

## RESEARCH SUMMARY AND RELATED GRANTS

### Materials Modelling

With modern computers, it is now possible to predict the properties of novel materials from first principles using advanced simulation techniques. This has the advantages of being both quicker and cheaper than a trial-and-error discovery process, and also yields detailed structural and dynamical information which can provide a stringent test of theoretical models. The computer modelling of materials can take place from the atomistic to the continuum level, and provides a powerful route for linking molecular-scale phenomena to complex emergent properties.

### Membranes and molecular tubes

A key component of redox fuel cells is the membrane which provides a physical barrier between the electrolytes, whilst allowing the passage of individual ions. By elucidating the motion of ions in the membrane using molecular dynamics, it is possible to predict the influence of environmental conditions on the resistivity and selectivity of the membrane, and thus improve the efficiency of the cell. Similar techniques allow the characterisation of the mechanical properties of carbon nanotubes, and their interactions with a polymer matrix when used as reinforcing fillers in composite materials

### Pharmaceutical Materials Science

A new frontier in Materials Science is the application of traditional knowledge about crystallisation and growth in small organic molecule and polymeric systems to biomedical problems. This requires extreme agility across time and length scales, and computer modelling is well placed to provide insights at all levels, from the prediction of the stability of different drug polymorphs to the optimum formulation of active ingredient and excipient to produce a stable form for drug delivery.

### Research Grants

RG34605 *Pfizer Institute for Pharmaceutical Materials Science*
Pfizer Inc., Co-investigator (£1.5 million share of £7.5 million total) [current]

RG38352 *Structural modelling of the biological interface with materials*
EPSRC, Principal investigator (£337,570) [current]

RG36886 *Artificial intelligence molecular dynamics approaches for simulating complex materials*
US Air Force Research Laboratories, Principal investigator (£188,864) [current]

RG38328 *Mechanisms of proton conduction in minimally hydrated ion-containing polymers*
EPSRC, Principal investigator (£119,493) [current]

RG34381 *Modelling of percolation in carbon nanotube polymer composites*
US Army Research Office, Principal investigator (£105,725) [completed]

RG28930 *New materials for innovative electrochemistry*
Regenesys Technologies Fuel Cell UTC, Collaborator (£492,570) [completed]

RG34761 *Computational modelling of carbon nanotubes*
DSTL, Co-investigator (£10,000) [completed]

Currently supervising 4 postdoctoral research associates (funded by Pfizer), 2 PDRAs (funded EPSRC) and 3 PhD students (US Army/Air Force/EPSRC).

**PUBLICATIONS & PRESENTATIONS**

**Refereed journal articles**

1. Fu, X., Elliott, J.A., Bentham, A.C., Hancock, B.C. and Cameron, R.E. "Application of X-ray microtomography and image processing to the investigation of a compacted granular system", *Particle & Particle Sys. Character.*, to appear (2006).
2. Tan, J.C., Elliott, J.A. and Clyne, T.W. "Analysis of tomography images of bonded fibre networks to measure distributions of fibre segment length and fibre orientation", *Adv. Eng. Mat.*, to appear in Special Issue for EUROMAT 2005, September 5-8, Prague (2006).
3. Wu, C.-Y., Hancock, B.C., Mills, A., Bentham, A.C., Best S.M. and Elliott, J.A. "Numerical and experimental investigation of capping mechanisms during pharmaceutical tablet compaction", *Powder Tech.*, to appear in Special Issue for "Particulate Processes in the Pharmaceutical Industry", June 26-30, 2005, Montreal (2006).
4. Paddison, S.J. and Elliott, J.A. "The effects of backbone conformation on hydration and proton transfer in the 'short-side-chain' perfluorosulfonic acid membrane" *Solid State Ionics*, to appear in Special Issue for 15th International Solid State Ionics meeting, July 17-22, 2005 Baden-Baden (2006).
5. Paddison, S.J. and Elliott, J.A. "The consequences of side chain flexibility and backbone conformation on hydration and proton transfer in perfluorosulphonic acid membranes", *Phys. Chem. Chem. Phys.*, **8**, 2193-2203 (2006).
6. Elliott, J.A., Hanna, S., J.N. Newton, Elliott, A.M.S. and Cooley, G.E. "The Elimination of Orientation in Perfluorinated Ionomer Membranes", *Polym. Eng. Sci.*, **46**, 228 (2006).
7. Rahatekar, S.S., Hamm, M., Shaffer, M.S.P. and Elliott, J.A. "Mesoscale modelling of electrical percolation in fibre-filled systems", *J. Chem. Phys.*, **123**, 134702 (2005).
8. Paddison, S.J. and Elliott, J.A. "Molecular modeling of the short-side-chain perfluorosulfonic acid membrane" *J. Phys. Chem. A*, **109**, 7583-7593 (2005).
9. Amer, M.S., Elliott, J.A., Maguire, J.F. and Windle, A.H. "Calculations of the Raman spectra of C60 interacting with water molecules" *Chem. Phys. Lett.*, **411**, 395-398 (2005).
10. Wu, C.-Y., Ruddy, O.M., Bentham, A.C., Hancock, B.C., Best S.M. and Elliott, J.A. "Modelling the mechanical behaviour of powders during compaction", *Powder Tech.*, **152**, 107-117 (2005).
11. Dutt, M., Hancock, B.C., Bentham, A.C. and Elliott, J.A. "An implementation of granular dynamics for simulating frictional elastic particles based on the DL_POLY code", *Comput. Phys. Comm.*, **166**, 26-44 (2005).
12. Elliott, J.A., Sandler, J.K., Windle, A.H., Young, R.J. and Shaffer, M.S.P. Reply to Comment on "The collapse of single-wall carbon nanotubes is diameter-dependent", *Phys. Rev. Lett.*, **93**, 149602 (2004).
13. Elliott, J.A., Sandler, J.K., Windle, A.H., Young, R.J. and Shaffer, M.S.P. "The collapse of single-wall carbon nanotubes is diameter-dependent", *Phys. Rev. Lett.*, **92**, 095501 (2004).
14. Elliott, J.A., Kelly, A. and Windle, A.H. "Recursive packing of dense particle mixtures" *J. Mat. Sci. Letters*, **21**, 1249-1251 (2002).
15. Elliott, J. A., Windle A. H., Hobdell, J.R., Eeckhaut, G., Olman, R. J., Ludwig, W., Boller, E., Cloetens, P., Baruchel, J. "In-situ deformation of an open-cell flexible

polyurethane foam characterised by 3D computed microtomography" *J. Mat. Sci.*, **37**, 1547-1555 (2002).

16. Elliott, J. A., James, P. J., McMaster, T. J., Newton, J. M., Elliott, A. M. S., Hanna, S. and Miles, M. J. "Hydrolysis of the Nafion precursor studied by X-ray scattering and in-situ AFM" *e-Polymers*, 22, (2001).
17. Elliott, J. A., Hanna, S., Elliott, A. M. S. and Cooley, G. E. "The swelling behaviour of perfluorinated ionomer membranes in ethanol/water mixtures" *Polymer*, **42**, 5, 2253-2255 (2001).
18. Elliott, J. A. and Windle, A. H. "A dissipative particle dynamics method for modelling the geometrical packing of filler particles in polymer composites" *J. Chem. Phys.*, **113**, 22, (2000).
19. James, P. J., Elliott, J. A., McMaster, T. J., Newton, J. M., Elliott, A. M. S., Hanna, S. and Miles, M. J. "Hydration of Nafion studied by AFM and X-ray scattering" *J. Mat. Sci.*, **35**, 20, 5111-5119 (2000).
20. Elliott, J. A., Hanna, S., Elliott, A. M. S. and Cooley, G. E. "Interpretation of the small angle X-ray scattering from swollen and oriented perfluorinated ionomer membranes" *Macromolecule*s, **33**, 11, 4161-4171 (2000).
21. Elliott, J. A. and Hanna, S. "A model-independent maximum-entropy method for the inversion of small angle X-ray diffraction patterns" *J. Appl. Cryst.*, **32**, 6, 1069-1083 (1999).
22. Elliott, J. A., Hanna, S., Elliott, A. M. S. and Cooley, G. E. "Atomistic simulation and molecular dynamics of model systems for perfluorinated ionomer membranes" *PCCP*, **1**, 20, 4855-4863 (1999).

**Selected recent conference publications**

- Elliott, J.A. "Multi-scale modelling of powder compaction: from granules to tablets", Highlighted oral presentation at the EUROMAT 2005 conference held in Prague, Czech Republic (2005).
- Benedict, M., Elliott, J.A. and Maguire, J.F. "Spherical Subdivision for Accurate Shape Representation in Mesoscale Computer Simulations of Granular Particulate Matter", Oral presentation at Intelligent Processing and Manufacturing of Materials (IPMM) conference held in Monterey, California, July 19–23 (2005).
- Elliott, J.A. and Paddison, S.J. "Multi-scale modelling of minimally hydrated perfluorosulphonic acid membranes", Oral presentation at the CCP5 Annual Meeting 2005, Keele, UK (2005).
- Elliott, J.A. "Multi-scale modelling of powder compaction: from tablets to granules", Invited oral presentation at the British Pharmaceutical Conference 2004, Manchester, UK (2004).
- Elliott, J.A. "Multi-scale modelling of powder compaction: from tablets to granules", Invited oral presentation at Cutting Edge Approaches for Drug Design, University of Bradford, UK (2004).
- Elliott, J. A. "Computational modeling and structural studies of perfluorosulfonate ionomer membranes", Invited oral presentation at NanoTech 2003, San Francisco, USA (2003).

**Other publications**

- Elliott, J.A., Book chapter entitled "Atomistic Modelling Of Perfluorosulphonate Ionomer Membrane Morphology", to appear in *Fuel Cell Modeling* (eds. S.J. Paddison, K. Promislow), Springer (2006).
- Elliott, J. A., Starikov, E., Crawshaw, J. C., Claiden, P. C., Nilsson, L., Windle, A. H. Book chapter entitled "Nucleation of polyglutamine amyloid fibres modelling using molecular dynamics", to appear in *Modern Methods For Theoretical Physical Chemistry Of Biopolymers* (eds. E. Starikov, J. Lewis, S. Tanaka), Elsevier, (2006).
- Elliott, J. A., Book chapters entitled "Monte Carlo and Molecular Dynamics Methods" and "Mesoscale Methods and Multiscale Modelling" in *Introduction to Materials Modelling* (ed. Z. H. Barber), Maney Publishing (2004).
- Elliott, J.A., Book review of "The Kinetic Theory of Gases: An Anthology of Classic
- Papers with Historical Commentary" (by S.G. Brush) *Contemporary Physics*, **45**, 5, 453-454 (2004).
- Elliott, J. A., Book review of "Polymers from the Inside Out. An Introduction to Macromolecules" (by A. E. Tonelli and M. Srinivasarao) *Contemporary Physics*, **43**, 1, 416-417 (2002).
- Elliott, J. A., Book review of "Soft Condensed Matter: Configurations, Dynamics and Functionality" (eds. A. T. Skjeltorp and S. F. Edwards) *Contemporary Physics*, **43**, 1, 40-41 (2001).
- Windle, A.H., Elliott, J.A., Oldman, R.J., Hobdell, J.R., Eeckhaut, G., Baruchel, J., Bouchet, S., Ludwig, W., Cloetens, P.and Boller, E. "In situ deformation of open-cell flexible foams using 3-D computed microtomography", ESRF Research Highlights 1999, pp. 87-88 (1999).
- Elliott, J. A. "X-ray diffraction and computer modelling of perfluorinated ionomer membranes", PhD thesis, University of Bristol (1998).

**TEACHING AND ADMINISTRATIVE RESPONSIBILITIES**

- University Lecturer in Materials Science, University of Cambridge.
  - Head of Year and Course Co-ordinator for IB Materials Science
  - Head of the *Materials Modelling* research group: 6 PDRAs, 3 PhDs, 1 MPhil
  - Senior Examiner for MPhil in Materials Modelling (2004, 2006)
  - MPhil 12 lecture course "Monte Carlo and Molecular Dynamics methods" (2001 to date)
  - MPhil 6 lecture course "Mesoscale Methods and Multiscale Modelling" (2001 to date)
  - MPhil 3 lectures on "Polymer Processing" (2001-2004)
  - Graduate lectures on "Model fitting and Data Analysis" (Lent Term 2006)
  - Part III undergraduate 16 lecture course "Particle Technology" (Lent Term2006)
  - Part III undergraduate 12 lecture course "Polymeric Materials" (Lent Term 2004 and 2005)
  - Supervising Part II courses "Polymers" and "Polymer Processing"
  - Chairman of Computing Committee
  - Member of Teaching, Research, X-ray and Graduate School committees

- College Lecturer in Materials Science, Fitzwilliam College, Cambridge.
    - Supervising IA Materials and Mineral Sciences
- Assistant Director of Studies in Natural Sciences (Physical)
- Member of Fitzwilliam College Committee (from January 2006)
- Senior Treasurer of Fitzwilliam College Boat Club
- Member of the Executive Trustees of Fitzwilliam College Junior Members Association
- Previously member of the Fitzwilliam New Buildings Committee (from January 2003 to December 2005)
- Previously supervised IA Natural Sciences course "*Mathematical Methods for Natural Scientists*" at Christ's College, Cambridge from 1998-2002.
- Completed a Postgraduate Teaching and Learning course, and passed the assessment exercise with distinction (credited at MEd level).
- Supervisor for a number of Part III, MPhil and MSci main research projects at the Universities of Cambridge and Bristol.

**COMPUTING SKILLS AND RESPONSIBILITIES**

- Chairman of Departmental Computing Committee (Materials Science & Metallurgy)
- System Administrator for 30 Unix/Linux workstations, 20 Windows XP and 2 Macintosh desktop computers in the Materials Modelling group, with responsibility for machine maintenance, system upgrades and weekly backups.
- Extensive experience of IRIX, Linux, Windows 9x/2000/XP and MacOS operating systems.
- Considerable experience of high performance parallel computing, in particular heavy usage of the High Performance Computing Facility in the University of Cambridge.
- Programming languages include FORTRAN 90/77, C/C++, PV-WAVE, IDL, Mathematica, MathCAD and Maple.