

**CURRICULUM VITAE**  
**CHARUSITA CHAKRAVARTY**

Department of Chemistry  
Indian Institute of Technology-Delhi  
Hauz Khas, New Delhi 110016  
Email: [charus@chemistry.iitd.ernet.in](mailto:charus@chemistry.iitd.ernet.in)  
Tel: +91 11 2659 1510  
Fax: +91 11 2686 2122

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**EDUCATION**

October '90      Ph.D in Chemistry  
Theoretical Chemistry Department, University of Cambridge, UK  
Thesis Title: *Open-shell van der Waals Complexes: Spectra and Dynamics of Ar-OH*  
Research Supervisor: Dr. D. C. Clary

June '87        B.A. (Hons.) in Natural Sciences (Chemistry, First Class)  
Queens' College, University of Cambridge, UK

July '85        B.Sc. (Hons.) in Chemistry (First Class)  
St. Stephens College, University of Delhi, India

**APPOINTMENTS**

Aug. '02 -      Associate Professor, Department of Chemistry  
Indian Institute of Technology, New Delhi, India.

Oct. '94 -      Assistant Professor, Department of Chemistry  
July '02        Indian Institute of Technology, New Delhi, India.

Sept. '93 -     Gulbenkian Junior Research Fellowship from Churchill College, Cambridge.  
Sept. '94        Affiliated to the Department of Chemistry, University of Cambridge, UK

Nov. '92 -      Department of Physics  
Aug. '93        Indian Institute of Technology-Delhi, India

March '91 -     Department of Chemistry, University of California, Santa Barbara, USA  
Sept. '92        Postdoctoral research associate with Prof. Horia Metiu

**AWARDS/PRIZES**

- Fellow of the Indian Academy of Sciences, Bangalore.
- Swarnajayanti Fellowship 2003-2004, Department of Science and Technology, New Delhi.
- Bronze Medal of the Chemical Research Society of India, 2004.
- B. M. Birla Science Award in Chemistry for 1999.
- Anil Kumar Bose Memorial Award for 1999, Indian National Science Academy, New Delhi.
- Associate Member of the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (1996-2003).
- INSA Medal for Young Scientists 1996, Indian National Science Academy, New Delhi.
- Associate of the Indian Academy of Sciences, Bangalore.

- Research Studentship, Churchill College, Cambridge (1987-90)
- Foundation Scholarship, Queens' College, Cambridge (1986-87)
- Hinduja Scholarship of the Cambridge Commonwealth Trust (1985-87)
- University Gold Medal for the B.Sc. Examination in Chemistry (1985)

#### PERSONAL DATA

- Date of Birth 5 May 1964
- Nationality: Indian
- Married

#### VISITING POSITIONS/MEMBERSHIP OF PROFESSIONAL SOCIETIES

- Visiting Fellow, Department of Chemical Engineering, Princeton University, U.S.A. (January-June 2005)
- Visiting Professor, Atomistic Simulation Group, The Queen's University, Belfast, U.K. (May-June 1998)
- Member, Royal Society of Chemistry
- Life Member, Chemical Research Society of India

#### RESEARCH INTERESTS

- Path Integral Monte Carlo Simulations  
Development of path integral simulation techniques for problems of chemical interest; applications to study quantum clusters, liquids and solids, specially with regard to quantum effects on melting and crystal-liquid nucleation.
- Classical Clusters and Liquids  
Classical Monte Carlo and molecular dynamics simulations applied in conjunction with potential energy landscape approaches to understand phase transitions and dynamics in atomic and hydrogen-bonded clusters and liquids. Systems of current interest are bulk Morse systems and water.
- Quantum and Classical Simulation Studies of Adsorption and Diffusion in Zeolites  
Using simulations to understand unusual diffusional behaviour, such as the effect of geometrical correlations and anomalous size dependences.
- Quantum Scattering and Spectroscopy  
Application of quantum scattering techniques to study spectroscopy and dynamics of van der Waals complexes

## PUBLICATIONS

### CITED JOURNALS

1. *Network Dynamics and the Diffusional Anomaly in Silica*  
Ruchi Sharma, Anirban Mudi and Charusita Chakravarty  
Journal of Chemical Physics (to be published).
2. *Spectral Characterization of Hydrogen Bond Network Dynamics in Water*  
Anirban Mudi, Charusita Chakravarty and Edoardo Milotti  
Journal of Chemical Physics (to be published).
3. *Effect of Ionic Solutes on the Hydrogen Bond Network Dynamics of Water: Power Spectral Analysis of Aqueous NaCl solutions*  
Anirban Mudi and Charusita Chakravarty  
Journal of Physical Chemistry B, **110**, 8422-8421 (2006).
4. *Diffusivity, Excess Entropy and the Potential Energy Landscape of Monoatomic Liquids*  
Somendra Nath Chakraborty and Charusita Chakravarty  
Journal of Chemical Physics, **124**, 014507-1 to 014507-10 (2006).
5. *Generating Inherent Structures of Liquids: Comparison of Local Minimization Algorithms*  
Charusita Chakravarty, Pablo G. Debenedetti and Frank H. Stillinger  
Journal of Chemical Physics, **123**, 206101-1 to 206101-2 (2005).
6. *Hybrid Monte Carlo Implementation of the Fourier Path Integral Algorithm*  
Charusita Chakravarty  
Journal of Chemical Physics, **123**, 024104-1 to 024104-12 (2005).
7. *Spectral Signatures of the Diffusional Anomaly in Water*  
Anirban Mudi, Charusita Chakravarty and Ramakrishna Ramaswamy  
Journal of Chemical Physics, **122**, 104507-1 to 104507-8 (2005).  
  
*Erratum: Spectral signatures of the diffusional anomaly in water (J. Chem. Phys., **122**, 104507 (2005))*  
Anirban Mudi, Charusita Chakravarty and Ramakrishna Ramaswamy  
Journal of Chemical Physics, **124**, 069902-1 to 069902-2 (2006).
8. *Multiple Time-scale Behaviour of the Hydrogen Bond Network in Water*  
Anirban Mudi and Charusita Chakravarty  
Journal of Physical Chemistry B, **108**, 19607-19613 (2004) (published in the Frank Stillinger Festschrift issue).  
  
*Correction to Multiple Time-scale Behaviour of the Hydrogen Bond Network in Water; Journal of Physical Chemistry B, Volume 108, page 19607 (2004).*  
Anirban Mudi and Charusita Chakravarty  
Journal of Physical Chemistry B, **110**, 4502 (2006).
9. *Melting of Atomic Solids: Effect of Range and Softness of Interaction Potentials*  
Somendra Nath Chakraborty, Nilanjan Ghosh, Pooja Shah and Charusita Chakravarty  
Molecular Physics, **102**, 909-918 (2004)  
(published in the special issue in honour of Ruth M. Lynden-Bell).

10. *Effect of the Berendsen thermostat on dynamical properties of water*  
Anirban Mudi and Charusita Chakravarty  
Molecular Physics, **102**, 681-685 (2004).
11. *Signatures of Multiple Time-scale Behaviour in the Power Spectra of Water*  
Anirban Mudi, Ramakrishna Ramaswamy and Charusita Chakravarty  
Chemical Physics Letters, **376**, 683-689 (2003).
12. *Melting of 55-atom Morse Clusters*  
Pooja Shah, Sharani Roy and Charusita Chakravarty  
Journal of Chemical Physics, **118**, 10671-10682 (2003).
13. *Quasi-saddles of liquids: Computational study of a bulk Lennard-Jones system*  
Pooja Shah and Charusita Chakravarty  
Journal of Chemical Physics, **118**, 2342-2348 (2003).
14. *Bond orientational order in clusters*  
Charusita Chakravarty  
Molecular Physics, **100**, 3777-3780 (2002).
15. *Potential Energy Landscapes of Simple Liquids*  
Pooja Shah and Charusita Chakravarty  
Physical Review Letters, **88**, 255501-1 to 255501-4 (2002).
16. *Instantaneous Normal Mode Analysis of Morse Liquids*  
Pooja Shah and Charusita Chakravarty  
Journal of Chemical Physics, **116**, 10825-10832 (2002).
17. *Path Integral Simulations of Quantum Lennard-Jones Solids*  
Charusita Chakravarty  
Journal of Chemical Physics, **116**, 8938-8947 (2002).
18. *Diffusional behaviour of Simple Sorbates in Zeolites: Effect of Anisotropic Frameworks and Geometrical Correlations*  
Sudeshna Kar and Charusita Chakravarty  
Chemical Physics Letters, **352**, 294-300 (2002).
19. *Comparison of inherent, instantaneous and saddle configurations of the bulk Lennard-Jones system*  
Pooja Shah and Charusita Chakravarty  
Journal of Chemical Physics, **115**, 8784-8794 (2001).
20. *Diffusional anisotropy of simple sorbates in silicalite*  
Sudeshna Kar and Charusita Chakravarty  
Journal of Physical Chemistry A, **105**, 5785-5793 (2001).
21. *Computational evaluation of Henry's constants and isosteric heats of sorption for Lennard-Jones sorbates in Na-Y zeolite*  
Sudeshna Kar and Charusita Chakravarty  
Molecular Physics, **99**, 1517-1521 (2001).
22. *Structure and Melting of Morse Solids*  
Pooja Shah, Piyalee Chakraborty and Charusita Chakravarty  
Molecular Physics, **99**, 573-583 (2001).

23. *Landau free energy curves for melting of quantum solids*  
C. Chakravarty and R. M. Lynden-Bell  
Journal of Chemical Physics, **113**, 9239-9247 (2000).
24. *Instantaneous Normal Mode Analysis of the Levitation Effect in Zeolites*  
S. Kar and C. Chakravarty  
Journal of Physical Chemistry B, **104**, 709-715 (2000).
25. *Melting of Quantum Solids: Comparison of Observable and Centroid Properties*  
C. Chakravarty  
Special issue on 'Contemporary Theoretical Chemistry Research in India' edited by N. Sathyamurthy,  
Indian Journal of Chemistry, **39A**,207 (2000).
26. *Response to "Comment on 'A comparison of the efficiency of Fourier- and discrete time-path integral Monte Carlo' "* C. Chakravarty, M. C. Gordillo, D. M. Ceperley  
Journal of Chemical Physics, **111**, 7687 (1999).
27. *Dynamics of Rare Gases in Zeolites: Instantaneous Normal Mode Analysis*  
V. Mehra, R. Basra, M. Khanna and C. Chakravarty  
Journal of Physical Chemistry B, **103**, 2740-2748 (1999).
28. *Isothermal-Isobaric Ensemble Simulations of Melting in Quantum Solids*  
C. Chakravarty  
Physical Review B, **59**, 3590-3598 (1999).
29. *A Comparison of the Efficiency of Fourier- and Discrete Time- Path Integral Monte Carlo*  
C. Chakravarty, M. C. Gordillo, D. M. Ceperley  
Journal of Chemical Physics, **109**, 2123-2134 (1998).
30. *Ab initio Path Integral Monte Carlo Simulations of Isolated Systems: Application to Small Lithium Clusters*  
R. Weht, J. Kohanoff, D. A. Estrin and C. Chakravarty  
Journal of Chemical Physics, **108**, 8848-8858 (1998).
31. *Path Integral Monte Carlo Simulations of Atomic and Molecular Systems*  
C. Chakravarty  
International Reviews in Physical Chemistry, **16**, 421-444 (1997).
32. *Effects of three-body (Axilrod-Teller) forces on the classical and quantum behaviour of rare gas trimers*  
C. Chakravarty, R. J. Hinde, D. L. Leitner and D. J. Wales  
Physical Review E, **56**, 363-377 (1997)
33. *Instantaneous Normal Mode Spectra of Quantum Clusters*  
C. Chakravarty and R. Ramaswamy  
Journal of Chemical Physics, **106**, 5564-5568 (1997).
34. *Quantum Adsorbates: Path Integral Monte Carlo Simulations of Helium in Silicalite*  
C. Chakravarty  
Journal of Physical Chemistry, **100**, 1878-1883 (1997).
35. *Cluster Analogues of Binary Isotopic Mixtures: Path Integral Monte Carlo Simulations*  
C. Chakravarty  
Journal of Chemical Physics, **104**, 7223-7232 (1996).

36. *Quantum Delocalisation and Cluster Melting*  
C. Chakravarty  
Journal of Chemical Physics, **103**, 10663-10668 (1995).
37. *Structure of Binary Quantum Clusters*  
C. Chakravarty  
Physical Review Letters, **75**, 1727-1730 (1995).
38. *The kinetics of H<sub>2</sub> chemisorption: The role of transients*  
C. Chakravarty and H. Metiu  
Journal of Chemical Physics, **102**, 8643-8655 (1995).
39. *1/f Spectra in Finite Atomic Clusters*  
S. K. Nayak, R. Ramaswamy and C. Chakravarty  
Physical Review Letters, **74**, 4181-4184 (1995).
40. *Fourier path integral simulations of para-H<sub>2</sub> and ortho-D<sub>2</sub> clusters*  
C. Chakravarty  
Molecular Physics, **84**, 845-852 (1995).
41. *Quantum Monte Carlo Methods in Chemistry*  
C. Chakravarty  
Current Science, **69**, 739-746 (1995).
42. *The maximal Lyapunov exponent in small Atomic clusters*  
S. K. Nayak, R. Ramaswamy and C. Chakravarty  
Physical Review E, **51**, 3376-3380 (1995)
43. *Melting of Quantum Neon Clusters: Path Integral Monte Carlo Simulations*  
C. Chakravarty  
Journal of Chemical Physics, **102**, 956-962 (1995)
44. *Particle exchange in the Fourier Path-Integral Monte Carlo Technique*  
C. Chakravarty  
Journal of Chemical Physics, **99**, 8038-8043 (1993).
45. *Refinement of the OH ( $A^2\Sigma^+, v=0$ ) + Ar Intermolecular Potential Energy Surface*  
M. I. Lester, R. A. Loomis, L. C. Giancarlo, M. T. Berry, C. Chakravarty and D. C. Clary  
Journal of Chemical Physics, **98**, 9320-9334 (1993).
46. *Calculations on Vibrational Predissociation of Ar-OH( $A^2\Sigma^+$ )*  
C. Chakravarty, D. C. Clary, A. D. Esposti and H.-J. Werner  
Journal of Chemical Physics, **95**, 8149-8165 (1991).
47. *Stimulated Emission Pumping of van der Waals vibrations in the ground electronic state of OH-Ar*  
M. T. Berry, M. R. Brustein, M. I. Lester, C. Chakravarty and D. C. Clary  
Chemical Physics Letters, **178**, 301-310 (1991).
48. *Rovibrational Spectra of Open-Shell van der Waals Complexes: Ar-OH ( $X^2\Pi$ )*  
C. Chakravarty and D. C. Clary  
Journal of Chemical Physics, **94**, 4149-4160 (1991).

49. *Electronic Spectrum of Ar-OH: Effect of Isotopic Substitution and Temperature*  
C. Chakravarty and D. C. Clary  
Chemical Physics Letters, **173**, 541-550 (1990).
50. *Calculation of the Electronic Spectrum of Ar-OH*  
C. Chakravarty, D. C. Clary, A. D. Esposti and H.-J. Werner  
Journal of Chemical Physics, **93**, 3367-3378 (1990).
51. *Ion-dipole fragmentations*  
C. Chakravarty and D. C. Clary  
Molecular Physics, **67**, 1099-1115 (1989).
52. *Reactions of  $N^+$  and  $H_3^+$  with structural isomers of  $C_2H_2Cl_2$*   
C. Rebrion, J. B. Marquette, B. R. Rowe, C. Chakravarty, D. C. Clary, N. G. Adams and D. Smith  
Journal of Physical Chemistry, **92**, 6572-6574 (1988).

#### ARTICLES IN BOOKS/CONFERENCE PROCEEDINGS

1. *Characterization of Hydrogen Bonded Network Dynamics in Water and Aqueous Salt Solutions*  
Anirban Mudi and Charusita Chakravarty  
Proceedings of the DAE-BRNS Symposium on Theoretical Chemistry held in Bhaba Atomic Research Centre, Mumbai, India from 9-12 December 2004.
2. *Potential Energy Landscapes of Supercooled Liquids*  
Somendra Nath Chakraborty and Charusita Chakravarty  
Proceedings of the DAE-BRNS Symposium on Theoretical Chemistry held in Bhaba Atomic Research Centre, Mumbai, India from 9-12 December 2004.
3. *Multiple Time-scale Behaviour and Hydrogen Bond Dynamics in Methanol*  
Ruchi Sharma and Charusita Chakravarty  
Proceedings of the DAE-BRNS Symposium on Theoretical Chemistry to be held in Bhaba Atomic Research Centre, Mumbai, India from 9-12 December 2004.
4. *Diffusion of Simple Sorbates in Silicalite: Effect of Anisotropic Frameworks and Geometrical Correlations*  
Sudeshna Kar and Charusita Chakravarty  
published in the Proceedings of the 13th International Zeolite Conference to be held in Montpellier, France from 8-13 July 2001.
5. *Size Matters: The Chemistry and Physics of Small Clusters*  
C. Chakravarty and R. Ramaswamy  
Chemistry Education Review, **14**, 10-18 (1999).
6. *Quantum Adsorbates: Helium in Zeolites*  
C. Chakravarty and K. V. Thiruvengadaravi  
published in proceedings of the conference on "Frontiers in Materials Modelling and Design", 20-23 August '96, Kalpakkam (Springer-Verlag, 1997).
7. *Parallelisation Strategies for Monte Carlo Methods: A Computational Chemistry Application*  
A. Agarwal, P. Mehra and C. Chakravarty  
published in the proceedings of the International Conference on High Performance Computing '95, New Delhi from 27 December '95 to 30 December '95.

8. *Stimulated Emission Pumping as a Probe of the OH ( $X^2\Pi$ ) + Ar Intermolecular Potential Energy Surface*  
M. I. Lester, W. H. Green, C. Chakravarty and D. C. Clary  
in *Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping*, edited by H.-L. Dai and R. W. Field ( World Scientific, Singapore, 1993).
9. *Predictions of Spectra for van der Waals molecules*  
D. C. Clary, C. Chakravarty and A. R. Tiller  
in *Dynamics of Polyatomic van der Waals Complexes*, edited by N. Halberstadt and K. C. Janda (Plenum Press, New York, 1991).

#### PAPERS COMMUNICATED

- *Entropy, Diffusivity and Structural Order in Liquids with Water-like Anomalies*  
Ruchi Sharma, Somendra Nath Chakraborty and Charusita Chakravarty

#### PAPERS IN PREPARATION

- *Lindemann Measures for the Solid-Liquid Phase Transition*  
Charusita Chakravarty, Pablo G. Debenedetti and Frank H. Stillinger
- *Multiple Time-scale Behaviour and Hydrogen Bond Dynamics in Methanol*  
Ruchi Sharma and Charusita Chakravarty
- *Landscape-based Criteria for Freezing*  
Somendra Nath Chakraborty and Charusita Chakravarty

#### RESEARCH PROJECTS

- **Title:** *Theoretical and Computational Aspects of Condensed-Phase Chemical Dynamics*  
**Principal Investigator:** Charusita Chakravarty  
**Funding agency:** Department of Science and Technology  
**Amount:** Rs. 3,24,000.0      **Duration:** November 1992 - August 1993
- **Title:** *Quantum Monte Carlo Simulations of Clusters*  
**Principal Investigator:** Charusita Chakravarty  
**Funding agency:** Department of Science and Technology, Govt. of India  
**Amount:** Rs. 7,35,000.0      **Duration:** February 1996 - February 1999
- **Title:** *Low Temperature Adsorption in Porous Media: Quantum and Classical Simulations*  
**Principal Investigator:** Charusita Chakravarty  
**Funding Agency:** Indian National Science Academy  
**Amount:** Rs. 5,00,000.0      **Duration:** October 1997 - October 2000.
- **Title:** *High Resolution X-ray Powder Diffractometer*  
**Principal Investigators:** Drs. A. Ramanan and A. K. Ganguli  
**Co-investigators:** Drs. C. Chakravarty, D. K. Bandhopadhyay, N. Pant, A. K. Singh and R. Prasad, Profs. H. M. Chawla and A. S. Brar.  
**Funding Agency:** Department of Science and Technology, Govt. of India.  
**Amount:** Rs. 47,00,000.0      **Duration:** March 2000- March 2003.



- **Title:** *Simulation of Rotational-vibrational spectra of molecular clusters*  
**Principal Investigator:** Charusita Chakravarty  
**Funding Agency:** Council of Scientific and Industrial Research (CSIR).  
**Amount:** Rs. 4,35,000.0     **Duration:** May 2000 - May 2003.
- **Title:** *Computer Simulations of Solid-Liquid Phase Equilibria*  
**Principal Investigator:** Charusita Chakravarty  
**Funding Agency:** Department of Science and Technology (DST).  
**Amount:** Rs. 25,65,800.0     **Duration:** May 2002 - May 2005.
- **Title:** **Phase Transitions, Energy Landscapes and Computer Simulations**  
**Principal Investigator:** Charusita Chakravarty  
**Funding Agency:** Department of Science and Technology (DST) as part of the Swarnajayanti Fellowship Award  
**Amount:** Rs. 56,00,000.0     **Duration:** November 2005 - November 2010.

#### CONFERENCE PRESENTATIONS (2000-2005)

1. Participant, 93<sup>rd</sup> Statistical Mechanics Conference held at Rutgers University from 15 to 17 May 2005.
2. Contributed Talk, STATPHYS22: 22nd International Conference on Statistical Physics of the International Union of Pure and Applied Physics held at the Indian Institute of Science, Bangalore, India from 4 to 9 July 2004.
3. Invited Speaker, "Unifying Concepts in Glass Physics III" held at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India from 28 June to 1 July 2004.
4. Invited Speaker, "Atomistic Simulation: A Symposium in Honour of Ruth Lynden-Bell" held at Queen's University, Belfast, U.K. on 21 May 2004.
5. Invited Speaker, CECAM Workshop on "Metastability and Landscapes in Complex Systems" held at Lyon, France from 22 to 24 May 2003.
6. Invited Speaker, "India and Abroad-III: A Conference on Condensed Matter Physics" held at S.N. Bose National Centre for Basic Sciences, Kolkata from 2 to 4 January 2003.
7. Poster presentation, "Fifth Liquid Matter Conference" organised by the European Physical Society at Konstanz, Germany from 14 to 18 September 2002.
8. Invited Speaker, Conference on "Slow Dynamics and Glass Transition" held at Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India from 6 to 9 January 2002.
9. Poster presentation, SIMU ESF Workshop on "Bridging the Time Scale Gap" held at Konstantz, Germany from 10 to 13 September 2001
10. Invited Speaker, SERC School on Concepts in Chemical Dynamics, held in I.I.T-Madras from 5 to 24 March 2001.
11. Invited Speaker, TC2K: Discussion Meeting on Theoretical Chemistry, held in I.I.T-Kanpur from 22 to 24 December 2000.
12. Co-organiser, SERC School on Statistical Mechanics and Simulation Techniques to be held during February 6-26, 2000 at Indian Institute of Technology, Kanpur, India.

## PH.D. STUDENTS

1. Sudeshna Kar (1998-2001)  
Thesis Title: *Molecular Dynamics Studies of Simple Sorbates in Zeolites*
2. Pooja Shah (1999-2003)  
Thesis Title: *Potential Energy Landscapes and Properties of Simple Liquids* (1999-2003)
3. Anirban Mudi (2001-2006)  
Thesis Title: *Computational Studies of Hydrogen Bond Network Dynamics in Water*
4. Somendra Nath Chakravarty (2002-present)
5. Ruchi Sharma (2003-present)
6. Manish Agarwal (2005-present)

## SEMINARS

Princeton University, U.S.A.; Michigan State University, U.S.A.; Daresbury Laboratory, CCLRC, U.K.; Imperial College, London, U.K.; University of Cambridge, U.K.; Johannes Gutenberg Universität, Mainz, Germany; Indian Institute of Science, Bangalore; Indian Association for the Cultivation of Science, Calcutta; Jawaharlal Nehru University, New Delhi; International Centre for Theoretical Physics, Trieste; Tata Institute of Fundamental Research, Bombay; Queen's University of Belfast, Belfast, U. K.; University College, London, U.K.; Indian Institute of Technology-Kanpur; Panjab University, Chandigarh; University of Firenze, Firenze, Italy; National Chemical Laboratory, Pune.

## REFEREES

- **Prof. D. C. Clary,**  
President, Magdalen College, Oxford OX1 4AU, U.K.  
e-mail: david.clary@magd.ox.ac.uk
- **Prof. R. M. Lynden-Bell,**  
Leverhulme Emeritus Fellow, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.  
e-mail: rmlb@cam.ac.uk
- **Prof. P. G. Debenedetti**  
Department of Chemical Engineering, Engineering Quadrangle, Princeton University, Princeton, New Jersey, NJ 08544, U.S.A.  
e-mail: pdebene@princeton.edu