Curriculum Vitae of M. Krishnan

Name	M. Krishnan
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Date of Birth	17th January 1977
Nationality	Indian
Marital Status	Single

Educational Qualifications

Ph. D	Thesis entitled "Phase Behaviour of Linear Molecular Crystals in Bulk and on Graphite: A Molecular Dynamics Simulation Study" to be submitted in April, 2005 at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
M. Sc (Physics) (I class)	The American College, Madurai Kamaraj University, Madurai, Tamil Nadu, India, 1999
B. Sc (Physics) (I class)	Madurai Kamaraj University, Madurai, Tamil Nadu, India, 1997

Computational Skills

Platform	Linux, Unix, Windows
Programming Languages	Fortran 90, C
Visual Softwares	xmovie, Chimera, Molden, dmovie, gimp
Scientific Softwares	Mathematica, Scilab
Plotting Softwares	xmgr, xmgrace
Molecular Dynamics (MD)	PINY_MD (Developed by G.J. Martyna, and M.E. Tuckerman) FIST (Developed by K. Bagchi, S. Balasubramanian, C.J. Mundy, and M.L. Klein) NEMD (Developed by C.J. Mundy, S. Balasubramanian and M.L. Klein) Own codes
Systems	Experience in using IBM SP and Beowulf clusters

Awards and Scholarships

Graduate Aptitude Test in Engineering (GATE), India (1999)

Lecturership, Council of Scientific & Industrial Research, India (2000)

Senior Research Fellowship (SRF), Council of Scientific & Industrial Research, India (2003)

Teaching

I have been a tutor for a graduate course on computational methods at the department of physics, Indian Institute of Science, Bangalore.

Publications

Phase Behaviour of Ultrathin Crystalline n-Heptane films on Graphite: An Atomistic Simulation Study
M. Krishnan and S. Balasubramanian
Physical Chemistry Chemical Physics (2005) (In press)

Thermal evolution of Conformation, Structure, and Dynamics in crystalline poly(ethylene oxide)
M. Krishnan and S. Balasubramanian
Journal of Chemical Physics (2004) (Submitted)

n-Heptane under Pressure: Structure and Dynamics from Molecular Simulations
M. Krishnan and S. Balasubramanian
Journal of Physical Chemistry B, **109**, 1936 (2005) (Appeared with cover art)

Order-disorder transitions and melting in a helical polymer crystal: Molecular dynamics calculations of model poly(ethylene oxide)
M. Krishnan and S. Balasubramanian
Chemical Physics Letters, **385**, 351 (2004)

Structure of solid monolayers and multilayers of n-hexane on graphite
M. Krishnan and S. Balasubramanian, and S. Clarke
Proceedings of Indian Academy of Sciences (Chemical Sciences), **115**, 663 (2003)

Vibrational dynamics of solid poly(ethylene oxide)
M. Krishnan and S. Balasubramanian
Physical Review B, **68**, 064304-1, (2003)

An atomistic simulation study of a solid monolayer and trilayer of n-hexane on graphite
M. Krishnan, S. Balasubramanian, and S. Clarke
Journal of Chemical Physics, **118**, 5082 (2003)

Computer simulation study of water using a fluctuating charge model
M. Krishnan, A. Verma, and S. Balasubramanian
Proceedings of the Indian Academy of Sciences (Chemical Sciences), **113**, 579 (2001)

Software Development

Software	Purpose
NMA	This code was developed to understand the vibrational behaviour of macromolecular systems using Normal Mode Analysis. We have derived the analytical Hessian matrix arising out of complex macromolecular interactions. This code was written in a modular way using Fortran-90 and has subroutines to compare the forces and Hessian components evaluated analytically against their numerical counterparts. This code has successfully been used to characterize the vibrational properties of crystalline poly(ethylene oxide) and n-heptane.
FIST	This molecular dynamics code, originally developed by S. Balasubramanian, K. Bagchi, C.J. Mundy, and M.L. Klein, incorporates extended system methods. I have worked with Prof. S. Balasubramanian in the implementation of the fluctuating charge model in the recent version of this code.
MD codes	I have written few codes to familiarize with the following MD concepts: **NVE Ensemble:** The code I wrote can handle both atomic and macromolecular systems. The SHAKE and RATTLE algorithms have been implemented in this code to constrain the bond lengths and bend-angles to be fixed. **NVT Ensemble:** I have implemented both Nose-Hoover and Nose-Hoover Chains algorithms to perform constant temperature MD simulation of atomic liquids interacting via Lennard-Jones potential. **NPT Ensemble:** I am familiar with Anderson's algorithm (For isotropic cell fluctuations) and Parrinello-Rahman method (For fully-flexible simulation cell) to perform isothermal-isobaric simulations. **Energy Minimization methods:** I have written minimization codes to compare the performance of steepest descent, conjugate gradient and simulated annealing methods for a system of Lennard-Jones particles. **Other Algorithms :** Multiple Time Step algorithms (RESPA), Ewald summation, Liouville operator methods of deriving integrators. Also, I am familiar with the basic methodology of Car-Parrinello molecular dynamics.
MPI	I have written parallel codes using MPI for calculating Radial Distribution Function (RDF), Velocity Auto-Correlation Function (VACF), Rotational Time Correlation Function (RTCF) and Mean Square Displacement (MSD) of molecular systems.
MC codes	To perform phase equilibria analysis of a system of Lennard-Jones particles, I have written a Monte Carlo code which uses the Gibbs Ensemble technique.

Workshops and Conferences Attended

- International Conference on "**Structure and Dynamics in Complex Chemical Systems**", held at Indian Institute of Science, Bangalore, India (2001)-poster presentation
- School on "**Computational Techniques for the Condensed Matter**", held at Indian Insti-

tute of Science, Bangalore, India (2001)

- "**First Conference of Asian Consortium for Computational Materials Science (ACCMS-1)**", Bangalore, Indian Institute of Science, Bangalore, India (2001)-poster presentation
- **Annual In-House Symposium**, JNCASR, Bangalore (2001)-poster presentation
- "**India and Abroad: A Conference on Condensed Matter Physics**", Bangalore, India (2002)
- "**Slow Dynamics and Glass Transition**", Bangalore, India (2002)
- "**Workshop on Advanced Materials -II**", Bangalore, India (2002)
- **Annual In-House Symposium**, JNCASR, Bangalore (2001)-oral presentation
- "**India and Abroad III: A Conference on Condensed Matter Physics**", Kolkata, India (2003)-poster presentation
- "**Unified Concepts in Glass Physics III**", Bangalore, India (2004)
- Oral presentation at the **Solid State and Structural Chemistry Unit**, Indian Institute of Science, Bangalore (2004)
- "**22nd International Conference on Statistical Physics**", Indian Institute of Science, Bangalore (2004)
- "**Symposium on Theoretical Chemistry (TCS-2004)**", Bhabha Atomic Research Centre, Bombay, India (2004)-poster presentation

Future Research Interests

Modelling of proteins, biomembranes, ion channels, bio-inspired molecular nanoscience, enhanced conformational sampling techniques, Car-Parrinello molecular dynamics, physical and chemical properties of complex molecular systems, drug design, free energy methods.

Thesis Title

Phase Behaviour of Linear Molecular Crystals in Bulk and on Graphite: A Molecular Dynamics Simulation Study

Thesis Advisor

Prof. S. Balasubramanian
Chemistry & Physics of Materials Unit,
Jawaharlal Nehru Centre for Advanced Scientific Research,
Bangalore-560064, India

Thesis Synopsis

The thesis entitled "Phase Behaviour of Linear Molecular Crystals in Bulk and on Graphite: A Molecular Dynamics Simulation Study" presents the results of investigations on linear molecular crystals under varied conditions of temperature and pressure. Classical molecular dynamics (MD) simulations were employed to characterize the microscopic structure, energetics and the dynamics of these systems while vibrational properties were studied using normal mode analysis (NMA) and other methods.

The characteristic features of chain molecules and their properties in condensed phases are introduced in **Chapter 1** and the need to understand their phase behaviour is stressed. A comprehensive survey of earlier studies on molecular crystals is presented. This chapter ends with a detailed description of the method of our choice, the molecular dynamics technique.

Chapter 2 covers the results obtained from the isothermal-isobaric MD simulations on the thermal behaviour of crystalline poly(ethylene oxide) (PEO). The possibility of a new, solid phase of PEO has been explored. This phase has been characterized to be partially disordered with a loss of long-range, in-plane orientational correlations between molecules. Across the premelting transition, the PEO oligomers continue to be oriented along the c-axis of the crystal with the retention of short-range helical conformational order. Interesting dynamical changes across this transition resulting in sliding diffusion and helical oscillations have been studied.

Results on the vibrational properties of crystalline PEO explored using NMA and from the MD trajectory are provided in **Chapter 3**. An efficient method to obtain the elements of the Hessian matrix arising out of complex macromolecular interactions is provided. Visual analyses of atomic displacements and group theoretical methods were employed to assign the vibrational features to specific modes. The model predictions on the PEO vibrations compare well with experiment.

Chapter 4 presents a study on the high-pressure phases of crystalline n-heptane using isothermal-isobaric molecular dynamics simulations. Structural and conformational changes associated with the solid-liquid transition upon decompression and within the solid phase with increasing pressures have been explored. Although the solid-liquid transition has clear signatures such as the formation of gauche defects along the molecular backbone, the simulations do not show any sign for a solid-solid transition at high pressures. However, interesting changes in the environment around methyl groups and in their dynamics are observed. These have been substantiated by calculations of the vibrational density of states obtained from a normal mode analysis and from the simulation trajectory.

The coverage dependent structural changes exhibited by ultrathin films of n-hexane adsorbed on graphite have been investigated in **Chapter 5**. Employing simulations that do not impose any particular periodicity on the adsorbed layer, the results of the present investigations are compared to neutron diffraction experiments. A structural transition from a uniaxially incommensurate lattice to a fully commensurate structure, on increasing the coverage from a monolayer to trilayer was observed. Additional simulations that employ regular periodic boundary conditions have also been performed to confirm the results.

Chapter 6 provides the outcome of investigations on the thermal behaviour of ultrathin n-heptane films physisorbed on graphite using constant temperature MD simulations. An uniaxially commensurate monolayer (UCM), an uniaxially commensurate bilayer (UCB) and a fully commensurate bilayer (FCB) of n-heptane have been studied in order to distinguish the contributions from coverage and in-plane density to the process of melting. The calculated intermolecular energy per molecule shows that the FCB structure is more stable than the UCB structure, consistent with x-ray and neutron scattering experiments. In all these systems, disordering processes in the solid state involves a fraction of molecules rotating about their backbone axes, in agreement with scanning tunneling microscopy studies. The molecules present in uniaxially commensurate structures (UCM and UCB) were found to be facile to rotate about their long axes, causing these adlayers to melt at lower temperatures compared to the fully commensurate structure. The importance of conformational defects for the melting of these quasi-two dimensional systems has also been explored.

References

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