

Curriculum Vitae

Pooja Shah, Ph.D.

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Summary

- Extensive programming and analytical skills
- Expertise in statistical modeling techniques
- SAS Basic Programmer certified
- Research career involved computer simulations at molecular and atomistic level
- Rich experience of interdisciplinary research involving interactions with chemists, chemical engineers, mathematicians, physicists and computer scientists
- Research work has been extensively published in peer reviewed international journals

Education

- PhD, Chemistry, Indian Institute of Technology (Delhi), India, 2003
- MS, Chemistry, Indian Institute of Technology (Delhi), India, 1999
- BS, Chemistry (Honors), Delhi University, Delhi, India, 1997

Professional Appointments

- Postdoctoral fellow, Dept. of Chem. Engg., University of Texas, Austin TX, 2003-2005
- Graduate research fellow, Dept. of Chemistry, IIT, Delhi, India, 1999-2003

Honors/Awards

- Senior research fellowship, Council of scientific and industrial research (CSIR), 2001-2003
- Junior research fellowship, Council of scientific and industrial research (CSIR), 1999-2001
- Dr. Khurana memorial award, Gargi College, Delhi University, 1996
- Awarded "Certificate of Merit" for highest GPA in Gargi College, Delhi University, 1995-1997
- Awarded "Certificate of Merit" for second highest GPA in Delhi University, 1995-1997

Leadership Positions

- Student council member, Ladies Hostel, IIT-Delhi (2001)
- Student representative, Chemical Society, Department of Chemistry, IIT-Delhi (2000-2001)
- Head Girl of Carmel Convent School (1992-1993)

Education

- PhD, Chemistry, Indian Institute of Technology (Delhi), India, 2003
Thesis title: "Potential energy landscapes and properties of simple liquids"
Advisor: Dr. Charusita Chakravarty (Professor)
- MS, Chemistry, Indian Institute of Technology (Delhi), India, 1999
Thesis title: "Synthesis of mixed valent polyoxovanadates"
Advisor: Dr. A. Ramanan (Professor)

Professional Appointments

- Postdoctoral fellow, University of Texas, Austin TX, 2003-2005 Advisor: Dr. Thomas M. Truskett

- Developed analytical model to predict protein stability and provide new insights into the mechanisms for pressure denaturation.
 - Explored intrinsic stability limits for ultrathin films using molecular simulations.
 - Constructed a landscape based theory for predicting the mechanical and thermal properties of thin films, including their vulnerability to failure.
- Graduate research fellow, Indian Institute of Technology, Delhi, India, 1999-2003
Advisor: Dr. Charusita Chakravarty
 - Explored the connection between the topography of the potential energy surface and properties of simple liquids.
 - Compared trends in melting behavior of bulk liquids and clusters with range of the interaction.
 - Proposed a convenient and interesting model to study properties of glasses.
- Research assistant, Indian Institute of Technology, Delhi, India, 1997-1999 Advisor: Dr. A. Ramanan
 - Synthesized, analyzed, and characterized mixed valent polyoxovanadates with layered structures.

Refereed Publications

1. J. Cheung, P. Shah, and T.M. Truskett, Hetero-polymer collapse theory for protein folding in the pressure-temperature plane, *Biophysical Journal* 91, 2427 (2006)
2. P. Shah and T.M. Truskett, Intrinsic vulnerabilities to mechanical failure in nanoscale films, *Mechanics of Material* 38, 924 (2006)
3. J. Mittal, P. Shah, and T. M. Truskett, Using energy landscapes to predict thin film properties, *J. Phys. Chem. B* 108, 19769 (2004).
4. S. Chakraborty, N. Ghosh, P. Shah, and C. Chakravarty, Melting point of Morse liquids using free energy methods, *Mol. Phys.* 102, 909 (2004).
5. P. Shah, S. Roy, and C. Chakravarty, Melting of 55-atom Morse clusters, *J. Chem. Phys.* 118, 10671 (2003)
6. P. Shah and C. Chakravarty, Quasi-saddles of liquids: Computational study of a bulk Lennard-Jones system, *J. Chem. Phys.* 118, 2342 (2003)
7. P. Shah and C. Chakravarty, Potential energy landscapes of simple liquids, *Phys. Rev. Lett.* 88, 255501-1 (2002)
8. P. Shah and C. Chakravarty, Instantaneous normal mode analysis of Morse liquids, *J. Chem. Phys.* 116, 10825 (2002)
9. P. Shah and C. Chakravarty, Comparison of inherent, instantaneous and saddle configurations of the bulk Lennard-Jones system, *J. Chem. Phys.* 115, 8784 (2001)
10. P. Shah, P. Chakrabarti, and C. Chakravarty, Structure and melting of Morse solids, *Mol. Phys.* 99, 573 (2001)

Talks/Conferences

- Pressure denaturation of proteins in water: Revisiting a Heteropolymer collapse model, 2004 Annual AIChE Meeting, Austin, Texas
- Intrinsic stability limits for glassy nanoscale films: Insights from the energy landscape, 2004 Annual AIChE Meeting, Austin, Texas
- An energy landscape based approach for studying supercooled liquid and glassy thin films, 2004 American Physical Society March Meeting, Montreal, Canada.

- Computational techniques for condensed matter, Jawahar Lal Nehru center for advanced scientific research, 2001
- SERC School on statistical mechanics and simulation techniques, IIT-Kanpur, 2000

Posters

- T.M. Truskett, J. Mittal, P. Shah, and V. Ganesan, Energy landscape perspectives for the properties of thin films, Tenth international conference on properties and phase equilibria for product and process design, Snowbird, Utah
- P. Shah and T. M. Truskett, An energy landscape based approach to study ultra thin films, NanoNight 2004, Center for nano- and molecular science and technology, University of Texas at Austin
- P. Shah and C. Chakravarty, Potential energy landscape of simple liquids, Fourth national symposium in chemistry, National Chemical Laboratory, India
- P. Shah and C. Chakravarty, Variations in melting behavior with range of potential, Theoretical chemistry meet (TC2K), IIT-Kanpur, India
- P. Shah and C. Chakravarty, Variations in melting behavior with range of potential, Science day, IIT-Delhi, India