Curriculum Vitae

Ronald Benjamin

UGC-FRP Assistant Professor,
Department of Physics,
Cochin University of Science and Technology,
Cochin University P.O.,
Cochin 682022,
Kerala, India.

Nationality: `Indian`
Phone: 91-9040000584
Email: `rbenjamin.phys@gmail.com`

Employment & Education

- **UGC-FRP Assistant Professor,** (February 2018 - Till date)
  Department of Physics,
  Cochin University P.O.,
  Cochin University of Science and Technology — Cochin, Kerala, India

- **Senior Postdoctoral Fellow,** (January 2017 - February 2018)
  TIFR Center for Insterdisciplinary Sciences — Hyderabad, India

- **Guest Scientist** (April 2016 - December 2016)
  Institute of Theoretical Physics II - Soft Matter,
  Heinrich Heine University — Duesseldorf, Germany

- **Postdoctoral Fellow** (November 2011 - March 2016)
  Institute of Theoretical Physics II - Soft Matter,
  Heinrich Heine University — Duesseldorf, Germany

- **DAAD Postdoctoral Fellow** (August 2009 - October 2011)
  Institute of Material Physics in Space,
  DLR (German Aerospace Center) — Cologne, Germany

- **Postdoctoral Fellow** (March 2009 - August 2009)
  Department of Chemical and Biological Engineering,
  University of Colorado at Boulder — Boulder, CO, USA

- **Phd in Physics** - 2008
  Outstanding Graduate Student Award
  Advanced Graduate Trainee (2005 - 2008)
  Department of Physics
  University of Alabama at Birmingham — Birmingham, AL, USA

- **MS Physics** 2005
  Graduate Student & Teaching Assistant (2003-2005)
  Department of Physics
  University of Oregon at Eugene Eugene, OR, USA

- **Diploma in Advanced Physics** (M.Phil Degree), 2002
  Research Scholar (2001-2003)
  Institute of Physics Bhubaneswar, Odisha, India

- **MSc Physics, 2001 (75%, 3^{rd} Rank in University)**
  MSc student (1999-2001)
  Department of Physics
  Utkal University, Vani Vihar Bhubaneswar, Odisha, India

- **BSc Physics (First Class Hons. with Distinction), 1999**
  (82.3%, 2^{nd} Rank in entire State)
  Awarded National Scholarship (1999-2001)
  Department of Physics
  Utkal University, Vani Vihar Bhubaneswar, Odisha, India
  B.Sc Student (1996-1999)

- **+2 Science (Higher Secondary Exam), 1996 (74%)**
  Awarded Senior College Merit Scholarship (1996-1999)
  Period of Study (1994-1996)
  B.J.B. College Bhubaneswar, Odisha, India
  Council of Higher Secondary Education Bhubaneswar, Odisha, India

- **ICSE Class 10th Exam (85.16%), 1994**
  Period of Schooling (1984-1994)
  Stewart School Bhubaneswar, Odisha, India
  The Council for Indian Certificate of Secondary Education New Delhi, India

Research Interest

Theoretical and Computational Condensed Matter Physics (Statistical Mechanics, Soft Matter, Theory and Simulations, Theoretical Physical Chemistry):

- Soft Matter Theory and Simulations
  - Nucleation and crystallization phenomena
  - Free-energy calculations
    - Computing interfacial free energies between different phases and absolute free energies of condensed phases using techniques such as *Thermodynamic integration, Metadynamics, Umbrella Sampling etc.*
    - Determination of Homogeneous and Heterogeneous nucleation free energy barriers of various monoatomic as well as binary systems.
  - Wetting behavior of solid-liquid and solid-solid interfaces.

  - Computing Phase diagrams of single and two-component systems using Monte Carlo and Molecular Dynamics Simulations

- Non-Equilibrium Statistical Mechanics and Thermodynamics
  - Kinetics and Thermodynamics of Brownian motors.
  - Non-Equilibrium Fluctuation theorems pertaining to work, heat and entropy in thermodynamic processes.
  - Stochastic phenomena in physical systems

Teaching Interests

Classical Mechanics; Thermodynamics; Statistical Mechanics; Electricity and Magnetism; Mathematical Methods; Quantum Mechanics; Numerical Methods; Computational Physics; Soft Matter Theory and simulation; Physical Chemistry.

Courses Taught

PostGraduate: Classical Mechanics, Mathematical Methods, Computational Physics
PhD: Research Methodology and Quantitative Techniques (Error Analysis Module)

Publications

h-index=8, i10-index=7 (From Google Scholar)

1.) *Diffusion and transport coherence of a Brownian particle driven by non-uniform temperature and subject to a piece-wise linear potential.*-**Ronald Benjamin** (to be submitted to PRE) [Paper presented at the DPG March 2012 meeting in Berlin, Germany].

2.) *Free energy cost of forming an interface between a crystal and its frozen version* -**Ronald Benjamin** and Juergen Horbach, Physical Review E **92**, 042408 (2015) .

3.) *Crystal growth kinetics in Lennard-Jones and Weeks-Chandler-Andersen systems along the solid-liquid coexistence line* -**Ronald Benjamin** and Juergen Horbach, J. Chem. Phys. **143**, 014702 (2015) .

4.) *Crystal-liquid interfacial free energy of hard spheres via novel thermodynamic integration scheme* - **Ronald Benjamin** and Juergen Horbach, Phys. Rev. E **91**, 032410 (2015) .

5.) *Excess free energy of supercooled liquids at disordered walls.*-**Ronald Benjamin** and Juergen Horbach, Phys. Rev. E **90**, 060101, [Rapid Communications] (2014).

6.) *Crystal-liquid interfacial free energy via thermodynamic integration.*- **Ronald Benjamin** and Juergen Horbach, J. Chem. Phys. **141**, 044715 (2014) .

7.) *Nucleation Barriers for the Liquid-to-crystal Transition in Simple Metals: Experiment vs. Simulation.*-J. Bokeloh, G. Wilde, R. E. Rozas, **Ronald Benjamin** and Juergen Horbach. European Physical Journal Special Topics **223**, 511 (2014).

8.) *Stochastic energetics of a Brownian motor and refrigerator driven by non-uniform temperature* - **Ronald Benjamin**. International Journal of Modern Physics B **28** , 1450055 (2014) .

9.) *Lennard-Jones systems near solid walls: Computing interfacial free energies from molecular simulation methods.*-**Ronald Benjamin** and Juergen Horbach. J. Chem. Phys. **139**, 084705 (2013) .

10.) *Wall-liquid and wall-crystal interfacial free energies via thermodynamic integration: A molecular dynamics simulation study.*-**Ronald Benjamin** and Juergen Horbach. J. Chem. Phys. **137**, 044707 (2012) .

11.) *Inertial Effects in Büttiker-Landauer Motor and Refrigerator at the Overdamped Limit.*-**Ronald Benjamin** and Ryoichi Kawai. Physical Review E, **77**, 051132 (2008) .

12.) *On and Off Membrane Dynamics of the ER-Golgi Tethering Factor p115 In Vivo.*- Elizabeth Brandon, Tomasz Szul, Cecilia Alvarez, Robert Grabski, **Ronald Benjamin**, Ryoichi Kawai, and Elizabeth Sztul, Molecular Biology of the Cell, Vol. 17, 2996 (2006) .

Manuscripts in preparation

1.) *Heat and entropy fluctuations in the Büttiker-Landauer Motor* -**Ronald Benjamin** [Paper presented at the DPG March 2012 meeting in Berlin, Germany].

2.) *Molecular dynamics simulation of the θ phase of Al-Cu alloy in molten and crystalline form*-**Ronald Benjamin** and Juergen Horbach [Paper presented at ANPHASES meeting in Haus der Universitaet, January 11, 2016].

3.) *Lennard-Jones crystal droplet in contact with a wall: Contact angle and heterogeneous nucleation*-**Ronald Benjamin** and Juergen Horbach.

4.) *Crystal-liquid interfacial free energy near fluid-fluid metastable critical point*- **Ronald Benjamin and Surajit Sengupta** [Paper presented at COMPLU 2017 meeting].

5.) *Free energy at glass-glass interfaces*- **Ronald Benjamin et al.**

Professional Service

Invited Journal Referee for Journal of Chemical Physics, Journal of Applied Physics, Journal of Statistical Physics, Acta Materialia, Computational Materials Science

Research Grants obtained

UGC Start-Up Grant worth Rs. 10 Lakh.

Academic Awards, Achievements and Honours

1.) Awarded the **"Outstanding Doctoral Student in Physics"** Award (2008) by the University of Alabama at Birmingham, USA.

2.) Awarded the prestigious **GAFP (Graduate Assistantship Fellowship Program)** Fellowship of University of Alabama at Birmingham from 2005-2008 for conducting research in the field of Non-Equilibrium Statistical Mechanics.

3.) **Earlier Selections as a Graduate Student with Fellowship** - i) **University of Southern California, LA, USA**, ii) **Tata Institute of Fundamental Research, Bombay, India**, iii.)Ohio University, Athens, USA, iv.)Montana State University, Bozeman, USA.,v)Wesleyan University, Middletown , Connecticut, USA.

4.) Got First position in the MSc Physics Entrance Exams, 1999, of Utkal University, Odisha, India and Ravenshaw College, Cuttack, India.

5.) **GATE- 2001 (Physics)** 99.46 percentile score. All India Rank- 10th out of approximately 20000 students (This is a national level test conducted by the Ministry of Human Resources Development, Government of India for fellowships to do Ph. D and M. Tech courses at the Indian Institutes of Technology and Indian Institute of Science, Bangalore.)

6.) **Qualified as UGC JRF&L, CSIR-UGC Exam of Govt. Of India** (I qualified this exam three times in December 2000, June 2001 and June 2002) - This is a national level eligibility test conducted by the Council of Scientific and Industrial Research under the Government of India, qualifying which is mandatory for being appointed for lecturership/professorship at any public university or Institute in India.

7.) **Ranked 1st in JEST 2001 (Joint Entrance Screening Test - 2001)** in entire State of Odisha (All India rank - 34). JEST is the entrance test to select students for Ph.d. positions in the various Research Institutes of India.

8.) Government of India post-graduate National scholarship (1999-2001) for obtaining 2nd Rank in the BSc Physics Honours Exam in entire State of Odisha.

9.) Senior college merit scholarship (1996-1999) for meritorious performance in the +2 Higher Secondary Exam, Odisha.

10.) **APS Travel Award** for three consecutive years for making oral presentations at SESAPS 2006 (Williamsburg, Virginia, USA), SESAPS 2007 (Nashville, Tennessee, USA) and SESAPS 2008 (Rayleigh, North Carolina, USA) (SESAPS-South Eastern Section of American Physical Society).

11.) **APS Travel Award** for making oral and poster presentations at APS March 2008 meeting in New Orleans, Louisiana, USA (APS-American Physical Society).

12.) Selected as a participant in the PHYSBIO 2006 Meeting held in St. Ettiene, France. This is a prestigious scientific workshop for training graduate students and postdocs in the Physics of stochastic processes.

13.) Awarded the prestigious **DAAD Scholarship** to pursue postdoctoral Research in Germany for two years at the Institute for Materials Physics in Space at the German Aerospace Center (DLR), Germany. The research involved investigating crystal growth and nucleation phenomena via molecular dynamics simulations.

14.) **Invited** to present a talk at SITGES XX11 Conference on "Energy Conversion: From nanomachines to Renewable Sources", in Sitges, Barcelona, Spain (June 2010).

15.) **Awarded Postdoctoral Fellowships at** (i)the University of Idaho, in Boise, Idaho, USA, (ii)Department of Applied Physics, Aalto university, Finland, (iii)**Indian Institute of Science, Bangalore, India**, (iv) Department of Physics, Nanyang Technological University, Singapore, (v)SN Bose National Center for Basic Sciences, Calcutta, West Bengal, India and (vi) Institute of Mathematical Sciences, Madras (India) (As I had committed myself to a postdoctoral position awarded by DAAD at DLR, I had to turn down these offers).

16.) **Awarded Graduate Student Travel Award** from University of Alabama at Birmingham, USA, to attend American Physical Society Conferences.

17.) Selected as Assistant Professor under UGC-FRP Programme (4th Batch, 2015).

Invited Talks at various Conferences and Seminars

1.) "Crystal-liquid interfacial free energy via thermodynamic integration"-April 15, 2014, Physics of Soft and Biological Matter, Homerton College, **Cambridge University**, Cambridge, UK.

2.) "Wall-liquid and wall-crystal interfacial free energies via thermodynamic integration: A molecular dynamics simulation study"- November 30, 2012, **CompPhys 2012, Leipzig, Germany**.

3.) "Stochastic energetics of the Büttiker-Landauer motor and refrigerator"- UAB (University of Alabama at Birmingham, USA) Physics Department Colloquium, August 22nd 2008.

4.) Invited Talk on "Molecular Simulation Study of the Solid-Liquid Phase Transition"- IIT BHU (Benares Hindu University), May 04th 2016.

5.) Invited Talk on "Investigating Statistical Mechanics problems via Molecular Simulations" - ICTS, Bangalore, 08th June, 2016.

6.) Invited Talk on "Molecular Simulation Study of the Thermodynamics of Buettiker-Landauer Brownian Motor" - Institute of Physics, Bhubaneswar, 04th July, 2016.

7.) Invited Talk on "Investigating Statistical Mechanics problems via Molecular Simulations" - Department of Physics, IIT Hyderabad, 21st July, 2016

8.) Invited Talk on "Investigating solids and liquids at interfaces via novel Molecular Simulation Techniques" - Department of Chemical Engineering, IIT Bombay, 28th July, 2016.

9.) Invited Talk at Department of Physics, IIT Patna, 17th August, 2016.

10.) Invited Talk at School of Basic Sciences, IIT Bhubaneswar, 01st September, 2016.

11.) Theoretical Physics Seminar Circuit (TPSC) talk at SN Bose National Center for Basic Sciences (Calcutta), 19th September, 2016.

12.) Invited Talk at School of Physics, IIT Indore, 21st September, 2016.

13.) TPSC Talk at Department of Physics, University of Pune, 24th September, 2016.

14.) Invited Talk at IMSC, Chennai, India, 19th October 2016.

15.) Invited Talk at TIFR, Hyderabad, India, 28th October 2016.

16.) Invited Talk at IIT Kharagpur, India, 10th November 2016.

17.) Invited Talk at IIT Gandhinar, India, 01st February 2017

18.) Invited Talk at BIT, Mesra, Ranchi, India, 25th March 2017.

19.) Invited Talk at Thapar University, Punjab, India, 21 June 2017.

Contributed Talks and Presentations at various Conferences and Seminars

1.) "Physics of Brownian ratchets." - Talk presented at SERC School on the Physics of Disordered Systems, April 2003, Institute of Mathematical Sciences, Chennai (Madras), India.

2.) Talk on "Modeling viscous incompressible flow in fluid dynamics" at University of Oregon, Eugene, Physics Department, Nov 2nd 2004.

3.) Talk on "Energetics and transport coherence of a Brownian heat engine in the underdamped regime"- SESAPS 2006 meeting in Williamsburg, Virginia, USA.

4.) Talk on "Study of a microscopic heat engine"- Feb 2007, Graduate Student Research Day at University of Alabama at Birmingham (Sponsored by **Sigma-Xi Research Society**).

5.) Talk on "Molecular Dynamics Simulation of a Büttiker-Landauer Refrigerator"- March **APS 2007** meeting held in Denver, Colorado, USA.

6.) Talk on "Molecular Dynamics Simulation of a Büttiker-Landauer ratchet"- SESAPS 2007 meeting in Nashville, Tennessee, USA.

7.) Talk on "Failure of overdamped models for Büttiker-Landauer Heat Engine" - March **APS 2008** meeting in New Orleans, Louisiana, USA.

8.) Poster on "Energetics and transport coherence of a Büttiker-Landauer heat engine"- March **APS 2007** meeting in Denver, Colorado, USA.

9.) Poster on "Energetics and transport coherence of a shifting-ratchet"- SESAPS 2007 meeting in Nashville, Tennessee.

10.) Poster on "Efficiency optimization of a Büttiker-Landauer Heat Engine and refrigerator"- March **APS 2008** meeting in New Orleans, Louisiana, USA.

11.) Talk on “Can a Brownian Motor reach Carnot efficiency?”- Feb 2008, Graduate Student Research Day at University of Alabama at Birmingham (Sponsored by **Sigma-Xi Research Society**).

12.) Talk on “Study of a Brownian heat engine”- March 2008, Annual Meeting of the Alabama Academy of Sciences at Samford University in Birmingham, Alabama, USA.

13.) Talk on “Stochastic energetics of a Brownian motor driven by position-dependent temperature"- SESAPS 2008 meeting in Raleigh, North Carolina, USA.

14.) Poster on “Energetics, coherent transport and work fluctuations of a Brownian particle driven by time dependent temperature" - SESAPS 2008 meeting in Raleigh, North Carolina, USA.

15.) Web talk on “Stochastic energetics of a Brownian motor and refrigerator driven by inhomogeneous temperature"- August 18 2009, Raman Research Institute, Bangalore, India.

16.) Talk on “Stochastic energetics of the Büttiker-Landauer Brownian Motor and Refrigerator"-March 16 2011, **DPG (German Physical Society) 2011** Meeting in Dresden, Germany.

17.) Poster on “Wall-fluid interfacial tensions via thermodynamic integration: a molecular dynamics simulation study"-September 6-10, 2011 **Liquid Matter Conference Vienna, Austria**.

18.) Talk and Poster on “Wall fluid interfacial tension via thermodynamic integration: A molecular dynamics simulation study"- September 28- 2011, SIMBIOMA 2011 in University of Konstanz, Germany.

19.) Talk on “Wall-liquid and wall-crystal interfacial excess free energies via thermodynamic integration: A molecular dynamics simulation study"-March 27, 2012, **DPG 2012** Meeting in Berlin, Germany.

20.) Talk on “Thermodynamics, fluctuation relations and transport in presence of state-dependent diffusion"-March 29, 2012, **DPG 2012** Meeting in Berlin Germany.

21.) Poster on “Wall-liquid and wall-crystal interfacial free energies via thermodynamic integration: A molecular dynamics simulation study."-19-21 September 2012, Statistical Mechanics: Interplay of Theory and Computer Simulations meeting in Johannes Gutenberg University, Mainz.

22.) Talk on “Wall-Liquid and Wall-crystal interfacial free energies via thermodynamic integration: A Molecular Dynamic simulation study."- September 24, 2012 in 10th International Symposium on crystallization in glasses and liquids in Goslar, Germany organized by TU Clausthal.

23.) Poster and talk on “Determination of partial wetting conditions for a Lennard Jones crystal in contact with a solid wall: A molecular dynamics study."-February 1-5 2013, Workshop and Tutorial on “SIMULATING ACTIVATED PROCESSES IN PHYSICS AND CHEMISTRY: THEORETICAL FOUNDATIONS" in Villars, Switzerland.

24.) Talk on “Excess free energy of supercooled liquids at disordered walls."-March 12, 2013 in **DPG 2013** Conference in Regensburg, Germany.

25.) Talk on “Lennard Jones systems near solid walls- A molecular dynamics simulation study"-July 15-19, 2013, SPP 2013 Meeting in Frankfurt, Germany.

26.) Talk on “Molecular simulation methods to compute interfacial free energies"-April 01, 2014, **DPG 2014** Meeting in Dresden, Germany.

27.) Talk on “Free energy cost of forming a solid-liquid interface"-March 2015, **DPG 2015** Meeting in Berlin, Germany.

28.) Talk on “Computing Crystal-Liquid interfacial free energies via Molecular Dynamics simulations"-December 2017, COMPFLU 2017 Meeting at IIT Madras, Chennai, India.

Memberships in Scientific Organizations

1.) Americal Physical Society.

2.) Alabama Academy of Sciences.

3.) German Physical Society (Deutsche Physikalische Gesselschaft).

Computer Skills

Software, Languages and Programming:
LaTeX, Shell scripting, Fortran 90, and 77, Molecular Dynamics Simulation, Open Office presentation, MPI, VMD (visualization software), Maple, Gnuplot, Xmgrace, Makefile, xemacs, vim, pico and kate text editors, queuing scripts on supercomputing clusters.
Operating Systems:
Windows 10/8/XP/Vista, Linux and Unix.

Referees

1.) Prof. Juergen Horbach,
Theoretical Physics II- Soft Matter,
Heinrich Heine University,
40225 Duesseldorf, Germany.
Tel: 0049 (211) 81-13699
Fax: 0049 (211) 81-10775
Email: `horbach@thphy.uni-duesseldorf.de`

2.) Prof. Ryoichi Kawai,
Department of Physics,
University of Alabama at Birmingham, USA.
Tel: 001 (205) 934-3931
Fax: 001 (205) 934-8042
Email: `kawai@uab.edu`

3.) Prof. Renato Camata,
Department of Physics,
University of Alabama at Birmingham, USA.
Tel: 001 (205) 934-8143
Fax: 001 (205) 934-8042
Email: `camata@uab.edu`

TEACHING STATEMENT

As a faculty at my Present Institute and prior to that as a postdoctoral scholar as well as a PhD student, I had numerous opportunities both official and informal in teaching many undergraduate and graduate students different Physics courses as well as topics pertaining to my research. During my tenure as an Assistant Professor I have taught Classical Mechanics, Mathematical Methods, Computational Physics and a module of the Research Methodology Course. During my postdoctoral research career, I have devised projects for a Computational Physics Course as well advised many undergraduate and graduate students regarding various topics on the physics of stochastic processes, computational methods and soft matter Physics.

During my PhD years at the University of Alabama at Birmingham, USA, I conducted several tutorial sessions helping Undergraduate level Physics students to solve Homework and Exam problems based **on a Classical Mechanics course and an Introductory Physics with Calculus Course**. As a Graduate Teaching Assistant at the University of Oregon, Eugene, USA, I had the opportunity to teach various Tutorial Classes and conduct help sessions for Undergraduate Physics students taking Calculus-based **Introductory Physics Courses** (at the level of Halliday-Resnick). I also taught the Lab version of this Introductory Physics Course. While preparing for the tutorial and Lab sessions, I was able to refresh my knowledge and obtain a deeper conceptual understanding of fundamental Physics. Interacting with students also helped me understand their learning problems and also honed by teaching skills such that at the end of two years of teaching I was able to reach out to the weakest students and help them to develop with their problem-solving skills and make them understand the basic concepts.

Based on my research interests and past teaching experience, I would be interested in teaching most Undergraduate Physics/Chemistry/Chemical Engineering Courses at your Institute as well as the core post-graduate courses. I am a theoretical Physicist and would prefer to teach theory courses, nevertheless, I would also be willing to teach undergraduate Physics Lab Courses. The Courses I would most like to teach are **Classical Mechanics, Heat & Thermodynamics, Electricity & Magnetism or Electrodynamics, Modern Physics, Quantum Mechanics, Quantum Chemistry, Statistical Mechanics, Chemical Thermodynamics, Mathematical Methods, Numerical Methods and Computational Physics**. Since my research involves topics related to Phase transitions, nucleation and surface phenomena, I would be very much interested in teaching a **Physical Chemistry course** as well as an advanced **course on Soft Matter Theory and Simulations**. I would also like to offer a **course on Molecular Simulations**, where various molecular simulations technique such as Monte Carlo and Molecular Dynamics are taught. The Soft Matter and Molecular Simulations course, would benefit students from various Science as well as Engineering disciplines. In addition to these courses, I would be also interested in teaching a **course on Non-Equilibrium Statistical Mechanics** with an emphasis on Stochastic processes and phase transitions.

I believe research and teaching go hand in hand and one of the ways to enhance the learning experience of students is to incorporate simple problems arising out of my research into the course-work so that they gain the knowledge and experience of solving a real world problem as well. This will also provide them with an impetus to try a research career if they are so inclined. Another novel teaching effort by me would be to integrate computational projects into the various courses that I teach, to help the students develop a deeper understanding of their problem and also help them in their pursuit of a career even beyond science and engineering, if they so desire. Through my mentoring of undergraduate and graduate students, I find teaching to be a rewarding experience and stimulating young minds to think creatively also benefits my research activity when they ask novel questions and find interesting and new ways of looking at a problem. My passion for my research and interest in teaching motivate me to pursue a academic career in your esteemed Institute.

STATEMENT OF RESEARCH INTERESTS

My research interests can be broadly classified under the field of Non-Equilibrium Statistical Mechanics and Thermodynamics and Soft Matter Theory and simulations, carried out using theoretical and computational approaches. I focus on: (1) studying nucleation, crystal growth and wetting phenomena involving condensed phases and, (2) investigating problems in non-equilibrium statistical mechanics and thermodynamics such as the physics of molecular motors and the recently derived fluctuation relations of thermodynamic variables like work, heat and entropy, using a combination of molecular simulations and analytical approaches based on the Fokker-Planck and Langevin equations.

In the following two sections, I describe the importance of these studies, my past and current research during my Doctoral and Post-Doctoral career pertaining to the investigating of such problems and my ***future research plans (indicated in italics)*** corresponding to each area of interest.

1.)Nucleation, crystal growth and wetting phenomena.

Nucleation and growth of a crystal from the melt is a phenomena of primary importance in many industrial and natural processes[1]. Understanding nucleation and crystallization processes is crucial to understanding the liquid-to-solid or the vapor-to-liquid phase transition. While considerable progress, both theoretical and experimental, has been made in understanding the vapor-to-liquid transition, nucleation and growth of a crystal from its co-existing liquid phase still remains a challenging problem for both theorists and experimentalists though in the past several years computer simulations have helped us obtain some insights on this problem. Till date, most theoretical understanding of nucleation processes comes from the classical nucleation theory[2] derived for macroscopic systems. However, understanding of crystal nucleation at a molecular level is still at a preliminary level. One of the major goals of statistical mechanics is to understand the microscopic behavior of such condensed-phase systems and their relationship with the macroscopic properties. As such atomistic simulations play a major role in investigating such processes at a molecular level.

Nucleation is the first step in the eventual formation of the crystal from its melt or the freezing of a liquid into a solid. According to classical nucleation theory, as a liquid is undercooled below its melting point there is a thermodynamic driving force towards forming the crystal phase since it is more thermodynamically favorable. However, the emergence of a new phase leads to the creation of an interface which costs energy. Competition between these two driving forces determines the free-energy barrier for homogeneous nucleation i.e. nucleation from a pure phase. The free energy cost of creating the crystal-liquid interface plays a crucial role in determining the rate of nucleation, the final morphology of the crystal as well as the nucleation mechanism. Hence, a knowledge of the crystal-liquid interfacial free energy is crucial to understand nucleation and crystallization phenomena.

If all nucleation were to occur only from a pure phase, we would have to freeze water to 40 degrees below its melting point of zero degrees Celsius before we could observe ice!![3] However, this is not so in real life and water indeed freezes at zero degrees Celsius on account of the presence of impurities. Such nucleation near a surface of an impurity or a wall is known as heterogeneous nucleation and the free-energy barrier for heterogeneous nucleation is smaller as compared to that for homogeneous nucleation, by a factor depending on the angle of contact that the crystal phase makes with the wall. The presence of a wall indicates the presence of two other interfaces, which is the wall-liquid interface and the wall-crystal interface. Consequently, two other interfacial free energies come into the picture i.e. the wall-liquid and wall-crystal interfacial free energies. Using the Young's equation[4], the three

interfacial free energies can be related to the contact angle, which describes the degree of wetting of the crystal phase by the wall.

The classical theories of crystal nucleation and the Young's equation are valid for macroscopic systems and have not been tested experimentally for the nucleation of nanoscopic droplets. In experiments it is difficult to maintain a stable interface between two condensed phases such as liquid and solids and the free energies can only be obtained indirectly by already assuming the validity of classical nucleation theory. In contrast, all system parameters can be controlled in molecular simulations and more importantly, free energies and contact angles can also be computed directly.

Several computational studies have been undertaken in the past and they have helped us to gain insights into the microscopic aspects of nucleation. Such studies have been undertaken for simple statistical mechanics models as well as for physical systems such as water, Nacl, metals and alloys. I have contributed to this field by developing simulation techniques to compute various interfacial free energies influencing the nucleation phenomena as well as the kinetics of crystal growth[7,8,9]. Using my simulation technique, a group at Oxford University, has recently calculated the interfacial free energy of water and ice in contact with different types of walls[10]. In recent years, simulation studies on nucleation have expanded greatly to include various aspects such as the effects of confinement on nucleation, nucleation from solution, polymorphism, etc. However, a detailed understanding is still incomplete due to the small length and time scales involved.

In this project, I plan to investigate the nucleation and crystal growth phenomena via molecular simulations. The goal of my research is to understand the static and dynamic phenomena which occur during a nucleation event at an atomic level by characterizing the structure of the crystal-liquid interface, determining the nucleation rate and computing the various free energy barriers, the contact angle as well as the various interfacial free energies independently across a range of parameters and for different materials. The parameters are the interaction potential between the particles and the degree of supercooling. The nucleation phenomena will be studied for various materials such as single component as well as multi-component systems, liquid crystals, passive as well as active particles and for monomers, dimers as well as polymers. I also plan to study nucleation under various conditions such as confinement as well as substances in a solutions. Determination of the various thermodynamic quantities such as the nucleation free energy barriers, nucleation rate and interfacial free energies will allow us to test the validity of classical theories of nucleation for various systems and lead to the development of better theoretical models, which can capture nucleation phenomena at the molecular level. The results obtained from our studies can also provide inputs to experimentalists, thereby acting as a bridge between theory and experiments.

Investigating nucleation and crystallization phenomena is a vast research field and in the next few years, I plan to study a few topics of interest to me in this field, which I list below:

(a)<u>Computing Solid-liquid Phase coexistence curves</u>

Determining the coexistence conditions for a substance and elucidating the nature of the liquid-to-solid phase transition is one of the fundamental problems in statistical mechanics and is crucial to understanding crystal nucleation and growth. While, the phase coexistence of one-component passive systems such as Hard Spheres (HS), Lennard -Jones (LJ), metals has been widely studied via computer simulations, comparatively less effort has been devoted to more complicated systems.

I first plan to study the nature of the freezing transition as well as determine the phase coexistence at various thermodynamic conditions for two component systems such as alloys, binary Hard spheres and binary Lennard Jones particles using Molecular Dynamics and Monte Carlo simulation techniques such as Thermodynamic integration, Gibbs-Duhem approach, phase switch Monte Carlo, Free solidification simulations, Semi-Grand-Canonical ensemble simulations, etc. While the nature of the freezing transition for one component systems is known in three and two dimensions there are hardly any results on two-component systems. Therefore, such studies will be undertaken for two dimensional systems as well. Later on, I will apply the techniques to compute phase diagrams of more complicated substances such as charged particles, self-propelled systems such as active particles, liquid crystals and polymers. The dependence of the coexistence temperature on the nature of the interaction potential will also be investigated for both one and two component systems. Melting points of solids in confinement will also be investigated.

(b) Study of the Crystal-liquid interface

The kinetics of crystal growth in contact with its own melt play an important role in determining the final structure of the crystal. While substantial effort has been invested to characterize the structure of the crystal-liquid interface as well as compute the growth kinetics for one-component passive systems which crystallize into the FCC structure, there are hardly any results for binary systems such as alloys or well-known statistical mechanics models such as binary HS and LJ particles or for one-component systems crystallizing into BCC or any other structure.

The nature of the crystal-liquid interface will depend on the crystal structure as well as the nature of interaction between the particles. My goal is to study the crystal-liquid interface and compute the growth kinetics for different crystal structures as well various kinds of interaction potentials ranging from purely repulsive such as HS and inverse power potentials to interactions with varying ranges of the attractive part of the potential. These studies will be carried out also for binary systems as well.

(c) Computation of interfacial free energies

Recently, I have worked to develop a molecular simulation technique based on Thermodynamic integration compute various interfacial free energies influencing homogeneous and heterogeneous nucleation. My next step is to further refine the Thermodynamic integration scheme developed by me and my collaborator [6], partly in order to optimize the computational time and also to adapt it for binary systems as well as other systems such as charged particles which interact via a long-range potential, liquid crystal systems, self-propelled particles etc.

One of the important liquid-solid phase transitions is that of water into ice. Despite its importance to the sustainment of life on this planet and many other important natural and artificial phenomena, it is only in the last few years that scientists have begun to study it using Computer simulations. One of my future projects is to compute the ice-water interfacial free energy as well as the interfacial free energies of ice and water in contact with walls with various simulation methods and compare it to existing data.

(d) Investigation of Heterogeneous nucleation

While crystal-liquid homogeneous nucleation of one-component systems has been studied extensively using molecular simulations, there are comparatively fewer studies on heterogeneous nucleation of a crystal in contact with different substrates. I plan to carry out simulation studies for

different model potentials in contact with various substrates and compute the free energy barrier from heterogeneous nucleation in order to test the predictions of classical nucleation theory. A direct determination of the contact angle will also be made and the validity of Young's equation will be tested. Such studies will initially be carried out for one-component systems and later on for complex systems such as binary HS and LJ, alloys, active or self-propelled particles, polymers, etc. In the next stage of the project, I plan to investigate ice nucleation on bacterial proteins, an important problem for the industry as well as the nucleation of ice on silver-iodide particles, a process used for cloud seeding.

Tools of Research and Research facilities

The tools of my research for investigation of nucleation, crystal growth and interfacial phenomena are Molecular Dynamics, Brownian Dynamics and Monte Carlo simulations in conjunction with such molecular simulation techniques as Thermodynamic Integration, Umbrella Sampling, Metadynamics[11], Tethered Monte Carlo[12] and other free-energy based methods. Since the work is primarily computational, I would need significant computational resources. Basically, I require a High Performance Computing cluster with at least 200 CPU cores and 2 GPU processors, with a processor speed of 2.4 GHz or above. As regards manpower, I would like to hire one or two PhD students to work with me on this topic.

2.)Non-Equilibrium Statistical Mechanics and Thermodynamics.

A.)Thermal noise-induced Phenomena .

Thermal noise is usually seen as a hindrance to be removed. However, in the past two decades it has been found that noise can play a beneficial role for some nonlinear systems. One important phenomena, which is of great interest to scientists in many different fields, is that of Brownian motors[13]. The Brownian motor phenomena refers to the unidirectional movement of particles in the absence of a global bias in the system. Such a directed current occurs on account of the interplay between non-equilibrium driving, thermal fluctuations and the asymmetry in the non-linear system. This effect is seen in microscopic or nanoscopic systems where thermal energy plays an important role.

During my Doctoral research, I investigated the thermodynamics of a Brownian motor driven by spatially inhomogeneous temperature, known as the Buettiker-Landauer motor[14]. Such a motor can also work as a microscopic heat pump or heat engine, when it works against an external load. In general, noise or stochastic phenomena is studied by the help of the Langevin and Fokker-Plank equations. In the high-friction limit one usually omits the inertial term from the Langevin equation since the dynamics become overdamped. However, my investigations showed that one has to take the inertial term into account to properly account for the various heat flows. I proved this by comparing numerical and analytical results from the Langevin equation with first-principles Molecular dynamics simulations[15]. My work was cited and commented upon by Ken Sekimoto, a pioneer in the field of Brownian motors and stochastic Phenomena, in his book *Stochastic Energetics (Springer, 2010)*. I also validated Onsager relations with the help of this model. Examining, the efficiency of this motor for different models, I found it to be very low. *A future work involves looking for models which deliver higher efficiency and power.*

The Brownian or molecular motor mechanism may also answer questions pertaining to biological transport within the cell and could also lead to the manufacturing of artificial nanomotors. In the next few years, I plan to work on the thermodynamic and transport features of various kinds of artificial and Biological Brownian motors as well as other noise-induced phenomena. A list of possible

projects that I am interested in is listed below.

(a)Physics of Brownian motors – Apart from artificial motors, such as the Buettiker-Landauer motor, the Brownian motor mechanism is important to describe the movement of biological motors such as myosin and kinesin, which are usually made of various proteins and powered by ATP hydrolysis[16]. A very challenging problem in this regard is to explain the high efficiency of energy conversion of such motors. However, current models of Brownian motors usually lead to very low efficiencies. Another aspect of such molecular motors which is not yet fully understood is their collective behavior since motor protein carrying molecular cargo do so collectively.

I plan to analyze various set-up of single and collective Brownian motors to explain the high efficiency of biological motors and also investigate how interaction between the Brownian particles impacts the transport and energetics of the system. I also plan to calculate the optimal potential to enhance the current and efficiency of the device, using variational calculus and other optimization algorithms. While, motor proteins operate in an over-damped environment, the under-damped regime of Brownian motors also displays interesting transport features such as absolute negative mobility, current reversals etc. I would also investigate the role of potential, noise and non-equilibrium driving on the transport of such inertial Brownian motors.

(b)*Other noise-induced phenomena such as stochastic resonance[17], noise-enhanced stability[18], resonant activation[19] - Thermal noise plays a beneficial role in many other phenomena as well such as stochastic resonance, where a weak sub-threshold signal can be amplified because of noise. Other phenomena include noise enhanced stability, where the system stays close to the potential well for a longer time as compared to the deterministic case and resonant activation, a phenomena where the mean first passage time for a Brownian particle escaping over a potential barrier shows a minimum as a function of some time-driven parameter.*

While such phenomena have been studied for single-particle systems an important area of study is the effect of interaction between many molecular motors. Such collective effects have shown interesting behavior in the past like phase transitions, spontaneous ratchet effect and negative mobility. Coupled Brownian particles also play an important role in the translocation of polymers through a nanopore[20], where various noise-induced phenomena are manifested. A future project is to investigate collective effects of coupled Brownian particles on such phenomena. Other lines of investigation are the role of inertia of the Brownian particle and the effect of non-thermal or non-Markovian thermal noise on such phenomena.

B.)Non-Equilibrium Thermodynamics of Small Systems.

While equilibrium thermodynamics is a well developed field, non-equilibrium thermodynamics and statistical mechanics has been a difficult area for theoretical physicists to tackle. Recently however, much progress has been made since the discovery of various fluctuation theorems by Evans and Searles[21], Jarzyski[22], Crooks[23], Seifert[24] and others. Such fluctuation theorems relate the probability of a physical quantity such as work, heat or entropy to its time reversed one and are valid even for a non-equilibrium process. One of the famous fluctuation theorems is the well-known Jarzynski equality, which relates the probability to obtain a certain value for the thermodynamic work in a non-equilibrium transformation between two thermodynamic states, to its time reversed counterpart. It converts the second law of thermodynamics, an inequality, which states that the work

done in any non-equilibrium thermodynamic process is always greater than the free energy, into an equality using which one can obtain the equilibrium free energy difference between two equilibrium states even from a non-equilibrium transformation.

Using the Jarzynski equality and molecular dynamics simulations, I have computed the interfacial free energies of liquid and crystal phases in contact with various kinds of solid walls (see discussion and reference in Section 1). However, a more interesting application of the Jarzynski equality is for systems, where the internal energy is of the same order as the thermal energy. Moreover, efficacy of such a non-equilibrium work method, depends on the amount of work that is dissipated during the transformation. In a non-equilibrium process such dissipated work is always positive, while for an equilibrium transformation the dissipation is zero. Hence, there is a necessity in devising optimal work protocols to obtain accurate values for the free energy.

I plan to investigate Brownian particles in harmonic as well as other non-harmonic potentials under the effect of various time-driven parameters. I also plan to illustrate the validity of the Jarzysnki equality as well as other fluctuation relations involving the work, heat and entropy by computing the probability distribution of such thermodynamic quantities. Such investigations will clarify our understanding of non-equilibrium thermodynamics for small scale systems, where thermal fluctuations play a dominant role. Finally, I will also study theoretically and computationally Thermodynamics of Brownian heat engines.

Tools of Research and Research facilities

Investigation of noise-induced phenomena and non-equilibrium thermodynamics of small systems will be carried out analytically and numerically. For analytical work, mathematical packages such as Maple and Mathematica would be very useful. While the existing computational facilities in the Institute might be adequate for numerical work, a HPC workstation with 20 cores (processor speed at least 2.4 GHz) will considerably speed up my research. I plan to hire 1-2 PhD students for this project.

References

1.)*Nucleation in Condensed Matter: Applications in Materials and Biology*, K. F. Kelton and A. L. Greer, (Elsevier, **2010**).
2.)*Nucleation*, D. Kaschiev, (Elsevier, **2000**).
3.)E. Sanz, *J. Am. Chem. Soc.*, **135** (15008), **2013.**
4.)*An Essay on the Cohesion of Fluids*, T. Young, *Phil. Trans. R. Soc. Lond.* **95** (65), **1805**.
5.)*Computer Simulations of Liquids*, M. P. Allen and D. J. Tildesley, (Clarendon, Oxford, **1987**).
6.)*Understanding Molecular Simulation*, D. Frenkel and B. Smit, (Academic, San Diego, **2002**).
7.)R. Benjamin and J. Horbach, *J. Chem. Phys.* **137**, 044707 (**2012**); *J. Chem. Phys.* **139**, 039901 (**2013**).
8.)R. Benjamin and J. Horbach, *J. Chem. Phys.* **139**, 084705 (**2013**).
9.)R. Benjamin and J. Horbach, *J. Chem. Phys.* **141**, 044715 (**2014**).
10.)A. Reinhardt and J.P.K. Doye, *J. Chem. Phys.* **141,** 084501 (**2014**).
11.)Laio, A.; Parrinello, M. *Proc. Nat. Ac. Sci.* **99**, 12562 (**2002**).
12.)L. A. Fernández *et al*., *Phys. Rev. Lett.* **108**, 165701 (**2012**).
13.)P. Reimann, Phys. Rep. **361,** 57 (**2002**).
14.)M. Büttiker, *Z. Phys. B: Condens. Matter* **68**, 161 (**1987**); R. Landauer, *J. Stat. Phys.* **5**3, 233 (**1988**).
15.)R. Benjamin and R. Kawai, *Phys. Rev. E.* **77,** 051132 (**2008**).

16.)A. Parmeggiani *et al.*, *Phys. Rev. E.* **60**, 2127 (**1999**).
17.)L. Gammaitoni *et al*., *Rev. Mod. Phys.* **70**, 223 (**1998**).
18.)B. Spagnolo *et al.*, *Acta Physica Polonica B,* **35**, 1419 (**2004**).
19.)C. R. Doering and J. C. Gadoua, *Phys. Rev. Lett.*, **69**, 2318 (**1992**).
20.)M. Muthukumar, *Polymer Translocation*, (CRC Press Inc, **2011**).
21.)D. J. Evans and D. J. Searles, *Phys. Rev. E,* **50,** 1645 (**2004**).
22.)C. Jarzynski, *Phys. Rev. E*, **78,** 2690 (**1997**).
23.)G. E. Crooks, *J. Stat. Phys.* **90**, 1481 (**1998**).
24.)U. Seifert, *Rep. Prog. Phys.* **75**, 126001, (**2012**).