Shubhadeep Nag
Curriculum Vitae

Address of correspondence:
Nanosensors and Biophysics Lab,
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Department of Biomedical Engineering,
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Permanent Address:
"Aswini Vatika", C2 1st Floor,
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Date of Birth : 7^{th} November, 1992
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Academic Qualification:

M.Sc. in Physics	2013-2015	70.1%	Rajabazar Science College	University of Calcutta, West Bengal, India.
B.Sc. in Physics (honours)	2010-2013	72.6%	Maulana Azad College	University of Calcutta, West Bengal, India.

Ph.D. Thesis Title : Novel and Fundamental Studies of Separation Methods Leading to Very High Degree of Separation of Molecular Mixtures and Related Studies.
Thesis advisor : Prof. Yashonath Subramanian (Supervisor) and Prof. Prabal K. Maiti (Co-Supervisor)
Institute : Solid State and Structural Chemistry Unit, IISc, Bengaluru - 560012, India.
Year of Award : September, 2021. Download from ResearchGate

Scholastic Achievements:

- Winner of the **Toulouse Medal** for the best Ph.D. thesis of SSCU, IISc for the academic year 2021-22.
- Winner of the **Lenovo AI Challenge** for 2018(Over the Asia Pacific Region) in Super Computing 2018 conference.
- Secured all India rank **106** (& **191**) in Joint Entrance Screening Test (JEST) 2013 & 2015.
- Secured all India rank **618** in Graduate Aptitude Test for Engineering (GATE) (2015) in Physics.

Work Experience:

- Currently working as a Post-Doctoral Fellow at the Department of Biomedical Engineering, Tel-Aviv University, Israel, October 2022 - Present(September 2023).
- Research Associate in Department of Physics, Indian Institute of Science, Bangalore, India, August 2021 - September 2022.
- Research Associate in Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India, April-July 2021.
- Guest Lecturer in Department of Physics, Bangabasi College (affiliated under University of Calcutta), Kolkata, India, July-December, 2015.
- Project assistant under Prof. Debnarayan Jana at the University of Calcutta, Kolkata, India, July-December 2015. **Project Title**: Spectroscopic Studies of Nanomaterial (CeLaO3).
- Project assistant under Prof. Amitava Ghorai at Maulana Azad College affiliated under the University of Calcutta, Kolkata, India, June-Jule 2012. **Project Title**: Effect of Electric Field on the Growth of Sprout Length of Ground Nut Seeds.

Teaching Assistant Experience:

- Served as teaching assistant for the integrated PhD and undergraduate course CD 214 (Basic Mathematics) at Indian Institute of Science, Bangalore, India, Aug-Dec 2017.

Technical Skills:

- *Asthira:* It is a NVT Monte Carlo simulation program written by me in Fortran-95 language(from scratch). This program can perform both equilibrium and non-equilibrium simulation of different systems such as
  (a) a system of single type hydrocarbon molecules,
  (b) a mixture of hydrocarbon molecules,
  (c) zeolite material,
  (d) a system of one type of hydrocarbon molecules in zeolite and
  (e) a mixture of hydrocarbon molecules in zeolitic material.
- C/C++, Fortran-95 MATLAB, Octave, LaTeX.
- Machine Learning (completed the course of Prof. Andrew Ng in Coursera and obtained the completion certificate)
- gnuplot, Origin, Xmgrace
- Classical and Quantum Monte Carlo, Classical Molecular Dynamics (LAMMPS, DL_POLY, VMD, PyRETIS, GROMACS), Gaussian, CP2K (Preliminary Experience), Packmol, Intermol.
- BET Isotherm, FTIR (Preliminary Experience)

Other Experiences:

- Worked as the main volunteer in the conference "Recent Advances in Molecular Simulations" during February 8-11, 2018 at the Indian Institute of Science (IISc) Bangalore, India.
- Worked as the main volunteer in the conference "Dynamics at the Interface of Chemistry and Biology" during February 19-21, 2019 at the Indian Institute of Science (IISc) Bangalore, India.
- Working voluntarily as an admin of the supercomputer (Thematic Unit of Excellence, SSCU) facility in IISc, Bangalore.

Publications:

Refereed Articles

1. Shubhadeep Nag, Jeet Majumdar, Bhalamurugan Sivaraman, Subramanian Yashonath, and Prabal K Maiti, Influence of the substrate on the density and infrared spectra of the adsorbed methanol ice of different thicknesses using molecular dynamics simulation, **Monthly Notices of the Royal Astronomical Society**, 2023, *522*, 3656. DOI Link
2. Shubhadip Basu*, Shubhadeep Nag*, Nihal B Kottan* and Bikramjit Basu, In silico study on probing atomistic insight into structural stability and tensile properties of Fe-doped hydroxyapatite single crystals, **Scientific Reports**, 2022, *12*, 20576. DOI Link
3. Shubhadeep Nag and Subramanian Yashonath, Separation of *n*-hexane from 2,2-dimethyl butane : Increase in octane number, **Advanced Theory and Simulations**, 2022, *5*, 2100204. DOI Link
4. Shubhadeep Nag and Subramanian Yashonath, Separation of hydrocarbon mixtures using NaY Zeolite : Large Distinct diffusivity, **Journal of Computational Chemistry**, 2022, *43* (10), 660. DOI Link
5. Shubhadeep Nag, Garani Ananthakrishna, Prabal K. Maiti and Subramanian Yashonath, High Purity Separation of *n*-pentane from neopentane using a Nano crystal of Zeolite Y, **The Journal of Chemical Physics**, 2021, *155*, 014702. DOI Link
6. Shubhadeep Nag, Prabal K. Maiti and Subramanian Yashonath, Separating a linear C_5 hydrocarbon from a branched C_6 hydrocarbon : 2,2 dimethyl butane from *n*-pentane using Levitation Blowtorch Method, 2021, **Phys. Chem. Chem. Phys.**, *23*, 18102. DOI Link
7. Shubhadeep Nag, Garani Ananthakrishna, Prabal K. Maiti and Subramanian Yashonath, Separating Hydrocarbon Mixtures by Driving the Components in Opposite Directions: High Degree of Separation Factor and Energy Efficiency, **Phys. Rev. Lett.**, 2020, *124*, 255901. DOI Link

8. Shubhadeep Nag, Manju Sharma and Subramanian Yashonath, Understanding fast diffusion of solutes in solid solutions: A molecular dynamics study of solutes in body centered cubic solid, **The Journal of Chemical Physics**, 2020, *153*(24), 244503. DOI Link

9. Angela Mary Thomas, Shubhadeep Nag, Dileep Kumar Yadav, Shrishti Uniyal, Sitharaman Uma and Yashonath Subramanian, A new empirical potential for zeolite with variable Si/Al ratio: Simulations vs. experiments, **Microporous and Mesoporous Materials**, 2020, *300*, 110119. DOI Link

Book Chapter

1. Shubhadeep Nag and Yashonath Subramanian, Anomalous Diffusivity in Porous Solids: Levitation Effect, Zeolites New Challenges, Edited by Karmen Margeta and Anamarija Farká , **IntechOpen**, 2020. DOI Link

Manuscripts To Be Communicated

1. Shubhadeep Nag, Titus van Erp, Enrico Riccardi and Subramanian Yashonath, Study of Levitation effect at a very low temperature: a Replica Exchange Transition Interface Sampling approach.

2. Shubhadeep Nag and Subramanian Yashonath, Influence of the localized hot zone on the potential energy landscape.

3. Parth V. Shah, Shubhadeep Nag, Debnath Pal and Subramanian Yashonath, Calculation of Velocity Auto-Correlation Function using parallel algorithms.

* = Equal Contribution

Poster Presentations:

- "Preparation and Characterization of La-doped Cerium Oxide by Solid State Reaction" at "National Workshop on Material Science and Technology" during December 10-12, 2015 at Maulana Azad College, Kolkata, India.

- "Classical Motion of Particles over Potential Barrier in Fluctuating Inhomogeneous System" at "Theoretical Chemistry Symposium" during December 14-17, 2016 at University of Hyderabad (UoH) Hyderabad, India.

- "Separation of Ideal Gas mixtures at Nano-scale" at 16 December 2021 at IISc, India.

- "Separation of Hydrocarbon Mixtures in zeolite NaY" at "Sorbonne-JNCASR School on Advanced Computational Materials Science (SJSACMS 2018)" during 29 January-2 February, 2018 at JNCASR Bangalore, India.

- "A non-equilibrium simulation of separation of molecular mixtures" at "Modern Approaches in Chemistry and Biology" during February 18-20, 2020 at JNCASR, Bangalore, India.
- "Pronounced Enhancement of Diffusion Anomaly in a confined system at Low Temperatures: a Transition Interface Sampling Study" at 14 December 2021 at IISc, India.

Oral Presentations:

- " Zeros of Grand Canonical Partition Function (Lee-yang Zeros)" at the department seminar at Solid State and Structural Chemistry Unit, IISc in 2017.
- " Casimir Effect" at the department seminar at Solid State and Structural Chemistry Unit, IISc in 2018.

Title:"Development of A Novel Method for Separation of Mixtures (A Combination of Levitation and Blow-torch Effect)"

- at "SERConnect - SERC Annual Workshop" during 19th March 2019 at Indian Institute of Science (IISc) Bangalore, India.
- at workshop "Transition Path Sampling Simulations via PyRETIS" during March 11-15 2019 at Leiden, the Netherlands.

Title: "The Study of Fast diffusion of solutes in bcc solid and its implication in metallurgy"

- at "Unit Day Symposium" organized at Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India
- at "Statistical Mechanics in Chemistry and Biology (SMCB 2021)" organized jointly by IIT Tirupati, IIT Goa and IISER Tirupati during January 23-26, 2021 (Live Presentation).

Title: "Green chemistry separation of linear hydrocarbon from branched hydrocarbon with high degree of separation factor by driving the components in opposite directions"

- at "ACS Spring 2021" during April 5-30, 2021 (Live Presentation).

Supervising and mentoring activities:

Assisted the following students with completing their Bachelor/Master projects:

- Parth Shah (2019, currently pursuing MTech from the University of Southern California, USA)
- Aditi Srinivas (2019)
- Aman Agarwal (2016, currently pursuing PhD from the University of Colorado Boulder, USA)