

SUNITA NEGI

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PERSONAL INFORMATION

Date of Birth: 20th September 1982
Present Position Assistant Professor at Cluster Innovation Centre (CIC), University of Delhi, INDIA since JULY 2012
Nationality: Indian
Marital Status: Married
Gender: Female
Office Address : Cluster Innovation Centre, University Stadium, University of Delhi, , Delhi - 110007
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CAREER OBJECTIVE

To accomplish high quality interdisciplinary research and teaching in area of computational biophysics, computational nanoscience and nanotechnology and material science in an open, team oriented and dynamic environment.

AREAS OF INTEREST

- Understanding and Solving problems related to the field of Computational bio-physics and biology.
- Problems related to Computational nanoscience, nanotechnology and Material science using Atomistic simulation techniques like Molecular Dynamics (MD),
- Data Analysis Techniques like FFT, SVD and Bispectral Analysis.
- Molecular Mechanics (MM), Density Functional Theory (DFT), Monte Carlo techniques etc.

WORK/RESEARCH EXPERIENCE

1) Working as an Assistant Professor at **CLUSTER INNOVATION CENTRE, UNIVERSITY OF DELHI**, Delhi - 110007 since July 2012. The main area of research and teaching includes Physics and Computational Biology.

2) Worked as a Post Doctoral Fellow at **FACULTY OF ENGINEERING & NATURAL SCIENCE, SABANCI UNIVERSITY**, Istanbul, Turkey from May 2011 - June 2012.

The research work involved doing Molecular Dynamics simulations of Calmodulin protein using the NAMD which is a parallel MD code for large biomolecular systems.

3) Worked as a Post Doctoral Fellow in **INSTITUTE FOR PLASMA RESEARCH, Gandhinagar**, Gujarat India from Dec 2010 – April 2011.

The area of interest included developing MD potentials using LAMMPS for metals like liquid sodium which play an important role in reactor physics.

ACADEMIC QUALIFICATION

Degree	Year	Institute / University
Ph.D.	2010	Institute for Plasma Reseach, BHAT, Gandhinagar, Gujarat, India
M. Sc (Physics)	2005	University of Delhi, Delhi, India
B. Sc. (Physics Honours)	2003	University of Delhi, Delhi, India
XII Standard	2000	Central Board of Secondary Education, New Delhi, India
X Standard	1998	Central Board of Secondary Education, New Delhi, India

THESIS TOPIC: MOLECULAR DYNAMICS SIMULATIONS OF NANOMETER SIZED DEVICES BASED ON CARBON NANOTUBES

THESIS SUPERVISOR: Dr. Shashank Chaturvedi,
Head, Computational Analysis Division,
Bhabha Atomic Research Center,
Autonagar,
Visakhapatnam, A.P - 530012, India

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PUBLICATIONS IN REFEREED JOURNALS

- **Sunita Negi**, "Effect of Calcium ion removal, Ionic Strength and Temperature on the conformation change in Calmodulin protein at physiological pH", **The Biophysics Journal (In press) 2014**
- **Sunita Negi**, Vivek Kumar Bhartiya and Shashank Chaturvedi, Charge Calculation Studies on a Single and Double Walled Carbon Nanotube Using Mopac, **Advance Science Letters, (Submitted, November 2014)**.
- **Sunita Negi**, Ayse Ozlem Aykut, Ali Rana Atilgan and Canan Atilgan, "Calmodulin Readily Switches Conformation upon Protonating High pKa Acidic Residues", **Journal of Physical Chemistry B, (2012)**, 116 (24), pp 7145–7153. <http://pubs.acs.org/doi/abs/10.1021/jp3032995>
- Canan Atilgan, Ayse Ozlem Aykut, Ali Rana Atilgan and **Sunita Negi**, Exploring pH dependent landscape shifts in proteins, **Biophysical Journal, (2012)**, vol. 102, issue 3, p. 450a. <http://www.sciencedirect.com/science/article/pii/S0006349511038148>
- **Sunita Negi**, Ali Rana Atilgan and Canan Atilgan, "Driving Calmodulin Protein towards Conformational Shift by Changing Ionization States of Select Residues", **Journal of Physics: Conference Series, 402** 012047 (2011). <http://iopscience.iop.org/1742-6596/402/1/012047>
- **S. Negi** and S. Chaturvedi, "Normal mode analysis of a Single-Walled Carbon nanotube based on Molecular Dynamics : A Singular Value Decomposition study", **International Journal of Nanoscience 9, 1-16 (2010)**. <http://www.worldscientific.com/doi/abs/10.1142/S0219581X10007125>
- **S. Negi**, M. Warriar and S. Chaturvedi, "Determination of useful parameter space for a nanometer scale motor stimulated by an external electric field", **Computational Material Science 50, 761-770 (2010)**. <http://www.sciencedirect.com/science/article/pii/S0927025610005677>
- **S. Negi**, M. Warriar, K. Nordlund and S. Chaturvedi. "Molecular Dynamic simulations of a double-walled carbon nanotube motor subjected to a sinusoidally varying electric field", **Computational Material Science 44, 979-987 (2009)**. <http://www.sciencedirect.com/science/article/pii/S0927025610005677>
- **S. Negi**, M. Warriar, K. Nordlund and S. Chaturvedi, "Molecular Dynamics simulations of carbon nanotubes interacting with a graphite surface", **J. Comput. Theor. Nanaosci 5, 318-353 (2008)**. <http://www.ingentaconnect.com/content/asp/jctn/2008/00000005/00000003/art00014>

PUBLICATIONS IN INTERNATIONAL CONFERENCES/WORKSHOPS

- **MESODIS 2006** (International Workshop on the physics of Mesoscopic and Disordered Materials), 04-08 December 1006, Department of Physics, **Indian Institute of Technology Kanpur, INDIA (Poster presentation)**
- **ICANAT – 2008**, International Conference on Advances in Nanotechnology, 06 – 08 November, 2008, Mats University, Raipur (CG) INDIA, **(Oral presentation)**
- **Indo-French Workshop cum International Conference on Nanoscience and Nanotechnology**, October 12-16, 2009, Ansal Institute of Technology, Gurgaon, India
- **Conference on Computational Physics (CCP2010)**, 24th - 27th June 2010, Trondheim, Norway **(Oral presentation)**
- **International Conference On Molecular Materials (MOLMAT2010)**, 4th - 8th July 2010, Montpellier, France **(Poster presentation)**
- **ICTP workshop on Nano-Opto-Electro-Mechanical Systems**, 6th - 10th September 2010, Trieste Italy **(Poster Presentation)**
- **18th Statistical Physics Days**, 30th June – 2nd July 2011, Sabanci University, Tuzla, Istanbul, Turkey

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(Oral Presentation)

- **19th Statistical Physics Days**, 28th June – 30th June 2012, Sabanci University, Tuzla, Istanbul, Turkey.
- **Conference on Computational Physics (CCP2011)**, 30th Oct - 4th Nov 2011, Tennessee, United States of America (**Oral presentation**)
- **INDO-GERMAN Workshop on Advanced Materials for Future Energy Requirements - 2012**, University of Delhi, November 29 - 30 2012.
- **International Conference on Protein Folding and Diseases I-ISC 2012**, December 08-10 2012, Jamia Millia Islamia, New Delhi.
- **International Conference on Recent Advances in Nanoscience & Nanotechnology (ICRANN-2014)**, Dec 14-15, 2014 (to be attended).
- **Biophysical Society Annual Meeting (BPS 2015)**, February 12-15, Baltimore, Maryland, USA (to be attended).

PUBLICATIONS IN NATIONAL CONFERENCES/WORKSHOPS

- **Workshop on nanotechnology – Current Status and Challenges**, March 17-18, 2007, **Indian Institute of Technology Delhi, New Delhi, INDIA**
- **52nd DAE Solid State Physics Symposium**, 27 – 31 December 2007, University of Mysore, Manasagangotri, Mysore, INDIA, (**Poster presentation**)
- **PSSI – 2007 (National Symposium on Plasma Science and Technology)**, IPR, Gandhinagar, Gujarat, INDIA (**Poster presentation**)
- **PSSI – 2008**, National Symposium on Plasma Science and Technology, **Bhabha Atomic Research Center**, Mumbai, INDIA (**Poster presentation**)
- **Workshop on Scientific Applications of the IUAC HPC Facility, Nov 22-23 2012 – Inter University Accelerator Centre, New Delhi**

EXPERTISED AREAS OF RESEARCH

- **Molecular Dynamic simulations** mainly classical MD.
- Extensive experience of handling **MD codes HCParCas (Hydrogen Carbon Parallel Cascade)**.
- Experience of solving problems with Molecular Dynamics code **LAMMPS**. Problems related to Carbon nanotubes studied extensively.
- Good experience of installing and handling **NAMD** code for biological molecules like proteins.
- **Docking of protein** structures with the external ligands and their simulations.
- Extensive experience of handling circuit design suite **MULTISIM**.
- Good experience of working on **MCCE (Multi-Conformation Continuum Electrostatics) program**. MCCE is a biophysics simulation program combining continuum electrostatics and molecular mechanics.
- Experience of implementing and solving problems with other Molecular Dynamic codes like **MOPAC (Molecular Orbital Package)**.
- Good Knowledge and experience of Data analysis techniques like **Fourier analysis, Singular Value Decomposition, Spectral analysis and Bi-spectral Analysis**.

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- Basic knowledge of other computational techniques like **Molecular Mechanics (MM)**, **Monte Carlo (MC)**, **Ab-initio (DFT) MD** etc.
- Basic knowledge of installing and using **GROMACS** code.

➤ EXPERTISED AREAS OF TEACHING

- Physics of Motion, Special and General Theory of relativity
- Computational Biology
- Digital Electronics

KNOWLEDGE OF PROGRAMMING TOOLS AND TECHNIQUES

- Good knowledge of programming in **Fortran F77 & F90**.
- Basic knowledge of programming in **C**.
- Very good experience of handling **Linux** operating system.
- Very good experience of using Visual Molecular Dynamics (**VMD**) program for the visualization of biological systems.
- Shell Programming: Experience of shell programming in Linux.
- Good experience of using **MATLAB** software extensively for numerical programming and plotting purposes.
- Knowledge of scientific softwares like **GNU PLOT**, **XFIG**, **YMOL**, **OPENDX**, **GIMP**, **Graph Pad Prism**, **ABPS** etc.
- Good experience of using operating system **Windows 98/2000/Vista**.

CO-CURRICULAR ACTIVITIES

- Lectures given on “**Basics concepts of Molecular Dynamics Simulations**” to the Summer School Training students at Institute of Plasma Research (IPR), 2008 batch.
- Talks delivered frequently in the group meetings.

TALKS DELIVERED

- The Accelerator Laboratory, University of Helsinki on 29th 2010.
- Thomas Young Centre for Theory and Simulation of Materials, Imperial College London on 31st Jan 2011
- The Atomistic Simulation Centre, Queen's University Belfast on 3rd February 2011

MEMBERSHIPS/AWARDS/RECOGNITIONS

- Young Scientists Award by **Department of Science and Technology (DST)**, Govt. of India (2013-2016).
- TUBA Doctoral-Research Program (TUBA-DSAP) (2011-2012), **Turkish Academy of Sciences**.
- Fellowship to visit Norway and France by **Department of Science and Technology**, Govt. of India (2010).
- Qualified UGC-CSIR **National Eligibility test** (2005).
- Life time member of **Plasma Science Society of India (PSSI)**.

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- Member of **Indian Biophysical Society (IBS)**.
- **Topper of Atma Ram Sanatan Dharma College**, University of Delhi, New Delhi , BSc Hons. (Physics).

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