Jhuma Das

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3097 Genetic Medicine Building,
Department of Biochemistry and Biophysics,
University of North Carolina, Chapel Hill, NC, 27599

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Research Interest

Computational/Theoretical Biophysics: Modeling of membrane proteins, phospholipid membrane, lipid-protein interactions, drug development, long range hydrophobic interaction between inhomogeneous biomembranes, water dynamics at water-bilayer interface, effect of cholesterol on membrane structure and function, lipid rafts, phase transition in mixed lipid bilayer.

Education

Ph. D. in Physics — Graduation
Department of Physics and Astronomy, **University of Missouri** — August, 2010
Thesis title: "Multiscale dynamics of biomaterials: channel proteins, phospholipid membranes and cellular aggregates" — Advisor: Dr. Ioan Kosztin

University of Pune, Maharashtra, India — 2001 – 2003
M. Sc. in Physics

Lady Brabourne College, Calcutta University, India — 1998 – 2001
B. Sc. in Physics

Professional Experiences

Research Consultant for Parion Sciences at Durham, NC — 2012 – present

Postdoctoral Research Associate — 2012 – present
Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill

Postdoctoral Research Associate — 2010 – 2012
Department of Chemistry, University of North Carolina at Chapel Hill

Graduate Research Assistant — 2005 – 2010
Department of Physics and Astronomy, University of Missouri

Graduate Teaching Assistant — 2005 – 2010
Department of Physics and Astronomy, University of Missouri

Project Assistant — 2003 – 2005
Saha Institute of Nuclear physics, Kolkata, India

Computational Skills

Operating Systems
Unix, Linux, Windows, Mac

Programming Languages
Proficient with: FORTRAN77, C, C shell script, Tool Command Language
Familiar with: C++, AWK, Perl, Python

Markup Language
LaTeX

Software Packages
Proficient with: NAMD, VMD, GROMACS, CHARMM, XMGRACE,

Mathematica, DMD, Medusadock, Pymol, Schrödinger
Familiar with: LAMMPS, GnuPlot, MATLAB

Awards

Director's Discretionary Program of Oak Ridge Leadership Computing Facility (USA) 6 million CPU-hours allocation **on Titan supercomputer (Cray/XK7)** — 2013

Director's Discretionary Program of Argonne National Laboratory (USA) 5 million CPU-hours allocation **on Intrepid supercomputer (Blue Gene/P)** — 2013

Director's Discretionary Program of Argonne National Laboratory (USA) 5 million CPU-hours allocation **on Vesta supercomputer (Blue Gene/Q)** — 2013

Honorable mention, 25th Annual Missouri Life Sciences Week, University of Missouri — Apr 2009

Physics Leader's Meeting Talks – 2nd Prize — Oct 2008
Department of Physics and Astronomy, University of Missouri

Donald K. Anderson Teaching Award Nomination, — Feb 2008
University of Missouri

Fellowships

O. M. Stewart Scholarship — Jun 2009, Jun 2007
Department of Physics and Astronomy, University of Missouri

Ernest W. Landen Fellowship — Jun 2008
Department of Physics and Astronomy, University of Missouri

Joint CSIR-UGC Junior Research Fellowship (JRF) and Eligibility for lectureship in Physical Sciences, National Eligibility Test, India — May 2005

Book-grant — Jan 2002
Department of Physics, University of Pune

Oral Presentations

International Graduate Research Training Group Annual Meeting 2011 (Self-Assembled Soft-Matter Nanostructures at Interfaces) — Oct 2011
"Restructuring of Hydrophobic Surfaces Created by Surfactant Adsorption to Negatively Charged Surfaces: All Atom and Coarse Grain Simulations"

Joint Condensed Matter/ECE/Biological Physics Seminar, **University of Missouri** — Jan 2009
Anomalous diffusion of lipid atoms and molecules in phospholipid bilayers: a combined Molecular Dynamics and theoretical study

Physics Leader's Meeting, University of Missouri — Oct 2008
Anomalous diffusion of lipid atoms and molecules in phospholipid bilayers:a combined molecular dynamics and theoretical study

Biophysical Society 52nd Annual Meeting, Long Beach, California — Feb 2008
Collective Dynamics of Phospholipid Bilayers: A Combined Neutron Scattering and Molecular Dynamics Study

Posters

Biochemistry Biophysics 2012 Research Retreat, Wrightsville, North Carolina — Oct 2012
Jhuma Das, Elizabeth A. Proctor, Kenneth L. Nesbitt, Andrei A. Aleksandrov, John R. Riordan, Nikolay V. Dokholyan,
"Effect of Charged Residues in Cytoplasmic Extensions of Transmembrane Helices on CFTR Pore Dynamics"

243rd ACS National Meeting & Exposition, San Diego, California — Mar 2012
Changsun Eun**, Jhuma Das**, Max Berkowitz
"A Computational Study of the Restructuring Process of Surfactant-coated Surfaces in Water"

Biophysical Society 55th Annual Meeting, Baltimore, Maryland — Feb 2011
Jhuma Das, Elijah Flenner, Maikel Rheinstädter and Ioan Kosztin
"Anomalous diffusion of water molecules in hydrated lipid bilayers"

Biophysical Society 54th Annual Meeting, San Francisco, California — Feb 2010
Jhuma Das, Elijah Flenner, Maikel Rheinstädter and Ioan Kosztin
"Anomalous diffusion of water molecules in hydrated lipid bilayers"

Nano Frontiers, Department of Life Sciences, University of Missouri, Columbia, Missouri — Nov 2009
Jhuma Das, Elijah Flenner, Maikel Rheinstädter and Ioan Kosztin
"Anomalous diffusion of lipid atoms and molecules in phospholipid bilayers: a combined molecular dynamics and theoretical study"

25th Annual Missouri Life Sciences Week, Columbia, Missouri — Apr 2009
Jhuma Das, Elijah Flenner, Maikel Rheinstädter and Ioan Kosztin
"Anomalous diffusion of lipid atoms and molecules in phospholipid bilayers: a combined molecular dynamics and theoretical study"

Biophysical Society 53rd Annual Meeting, Boston, Massachusetts — Feb 2009
Jhuma Das, Elijah Flenner, Maikel Rheinstädter and Ioan Kosztin
"Anomalous diffusion of lipid atoms and molecules in phospholipid bilayers: a combined molecular dynamics and theoretical study"

Biophysical Society 53rd Annual Meeting, Boston, Massachusetts — Feb 2009
Bogdan Barz, **Jhuma Das**, Elijah Flenner, Francoise Marga, Cyrille Norote, Gabor Forgacs, Ioan Kosztin
"Cellular particle dynamics simulation of bioprinted 3D tissue constructs"

23rd Annual Missouri Life Sciences Week, Columbia, Missouri — Apr 2007
Jhuma Das, Lorant Janosi, Ioan Kosztin
"Water permeation through GlpF protein channel using FR method"

Biophysical Society 51st Annual Meeting, Baltimore, Maryland — Feb 2007
Jhuma Das, Lorant Janosi, Ioan Kosztin
"Water permeation through GlpF protein channel using FR method"

Saha Institute of Nuclear Physics, Kolkata, India — 2004
Jhuma Das, Dhananjay Bhattacharyya, Shayantani Mukherjee, Abhijit Mitra
"Non Watson-Crick Base Pairs in RNA: Structure, Occurrence and Stabilities"

Workshop(s)

NSF-FIBR grant meeting, Salt Lake City — Feb 2009

NSF-FIBR grant meeting Charleston, South Carolina Jan 2008

Affiliations

American Physical Society since 2009

Biophysical Society since 2006

Physics and Astronomy Graduate Student Association,
University of Missouri 2005 – 2010

Chemistry Department Postdoctoral Association
University of North Carolina-Chapel Hill 2010-2012

University of North Carolina postdoc association
University of North Carolina-Chapel Hill 2010-present

Graduate Student Association, University of Missouri Since 2005

Referred Publications

D. M. Cholon, N. L. Quinney, M. L. Fulcher, C. R. Esther, **J. Das,** S. H. Randell, N. V. Dokholyan, R. C. Boucher, and M. Gentzsch
Potentiator ivacaftor abrogates pharmacological correction of ΔF508 CFTR in cystic fibrosis
Science Translational Medicine, 6:246ra96, (**2014**)

J. Das, E. J. Flenner, and I. Kosztin
Anomalous Diffusion of Water Molecules in Hydrated Lipid Bilayers
Journal of Chemical Physics, 139, *065102* (**2013**)

C. Eun*, **J. Das***, and M. L. Berkowitz
Restructuring of a Model Hydrophobic Surface: Monte Carlo Simulations using a Simple Coarse-grained Model, **Journal of Physical Chemistry B**, *in press* (**2013**) (* These authors contributed equally to this manuscript)

J. Das, C. Eun, S. Perkin and M. L. Berkowitz
Restructuring of Hydrophobic Surfaces Created by Surfactant Adsorption to Mica Surfaces
Langmuir, 79, 011907-1 - 011907-11 (**2011**).

E. J. Flenner, **J. Das**, M. C. Rheinstädter, and I. Kosztin
Subdiffusion and lateral diffusion coefficient of lipid atoms and molecules
in phospholipid bilayers
Physical Review E, 79, 011907-1 - 011907-11 (**2009**).
-Selected for the January 15, 2009 issue of **Virtual Journal of Biological Physics Research** and for the February 2009 issue of *Virtual Journal of Ultrafast Science*

M. C. Rheinstädter, **J. Das**, E. Flenner and I. Kosztin
Motional Coherence in Fluid Phospholipid Membranes
Physical Review Letters, 101, 248106-1 - 248106-4 (**2008**).

M. C. Rheinstädter, **J. Das**, E. J. Flenner, B. Brüning, T. Seydel, and I. Kosztin
Motional Coherence in Fluid Phospholipid Membranes
Scientific Highlight, ILL Annual Report (**2008**).

J. Das, S. Mukherjee, A. Mitra and D. Bhattacharyya,
Non-Canonical Base Pairs and Higher Order Structures in Nucleic Acids: Crystal Structure Database Analysis
J. Biomol. Struct. Dynam., 24, 149 – 162 (2006).
(http://www.saha.ac.in/biop/www/db/local/RNAbase-pair.html).

Manuscripts in preparation

J. Das, A. A. Aleksandrov, L. He, L. Cui, J. R. Riordan, N. V. Dokholyan
Molecular Modeling of the conducting and non-conducting states of CFTR protein: A combined experimental and computational approach (to be submitted)

S. E. Sinnett, **J. Das**, N. V. Dokholyan, J. E. Brenman
PT1 can act as an ADP-mimetic that binds the regulatory region of AMP-activated protein kinase (AMPK) (submitted)

E. A. Proctor*, **J. Das***, K. L. Nesbitt, A. A. Aleksandrov, J. R. Riordan, N. V. Dokholyan (* these authors contributed equally to this work)
Ring of Fire: Charged Residues that Control Channel Conductance, Open Probability, and Pore Dynamics of Cystic Fibrosis Transmembrane Regulator (submitted)

J. Das, E. J. Flenner, M. Rheinstadter and I. Kosztin
Calculating Diffusion Coefficient from Dynamic Structure Factor Using Memory Function Approach