Jaydeb Chakrabarti

Professor
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Prof. Jaydeb Chakrabarti works in the area of soft matter physics. He completed his PhD from IISc, Bangalore in 1995. He did his post-doctoral research at FOM, AMOLF, Amsterdam, The Netherlands and TUE, Eindhoven, The Netherlads.

Supervision of Research / Students

Ph.D. Students

1. Samapan Sikdar; 'Microiscopic description of protein-ligand and protein-protein interaction (completed)
2. Suman Dutta (ongoing)
3. Sutapa Dutta (ongoing)
4. Arunava Adhikary (ongoing)
5. Piya Patra (external, ongoing)

Post Doctoral Research Scientists

1. Manas Mandal
2. Lakshmi Maganti

Teaching activities at the Centre

1. Phy 201: Basic Statistical Mechanics

Publications in Journals

1. Paramita Saha, Samapan Sikdar, Camelia Manna, **Jaydeb Chakrabarti** and Mahua Ghosh; *SDS induced dissociation of STY3178 oligomer: experimental and molecular dynamics studies;* RSC advances; 2017; **7**; 6209-6214.
2. Sutapa Dutta, Mahua Ghosh and **J. Chakrabarti;** *Spatio-temporal coordination among functional residues in protein*; Sci Rep.; 2017; **7**; 40439; doi:10.1038/srep40439.
3. Paramita Saha, Samapan Sikdar, **Jaydeb Chakrabarti** and Mahua Ghosh; *Response to chemical induced changes and their implication in yfdX proteins;* RSC advances; 2016; **6;** 91256-91264.
4. P. Saha, C. Manna, **Jaydeb Chakrabarti** and Mahua Ghosh; *Reversible thermal unfolding of a yfdX protein with chaperone-like activity*; Sci Rep.; 2016, **6**; 29541; doi:10.1038/srep29541.
5. S Sikdar, M Ghosh, M De Raychaudhury and **J Chakrabarti;** *Quantum chemical studies on nucleophilic sites in calcium ion bound Zwitterionic calmodulin loops*, RSC. Adv.; 2016; **6**; 54608-54614.
6. S. Dutta and **J. Chakrabarti;** *Anomalous dynamical responses in a driven system;* Europhys. Lett.; 2016; **116**; 38001.
7. B. Ash, **J. Chakrabarti** and A. Ghosal; *Spatio-temporal correlations in Coulomb clusters;* Europhys. Lett; 2016; **114;** 46001.

Lectures Delivered

1. Presented Poster by Sutapa Dutta in "Statphys Kolkata IX" at SINP, Kolkata during December, 2016.
2. Presented Poster by Sutapa Dutta in International Conference on "Advances in Biological System and Material Science in NanoWorld" at IIT BHU, during February 2017.
3. Oral presentation by Sutapa Dutta in "Mini Conference on Statistical Physics" at University of Calcutta during March, 2017.
4. Oral presentation by Sutapa Dutta in Bose Fest organized by SNBNCBS, March 2017.
5. C. K. Majumdar Summer workshop, May 2016, two lectures.

Sponsored Projects

1. Microscopic calculations of metal ion binding to proteins, DST, 2013-2016.

Collaborations including publications (Sl. No. of paper/s listed in 'Publications in Journals' jointly published with collaborators)

National

1. 2 (Sl. No. 5 and 7)

Significant research output / development during last one year

General research areas and problems worked on

- Statistical mechanics of soft matter systems
- Computational physics of bio-molecular systems

Interesting results obtained

1. Anomalous Dynamical Responses in a Driven System

The interplay between structure and dynamics in non-equilibrium steady-state is far from understood. We address this issue by tracking Brownian Dynamics trajectories of particles in a binary colloid of opposite charges in an external electric field. The particles show cross-over from homogeneous to lane state, a prototype of heterogeneous structure formation in non-equilibrium systems. We show that the length scale of structural correlations controls heterogeneity in diffusion and consequent anomalous dynamic responses, like the exponential tail in probability distributions of particle displacements and stretched exponential structural relaxation. We generalize our observations using equations for steady state density which may help to understand microscopic basis of heterogeneous diffusion in condensed matter systems.

2. Spatio-temporal correlations among functional residues of protein

The microscopic basis of communication among the functional sites in bio-macromolecules is a fundamental challenge in uncovering their functions. We study the communication through temporal cross-correlation among the binding sites. We illustrate via Molecular Dynamics simulations the properties of the temporal cross-correlation between the dihedrals of a small protein, ubiquitin which participates in protein degradation in eukaryotes. We show that the dihedral angles of the residues possess non-trivial temporal cross-correlations with asymmetry with respect to exchange of the dihedrals, having peaks at low frequencies with time scales in nano-seconds and an algebraic tail with a universal exponent for large frequencies. We show the existence of path for temporally correlated degrees of freedom among the functional residues. We explain the qualitative features of the cross-correlations through a general mathematical model. The generality of our analysis suggests that temporal cross-correlation functions may provide convenient theoretical framework to understand bio-molecular functions on microscopic basis.

Proposed research activities for the coming year

The primary focus of my research would be as follows:

a) **Kinetics of bio-molecular processes:** We shall look into coarse-grained model of proteins to calculate factors affecting rates of folding of proteins into native structures and that of aggregation of misfolded proteins. Such calculations would be based on Brownian dynamics simulations. These results are expected to throw lights on energy landscapes governing folding and aggregation in systems having large number of degrees of freedom.

b) **Microscopic theory of aggregation in driven systems:** Recent experiments suggest that thermo-phoretic motion of nanometer sized particles often drive their aggregation. We shall try to understand the mechanism of such cluster formation through Brownian Dynamics simulations and mean field calculations.

c) **Microscopic description of metal ion coordination to proteins:** This project involves ab-initio simulation of metal ion and peptide fragments. The main objective is to understand how ion induced polarization affect the stability of peptides in an aqueous medium.