Jaydeb Chakrabarti

Senior Professor
CBMS
jaydeb@bose.res.in

Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Sashthi Charan Mandal; Biophysics; Under progress
2. Edwine Tendong; Soft matter physics; Under progress; Tanusri Saha-Dasgupta (Supervisor)
3. Abhik Ghosh Moulik; Biophysics; Under progress
4. Rahul Karmakar; Soft matter physics; Under progress
5. Anirban Pal; Biophysics; Under progress
6. Suravi Pal; Soft matter physics; Under progress
7. Avik Sasmal; Not decided; Under progress
8. Konika Kole; Not decided; Under progress

b) Post-Docs

1. Ayatti Mallik; Biophysics

Teaching

1. Autumn semester; CB523; PhD; 5 students; with 1 (Gautam Gangopadhyay) co-teacher
2. Spring semester; PHY201; Integrated PhD

Publications

a) In journals

1. Satyabrata Maiti, Debasish Mukherjee, Parthajit Roy, **Jaydeb Chakrabarti** and Dhananjay Bhattacharyya, *Stacking geometry between two sheared Watson-Crick basepairs: Computational chemistry and bioinformatics based prediction*, Biochimica et Biophysica Acta (BBA) - General Subjects, 1864, 129600, 2020
2. Takashi Yoshimoto, Hisako Hashimoto, Mausumi Ray, Naoki Hayakawa, Tsukasa Matsuo, **Jaydeb Chakrabarti** and Hiromi Tobita, *Products of [2 + 2] Cycloaddition between a W≡Si Triple-bonded Complex and Alkynes: Isolation, Structure, and Non-classical Bonding Interaction*, Chemistry Letters, 49, 311-314, 2020
3. E Tendong, T Saha Dasgupta and **J Chakrabarti**, *Dynamics of water trapped in transition metal oxide-graphene nano-confinement*, Journal of Physics: Condensed Matter, 32, 325101, 2020
4. Piya Patra, Raja Banerjee and **Jaydeb Chakrabarti**, *Control of solvent exposure of cationic polypeptides in anionic environment*, Chemical Physics Letters, 750, 137503, 2020
5. Suman Dutta and **J. Chakrabarti**, *Length-scales of dynamic heterogeneity in a driven binary colloid*, Physical Chemistry Chemical Physics, 22, 17731-17737, 2020
6. Sasthi Charan Mandal, Lakshmi Maganti, Manas Mondal, **Jaydeb Chakrabarti**, *Microscopic insight to specificity of metal ion cofactor in DNA cleavage by restriction endonuclease EcoRV*, Biopolymers, 111, e23396, 2020
7. Aayatti Mallick Gupta, **Jaydeb Chakrabarti** and Sukhendu Mandal, *Non-synonymous mutations of*

SARS-CoV-2 leads epitope loss and segregates its variants, Microbes and Infection, 22, 598 – 607, 2020

Administrative duties

1. Head of the Department, CBMS
2. Convenor, SCOLP

Scientific collaborations with other national / international institutions (based on joint publications)

1. D. Bhattacharya's group, SINP; Sl. No. 1; International

Areas of Research

Statistical mechanics of soft matter and biological systems

Length scale of dynamic heterogeneity:

Here we study by Brownian Dynamics simulations a system of oppositely charged colloid subject to a constant electric field. We consider sufficiently strong electric field where the like charges in the system form macroscopic lanes. We examine spatial correlation lengths characterizing structural order and that between particles of different mobility. We find that the correlation lengths show dependence on the observation time. Moreover, slow particles are responsible for formation of lanes and offer independent length-scale in the steady states.[Ref: Physcial Chemistry Chemical Physics, 22, 17731-17737, 2020.

Microscopic insight to specificity of metal ion cofactor in DNA cleavage by restriction endonuclease EcoRV

Restriction endonucleases protect bacterial cells against bacteriophage infection by cleaving the incoming foreign DNA into fragments. In presence of Mg^{2+} ions, EcoRV is able to cleave the DNA but not in presence of Ca^{2+}. We make an attempt to understand this difference using conformational thermodynamics. We calculate the changes in conformational free energy and entropy of conformational degrees of freedom, like DNA base pair steps and dihedral angles of protein residues in Mg^{2+}-EcoRV-DNA complex compared to Ca2+-EcoRV-DNA complex using all-atom Molecular Dynamics (MD) trajectories. We find that the base pairs in cleavage region are highly disordered compared to Mg2+-EcoRV-DNA. One of the acidic residues ASP90, co-ordinating to the metal ion, is conformationally destabilized and disordered, while basic residue LYS92 gets conformational stability and order. The changes in conformational stability and order of the base pair steps and the residues lead to cofactor sensitivity of the enzyme. [Ref: Biopolymers, 2020; e23396.]

Plan of Future Work Including Project

1. Modification membrane properties in presence of short biomolecules, like polypetide, Hyaluronic acid and so forth.
2. Phase behaviour of ligand capped nanoparticles
3. Manipulation of reverse osmosis membranes
4. Time dependent perturbation of colloidal structures