

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE
2A & 2B, Raja S.C. Mullick Road, Jadavpur, Kolkata-700032, India

Seminar Notice

Speaker: Dr. Suman Majumdar, Institut für Theoretische Physik, Universität Leipzig, Germany

Date & time: 25 Feb (Tuesday), 3:45 pm

Venue: C-406, Theo. Phys. Seminar Room, Centenary Building

Title: Out of equilibrium dynamics of Macromolecular transition

Abstract: Understanding the dynamics of collapse transition of a polymer is intriguing considering the fact that collapse of the backbone polypeptide forms an integral part of the overall folding of a protein. Although, the equilibrium aspects of this transition have been extensively studied, the nonequilibrium kinetic pathways of collapse has received lesser attention. In my talk, I will demonstrate how to explore this kinetic pathways by drawing analogies with the usual coarsening phenomenon popular in spin (magnetic) or particle (fluid) systems. Thus, borrowing corresponding tools one can easily understand the kinetics in terms of various scaling laws related to the collapse time, growth of a relevant length scale, etc. As a step further, this also provided evidence of aging and corresponding dynamical scaling during collapse. In the early part of my talk I will discuss all these while presenting simulation results obtained from simple model homopolymers with implicit solvent. In the latter part, I will show that how these understandings can be extended to real biological polymers via all-atom molecular dynamics simulations of real polypeptides in water.

Selected References

- S. Majumder and W. Janke, Phys. Rev. E **93**, 032506 (2016)
- S. Majumder, J. Zierenberg, and W. Janke, Soft Matter **13**, 1276 (2017)
- H. Christiansen, S. Majumder, and W. Janke, J. Chem. Phys. **147**, 094902 (2017)
- S. Majumder, U.H.E. Hansmann, and W. Janke, Macromolecules **52**, 5491 (2019)
- S. Majumder, H. Christiansen, and W. Janke, arXiv:1910.03394 (2019)

All are cordially invited to attend the seminar