Dr Debashish Mukherji

Max-Planck Institut für Polymerforschung

Mainz, Germany

Debashish Mukherji is a Computational Soft Matter Physicist. He studied Physics at the Banaras Hindu University, completing a Masters degree in 2001. For his doctoral studies he moved to the University of Western Ontario, Canada, where he investigated the effects of surface roughness and commensurability on the dynamics of polymers in high geometric confinements using molecular dynamics simulations. He was then appointed as a research associate in the Army Material Center of Excellence at Drexel University, USA, where he designed and fabricated advanced glassy network polymeric materials. Recently, he joined the theory group of the Max-Planck Institute for Polymer Research in Mainz, Germany. He is the recipient of numerous research and teaching awards.

Plenary Lecture:
Soft Matter Properties: What can we learn from computer simulations?

I will present three unrelated examples in which efficient computer simulations have been employed to address soft matter properties. The first example will deal with the dynamics of polymers near surfaces. Despite the significant progress within the last decade, in particular on the structure and thermodynamic properties in confinement, their dynamics remained an active field of research. Unlike some of the prior studies, we introduced atomic scale roughness of the confining surface(s) while abstaining from introducing any artificially-imposed divergent obstacles. Because of this type of modeling, we could reproduce the scaling of the single polymer dynamics near attractive surface and relate the dynamics of adsorbed polymer films with the degree with which they interlock with the surface. The second example will explore the mechanical behavior of highly cross-linked polymer (HCP) glasses; such as epoxy and vinyl-ester thermosets, which are used as both high-strength adhesives and as composite matrices. One particular property of HCPs which limits their usefulness is their lack of toughness. Fully cured epoxies, for example, can have about 2 GPa of tensile strength but are brittle, failing at about 1% strain. Using computer simulations, we were able to devise ways of toughening the HCP networks by introducing engineered micro-voids. We have also performed experiments on amine cured epoxy networks by introducing voids using reactive encapsulation of nonreactive solvent tetrahydrofuran. The experiments were consistent with our prediction. Lastly, as the third example, I will briefly mention our recent work on the solvation properties of liquid mixtures using an Adaptive Resolution Molecular Dynamics Scheme in which particles can change their resolution (atomic or coarse-grained) on the fly.