Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

TIFR-UoH (Chemistry) Seminar Series

Paracetamol Aggregation in Biocompatible Polymers - Role of Interactions and Topology

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Heterogeneous nucleation of molecular systems in solution is a grand challenge. The current understanding of heterogeneous nucleation is limited only to simple, model systems like Lennard-Jones particles due to lack of apriori knowledge of reaction coordinates and simulation techniques to explore heterogeneous nucleation of complex molecules in solution. We proposed that direct molecular dynamics simulations techniques could be employed to study the factors that effect aggregation (pre-nucleation) in complex systems and could be correlated with factors that control nucleation. In this direction, we elucidated the role of topology and interactions in the formation of pre-nucleation aggregates of paracetamol in porous, polyethyelene glycol diacrylate (PEGDA) polymers and thin films of cellulose derivatives using direct molecular dynamics simulations techniques. The simulation results for probabilites of formation of paracetamol aggregates are consistent with experimentally observed rates of paracetamol nucleation in different polymers. The study of pre-nucleation stages using direct molecular dynamics simulation techniques could provide a faster route to generate libraries of polymers that could be employed to enhance heterogeneous nucleation of paracetamol.

Tuesday, Jan 30th 2018

04:00 PM (Tea/Coffee at 03:30 PM)

Auditorium, TIFR-H