

Seminar

What is the structure of a simple liquid?

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We present a simple geometric method for structural characterization of heterogeneous dynamics observed in soft materials. A simple mono-disperse Lennard-Jones system in two dimensions is considered as a model system. At a fixed temperature, spatio-temporal heterogeneity is demonstrated by the spatial map of mobility of individual particles, computed from the simulated trajectories for a range of densities. Nearest neighbor shell of each particle is identified using an adaptive solid angle based method. Quantifying the shape of these shells reveals three geometric populations with distinct thermodynamic and dynamic properties consistent across all densities and thus, identifies the key structural components of dynamical heterogeneity. Such a characterization can be extremely useful to answer the long-standing question of structure-dynamics relation in much complex systems, such as glassy materials.

Wednesday, Mar 28th 2018

4:00 PM (Tea/Coffee at 03:30 PM)

Auditorium, TIFR-H