MONDAY

COLLOQUIUM

Machine learning phase and glass transitions

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8 Sep 2025 (Monday) | 16:00 Hrs (Tea / Coffee 15:45 Hrs) | Venue: TIFRH Auditorium

The phase behaviour of complex mixtures is important in many applications and understanding them from a molecular perspective is of fundamental importance. Molecular simulation of complex fluids has become feasible, but elucidating the phase behaviour is difficult. In this work we describe machine learning (ML) methods for the phase behaviour of complex fluids. We show that with a robust input feature, unsupervised machine learning methods can predict the phase behaviour of a variety of lattice and continuous-space models in quantitative agreement with conventional simulations. The method can also be extended to study the dynamics and is applied to the glass transition in model glass formers.

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