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Simulation studies of glassy nanoclusters

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Glassy materials are amorphous solids usually formed by rapidly cooling a liquid below its equilibrium freezing temperature, trapping the particles in a liquid-like structure at the glass transition temperature. While appearing throughout nature and industry, these systems continue to challenge the way we think about the dynamics and thermodynamics of condensed matter and a fundamental understanding of the glass state remains elusive. This talk describes molecular simulation studies of glassy behaviour in binary Lennard–Jones nanoclusters. We show that the relaxation dynamics of the clusters is nonuniform and the core of the cluster goes through a glass transition at higher temperatures than at the surface. As the nanoclusters are cooled, they also exhibit a fragile–strong crossover in their dynamics and we explore how this phenomena is linked to the potential energy landscape of the clusters. Finally, we compare the properties of nanoclusters formed through vapour condensation, directly to the glassy state, with those of glassy clusters formed through traditional supercooling. The condensation clusters are shown to form ultra-stable glassy states analogous to the ultra-stable glasses formed by thin film vapour deposition onto a cold substrate. In all, our work suggests that nanoscale clusters exhibit some unique glassy features, while also offering potential insights into the fundamental nature of the glass transition.