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Phase behavior of the 38-atom Lennard-Jones cluster RAY SEHGAL, DAVID FORD, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We have developed a coarse-grained description of the phase behavior of the isolated 38-atom Lennard-Jones cluster (LJ_{38}). The model captures both the solid-solid polymorphic transitions that the cluster undergoes at low temperatures and the complex cluster breakup and melting transitions at higher temperatures. For this coarse model development, we employ the manifold learning technique of diffusion mapping. The outcome of the diffusion mapping analysis over a broad temperature range indicates that two order parameters are sufficient to describe the cluster's phase behavior; we have chosen two such appropriate order parameters that are metrics of condensation and overall crystallinity. In this well-justified coarse-variable space, we calculate the cluster's free energy landscape (FEL) as a function of temperature, employing Monte Carlo umbrella sampling. These FELs are used to quantify the phase behavior and onsets of phase transitions of the LJ_{38} cluster.

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