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Molecular simulation of crystal nucleation of an n-alkane PENG YI[1], GREGORY RUTLEDGE[2], Massachusetts Institute of Technology — We report the results of molecular simulations to study crystal nucleation of n-octane from the melt. A realistic united atom force field was employed for n-octane. The melting behavior was first determined by ramping temperature in a set of Monte Carlo simulations. The adiabatic nucleation trajectory was then sampled using the umbrella sampling technique with a set of proposed global and local order parameters, and analyzed for selection of best order parameter. The transition state ensemble has been verified by molecular dynamics simulation. The structure of critical nuclei in the nucleation process is analyzed and the effect of intermediate phases discussed.

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