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Title: Analysis of homogeneous droplet nucleation for anisotropic particles using molecular dynamics simulations

Annotation:

Nucleation is an initial molecular level phenomenon of the first order phase transition and it has been investigated more than a half-century. However, a large gap between experiment and theory exists when appraising the nucleation rate because the classical nucleation theory (CNT) with all its modifications, assuming the spherical droplet for instance, still cannot fully incorporate the dynamics of homogeneous nucleation. This molecular dynamics study focuses on the uniaxial anisotropic particles and analyzes the nucleation rate difference and cluster formation process using alkane molecules and uniaxial anisotropic particles like liquid crystal.