MIT Chemical Engineering Department

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Solute precipitate nucleation: toward reliable theories and processes

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3:00pm, refreshments at 2:45pm

66-110

Abstract:

Nucleation is the activated process by which stable embryos are born to initiate a phase transition. Following an introduction to nucleation theory and simulation methods, I will highlight special challenges posed by solute precipitate nucleation. For homogeneous solute precipitate nucleation, these challenges have been partly overcome by new seeding methods and specialized rare events tools. In practice, nucleation rates remain difficult to predict and control due to heterogeneous nucleation events at sites with unknown characteristics. There are two potential strategies to promote the more predictable homogeneous nucleation pathway: (i) use soluble nucleants that accelerate nucleation by binding to surfaces and thereby lowering interfacial free energies, or (ii) use *in situ* solute (or anti-solvent) generation reactions to drive a LaMer burst, i.e. a sudden surge of homogeneous nucleation events. Theoretical models for both strategies will be compared to data from simulations and experiments.