



**Professor
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*Solute Precipitate Nucleation: Advances in
Theory and Simulation Methods*

Nucleation is the stochastic process that creates the first stable embryo of a new phase to initiate a phase transition. The mechanism is poorly understood because rare event processes like nucleation present special challenges to both experiments and simulations. The difficulties are particularly acute for multi-component condensed phase nucleation processes. New rare events approaches that reveal how thermodynamic and dynamical factors in nucleation will be presented. Particular emphasis will be given to the factors that influence polymorph selection including disparate growth rates of competing polymorphs, and the effects of additives on the free energy landscape. Finally, we will examine assumptions about interfacial free energies as a possible origin for continuing discrepancies between experimental and theoretical nucleation rates.

**Monday, April 4, 2016
4:00 P.M.
2033 Young Hall**