

Keynote Lecture

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Atomistic Modeling of Crystal Nucleation and Growth

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Understanding crystal growth from solution is crucial to control the development of crystal morphologies. Since the interaction of crystals with their environment occurs through their surface, their shape controls a wide variety of properties. This is particularly important not only in nanotechnology, where shape-function relations play a key role, but also in medicine where, e.g., changing the morphology of particles allows for a better targeting of cancer cells. In this work we combine experiments, molecular simulations and theory to examine the morphology of urea crystals grown in different solutions. In order to get a rational representation of all the possible habits we introduce a Shape Diagram in which the habit dependence on the relative growth rates is displayed. A wide portion of the habit space can be experimentally explored by varying the composition of the mother solution. By doing so we obtain morphologies ranging from the paradigmatic needle-like habit obtained in water to regular tetrahedra obtained in acetonitrile/biuret mixtures. By combining advanced molecular simulation techniques and theory we can predict urea steady state crystal habits and their dependence on additive concentration and/or supersaturation, paving the way towards a rational control of the habit of crystals grown from solution. We present also some other example of nucleation processes which will lead to some rather surprising results even in the case of humble NaCl. Finally we discuss some recent advances that allow us to calculate nucleation rates.

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