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Vapor and Condensed Phase Clusters¹ SHAWN KATHMANN, Pacific Northwest National Laboratory

Given the difficulty of directly observing clustering mechanisms underlying nucleation, classical and *ab initio* statistical mechanics provide crucial insight into the thermodynamics and kinetics of these processes. Recent experiments have shown nucleation can emit (e.g., crystalloluminescence) and be induced (e.g., IR lasers) by electromagnetic radiation. This opens up the possibility of using luminescence as an exquisite probe of the nucleation mechanism in addition to doing the reverse process by imposing external electromagnetic fields to activate specific modes of nucleation. The inclusion of electronic degrees of freedom as well as excited electronic states lies beyond classical theory. In addition, the osmotic coefficients of sub- and supersaturated aqueous electrolytes may provide quantitative insights into salt cluster distribution functions and free energies of crystal formation. Here we outline the chemical physics relevant to these findings and their consequences on how we understand and model nucleation to control and exploit the synthesis of matter.

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