The Birth and Growth of Salt Crystals: Insights from Molecular Dynamics Simulations

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Molecular dynamics simulations are used to investigate the factors that influence the nucleation of salt crystals in supersaturated aqueous solution. Two salts, NaCl and LiF, will be considered. We describe a methodology for detecting solid-like clusters and following their evolution in time until they achieve nucleation or dissolve back into solution. Through an analysis of cluster lifetimes and multiple nucleation events, we demonstrate that for NaCl cluster size is not the only property that influences cluster stability and the probability of achieving nucleation. We define a parameter called the cluster crystallinity, which is a measure of the solid-like order of a particular cluster. We demonstrate that the cluster order has a strong influence on the lifetime and nucleation probability of clusters of equal size, with the lifetime and probability of nucleation increasing with increasing crystallinity. These observations remain true for clusters as small as six ions indicating that the structural factors are important even at the very earliest stages of crystal birth. For LiF, we show that ion solvation has a dominate influence on the rates of crystal nucleation and growth.