

The Effect of Urea on the Morphology of NaCl Crystals: a Combined Theoretical and Simulation Study

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It has been known for over a century that the presence of cosolvents such as urea and formamide can alter the morphology of NaCl crystals grown from solution. To help understand this effect we have been developing a theoretical approach based on the Kirkwood-Buff (KB) theory of solutions, and combine this with computer simulations of the interaction of urea with different crystal faces of NaCl. In this way one can predict the effect of urea on the thermodynamic stability of different NaCl faces, with atomic level detail provide by the simulations. We observe that urea is preferentially excluded from 100 and 111 crystal faces, but is less excluded from 111 faces which present chloride ions at the surface. This helps to explain why the 111 face is stabilized in urea solutions and promotes the formation of octahedral over cubic NaCl crystals. The approach is totally general and can be applied to understand a variety of interfacial properties.