



## *Freezing Water: Thinking Outside the Box*

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“The box” represents classical nucleation theory, CNT, a conceptually simple and at first appealing mechanism in which the interfacial energy between an initial, unstable phase (liquid water, here) and a stable one (ice) constitutes an energy barrier against the stable one’s first appearance. Ice nucleation obviously involves crystal growth, but the theory of CNT in general has been based upon thermodynamics and chemical reaction theory, independent of crystal structure. Outside the box here is treating crystal growth and nucleation in terms of growth of the known hydrogen-bond network of ice: the ice crystal structure and its tetrahedral bonding. The initial context here was trying to explain the observed correlations between ice crystal growth in liquid water and the ice crystal structure, part of which appeared to involve two-dimensional nucleation of new molecular layers at an interface between ice and liquid water. This explanation turned out not to work well whereas a simple model of growth of the bonding network does seem to provide conceptual understanding. A bonding-network approach to homogeneous nucleation is unwieldy but interesting, and from that point of view, CNT (for nucleating ice) seems dubious. The actual mechanism may be dominated by structural effects, not interfacial energy.

*This seminar will be webcast live at:*

*<http://ucarconnect.ucar.edu/live>*

*Recorded seminar link can be viewed here:*

*<https://www.mmm.ucar.edu/events/seminars>*

**Thursday, 22 March 2018, 3:30 PM**

Refreshments 3:15 PM

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