



Seminar

Simulating ice nucleation one molecule at a time: from the smallest piece of ice to five sided snowflakes!



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- **Time: 13:30, Dec. 9, 2010 (Thursday)**
- **Venue: Conference Room A (607), No. 5 Science Building**

Abstract

Water is not easy to freeze! The homogeneous freezing point of pure water is some 30-40 degrees below zero. Invariably then when water freezes it does so heterogeneously on the surface of some foreign particle. In this talk I will discuss our recent first principles simulations of such heterogeneous ice nucleation events on a variety of solid surfaces. I will show how the subtle interplay of bonding within the overlayers and to the substrate conspires to yield a rich variety of structures, including even ice structures built from pentagons. I will also show how surprisingly strong quantum nuclear effects can lead to hydrogen bond symmetrisation in certain ice overlayers on metal surfaces [1-5].

1. A. Michaelides and K. Morgenstern, *Nature Mater.* 6, 597 (2007)
2. D. Pan et al., *Phys. Rev. Lett.* 101, 155709 (2008)
3. H. Gawronski et al. *Phys. Rev. Lett.* 101, 136102 (2008)
4. J. Carrasco et al. *Nature Mater.* 8, 427 (2009)
5. X.-Z. Li et al. *Phys. Rev. Lett.* 104, 066102 (2010)