

## A molecule's eye view of water at interfaces

Angelos Michaelides, London Centre for Nanotechnology, University College London  
[www.chem.ucl.ac.uk/ice](http://www.chem.ucl.ac.uk/ice)

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].

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