

O 16 Invited talk Michaelides

Time: Tuesday 10:15–11:00

Room: TRE Phys

Invited Talk

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Ab initio Ice Growth at Metal Surfaces — ●ANGELOS MICHAELIDES — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Few physical processes are as ubiquitous or feature more prominently in our daily lives than the nucleation of water into ice. Typically this process is aided by a so-called ice nucleating agent; a microscopic substrate that in essence catalyses the nucleation process. Remarkably little is known, however, about these seemingly simple "catalytic" processes, particularly at the all-important atomic and molecular level.

Here we present the results of density-functional theory simulations for ice nucleation on model (metal) substrates, which aim to put our understanding of catalysed ice nucleation on a much firmer footing. A particular focus will be placed on how the competing influences of substrate reactivity and water cluster-substrate epitaxial mismatch conspire to yield a rich variety of (novel) ice-like structures. Moreover, the key molecular clusters that are accessed en route to ice crystal growth will be presented and how these differ from gas phase water clusters discussed.

This work has been performed in collaboration with Matthias Scheffler