

WIENER PHYSIKALISCHES KOLLOQUIUM

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Einladung zum Vortrag von

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www.chem.ucl.ac.uk/ice

Structure and dynamics of water at interfaces: “Surfing” water droplets and ice formation

Water/solid interfaces are relevant to a broad range of physicochemical phenomena and technological processes such as corrosion, lubrication, heterogeneous catalysis and electrochemistry (Nature Mater 11, 667 (2012)). In this talk some of our recent computer simulation work in this area will be covered. Specifically results on water droplet diffusion on the surfaces of layered materials will be presented and a novel “surfing” mechanism for droplet diffusion discussed (Nature Mater, in press). In addition, simulations of ice nucleation on various nanoparticles with different physicochemical characteristics will be presented and the fundamental insight obtained from these into heterogeneous ice nucleation discussed (J. Am. Chem. Soc., in press). Time permitting some recent ab initio molecular dynamics results at wet interfaces in which rapid proton transfer is observed will also be discussed.

November 16th, 2015, 17:30 hrs

TU Wien-Freihaus, Hörsaal 5, 2. Stock, grüner Bereich

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