Ben Slater (UCL)

“From ices in space, to space in ices to functional framework materials”

2pm 4 Mar 2015 / Ingram Lecture Theatre

In this talk, I will present something of a smorgasbord of my research: work in my group has two broad themes, characterisation of water ices and functional porous materials (primarily zeolitic and metal-organic frameworks) using computational approaches, see publications at http://www.ucl.ac.uk/chemistry/staff/academic_pages/ben_slater. Water ice has a rich and increasingly structurally diverse phase diagram [1] and has structural analogues in the zeolite family (nanoporous framework silicates/aluminosilicates) [2] but these materials have wholly distinct functionality. Ice has a key role in regulating albedo on earth, it can catalyse atmospheric reactions and ice on interstellar dust particles are thought to be important in the formation of the basic building-block molecules of the universe, such as simple sugars [3]. Many ice phases, including ordinary hexagonal ice, are surprisingly hard to characterise experimentally and I will show how computational approaches can shed light on the structure of ices [4, 5] and predict unforeseen properties, such as the surface of crystalline ice has an amorphous character [6]. I will then turn to porous functional materials and briefly describe results on the prediction of acid sites and their acidity, in and on the widely used zeolite catalyst ZSM-5. Finally, I will discuss work on metal organic frameworks drawing on a recent report of a MOF with extremely high porosity and chemical stability, that owes its unique properties to a combination of ligands, which is explained through modelling [7].

[1] Falenty, Hansen, Kuhs, Nature 2014, doi:10.1038/nature14014
[2] Tribello, Zwijnenburg, Slater, Bell, Phys. Chem. Chem. Phys. 2010, doi:10.1039/b916367k.
[3] Woods et al., Astrophysical Journal, 2010, doi:10.1088/0004-637X/777/2/90.
[4] Del Ben et al., J. Phys. Chem. Lett., 2014, DOI: 10.1021/jz501985w
[5] Slater, Quigley, Nat. Mater., 2014, doi:10.1038/nmat4017
[6] Watkins et al., Nat Mater., 2011, doi:10.1038/nmat3096
[7] Kalindi et al., Ange. Chemie. Int. Ed., 2014, doi:10.1002/ange.201406