Simulation Strategies Versus Experiment in Hybrid Organic-Inorganic Frameworks

Professor Caroline Mellot
University College, London

The field of hybrid inorganic-organic materials is one of the major growth areas of materials chemistry. Hybrid frameworks show an enormous diversity of chemical and structural types, and surface properties, including flexible structures exhibiting guest-induced solid-state transformations upon gas adsorption. In such a rich context, simulations have a crucial role to play in guiding the development of the field. Here, we present how simulations, when combined with experiment, can address a variety of issues such as the structure solution and energetics of highly complex crystal structures [1], the guest-induced transformations of hybrid frameworks [2] and the related thermodynamics of adsorption [3] while being the most powerful approach in the area of structure prediction and design [4].

[1] C. Mellot-Draznieks J. Mater. Chem. 2007, 17, 4348. AJ Bailey, C. Lee, R.K. Feller, Orton JB,A. Navrotsky, C. Mellot-Draznieks, W.T.A. Harrison, MC Grossel, A. K. Cheetham, Angew. Chem. Int. Ed. 2008, 47, 8634.
[2] C. Serre, C. Mellot-Draznieks, S. Surblé et al. Science, 2007, 315, 1828. D.S. Coombes, F. Cora, C. Mellot-Draznieks, R. G. Bell, J. Phys. Chem. 2009, 113, 544. F. Salles, A. Ghoufi A, G. Maurin, R.G. Bell, C. Mellot-Draznieks, G. Ferey, Angew. Chem. Int. Ed., 2008, 47, 8487.
[3] F.X Coudert, M. Jeoffroy, A. H. Fuchs, A. Boutin, C. Mellot-Draznieks, J. Amer. Chem. Soc. 2008, 130, 14294.
[4] C. Mellot-Draznieks, J. Dutour and G. Férey, Angew. Chem. Int. Ed. 2004, 43, 6290. A. Torrisi, C. Mellot-Draznieks, R.G. Bell, J. Chem. Phys, 2009, 194703.