KN15 **Computational Crystallography.** Björn Winkler[a]
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Atomistic model calculations are now an established approach for the studies of structure-property relations. While for inorganic compounds, density functional theory-based calculations dominate, computationally more efficient "force field" models continue to maintain to play an important role as they allow to follow the trajectory of millions of atoms as a function of time.

In this contribution, I will summarize some recent studies which represent the current state-of-the-art of investigations of structure-property relations of crystals with atomistic models. The emphasis will place on explaining how atomistic model calculations complement more traditional crystallographic investigations, and to compare advantages and limitations of various approaches.

Keywords: computational crystallography

KN16 **Metal-Organic Frameworks: Synthesis and Applications.** Neil R. Champness,[a] [a]*School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK.*
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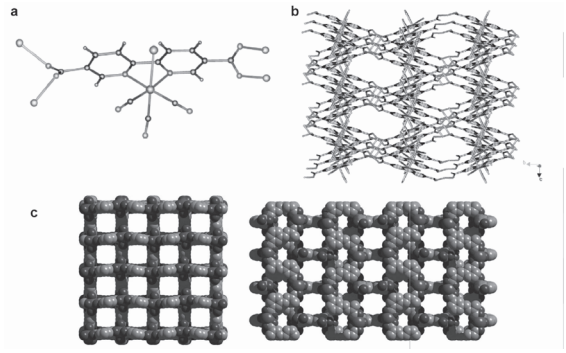
Non-covalent directional intermolecular interactions provide a pre-determined recognition pathway which has been widely exploited in supramolecular chemistry to form functional nanostructures in both solution and in the solid-state. One particular area of extensive current interest has been the exploitation of coordination bonds to prepare solid-state polymeric architectures. By controlling the geometry of the polymer components, metal cation and ligand, the structure of the resulting material can, to some extent, be predicted and controlled. As a result it is possible to design materials with specific properties [1], notably porosity for gas storage applications [2].

This lecture will present the successful application of the 'building-block' methodology [3] in preparing a range of solid-state structures commonly known as coordination polymers or metal-organic frameworks (MOFs). The talk will highlight the use of MOFs to host photoactive species [4] modifying the properties of the incorporated species (see Fig. a,b) and allowing direct crystallographic characterisation of structural transformations upon photoexcitation. Particular focus will be given to our recent efforts in preparing porous MOFs for gas storage applications [2,5,6]. Examples will focus predominantly on the storage of H_2 gas for ultimate application in the automobile industry, illustrating the influence of pore framework structure [5] and introduce the concept of using anionic MOFs to control hysteresis in gas adsorption (see Fig. c) [6].



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Keywords: Metal-Organic Framework, Hydrogen Storage, Photochemistry