Modelling gas adsorption on zeolite-like metal organic frameworks

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Abstract
In order to slow down the process of global warming it is crucial to find new routes to capture CO2 and green-house gases produced during different processes such as steam reforming of natural gas or liquid hydrocarbons to produce hydrogen. For these applications Zeolitic Imidazolate Framework (ZIF) structures incorporating transition metal ions and a great variety of functionalised organic linkers, have been recently proposed because of their interesting selective adsorption and molecular sieving properties [1]. One of the most important aspects that make ZIFs special is the fact that preferential adsorption sites are located close to organic linkers instead of metal oxides as it commonly occurs on "traditional" MOF structures [2]. This fact may explain why traditional force fields (Dreiding, UFF, etc) overestimate the gas adsorption behaviour on several of these materials. We have recently produced new experimental adsorption isotherms of gases on different solid structures which allowed us to develop a new transferable force field that takes into account this specificity [3]. The agreement between experimental and simulation data allows us to use simulations as a reliable tool for predicting adsorption properties of other ZIF materials. We will discuss the combined effect of pore size and linker chemistry upon green house gas adsorption on different ZIFs. General trends about the characteristics of an ideal adsorbent material are proposed.

[1] Hayashi, H.;Côté, P. A.; Furukawa, H.; O'Keeffe, M.; Yaghi, O. M. Nature, 2008, 453, 207-212
[2] Wu, H.; Zhou, W.; Yildirim, T., J. Am. Chem. Soc., 2007, 129, 5314-5315
[3] Perez-Pellitero, J; Amrouche, H.; Sipertstein, F.; Nieto-Draghi, C.; Pirngruber, G.; Bazer-Bachi, D.; Peralta, D.; Bats, N., in preparation.