Center for Molecular Modeling, Ghent University
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Lecture in the framework of **IAP P7/05**

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Hydrogen adsorption in metal-organic frameworks

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Talk

Hydrogen adsorption in metal-organic frameworks

Abstract

A new family of nanoporous materials is that formed by Metal-Organic Frameworks (MOFs). MOFs contain two basic secondary building units made by the metallic clusters linked through organic ligands forming a structure encompasing large pores in its interior. The large variety of metallic clusters and organic ligands and their combination rules allows a plethora of MOFs to be synthesised. The computational aided synthesis and the subsequent exploration of the existing possibilities as well as the computational assessment of their physico-chemical properties are the two main points that will be addressed in this talk. Since their discovery in 1999, the properties of MOFs as excellent absorbents were obvious and they currently compete with existing commercial processes. Separation of CO_2 from a stream of hydrocarbons coming from natural feedstocks, or hydrogen storage are applications where MOFs are good candidates to improve existing technologies. The absorption properties of MOFs are influenced, in different ways yet to be fully understood, by the metallic and the organic part depending on the gas concentration and temperature. The present talk also aims to contribute to unveil the mechanisms and intermolecular forces that govern these processes by using computational chemistry techniques.