

Séminaire du CETHIL

Jeudi 20/10/2016 à 13h30

Salle 230, bâtiment Carnot

Investigating the molecular behaviour of water in nanostructures for thermal storage and molecular separation

Auteur :

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Sujet du séminaire :

When water is confined in nanostructures, or forced to pass thorough them, it reveals some peculiar behaviour due to its underlying molecular nature. Taking into account such effect may be problematic, but it offers also novel opportunities. In this talk, I will discuss two examples based on zeolites.

First of all, we will investigate the possibility to use zeolites for thermal storage. I will present a hybrid (molecular dynamical + Monte Carlo) numerical approach, validated against experimental data from literature, for predicting both adsorption and infiltration isotherms of zeolite-water pairs. The approach is general and it can be used for other pairs as well. Adsorption isotherm data are critical for designing optimal sorption heat storage cycles.

Secondly, I will present the challenges for molecular separation by zeolite-based membranes. Infiltration isotherms are essential for assessing the performances of molecular sieve for next-future desalination (or other separation) processes. Numerical evidences show that a simple Dubinin-Astakhov model can be safely used (and physically interpreted) for describing the infiltration process. However, from the practical point of view, the role of surface barriers remains elusive.

Invité par :

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