Contribution ID: **805** Type: **Oral 20 Minutes**

Adsorption and Transport in Multiscale Porous Media

Wednesday, 16 May 2018 11:35 (15 minutes)

Hierarchical porous materials such as hierarchical zeolites, which combine several porosity scales, are widely used in industry (adsorption, separation, catalysis) to overcome slow diffusion in microporous solids (< 2 nm) and enhance access to their large surface area. Available modeling approaches for adsorption and transport in such multiscale porous media are limited to empirical parameters which cannot be derived from molecular coefficients. In particular, existing approaches do not offer the ground for a bottom up model of adsorption/transport in multiscale materials as (1) they describe empirically the adsorption/transport interplay and (2) they do not account for the breakdown of hydrodynamics at the nm scale.
In this talk, I will present a multiscale model of adsorption and transport in hierarchical materials obtained by adding mesopores (~ few nm) and macropores (> 10 nm) to existing microporous crystals [1]. I will first show how adsorption, permeance, and transport in such media can be described without having to rely on macroscopic concepts such as hydrodynamics [2,3]. Using fundamental parameters and coefficients available to simple experiments, we will see how transport coefficients can be rigorously obtained from simple models in the framework of Statistical Mechanics. Then, I will present a multiscale model of adsorption and transport in hierarchical materials [4]. This approach consists of upscaling accurate molecular simulations in a lattice model. Thanks to the use of atom-scale simulations, which capture the different adsorption and transport regimes upon varying the temperature, pore size, pressure, etc. this bottom-up model does not rely on hydrodynamics and, hence, does not require assuming a given adsorption or flow type. I will also discuss NMR experimental results on transport in hierarchical zeolites [5].

References

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Session Classification: Parallel 7-G

Track Classification: GS 1: Fundamental theories of porous media