Contribution ID: **14** Type: **Oral Presentation**

Unusual coexisting adsorption and structural transformations mechanism in Nano-Porous Materials

Monday, May 20, 2024 2:50 PM (20 minutes)

The phase behavior of confined fluids adsorbed in nanopores differs significantly from their bulk counterparts and depends on the chemical and structural properties of the confining structures. In general, phase transitions in nanoconfined fluids are reflected in stepwise adsorption isotherms with a pronounced hysteresis. Here, we show experimental evidence and an in-silico interpretation of the reversible stepwise adsorption isotherm which is observed when methane is adsorbed in the rigid, crystalline metal– organic framework IRMOF-1 (MOF-5) [1]. In a very narrow range of pressures, the adsorbed fluid undergoes a structural and highly cooperative reconstruction and transition between low-density and high-density nanophases, as a result of the competition between the fluid–framework and fluid–fluid interactions. This mechanism evolves with temperature: below 110 K, a reversible stepwise isotherm is observed, which is a result of the bimodal distribution of the coexisting nanophases. This temperature may be considered as a critical temperature of methane confined to nanopores of IRMOF-1. Above 110 K, as the entropy contribution increases, the isotherm shape transforms to a common continuous S-shaped form [2] that is characteristic to a gradual densification of the adsorbed phase as the pressure increases. The other IRMOF structures have been also modeled and the results compared to the IRMOF-1 case. The density distribution shows symmetric structures which structural properties evolve in a function of uptake and temperature [3]..

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Session Classification: Monday

Track Classification: Oral Presentations