Contribution ID: **221** Type: **Oral 20 Minutes**

Adsorption induced transformations of methane adsorbed in MOF-5

Tuesday, 15 May 2018 10:26 (15 minutes)

At the nanoscale the positions of coexistence lines on the phase diagrams are shifted and their new locations depend mainly on the size and shape of the nano-confinement, the structure of the confining walls, and their interaction with the confined substance. Here we show that it is possible to induce structural transformations in a confined system by simply varying the number of molecules adsorbed in the pore. We found that the mechanism of these novel, adsorption-induced structural transformation in nano-pores differs from the capillary condensation. First, the structure of the confined gas is determined by a competition between adsorption sites attractive forces and intermolecular interaction. Second, at low temperature, the transformation is discontinuous because it is defined by limited number of adsorption sites [1,2].
The confined, equilibrium structures are not characterized by mean positions of molecules but rather by a probability distribution of molecular positions around adsorption centres. This distribution changes when the number of molecules in the pore increases. The character of transformation is temperature dependent: strongly discontinuous at low temperature, it evolves into a continuous transition when the temperature increases. The mechanism of the transformation is also modified when the size of the gas molecules and types of interaction change. In particular, we report the existence of the intermediate phase, observed only above a critical strength of the attractive interactions.

References

1. Heterogeneous melting of methane confined in nano-pores. Dundar, E.; Boulet, P.; Wexler, C.; et al. JOURNAL OF CHEMICAL PHYSICS Volume: 145 Issue: 14 Article Number: 144704 Published: OCT 14 2016
2. Adsorption-Induced Structural Phase Transformation in Nanopores. Kuchta, Bogdan; Dundar, Ege; Formalik, Filip; et al. Angewandte Chemie Published: 2017-Nov-01 (Epub 2017 Nov 01)

Acceptance of Terms and Conditions

Click here to agree

Primary authors: Prof. KUCHTA, Bogdan (Aix-Marseille University); Mr FORMALIK, Filip (Wrocław University of Technology Faculty of Chemistry Group of Bioprocess and Biomedical Engineering); Prof. FIRLEJ, Lucyna (University of Montpellier); Dr LLEWELLYN, Philip (Aix-Marseille University)

Presenter: Prof. KUCHTA, Bogdan (Aix-Marseille University)

Session Classification: Parallel 3-E

Track Classification: MS 1.12: Fluids in Nanoporous Media