

Contribution ID: 26 Contribution code: **Board 59**Type: **Poster Presentation**

In-Silico Analysis of the Mechanical Properties of Fluid-Saturated Zeolites

Monday, May 20, 2024 7:10 PM (20 minutes)

Fluids exhibit different thermodynamic properties in confinement compared to their bulk state. Their boiling and melting temperatures shift, their densities are lower than their bulk phase, and their mechanical properties, such as the elastic modulus, alter depending on the pore size [1]. These phenomena have been analyzed previously through computational models, such as molecular simulations, although the focus on understanding the altered mechanical properties in confinement has primarily centered on mesopores rather than micropores. There were previously only several attempts to study such effects in micropores, including Dobrzanski et al. [2], who analyzed how variations in pore geometry and size influence the mechanical properties of fluids confined in micropores. However, due to the distribution of fluid molecules, when confined in a micropore, being far from the normal distribution, these studies presented a challenge for applying a fluctuation theory to calculate the mechanical properties of a fluid through molecular simulations.

In this work, we studied the elastic properties of nitrogen and carbon dioxide adsorbed in micropores. As a model system, we focused on a recent molecular simulation study of gas adsorption in LTA4A and NaX zeolites [3]. We extended the results obtained in [3] by calculating the mechanical properties of adsorbed nitrogen and carbon dioxide using the fluctuation theory. We found that the enhancement of the elastic modulus is observed in micropores, even when the densities of the adsorbed fluid are lower than in the bulk phase. We concluded that this effect is due to reduced fluctuations in the adsorption of the fluid. We showed that similar calculations can be applied to any fluid adsorbed in a micropore. Therefore, our results bring a deeper insight into the characterization of confined fluids in micropores.

References:

1. C.D. Dobrzanski, B. Gurevich, G. Y. Gor, Elastic Properties of Confined Fluids from Molecular Modeling to Ultrasonic Experiments on Porous Solids, *Applied Physics Reviews*, 8 (2021) 021317.
2. C.D. Dobrzanski, M. A. Maximov, G. Y. Gor, Effect of Pore Geometry on the Compressibility of a Confined Simple Fluid, *The Journal of Chemical Physics*, 148 (2018) 054503.
3. A. Emelianova, C. Balzer, G. Reichenauer, G. Y. Gor, Adsorption-Induced Deformation of Zeolites 4A and 13X: Experimental and Molecular Simulation Study, *Langmuir*, 39(2023) 11388-11397.

Primary author: Mr FLORES ROMAN, Santiago (New Jersey Institute of Technology)

Co-authors: Dr EMELIANOVA, Alina (Princeton University); Prof. GOR, Gennady (Princeton University, NJIT)

Presenter: Mr FLORES ROMAN, Santiago (New Jersey Institute of Technology)

Session Classification: Poster Session

Track Classification: Poster Presentations