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Acoustic Response of Fluid Adsorption in Nanoporous Materials

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Fluid adsorption and transport in nanoporous materials are at the heart of efficient technologies impacting our economy/ecology: energy storage/conversion, environment protection, health/human welfare, agribusiness/food science, etc. In particular, nanoporous solids shaped as membranes are expected to play a leading role in the "seven key chemical separations to change the world"1 but also to address increasingly complex problems such as bio/agropollutants removal, greenhouse gas mitigation, drinkable water production, etc. With the goal to design efficient processes based on an appropriate nanoporous material for a given application, the characterization of its textural and physicochemical properties is essential to establish reliable structure/property relationships. In this context, despite its generalized use in materials science, acoustics is often assumed to be unsuited for nanoporous due to their large wavelength compared to the pore size in this class of materials. Yet, the adsorption/permeation footprint of a nanoconfined fluid is included in an average way in the signal emitted by the system subjected to fluid pressure or acoustic excitation2 (see also recent review paper by Gor and coworkers on the elastic properties of confined fluids as probed using molecular modeling and ultrasonic experiments)3.

In this work, we employ molecular modeling and theoretical approaches to unravel the acoustic signature of adsorption in nanoporous materials. Different fluid models (coarse-grained versus molecular descriptions) and with different interactions (CH_4 versus CO_2) are studied in a prototypical nanoporous material (zeolite) to probe pore size/interaction effects. We investigate the molecular mechanisms through which sound propagation and attenuation in nanoporous materials occur when subjected to fluid adsorption. Both dynamic structure factors and vibrational density of states for the fluid and solid phases are assessed to unravel the complex fluid/solid coupling at their interface and its impact on phonon modes (including their scattering which lead to sound attenuation). We will also discuss the implication of the acoustic signature of fluid adsorption for the characterization of nanoporous materials.

References:

[1] D. Sholl, R. Lively, Nature 532, 435-437 (2016).
[2] M. Miansari, J. Friend, Advanced Functional Materials 26(43) (2016).
[3] C. D. Dobrzanski, B. Gurevich, G. Y. Gor, Appl. Phys. Rev. 8, 021317 (2021)

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