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Incorporating material flexibility effects into adsorption modeling using non-local Density Functional Theory

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Among theoretical developments, the molecular density functional theory (DFT) has emerged as one of the most powerful and convenient molecular approach for the description of the thermodynamic properties of inhomogeneous fluids. The development of DFT for classical fluids originates in the late 70's [1] and its use is nowadays widespread for the description of fluid interfaces or fluids confined in nanopores, the characterization of porous materials [2], etc. The success of DFT approaches is explained by the fact that they preserve detailed information on the microstructure of inhomogeneous fluids but with a much lower computational expense than molecular simulations. Much progress has been made in recent years in the development of both: i) the formulation of more realistic free energy functionals, necessary to account for complex fluids [3], ii) and more efficient numerical algorithms to apply DFT to complex geometries [4]. DFT framework is naturally derived in the Grand Canonical ensemble, which is suitable for fluid adsorption in rigid frameworks while the appropriate thermodynamic ensemble for the treatment of adsorption in flexible porous materials is the osmotic statistical ensemble. Hence, only a very limited number of DFT-based studies addressed the flexibility of the porous network [5,6]. Few years ago, Coudert et al. [7] proposed a simplification of the osmotic configurational partition function leading to a tractable formulation of the osmotic potential to study the adsorption in flexible porous materials with molecular simulations. In this work, we use this strategy to address the adsorption of fluids in breathing adsorbents with a NLDFT framework. In particular, the adsorption in a material presenting two distinct shapes (large-pore and narrow-pore) is investigated as a representative example of breathing metal-organic framework (such as MIL-53).

Primary author: MIQUEU, Christelle (Université de Pau et des Pays de l'Adour)

Co-author: LABEYRIE, Raphael

Presenter: MIQUEU, Christelle (Université de Pau et des Pays de l'Adour)

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