Computational Investigation of Gas Pollutants Adsorption on Copper Squarate

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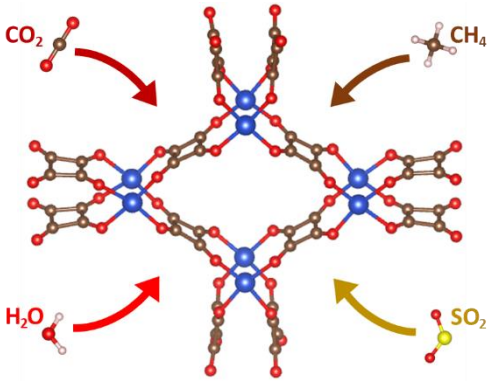

Copper squarate is a metal-organic framework (MOF) that is recognized for its potential in adsorbing gas pollutants due to its porous structure [1-3]. This study explores the adsorption of CO_2, CH_4, SO_2, and H_2O by copper squarate using density functional theory (DFT) calculations performed with the TURBOMOLE program. Following approaches [4] for other MOFs, we explore cluster representations of copper squarate. The structures of different cluster models with and without adsorbed pollutants were optimized, followed by frequency calculations to confirm their stability. Adsorption energies were then computed to assess the interaction strength, alongside an analysis of the adsorption nature. Our findings offer valuable insights into the adsorption behavior of copper squarate and pave the way for more advanced simulations, such as IR spectra and the temperature dependence of adsorption and desorption. These advancements are crucial for enhancing pollutant capture and demonstrating its potential for gas separation in environmental applications.

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