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The role of Water in Physisorption and Chemisorption of Pollutants within Copper Squarate: A DFT cluster study

Celia Adjal[1,2, †], Nabila Guechtouli[1,3], Vicente Timón[2]

[1] USTHB, Laboratory of Thermodynamics and Molecular Modeling, Faculty of Chemistry, BP32, El Alia, 16111, Bab Ezzouar, Algiers; Algeria.
[2] Instituto de Estructura de la Materia, CSIC, Serrano 121, Madrid 28006, Spain.
[3] University of M'hamed Bougara, UMMB, Faculty of Sciences, 35000 Boumerdes, Algeria.
Presenter's email address: vicente.timon@csic.es
[†] Present address (Department of Chemistry, McGill University, 801 Sherbrooke Street West, Montreal, Quebec H3A 0B8, Canada)

The global escalation of atmospheric pollutants presents a critical challenge to public health and biodiversity. To combat this, Metal-Organic Frameworks (MOFs) have emerged as first candidates due to their exceptional adsorption mechanisms skills on various pollutants [1].

We modeled our structures using Density Functional Theory (DFT) at the B3LYP-GD3(BJ) level of theory. To ensure high precision, we employed the LANL2DZ pseudopotential for Cu atoms and the 6-31G** basis set for light atoms, with all adsorption energies refined via the Basis Set Superposition Error (BSSE) counterpoise correction [2]. Our analysis explores energetic profiles by calculation of adsorption energies in both dry and humid environments of CO_2 and SO_2 pollutants to simulate real-world conditions. Structural Parameters as well as vibrational Analysis, with comparison of theoretical IR spectra with experimental data to validate the host-guest interactions.

The results reveal a nuanced interplay between physisorption and chemisorption—details often overlooked in periodic solid-state simulations. By elucidating these distinct capture mechanisms within the framework cavities, this work demonstrates the high efficiency of Copper Squarate as a robust material for targeted pollutant sequestration [3].

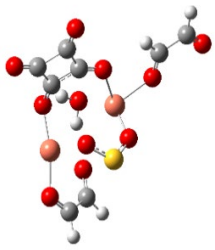

Figure 1: Optimised structure of SO_2 captured by molecular Copper Squarate and water.

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