Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information for

Adsorption of Hydrogen Sulfide on Metal-Organics Frameworks

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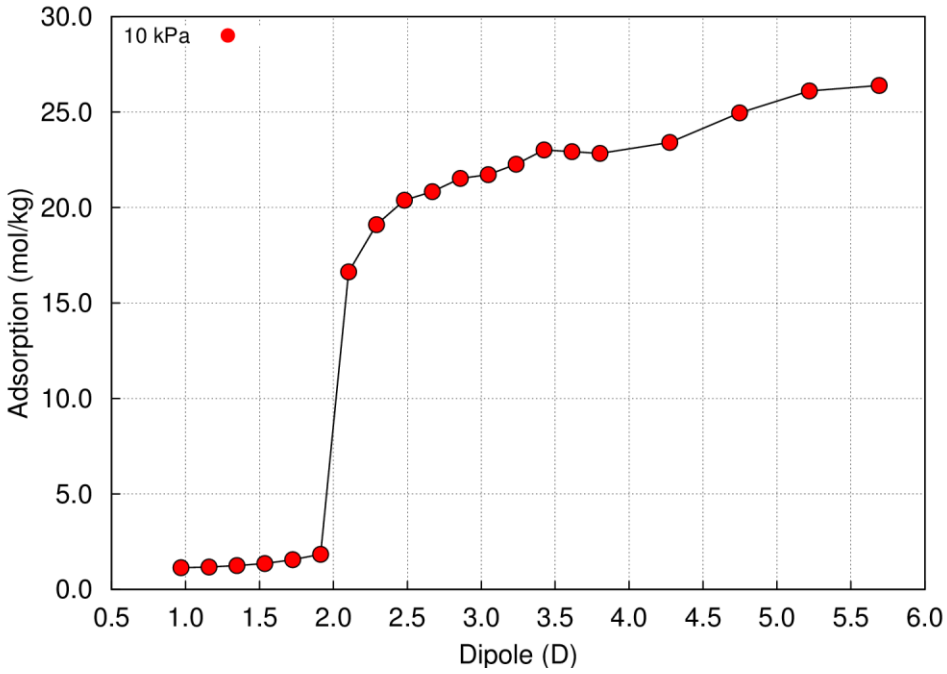
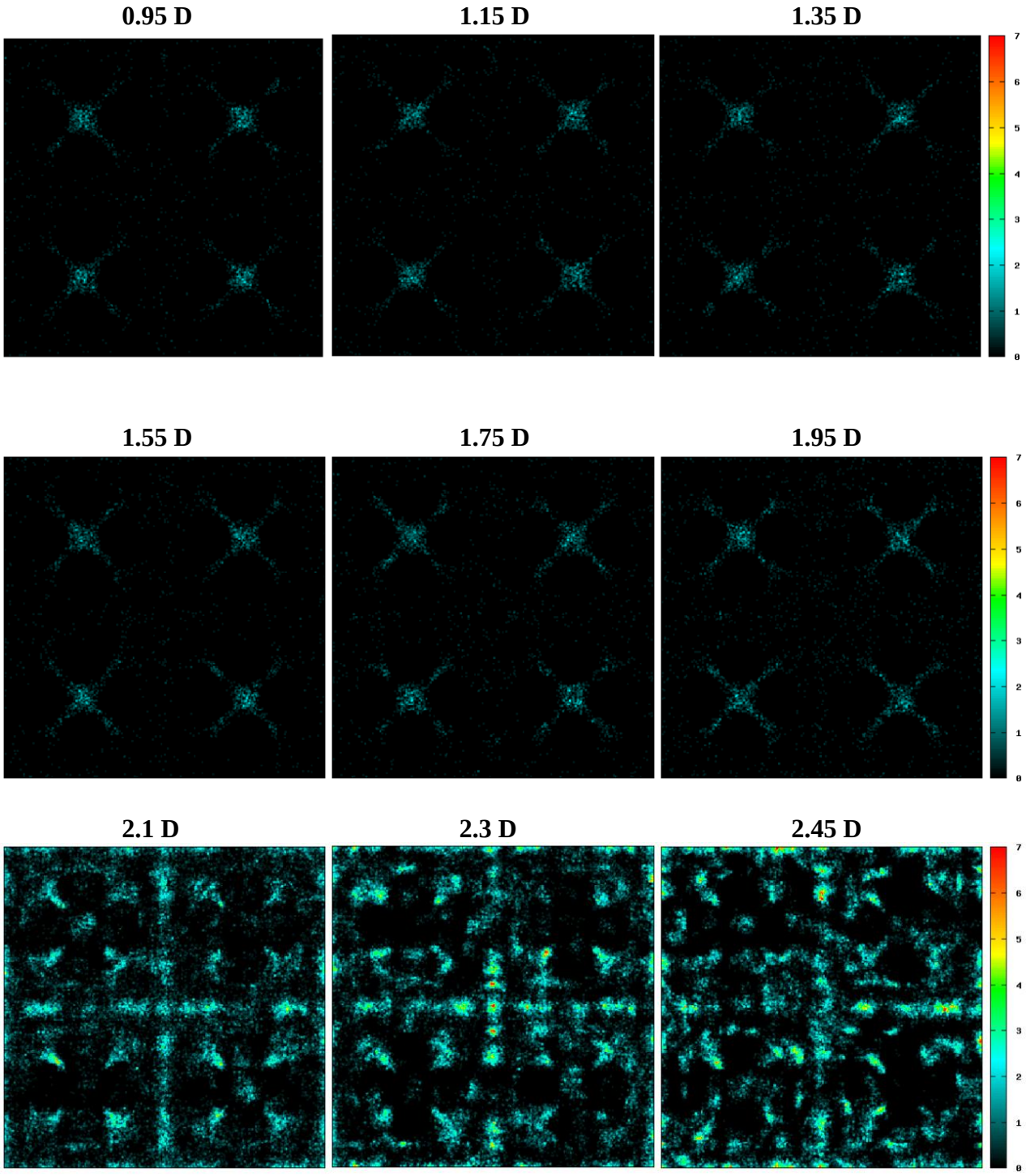
Table of Contents

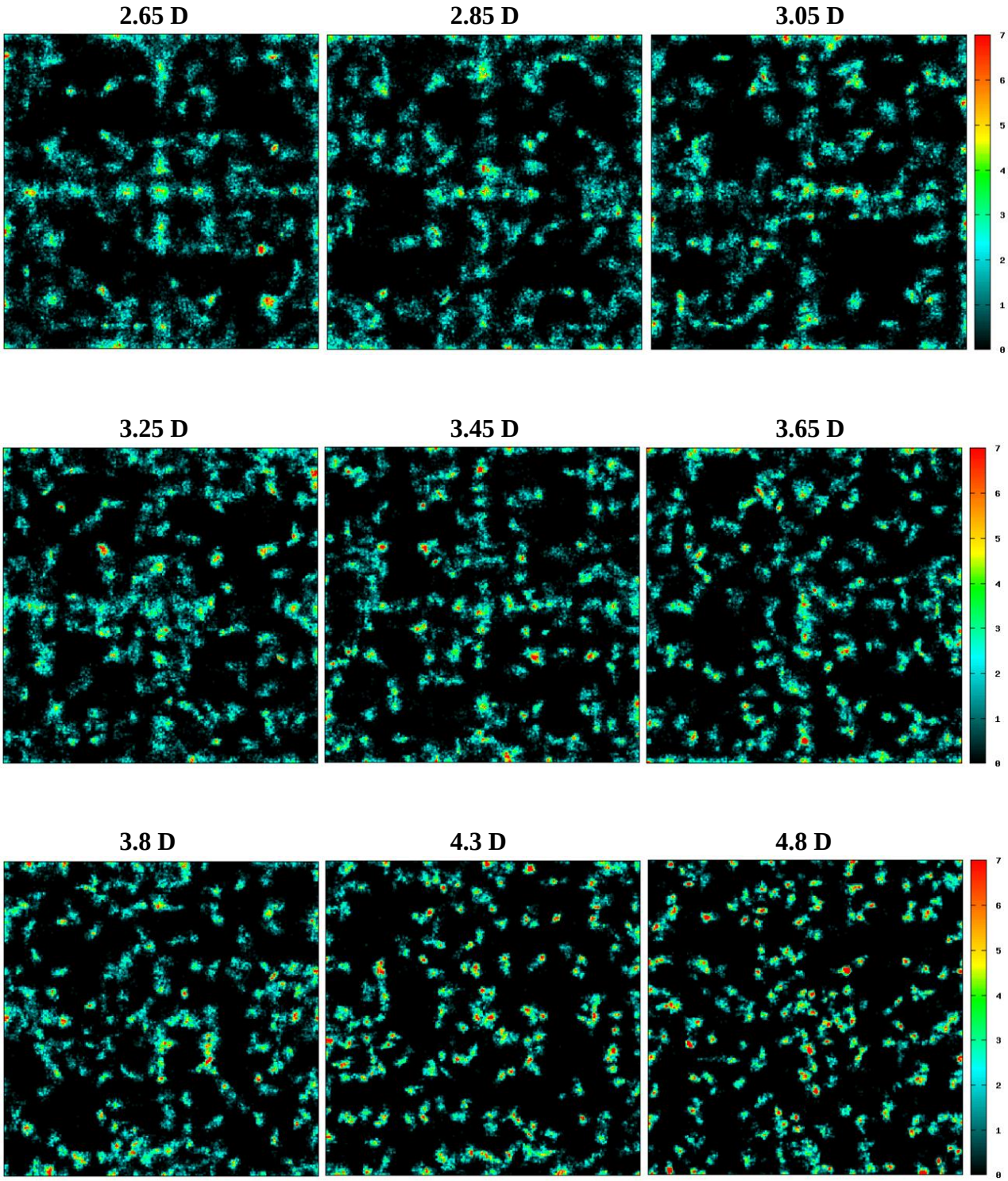
S1. Influence of the molecular dipole on the adsorption

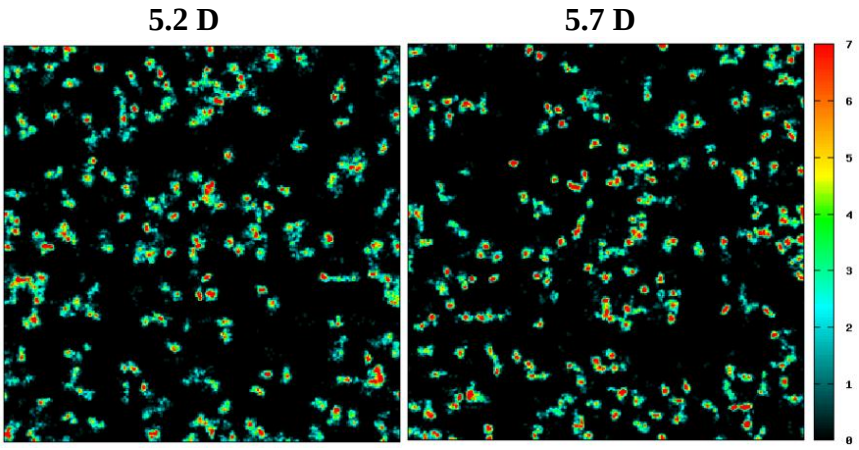


Adsorption of H_2S in Cu-BTC as a function of the dipole moment of the molecule, employing the 5S force field. The temperature is 300 K and the pressure is 10 kPa.

S2. Variation of the average occupation profile with the molecular dipole

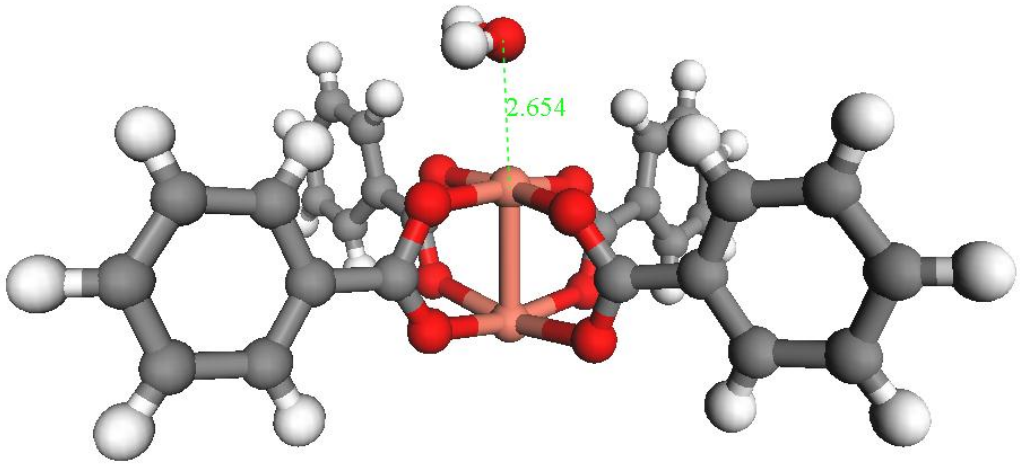




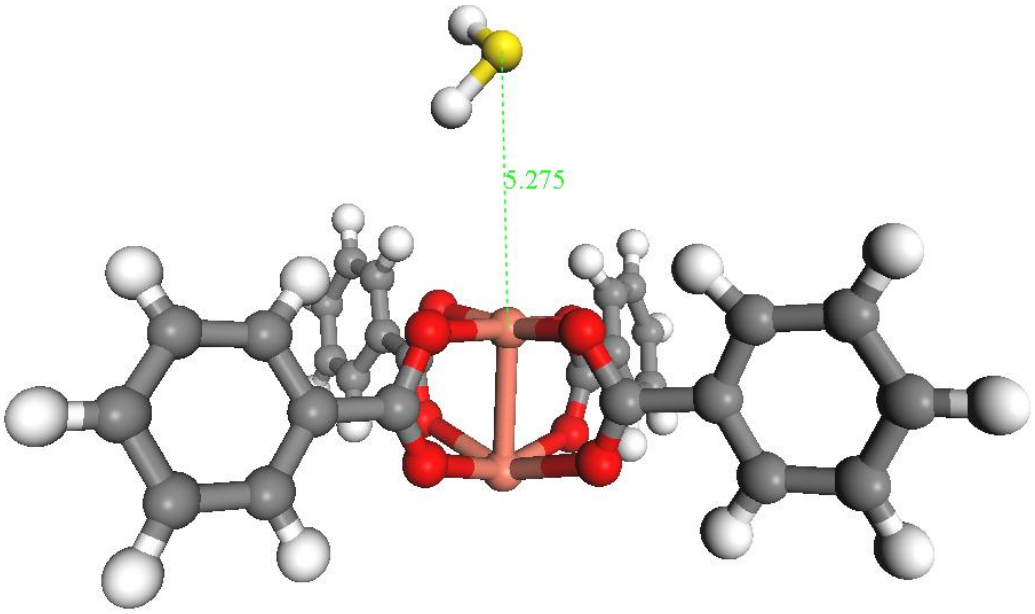


Variation of the average occupation profiles of the H_2S centers of mass (at 10 kPa and 300 K) in Cu-BTC, as the molecular dipole changes from 0.95 D to 5.7 D. The force field employed is the five-sites 5S.

S3. Snapshots of *ab initio* Molecular Dynamics simulations of H_2S and H_2O adsorbed on a cluster model of Cu-BTC



a)



b)

Snapshots of ab initio Molecular Dynamics simulations of H_2O (a) and H_2S (b) adsorbed on a cluster model of Cu-BTC. The simulations are carried out employing the Gaussian 09 code, with the Atom Centered Density Matrix Propagation molecular dynamics method. The level of theory used is HF/LanL2MB. The calculations were 3 ps long, with a time step was 0.1 fs, and the temperature was 300 K.