Effect of Magnesium alkoxide group on the CO_2 adsorption in Metal-Organic Frameworks.

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Ab-initio calculations and Grand Canonical Monte Carlo (GCMC) simulations were performed in order to study the CO_2 adsorption in Mg modified Isoreticular Metal-Organic Framework-10 (IRMOF-10). Mg cations were introduced in the linker of IRMOF-10 by creating Mg alkoxide groups on the linker of IRMOF-10. MP2 calculations on the Mg alkoxide linker showed that up to 4 CO_2 molecules were able to interact simultaneously with the Mg alkoxide group on the linker. The corresponding binding energies of the CO_2 molecules ranged from -13,6 kcal/mol to -8,9 kcal/mol. GCMC simulations were also performed with a modified 12-6 Lennard-Jones potential in order to predict the CO_2 adsorption isotherms at 300K and up to 40 bar. The predicted isotherms showed a clear enhancement of the CO_2 uptake up introduction of one and two Mg alkoxide groups on the linker with respect to the unmodified IRMOF-10, which is more pronounced at low pressures. The calculated isosteric heat of adsorption also showed that the introduction of Mg alkoxide groups on the linker greatly enhances the fluid – solid interactions between CO_2 and modified IRMOF-10.

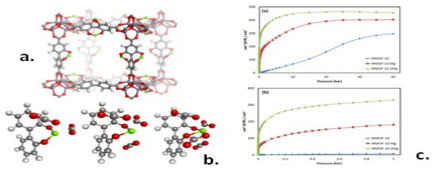

Figure 1: a. Mg alkoxide IRMOF-10 cell; b. stationary points of multiple CO_2 addition on Mg alkoxide group; c. excess volumetric adsorption isotherms of CO_2 adsorption in Mg alkoxide IRMOF-10 at room temperature.

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