Theoretical Study of CO_2 adsorption in functionalized MOFs

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As carbon dioxide is the primary greenhouse gas contributing to global warming, its storage and conversion has attract great attention in the scientific community. Many materials have been investigated for CO_2 adsorption[1]. Among all these types of materials Metal Organic Frameworks (MOFs)[2] have been attracting the major scientific interest. MOFs are organic-inorganic hybrid materials made of metal ions or clusters interconnected through an organic linker.

In present work we study the interactions between carbon dioxide and a range of functionalized aromatic molecules by using quantum chemistry methods (MP2). This study focus on design of linker molecules which could be the organic part of new metal organic framework, with the aim of improving the CO_2 adsorption capacity of the material[3].

Møller–Plesset perturbation theory within ri aproximation using the def2-TZVPP basis sets was used to compute the interaction energy between CO_2 and the various molecular functional groups. From a total of forty-four different functional groups the ten substituents with the best binding energies are**:**

OLi>OSO_3H>CNH_2NOH>SO_3H>CHNOH>OOH>SOOH>COOH>$CONH_2$>CH2OH

The results indicate that the incorporation of the OLi (8.6 kcal/mol) and OSO_3H (4.7kcal/mol) substituents in the MOF structure increases the interaction energy of the molecule with CO_2 at the most.

This research has been co-financed by the European Union (European Social Fund–ESF) and Greek national funds through the Operational Program"Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: Heracleitus II. Investing in knowledge society through the European Social Fund

1 J.C.M. Pires,F.G. Martins, M.C.M. Alvim-Ferraz, M. Simões Chemical Engineering research and design **89** 1446–1460 (2011)

2 Deanna M. D Alessandro,Berend Smit, and Jeffrey R. Long, Angew. Chem. Int. Ed. **49**, 6058 – 6082 (2010)

3 Maria G. Frysali, Emmanuel Klontzas and George. E. Froudakis ChemPhysChem **15**, 905-911 (2014)