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TITLE: Interaction between CO2 and organic-metal frameworks

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Abstract

We study trends in the binding between CO_2 and MIL-47(V) (see bottom figure) as an open-metal site (OMS) metal-organic framework (MOF) using van der Waals-corrected density functional theory. The latter method is same Grimme's functional including dispersion on periodic boundary DFT that call usually DFT-D2 .

We find that the OMS-MOF based on vanadium (V) with terephthalic acid as its linker has large CO_2 binding energies and show that for these cation, the CO_2 binding energies are twice the value expected based on pure electrostatics. We associate this adsorption behavior with the specific electronic configuration of the divalent cations and symmetry of the Zn and Fe site in same organic linker upon CO_2 binding. In the last investigations, the grand canonical Monte-Carlo (GCMC) and molecular dynamics (MD) simulations based on REPEAT electrostatic charges are presented to demonstrate that physical bond and electrostatic interactions can be used to predict trends of CO_2 binding affinities to OMS-MOFs with transition-metal cations which are filling their *d* orbitals.

Keywords:MOF, MD simulation, Adsorption, DFT, GCMC simulation.

1 Introduction and overview

For the creation of infinite structures of the framework, metal-ligand cords and ligaments between the donor molecules and the hydrogen bonding receptor are used. The variety of infinite networks achieved is remarkable. Olafhi and Ookifhe have suggested that these frameworks will presumably create spatial structures of a network that can be connected to the vertices of each other [1].

Most of the ligands used in organic-metallic chemistry are ligands based on bipyridine or carboxylate. Pyridine is an interconnected pyridine. The carboxylate group COO is a negative charge, some of which are shown in the figure below [2].

1-1Characteristics of organic frameworks - metal

1-1-1 High design capability

1-1-2 The order and the rule

1-1-3 Flexibility and dynamism

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To investigate the interaction of CO2 with MIL_47, a molecular cloud has been used. In this method, the energy of interaction is obtained in the form of a difference between the complex energy of the energy of one of the component constituents.

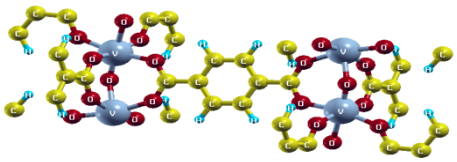


Figure 1: A view of the MIL_47 cell

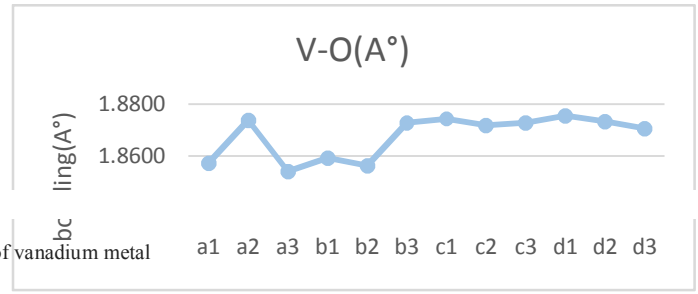
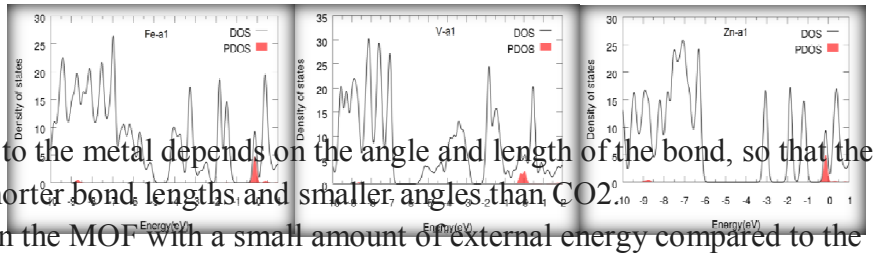


Fig2 The average length of oxygen bond between two atoms of vanadium metal

1-1-1 Checking Density (DOS)

The state density is the number of states whose energy is between E and E d, that is, the number of states available per unit of energy, the state density is called. Due to the presence of symmetry, it is sufficient to obtain the state density in the first region of the braille.



2 -Conclusions

The energy of CO2 binding to the metal depends on the angle and length of the bond, so that the larger binding energy has shorter bond lengths and smaller angles than CO2. Examining all orbital CO2 in the MOF with a small amount of external energy compared to the isolated CO2 indicates that the main source of CO2 binding to the MOF is due to the positive load of the metal sites open

Recent reports show that using DFT with reformatting algorithms is very useful for non-saturated web sites in MOFs in the process of describing operations. It can be easily demonstrated that the DFT + D2 method can have credible results in comparison with the analyst.

The amount of CO2 penetration in MIL_47 decreases with increasing temperature and pressure. The optimal temperature and pressure for these calculations are K200 and atm10, respectively. On the other hand, with increasing pressure and temperature, the excess error decreases and in some cases disappears.

From the two atoms of the CO2 molecule, the oxygen atom, due to its small negative charge and the pair of unbound electrons, has the most presence in the vanadium metal since the framework since the vanadium metal has a positive and anomalous amount of d in its capacity layer and

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This has improved the absorption in this area.

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(2) **Rosseinsky,M.J. Recent developments in metal-organic framework chemistry : desing , discovery ,permanent porosity and flexibility;Mesoporous and Microporous Meterials. Science 73,2004,15-30.**

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