Adsorption of Drugs in Metal-Organic Frameworks: A Combined Grand Canonical Monte Carlo and DFT-D Study.

Júlio C. S. Da Silva [a] (PQ), Amanda L.[a] (PG), Roberta P. Dias[b] (PQ) and Thereza A. S.[a] (PQ)

[a] *Departamento de Química Fundamental, UFPE.*
[b] *Centro Acadêmico do Agreste, UFPE.*

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INTRODUCTION

Metal–organic frameworks (MOFs) have drawn considerable attention in recent years due to their promising applications in gas technology, catalysis, sensors, electronic devices, and more recently, drug delivery.[1] In general, MOFs have excellent biodegradability, biocompatibility and guests loading capability, endowing promising candidates as nano-carrier platforms for drug delivery. Given the fact of the existence of many different MOF structures, a systematic study of their performance in drug delivery is crucial for identification of new promising structures. In order to get a detailed understanding about the adsorption of drugs in MOFs, is essential to get information about the nature of the interactions between the drug and specific sites of the material. Inside this context, molecular simulations emerge as an outstanding approach to predict the performance of the MOFs for drug delivery from the quantitative predictions with additional molecular level insight.[2]

METHODS

Grand Canonical Monte Carlo simulations were carried out to investigate the adsorption mechanism of some drugs (5-fluoracil, ibuprofen, cis-platinum and carbo-platinum) in different Metalo-Organic Frameworks (MOFs) (three new nanocage-based MOFs of Zn, Cu, Sm and HKUST-1). Some configurations obtained during the GCMC simulations were used to estimate the binding energy of the drugs from DFT-D calculations.

RESULTS AND DISCUSSION

Figure 1(a), 1(b) and 1(c) shows some snapshots taken from GCMC simulation of the adsorption of 5-fluoracil (5-FU) in **ZnMOF**, **CuMOF** and **SmMOF** MOFs, respectively.

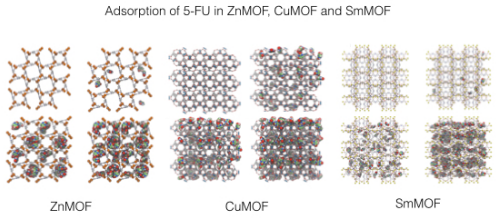

Figure 1. Snapshots of 5-FU in ZnMOF (a), CuMOF (b) and SmMOF (c).

According our GCMC results the 5-FU adsorption to **ZnMOF**, should occurs in two steps: (1) 5-FU molecules fill up the larger pore, forming well-structured aggregates. (2) Once the larger pores are occupied, 5-FU molecules bind to the smaller pore albeit in much smaller numbers. Our results also suggest that 5-FU binding preferences to **ZnMOF, CuMOF** and **SmMOF** reflect the diversity in pore types, chemical nature and size. The calculated drug payloads indicate that capacity of each material in adsorb the 5-FU is more related to the accessible volume than to the pore size. We calculated the bind energy of the drugs in the materials from DFT-D calculations performed with molecular models built from some configurations generated in the GCMC simulations. Details about these calculations as well as the results obtained will be presented and discussed during the event.

CONCLUSIONS

The GCMC simulations and DFT-D calculations carried out in this work revealed some insights into the fundamental aspects related to adsorption mechanism of some drugs in different Metal-Organic Frameworks.

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[1] MOFs special issue: Chem. Rev., 112, 2 (2012).
[2] R. Q. Snurr, et al, J. Mater. Chem. B, 2, 766-774, (2014).