Theoretical study of Covalent Organic Frameworks based on C_3-symmetric Central Cores

Sergio Gámez-Valenzuela,[a] Berta Gómez-Lor,[b] M. Carmen Ruiz Delgado,*[a] José Ignacio Martínez Ruiz *[b]

a) Department of Physical Chemistry, University of Málaga, Campus de Teatinos, 29071, Spain.

b) Instituto de Ciencia de los Materiales de Madrid (ICMM), Consejo Superior de Investigaciones Científicas (CSIC), Sor Juana Inés de la Cruz 3, 28049, Madrid (Spain)

In recent years, the design and synthesis of COFs (covalent organic frameworks) has been deeply investigated. These materials are constructed from the union of different covalently linked conjugated platforms and they have a wide range of analytical applications, such as adsorption and / or separation of certain compounds, catalysis or identification of analytes, among others.[1] On the other hand, the π-conjugated nature of these systems together with their extended 3D nature make them excellent candidates to be used in organic electronics.[2] Recently, in collaboration with the group of Dr. Berta Gómez-Lor, we have studied the electronic and optical properties of four new porous truxene-based polymers.[3] The results of this work opens the door to the control of the degree of π-conjugation and therefore to the optoelectronic properties of these materials (*i.e.*, their potential as nitroaromatic compound sensors) through the substitution position of the truxene units. Here we propose to expand this study to COFs (Figure 1) derived from platforms with C_3 symmetry based not only on truxene (X=C) but also on triindole (X=N) and truxenone (X=CO) units by means of periodic DFT-calculations (see Figure 1). Specifically, we study how the different structural modifications affect the intra- and intermolecular properties of the systems for their subsequent synthesis and real application in organic electronic devices.

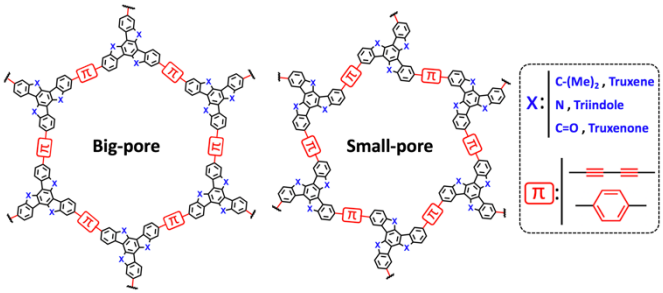

Figure 1. Chemical structure of COFs under study.

References

1. Côté, A. P.; El-Kaderi, H. M.; Furukawa, H.; Hunt, J. R.; Yaghi, O. M, JACS. 2007, **129**, 12914.
2. Tilford, R. W.; Mugavero III, S. J.; Pellechia, P. J.; Lavigne, J. J. Adv. Mat. 2008, **20**, 2741.
3. Echeverri, M.; Gámez-Valenzuela, S.; González-Cano, R. C.; Guadalupe, J.; Cortijo- Campos, S.; López Navarrete, J. T.; Iglesias, M.; Ruiz Delgado, M. C.; Gómez-Lor, B. Chem. Mat. 2019, **17**, 6971.
4. Albacete, P.; Martínez, J. I.; Li, X.; López-Moreno, A.; Mena-Hernando, S. a.; Platero-Prats, A. E.; Montoro, C.; Loh, K. P.; Pérez, E. M.; Zamora, F. JACS. 2018, **140**, 12922.