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seminar

Friday 3rd February

c/Faraday, 9
Conference Hall
Imdea Nanociencia
Ciudad Universitaria de Cantoblanco

12:00h

Structural and Electronic Characteristics of Conjugated Materials: The key Role of DFT calculations

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The use of organic materials to design electronic devices constitute an ecological and suitable resource for our current "electronic world". Actually these materials have been implemented into electronic devices, like organic light-emitting diodes (OLEDs), organic solar cells (OSCs), and organic field-effect transistors (OFETs). These materials provide several advantages (low cost, light weight, good flexibility and solubility to be easily printed) that cannot be afforded with silicium.1 They can also potentially interact with biological systems, something impossible with inorganic devices.2 Between these materials we can include small molecules, polymers, fullerenes, nanotubes, graphene, other carbon-based molecular structures and hybrid materials.

Here we analyze the electronic and molecular characteristics of different π-conjugated structures. Specifically, we focus on the study of materials ranging from small oligomers to polymers and carbon nanostructures (see Figure 1), with different backbone configurations: (i) donor-acceptor configuration, (ii) 1D lineal or 2D branched conjugated backbones, and (iii) encapsulated systems, among others.3 The key role of DFT calculations for an accurate interpretation of the experimental results is highlighted, showing their potential in helping guide the design of new materials for organic electronics.

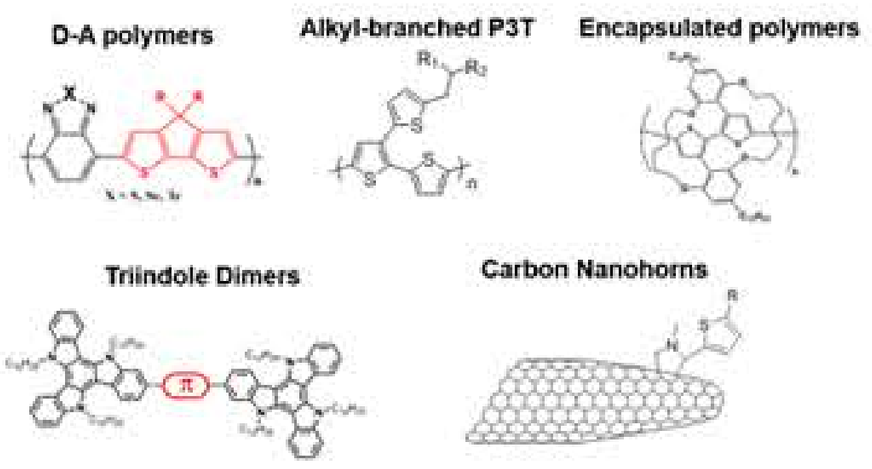

Figure 1. Chemical structures of different types of π-conjugated materials under studyzz

References
1. J. Z. Low, S. N. Sanders, Luis M. Campos Chem. Mater., 2015, 27, 5453–5463.
2. H. A. M. Ardoña, John D. Tovar, Bioconjugate Chem., 2015, 26, 2290–2302.
3. a) C. Ruiz, J.T. Lo□pez Navarrete, M.C.Ruiz Delgado, B. Go□mez-Lor, Org. Lett. 2015, 17, 2258–2261. b) M. Scheuble, Y. M. Gross, D. Trefz, M. Brinkmann, J. T. López Navarrete, M. C. Ruiz Delgado, and S. Ludwigs, Macromolecules, 2015, 48, 7049.. c) C. Ruiz, A. Monge, E. Gutiérrez-Puebla, I. Alkorta, J. Elguero, J. T. López Navarrete, M.C. Ruiz Delgado and B. Gómez-Lor, Chem. Eur. J. 2016, 22, 10651 – 10660

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