MOLECULAR AND ELECTRONIC STRUCTURE INVESTIGATION OF ENCAPSULATED POLYTHIOPHENES

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Insulated molecular wires (IMWs) are expected to be applied to various optoelectronic applications due to their unique photophysical, electronic, and mechanical properties which originate from the absence of π-stacking.[1] Kazunori et al have succeeded in the synthesis of a self-threading polythiophene with a polyrotaxane-like 3D architecture (PSTB, see Figure 1a), for which an intrawire hole mobility of 0.9 $cm^2\ V^{-1}\ s^{-1}$ has been measured.[2] In this study we aim to evaluate for the first time the extension of the π-conjugation in encapsulated polythiophenes. A comparison between the experimental Raman spectra of the self-threading PSTB polymer with their correspondent oligomers (*i.e.* 2STB-5STB) suggests that the effective conjugation length in the polymer is longer than five monomer units. Whether the effective conjugation length of the polymer is better described by using the long oligomer extrapolation approach or periodic DFT calculations of the polymer is discussed in detailed by exploiting the very recent potentialities of state-of-the-art quantum chemical simulations of vibrational properties for crystalline solids.

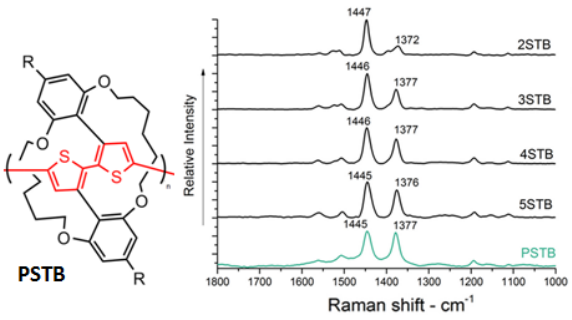

Figura 1. Chemical structures and Raman spectra of the encapsulated polythiophenes.

Referencias

[1] C.Pan, C.Zhao, M. Takeuchi and Kazunori Sugiyasu, Chem. Asian J, 2015, 10, 1820.

[2] Sugiyasu, K.; Honsho, Y.; Harrison, R. M.; Sato, A.; Yasuda, T.; Seki, S.; Takeuchi, M. J. Am. Chem. Soc. 2010, 132, 14754.

[3] M. C. Ruiz Delgado, S.Mosca, C. Capel Ferrón, V. Hernández, J.T. López Navarrete, L. Brambilla, M. Tommasini, A. Milani, C. Castiglioni, K. Sugiyasu, *in preparation*