Evaluating the Role of Intermolecular Interactions in π-conjugated Materials: What can we learn from DFT calculations and Raman Spectroscopy

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For practical applications in sensors, dynamic covalent chemistry and molecular (photochromic) switches, soft conjugated materials can be envisaged as promising functional materials.[1] To advance in this research field, deciphering the mechanisms involved on how sensitive the structural and electronic properties are to specific molecular ordering is essential. In stimuli responsive materials, such as piezochromic materials, the molecular orientation and intermolecular interactions can change upon mechanical grinding. In this context, Raman spectroscopy can help to clarify how organic molecular solids respond to high pressure, for instance, by reducing intermolecular interactions and/or changing molecular conformations.[2]

On the other hand, DFT calculations can help us to rationalize the nature and stability of the formation of aggregates and complexes, allowing the evaluation of the effects of the surrounding media on different molecular properties.[3] Thus, we propose here a combined Raman spectroscopy and DFT study of molecular crystals and/or aggregates upon soft external stimuli that can be envisaged as a very sensitive approach to understand the structural effects causing any chromic changes. To this end, we focus on different families of π-conjugated materials with potential application in organic electronics, ranging from cyclophane aggregates to tetrathiazolylthiophenes crystals (Figure 1).[2-3]

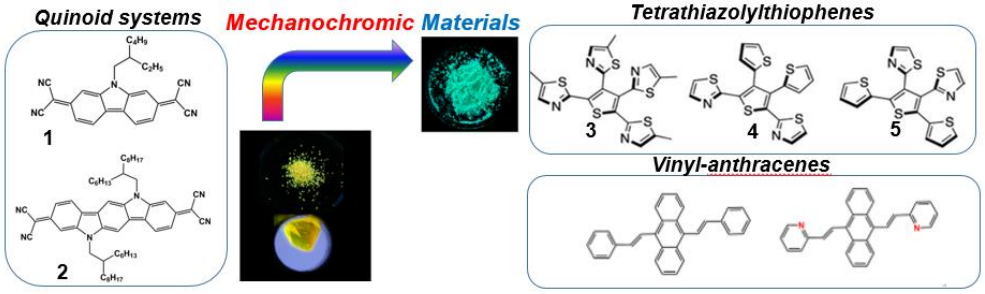

Figure 1. Chemical structures of π-conjugated materials under study

Referencias

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