THEORETICAL INVESTIGATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF TRUXENE-BASED 2D POLYMERS

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Recently, significant attention has been devoted to the design and synthesis of covalent organic frameworks (COFs) as semiconductor materials, which has emerged as an effective strategy to provide large electron delocalization. The extended π-conjugated nature of these systems together with their 2D nature can lead to strong electronic interactions between the 2D COF layers, making them highly applicable to a wide range of potential applications in energy storage, photocatalysis, gas storage or identification of analytes, among others.[1] Recently, in collaboration with the group of Dr. Berta Gómez-Lor, we have studied the relationships between the chemical structure and electronic properties of several C_3-symmetric truxene-based semiconductors[2] and 2D polymers with different π-substituted bridges connecting the cores.[3] This systematic study provides a powerful protocol for the pre-filtering of new candidate materials to guide the design of new optimized 2D materials.[3] In our previous theoretical study shows that the most promising charge transport properties were predicted for 2D COFs based on hexa-substituted truxene cores with alkyne bridges. As a novelty, now in this work we wanted to explore how an increasing number of alkyne bridges can influence the electronic and charge transport properties of these 2D conjugated polymers.

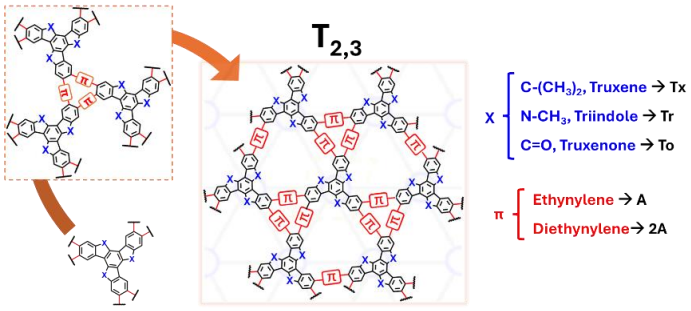

Figure 1. Chemical structures of 2D polymers under study.

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