IN SILICO DESIGN AND RAMAN SPECTROSCOPY FOR A BETTER UNDERSTANDING OF THE ELECTRONIC PROPERTIES OF 2D POLYMERS

2D organic semiconducting polymers have emerged as an important class of materials that offer high potential for a variety of applications, such as energy storage, sensing or organic electronics. However, the design of novel materials generally involves an expensive and environmentally unfriendly methodology that strongly contrasts with the ecological transition spirit. In this sense, computational design offers a green alternative to experimental laboratory research. On the other hand, Raman spectroscopy is a fast and nondestructive characterization tool widely used to evaluate the structural and electronic properties of pi-conjugated materials. In this study, we combine an experimental and theoretical approach that links DFT calculations with Raman spectroscopy aiming to control the electronic and structural properties of conjugated materials. Overall, our findings open the door to the control of the degree of the π-conjugation of 2D organic polymers for their subsequent synthesis and real applications ranging from sensing to electronics.