

Evaluating the Structural and Electronic Properties of 1D and 2D Conjugated Polymers

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The emergence of 1D and 2D organic semiconducting polymers has led to a plethora of potential applications, including energy storage, sensing, and organic electronics. In these applications, the chemical structure and intermolecular organisation of π -conjugated materials can exert a pronounced influence on their properties, thereby impacting the performance of the device. Consequently, elucidating the mechanisms by which structural and electronic properties are sensitive to specific chemical structural changes and molecular ordering is imperative.[1] However, the design of novel materials typically necessitates an expensive and environmentally unfriendly methodology that is incongruent with the principles of ecological transition. In this regard, computational design offers a green alternative to experimental laboratory research. Raman spectroscopy is a fast and non-destructive characterisation tool that is widely used to evaluate the structural and electronic properties of π -conjugated materials. In our research group we have a wide experience in evaluating the electronic and structural properties of conjugated organic materials by combining Raman spectroscopy with theoretical calculations.[2] In particular, here we show our most recent studies in the field of 1D and 2D polymers, which aim to decipher the complex structure-property relationship of these materials.

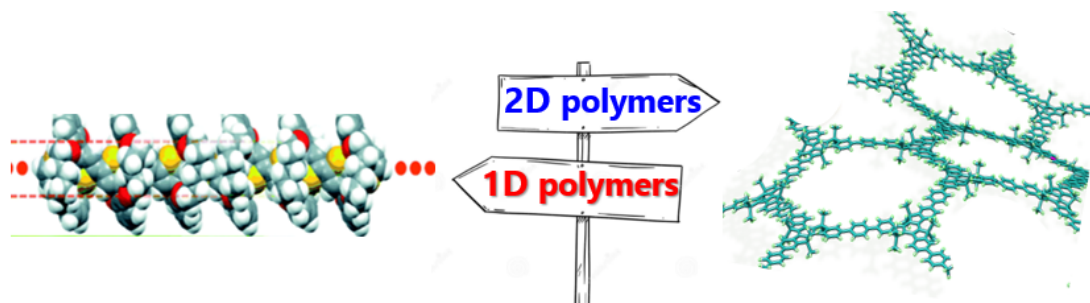


Figure 1. Examples of the 1D and 2D conjugated materials.

References

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