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INSIDE PEF: CHAIN CONFORMATION AND DYNAMICS IN CRYSTALLINE AND AMORPHOUS DOMAINS

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A thorough vibrational spectroscopy and molecular modelling study on poly (ethylene 2, 5-furandicarboxylate) (PEF) explores its conformational preferences, in the amorphous and crystalline regions, while clarifying structure–property correlations. Despite the increasing relevance of PEF as a sustainable polymer, some of its unique characteristics are not yet fully understood and benefit from a deeper comprehension of its microstructure and intermolecular bonding. Results show that in the amorphous domains, where intermolecular interactions are weak, PEF chains favour a helical conformation. Prior to crystallization, polymeric chains undergo internal rotations extending their shape in a zigzag pattern-an energetically unfavourable geometry which is stabilized by C–H•••O bonds among adjacent chain segments. The zigzag conformation is the crystalline motif present in α- and β-PEF polymorphs. The energy difference among the amorphous and crystalline chains of PEF is higher than in PET poly (ethylene terephthalate) and contributes to PEF's higher crystallization temperature. The 3D arrangement of PEF chains was probed using inelastic neutron scattering (INS) spectroscopy and periodic DFT calculations. Comparing the INS spectra of PEF with that of poly (ethylene terephthalate)-PET revealed structure–property correlations. Several low-frequency vibrational modes support the current view that PEF chains are less flexible than those of PET, posing greater resistance to gas penetration and resulting in enhanced barrier properties. The vibrational assignment of PEF's INS spectrum is a useful guide for future studies on advanced materials based on PEF.

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