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DFT study on intermolecular interactions of MDI-BDO-PCL urethane molecules

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The packing arrangements of polyurethane chains in the crystalline and amorphous regions are responsible for several physicochemical and mechanical properties such as melting temperature, rigidity, abrasion resistance, and tensile strength. In this study, a model of (1,7)-Polyoxepan-2-one (PCL), 1,1'-Methylenebis(4-isocyanatobenzene) (MDI), and Butane-1,4-diol (BDO), (MDI-BDO-PCL) has been developed computationally, and it was used to study the packing arrangements and intermolecular interactions using DFT/B3LYP-6-31G(d). Out of the four possible intermolecular hydrogen bonding patterns for urethane chain, only the H-bond interactions between carbonyl oxygen (hard segment) and a hydrogen atom attached to the nitrogen (urethane linkage in the hard segment) were observed. The average H-bond distance is 2.04 Å. Therefore, hard segment crystallization was predicted due to the hard segment-hard segment H-bond interactions. In the crystallized region, hard segments are packed together, showing zig-zag orientation. The planer nature of the urethane group and benzene ring in the hard segment reduces steric hindrance and increases the crystallinity. The findings of this study have shed new light on the atomistic level understanding of the microstructure of the urethane matrix.

Keywords: Polyurethanes, hard segment, soft segment, hydrogen-bonding interactions

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