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Local segmental dynamics of cis-1,4-polybutadiene, polypropylene, and polyethylene terephthalate via molecular dynamics simulations
DAVID WHITLEY, DAVID ADOLF, University of Leeds, UK — NPT molecular dynamics simulations of cis-1,4-polybutadiene, polypropylene, and polyethylene terephthalate have been performed. The simulation pressure was 1 atmosphere for all systems, with all simulation temperatures being well above each polymer's glass transition temperature. The trajectories have been analysed via autocorrelation functions (ACFs) of chord vectors spanning different numbers of chain backbone bonds. Inverse Laplace transformations of these ACFs using the CONTIN algorithm afforded the corresponding distributions of relaxation times (DRTs) for the simulated dynamics. All DRTs illustrated a peak on fast time scales corresponding to short length scale segmental motion and a peak at longer time scales corresponding to longer length scale relaxations. An intermediate peak between the fast and slow peaks appears as the relaxation dynamics of longer chord vectors are analysed. The temperature dependence of the relaxation dynamics has also been investigated.

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