Electronic Supplementary Information: A comparative study of electronic properties of disordered conjugated polymers

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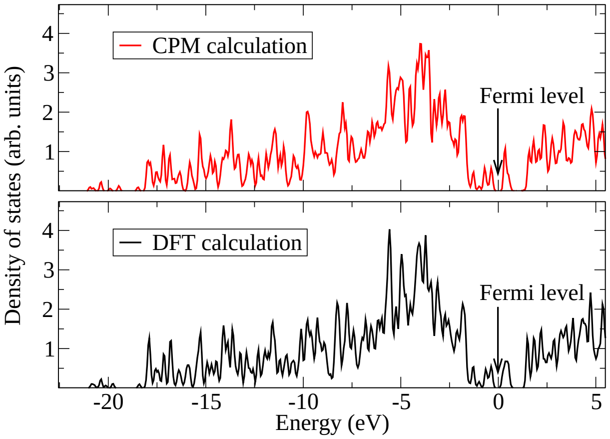

Fig. 1 The comparison of the density of states of the 462 atom APFO3 polymer system calculated using the direct DFT/LDA calculation and the CPM. The system consists of 3 chains, each is 2 monomers long, with pentyl side chains. A good agreement between the results obtained by the two methods verifies that CPM provides the accuracy similar to that of DFT/LDA.

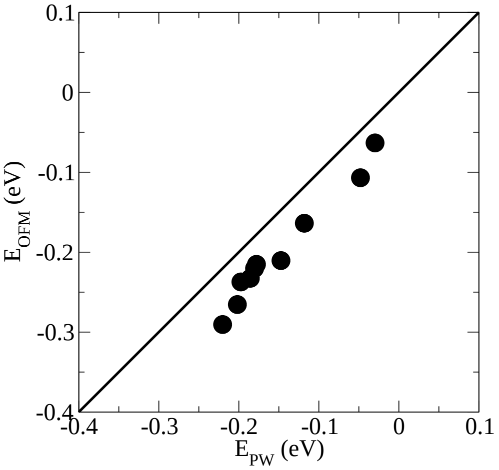

Fig. 2 The comparison of eigenenergies obtained by diagonalization in the plane wave basis (E_{PW}) and the ones obtained by the OFM (E_{OFM}). The comparison was performed for a 2360 atom APFO3 polymer system (5 chains, each 5 monomers long, with octyl side chains) where plane wave diagonalization is still feasible. The basis set consisting of one HOMO orbital per fragment was used in OFM calculations. The comparison shows that the OFM provides satisfactorily accurate eigenenergies.

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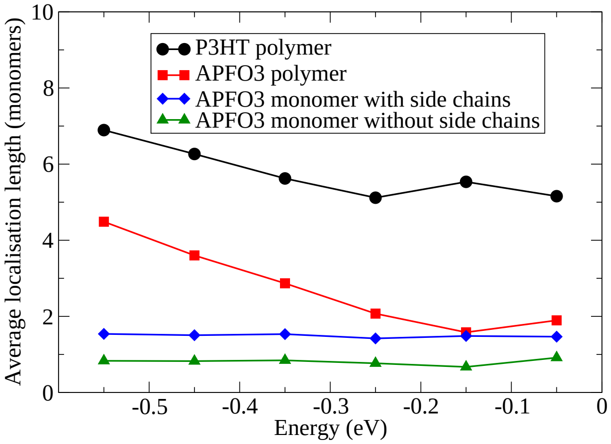

Fig. 3 The dependence of average wave function localisation length on energy for the materials studied in this work. Wave function localisation length was calculated using the procedure described in Ref. 30 of the main text. The average localisation length at energy E was then calculated as the average of localisation lengths of all states within the interval $(E - 50\,\mathrm{meV}, E + 50\,\mathrm{meV})$.

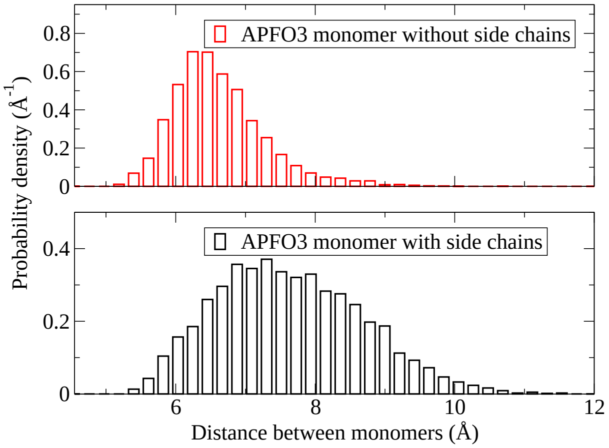

Fig. 4 Distribution of distances between nearest neighbour monomers for materials based on APFO3 monomers with and without alkyl side chains. The distance between two monomers was defined as the distance between atoms labelled as 7 in Fig. 1 in the main part of the paper. The figure demonstrates that the distances between nearest neighbour monomers in material without alkyl side chains are smaller than in the case of the material with alkyl side chains.

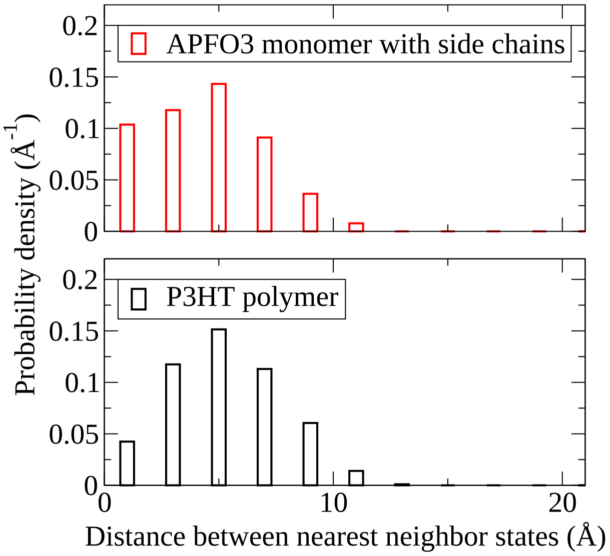

Fig. 5 Distribution of distances between nearest neighbour hole states for materials based on P3HT polymers and APFO3 monomers with alkyl side chains. The figure demonstrates that the distribution of distances between a hole state and its nearest neighbour state is similar in these materials. The distance between hole states was defined as the distance between the centres of mass of the corresponding wave functions. The states spanning the spectral region of first 0.2 eV below the top of the valence band were included in the distribution.

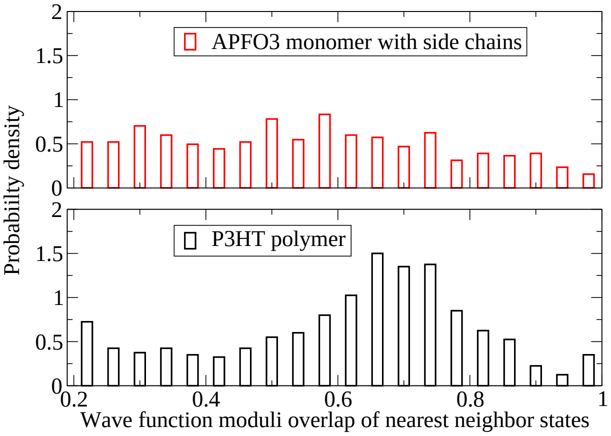

Fig. 6 Distribution of wave function moduli overlaps between nearest neighbour hole states for materials based on P3HT polymers and APFO3 monomers with alkyl side chains. The figure demonstrates that the wave function overlaps are better in the material based on P3HT polymers. The distance between hole states was defined as the distance between the centres of mass of the corresponding wave functions. The states spanning the spectral region of first 0.2 eV below the top of the valence band were included in the distribution.