Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials

Unraveling the real structures of solution-based and surface-bound poly(3-hexylthiophene) P3HT oligomers: a combined theoretical and experimental study

Dalila Khlaifia[1,2], Christopher P Ewels[2], Florian Massuyeau[2],Mourad Chemek[1], Eric Faulques[2], Jean-Luc Duvail[2*], Kamel Alimi[1*]

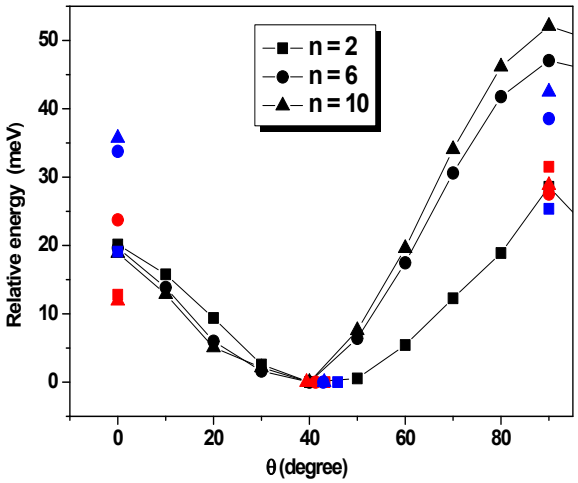

Figure S1. Torsional potential energy per monomer curves of P3HT oligomers containing two, six and ten monomer units as a function of the inter-ring torsional angle θ, using three different exchange-correlation functionals: B3LYP (black symbols), CAM-B3LYP (blue symbols), and WB97X(D) (red symbols). Note the excellent qualitative agreement between them, with the global minimum located at 40°±5° in each case.

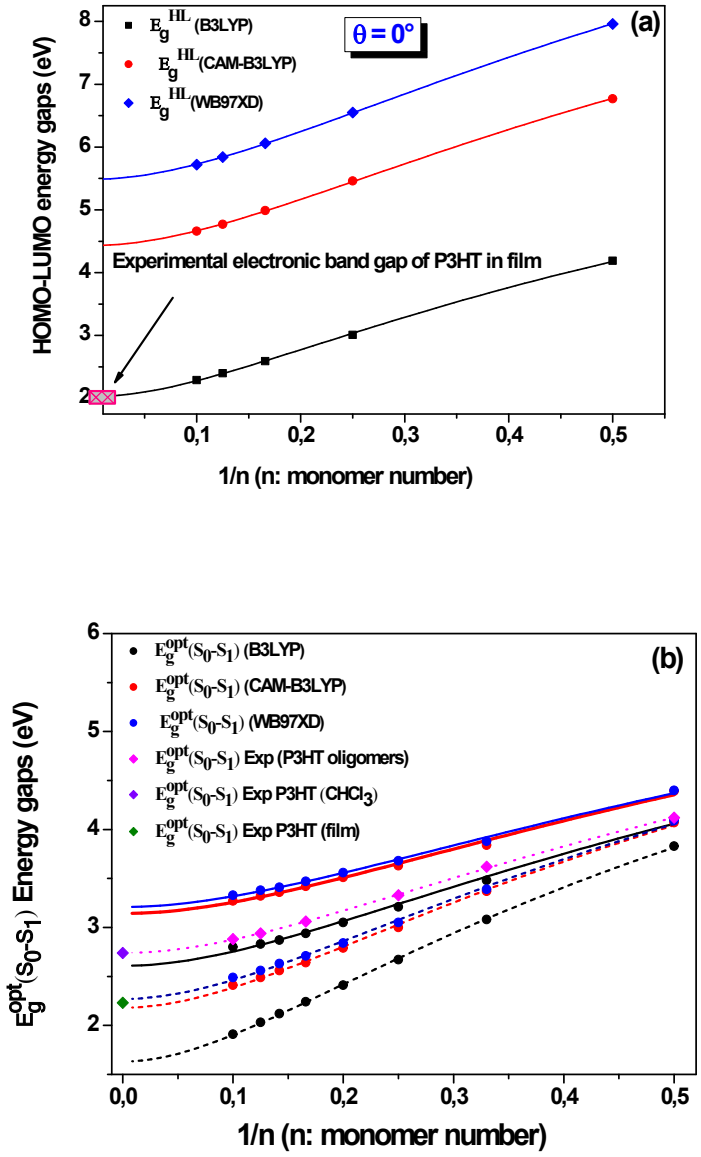

Figure S2. E_g^{HL} energy gaps in the planar conformations (θ=0°)(a) and $E_g^{opt}(S_0 - S_1)$ energy gaps in the planar conformations (θ=0°) (dashed lines) and twisted conformations (θ=40°) (solid lines) of P3HT oligomers as a function of reciprocal chain length, calculated with the three different exchange-correlation functionals (B3LYP: black, CAM-B3LYP: red and WB97X(D): blue). In (a), the pink square is the value of the experimental electronic band gap of P3HT in thin film. In (b), the pink, violet and green colored diamond symbols (dotted line) represent the experimental band gap $E_g^{opt} = E(S_0 - S_1)$ of P3HT oligomers in chloroform taken from ref [30] and those of P3HT in chloroform and in thin film, respectively.