Ab-initio study of singlet and triplet excitation energies in oligothiophenes [phys. stat. sol. (c)1, No. 3, 539–542 (2004)]

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Erratum

Ab-initio study of singlet and triplet excitation energies in oligothiophenes

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The authors report an error in the fit for the ^3A state shown in Fig. 1 of their article and present a new corrected figure.

In Fig. 1 we reported linear fits of the calculated excitation energies for T1,T2,T3, and T4 and compared them with experimental results. We have now found that the fit for the ^3A state is not valid because the ^3A state of the monomer has a different character as compared to its oligomers. Here we report in Fig. 1 the new linear fits for all the states considering only excitation energies for T2,T3, and T4. While similar results are obtained for the ^1B and ^3B states, a qualitatively different behavior is found for ^3A state: the second triplet excited-state lies energetically below the first singlet excited-state for long oligomers. In order to verify this trend, we have calculated the excitation energies of pentathiophene (T5) and we found that the ^3A state lies indeed 0.26 eV below the ^1B state. This new finding shows a discrepancy between the theoretical and the experimental evolution with the number of monomers of the ^3A state. However all the other results and conclusions of the article are still valid due to the very small energetical difference between the ^1B and ^3A states.

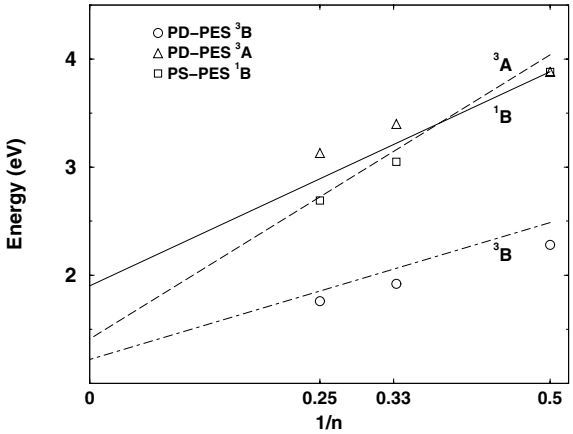

Fig. 1 Theoretical (lines) and experimental (points) energy of the ^1B, ^3B and ^3A excited states as a function of inverse of oligomer size $1/n$.

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