

Abstract Submitted
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An ab initio approach to organic photovoltaics VINCENT GOSSELIN, NICOLAS BÉRUBÉ, JOSIANE GAUDREAU, MICHEL CÔTÉ, Univ of Montreal — Within the recent years, we have witnessed continual improvements in the Power Conversion Efficiencies (PCE) of organic photovoltaic devices. These improvements have been achieved by the discovery of new polymers which are being synthesised and their performance assessed experimentally. Scharber has introduced a simple model which determines the desired properties of polymers in order to achieve high PCE. An appealing alternative to the lengthy process of polymer synthesis consists in using ab initio calculations in order to predict the electronic structure of polymer candidates and evaluate the relevant properties in the determination of their PCE. In this work, Density Functional Theory (DFT) is being used to compute the optical band gap and HOMO / LUMO levels which, in conjunction with Scharber's model, allows to predict the efficiency of various polymer - fullerene blends. In order to assess the quality of such calculations and the validity of the model, we first compare the predictions with experimental device performances. We find that the model offers an indication as to what one should expect in terms of the maximum efficiency attainable experimentally. Lastly, we present new unsynthesised polymers which have shown promising results within this framework.

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