Abstract Submitted
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Ab initio study of a promizing class of copolymers for application to high-efficiency photovoltaics JEAN FRÉDÉRIC LAPRADE, MICHEL CÔTÉ, Département de physique and Regroupement québécois sur les maériaux de pointe (RQMP), Université de Montréal, Canada — In order to achieve high power conversion efficiency in bulk-heterojunction solar cells using PCBM as electron acceptor, it is essential to identify an electron donor polymer which i) harvests the largest part of the solar spectrum and ii) shows an electronic structure appropriate to PCBM. In the last few years, different groups synthetized copolymers based on either fluorene[i], carbazole[ii] or dibenzosilole[iii] with interesting results. This presentation will report the results of density-functional theory (DFT) and time-dependant density-functional theory (TDDFT) calculations on those copolymers and their units in order to better assess the impact of changing the fluorene's 9-atom on the electronic properties. We will focus our discussion on the interplay of the counits on the energy levels and on the oscillator strength of the oligomers. [i] O. Inganäs & *al.* *Appl. Phys. A*, **2004**, 79, 31 [ii] N. Blouin & *al.*, *Adv. Mater.*, **2007**, 19, 2295 [iii] P.L.T. Boudreault & *al*, Macromol. Rapid Commun., **2007**, 28, 2176

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