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**Design of low band gap polymers for photovoltaic applications: a theoretical study** NICOLAS BERUBE, MICHEL COTE, Departement de physique, Universite de Montreal — Organic photovoltaic cells received a great interest in the last few years as they offer an environmentally clean and low-cost solution to the world's rising energy needs. Studies show that this technology holds the potential to reach a power conversion efficiency of 10 %, which would hold on as a competitor to actual inorganic devices based on silicon. Experimental results of solar cells using PCPDTBT (pentadithiophene-benzothiadiazole) or DPP (diketo-pyrrolo-pyrrole) as the electron donor and PCBM as the acceptor already show power conversion efficiencies of over 5 %. Those results are limited mostly by a misalignment of the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) energy level of the different components of the solar cell. In this presentation, we will discuss how different modifications on those polymers can affect and improve their electronic properties. Our calculations based on density-functional theory using the B3LYP functional on a DPP-based copolymer with a ITN (isothianaphtene) unit, indicate a bandgap as low as 1.2 eV and a HOMO level comparable to P3HT, making a promising candidate for photovoltaic applications.

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