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Electronic structure study of Diketo-Pyrrolo-Pyrrole Polymers for Photovoltaic Applications[1] SIMON LEVESQUE, PAOLO E. TREVISANUTTO, JEAN FREDERIC LAPRADE, MICHEL COTE, Universite de Montreal et regroupement quebecois sur les materiaux de pointes (RQMP) — Using density-functional theory, we investigate the electronic properties of polymers that contain diketo-pyrrolo-pyrrole (DPP) in the repeating units. We will present our calculated results for the band gap and LUMO energy levels that can be related to the measured optical gap and electron affinity. Some of the polymers studied have LUMO energy similar to the C70-PCBM, or even lower, making them promising candidates for electron transport in organic photovoltaic devices. The homopolymer of DPP is predicted to have a band gap around 1.2 eV and shows a good dispersion of the conduction band, suggesting it should be a good charge carrier. Finally, we use approximations of the quantum field theory of many-body systems to get more accurate results and obtain the absorption spectrum of some polymers.

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