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Ab initio **Study of Diketo-Pyrrolo-Pyrrole Polymers for Photovoltaïc Applications**[1] SIMON LÉVESQUE, JEAN FRÉDÉRIC LAPRADE, MICHEL CÔTÉ, Departement de physique et Regroupement quebecois sur les materiaux de pointe (RQMP), Universite de Montreal, Canada — Using density functional theory with the hybrid functional B3LYP, we investigate the electrical and optical properties of polymers made with diketo-pyrrolo-pyrrole. It is found that the value of the band gap can be tuned by varying the number of thiophene units within the polymer. Band structure and time-dependent density functional theory results will also be presented.

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