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First principles electronic properties investigation of polythienoacene and its derivatives[1] SIMON PESANT, PAUL BOULANGER, GUILLAUME DUMONT, MICHEL CÔTÉ, Département de physique et Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — The electronic properties of ladder-type polythiophene (polythienoacene) and its derivatives are studied using density functional theory. Upon an analysis of the variation of the band gap when comparing the non-ladder and the ladder-type polymers, a discrepancy is found between the thiophene and the pyrrole(nitrogen-substituted thiophene) polymer families. The polythienoacene has a larger band gap than the polythiophene whereas the opposite is found for the pyrrole polymers. Also, it is found that a simple alternation of the sulfur atom in polythienoacene structure by nitrogen or boron atoms can lead to small band gap polymers. The excitations of these polythienoacene's derivatives are investigated using time-dependent density functional theory.

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