

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Ab initio study of ladder-type metallic polymers SIMON PESANT, GUILLAUME DUMONT, SEBASTIEN LANGEVIN, MICHEL COTE, Departement de physique, Universite de Montreal — The electronic structure of recently synthesized ladder-type polythiophene polymer is studied with density-functional theory based calculations. It is found, in the local density approximation (LDA) that upon a simple substitution of the sulfur atoms by nitrogen and boron atoms, the band structure of the resulting polymer (called LPPyB) exhibits bands overlap between the occupied and the unoccupied states that is characteristic of metallic systems. The band structure is further validated by GW calculations confirming the assessment of the LDA results. Calculations using the B3LYP functional, which contains exact exchange, show a different electronic behavior, a small HOMO-LUMO band gap of 0.67 eV is obtained. In order to better assess the energy gap of the polymer, a TDDFT (Time-dependent density-functional theory) study of the LP-PyB was performed on oligomers and verifies the metallic structure of this polymer. Other calculations were done using TDDFT on different polymers to validate the last result. In parallel, similar electronic properties were computed on an isoelectronic polymer of LPPyB, having the atomic structure of the ladder-type polythiophene, with only one sulfur atom replaced by a boron atom.

Simon Pesant
Departement de physique, Universite de Montreal

Date submitted: 17 Nov 2006

Electronic form version 1.4