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Density-functional study of Peierls instability in carbon nanotubes using hybrid functionals GUILLAUME DUMONT, PAUL BOULANGER, MICHEL COTE, Departement de physique, Universite de Montreal, MATTHIAS ERNZERHOF, Departement de chimie, Universite de Montreal — We present a first-principles study of Peierls distortions in *trans*-polyacetylene, polyacene and armchair (n, n) carbon nanotubes. All calculations were done within density- functional theory using a gaussian basis set. We show that while density only functionals (LDA, GGA) cannot reproduce the experimentally mesured dimerization in *trans*- polyactetylene, hybrid functionals including Hartree-Fock exchange can give the correct geometry. These findings suggest that armchair (n, n) carbon nanotubes could have a nonsymmetric ground state; in contradiction with what is commonly accepted. Indeed, the B3LYP functional (which includes 20% of exact exchange) opens a gap of 0.26 eV and 0.12 eV for the $(3, 3)$ and $(6, 6)$ carbon nanotubes respectively. Accordingly, dimerization amplitudes of 0.005 Å and 0.002 Å are obtained. It is found that the dimerization and the band gap are proportional to the the amount of exact exchange included in the functional.

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