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**Physisorption of Nucleobases on C(9,1) and C(6,5) Single-Wall Carbon Nanotubes: A Density Functional Theory Study** BRAHIM AKDIM, RUTH PACHTER, Wright Patterson Air Force Base, OH — Selective enrichment of single-wall carbon nanotubes (SWCNTs) of a specific chirality by single-stranded DNA sequences has been shown experimentally by Zheng et al. [JACS 2007, 129, 6084], where a larger enrichment of C(6,5) as compared to C(9,1), which are SWCNTs of the same diameter but different chirality, was demonstrated with alternating guanine and thymine (GT) bases. In this work, we report density functional (DFT) calculations of (G) and (T) nucleobase adsorption on C(6,5) and C(9,1) SWCNTs, in order to gain an understanding of the selective sorting, specifically regarding adsorption characteristics, interface energetics, and electronic structures, as dependent on the tube chirality, also including specifically an empirical dispersion correction in the DFT functional.

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