

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Single-walled (5,3) gold nanotube-a theoretical study¹ CHIH-KAI YANG, Chang Gung University — Total-energy calculations based on first principles reveal that a (5,3) gold nanotube has a helical pitch of 10.05 nm or a natural length of 20.1 per unit cell at the minimum total energy. The figure is about 9.5 % shorter than the experimental pitch of 11.0 nm under stress from the experimental setup. Energy bands for both pitches are similar, giving five units of quantum conductance. The calculations indicate that the single-walled gold (5,3) nanotube is a robust and stable conducting wire suitable for nanoelectronic applications.

¹Supported by the National Science Council of the Republic of China

Chih-Kai Yang
Chang Gung University

Date submitted: 29 Nov 2004

Electronic form version 1.4