Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Structural and electronic properties of few-layer graphenes from frist-principles[1] M.-H. TSAI, J.-R. HUANG, J.-Y. LIN, B.-H. CHEN, National Sun Yat-Sen University — Using first-principles calculation method, it is found that the calculated layer spacing for the two-layer AB stacked FLG is only 2.725Å, which is substantially reduced from the calculated value of 3.257Å for bulk graphite. The average interlayer spacing for 2-, 3-, 4-, 5-, 6-, 7- and 8-layer FLG's are found to oscillate and approach that of the bulk graphite. The two-layer AA stacked FLG is found to remain metallic for the external electric potential up to 4.5Volts considered in this study. In contrast, the two-layer AB stacked FLG is found to exhibit a semi-metal-semiconductor transition under an external electric potential qualitatively in agreement with previous theoretical studies. However, the energy gap is not limited at 0.3eV as obtained in previous first-principles calculation due to the substantially reduced interlayer spacing. The threshold of the semi-metal-semiconductor transition is 0.04 Volts. The external electric potential also induced energy gaps in 3- and 4-layer AB stacked FLG's. However, in these two thicker FLG's, the induced energy gaps are small within 0.1eV. Based on this study, only the two-layer FLG is useful as a nanoscale electronic switch.

[1]Supported by National Center for Theoretical Sciences (South) of Taiwan

Min-Hsiung Tsai
National Sun Yat-Sen University

Date submitted: 22 Nov 2007 Electronic form version 1.4