Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic structure of graphene nanoflakes: band gap evolution with increasing size E. MARTINEZ-GUERRA, M.E. CIFUENTES-QUINTAL, Departamento de Fisica Aplicada, Cinvestav-Merida, Yucatan, Mexico, I. RODRIGUEZ-VARGAS, S. VLAEV, Unidad Academica de Fisica, Universidad Autonoma de Zacatecas, Mexico, R. DE COSS, Departamento de Fisica Aplicada, Cinvestav-Merida, Yucatan, Mexico — Graphene has unusual electronic properties which make it a promising material for electronic devices. Neverthless, the absence of a band gap sets limitations on its applications. Thus, it is crucial to tune the band gap of systems based on graphene. In this way, we explore to modulate the electronic properties of graphene through the size system. In particular, we studied the evolution of the electronic structure of graphene nanoflakes ($C_{6n2}H_{6n}$) as a function of size. The calculations were performed using the pseudopotential LCAO method with a Generalized Gradient Approximation for the exchange-correlation functional. We found that the energy gap decreases as the diameter of the nanoflakes increases. From a tight-binding analysis, we show that the energy gap reduction is due to an HOMO-LUMO bands widening. This effect results from the fact that as nanoflakes size increases the ratio between the number of internal and periferical atoms decreases. Thus, we found that controlling the size of graphene nanoflakes is a useful way for the electronic modulation. Supported from CONACyT Grant 83604.

E. Martinez-Guerra
Departamento de Fisica Aplicada, Cinvestav-Merida, Yucatan, Mexico

Date submitted: 09 Dec 2008 Electronic form version 1.4