Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Density functional study of the mechanical properties in single-layered graphene sheet[1] JORGE TAPIA, FRANCIS AVILES, RICARDO PEON, FI-UADY, GABRIEL CANTO, CICORR-UAC, MMS-NM TEAM — By means of the density functional theory, we studied the structural and mechanical properties (the Young's modulus, shear modulus and Poisson's ratio) of single-layered graphene sheets (SLGS). The calculations were performed with a linear combination of atomic orbitals method using pseudopotentials and the generalized gradient approximation for the exchange-correlation potential. The uniaxial stress is applied along the one preferential direction for the range of $\pm 10\%$ in the unitary deformation. We found that the bond lengths between carbon atoms in SLGS are larger than the experimental value of graphite and the mechanical properties showed good agreements with the data available in the literature.

[1]This research was supported by SEP under Grants: PROMEP/103.5/07/2595, PROMEP/103.5/08/2971 and CONACYT under Grants: No. 82497 and No. 60534.

Jorge Tapia
FI-UADY

Date submitted: 19 Nov 2010 Electronic form version 1.4