Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electric-Field Dependence of the Effective Dieletric Constant in Graphene Materials[1] ELTON SANTOS, School of Engineering and Applied Sciences, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — The dielectric constant of a material is one of the fundamental features used to characterize its electrostatic properties such as capacitance, charge screening, and energy storage capability. Here we address the issue of the effective dielectric constant (ε_G) in a few-layer graphene materials (e.g. graphene, MoS_2, WS_2, etc.) subjected to an external electric field. In particular for graphene, the value of ε_G has attracted interest due to contradictory reports from theoretical and experimental studies. Through extensive first-principles electronic structure calculations, including van der Waals interactions, we show that the graphene dielectric constant depends on the value of the external field (E_{ext}): it is nearly constant at $\varepsilon_G \sim 3$ for low fields ($E_{\text{ext}} < 0.1$ V/Å) but increases at higher fields, reaching ε_G=4.5 at $E_{\text{ext}} = 1.7$ V/Å. Further increase of E_{ext} drives the system to an unstable state where the layers are decoupled and can be easily separated. Calculations performed for other layered materials follow the same trend. Our results point to a promising way of understanding and controlling the screening properties of few-layer graphene materials via electrical means.

[1]Supported by NSF grant numbers TG-DMR120049, TG-PHY120021, TG-DMR120073 (XSEDE)

Elton Santos
School of Engineering and Applied Sciences, Harvard University

Date submitted: 09 Nov 2012 Electronic form version 1.4