Theoretical and experimental studies of electronic properties of nanostructured graphene and related layered materials

Efthimios Kaxiras,
Wei Li Wang, Elton J. G. Santos,
Brad Malone, Georgios Tritsaris

Department of Physics
School of Engineering and Applied Sciences
Harvard University

NN13 – Thessaloniki – July 9-12, 2013
- Graphene Nano Flakes (GFN’s): magnetic properties (theory : WW) – NN08
- Ripples in graphene: real-space imaging (exp.+th. : WW) – NN12
- Functionalized graphene: optical, magnetic properties (theory : WW, ES) – NN12
- Graphene: dielectric response, hybrid 2D layered devices (theory : ES,WW,BM) – NN13
- Single-atom chisel for graphene sculpting (exp.+th. : WW, ES) – NN13
- Graphene as functional substrate: organic PV’s (theory : WW, ES,GT)
Dielectric response of graphene

Capacitance, screening, electrical displacement, polarization, compressibility, etc.

Nature of electron-electron interactions in layered system under external fields

Dielectric constant, $\varepsilon(k, \omega)$

A. F. Young et al. PRB (2012), 85, 235458
Graphene subjected to static electric fields

\( \varepsilon_G \) different values reported by different groups (2 to 15)

- Geim's group
- Lanzara's group
- Jarillo-Herrero's group
- Abbamonte's group
- Ruof's group
- Yacoby's group
- Das Sarma's group
- Guinea's group
- MacDonald's group

\( E_{\text{ext}} \)

*ab initio* calculations of electrostatic response (including vdW's interactions)
Electric Field Dependence of the Effective Dielectric Constant (in-plane and out-of-plane)
Inter-layer electric field is not constant

\[ \varepsilon_G = \frac{E_{\text{ext}}}{E_{\text{eff}}} \]
Polarization charge is field dependent

\[ E_{\text{tot}} = E_{\text{ext}} - E_{\rho} \]
Electric-field control of the static dielectric constant in MoS$_2$
Similar behavior as in multilayer graphene

The polarization charge and the response field depend on external field
Graphene-MoS$_2$ devices

MoS$_2$ n–doped

1. Graphene/1.MoS$_2$
2. Graphene/2.MoS$_2$

_interface

In collaboration with
- P. Kim (Columbia)
- T. Palacios (MIT)
Graphene Nano Flakes (GNFs) as building blocks for spintronic devices

Spin splitting

SOMOs on majority lattice

E-E_f (eV)

DOS (arb. u.)

Net spin increases with GNF size

\[ \frac{[\rho_u(r) - \rho_d(r)]}{2} = 0.0025/Å^3 \]

Spin orbitals in bowtie GNFs

How can one “carve out” such features (e.g. flakes, pores) in graphene?

Frustration on both sub-lattices

Depends sensitively on shape
Graphene nano-pores for biological and membrane applications (DNA sequencing, sifting, purification)

Need precise control of pore size
Sculpting suspended graphene

Images obtained at the Berkeley National Lab’s STEM facility (by W.L. Wang)
Punching nanopore with STEM

ADF Cs STEM Image at 200 KV

Imaging at 80 KV
Cs TEM Image

30 nm

5 nm
Cutting graphene edges
An atomic-scale chisel for sculpting graphene

By Wei Li Wang
Expts. carried out at LBNL’s NCEM
Reconstructed image

Ball-and-stick model

Equilibrium configurations

Action on edges
\[ a = r_p - r_{Si} \]

edge atom

\[ b = r_m - r_{Si} \]

removed atom
Simulation of C atom removal from G and $\overline{G}$ (edges) with and without Si impurities
Sculpting of graphene with atomic scale precision clearly feasible!

Many possibilities for new physics and devices

Theory:
- Dr. Wei Li Wang
- Dr. Elton Gomes Santos
- Dr. Brad Malone
- Dr. Georgios Tritsaris

Experiment:
- Dr. Wei Li Wang (Harvard-UCB)
- Prof. Robert Westervelt (Harvard)
- Dr. David Bell (Harvard, CNS)
- Samples from Graphenea (thanks to Amaia Zurutuza)

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