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

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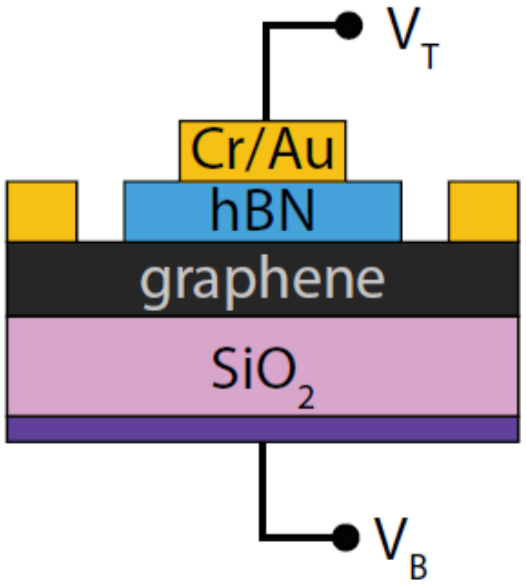
- Graphene Nano Flakes (GFN's): magnetic properties
  (theory : WW) – NN08
- Ripples in graphene: real-space imaging
  (exp.+th. : WW) – NN12
- Functionalized graphene: optical, magnetic properties
  (theory : WW, ES) – NN12
- Graphene: dielectric response, hybrid 2D layered devices
  (theory : ES,WW,BM)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

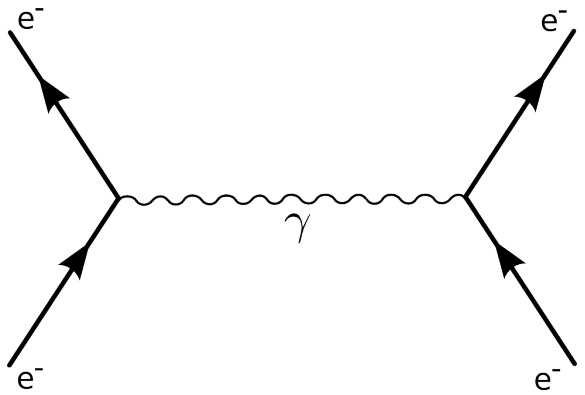
Dielectric response of graphene



A. F. Young et al. *PRB* (2012), **85**, 235458

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

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



Dielectric constant, $\varepsilon(\mathbf{k},\omega)$

Graphene subjected to static electric fields

ε_G different values reported by different groups (2 to 15)

Geim's group

Lanzara's group

Jarillo-Herrero's group

Das Sarma's group

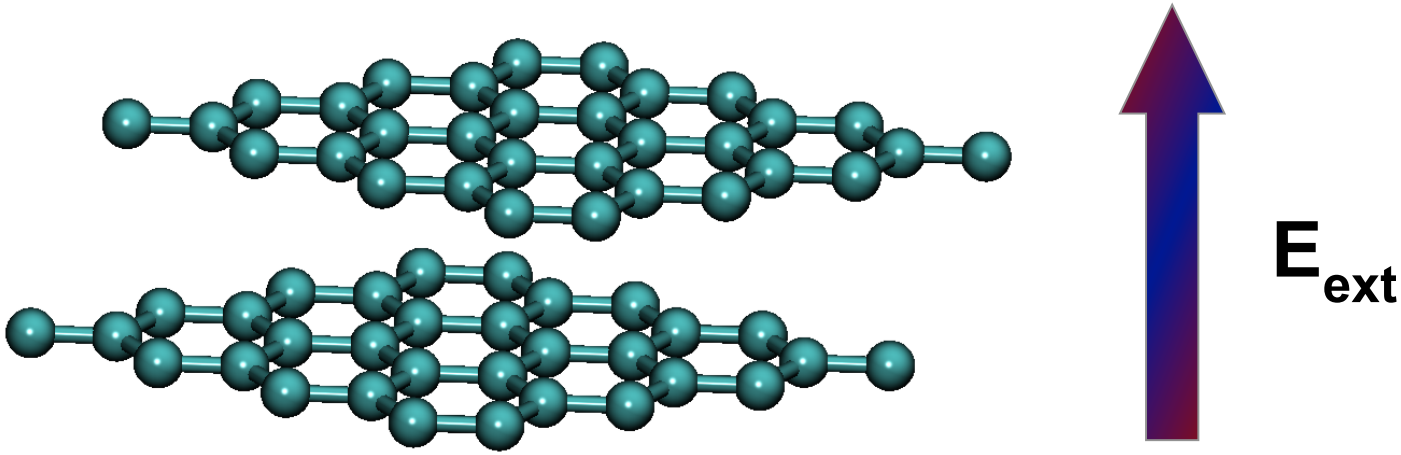
Guinea's group

Abbamonte's group

Ruof's group

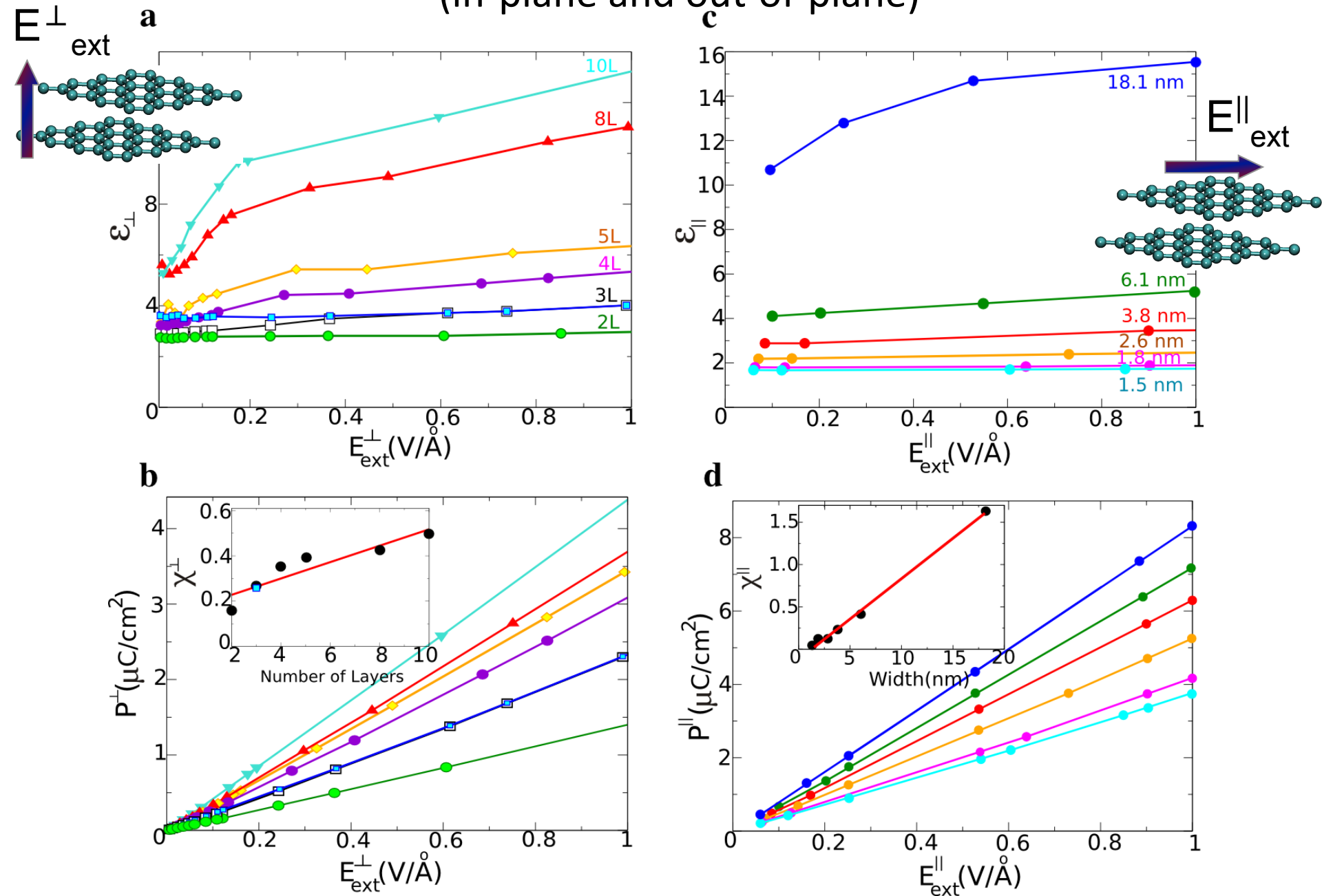
Yacoby's group

MacDonald's group



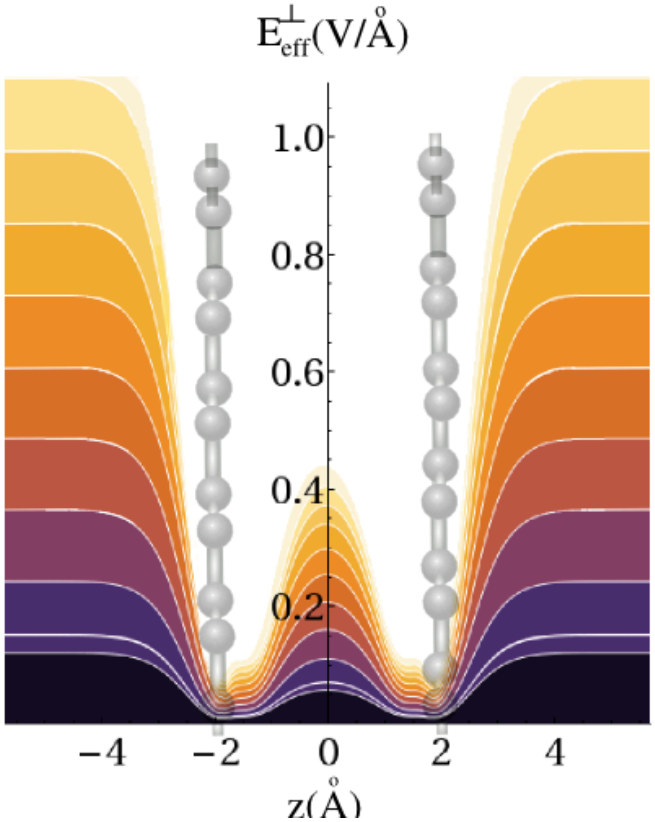
ab initio calculations of electrostatic response (including vdW's interactions)

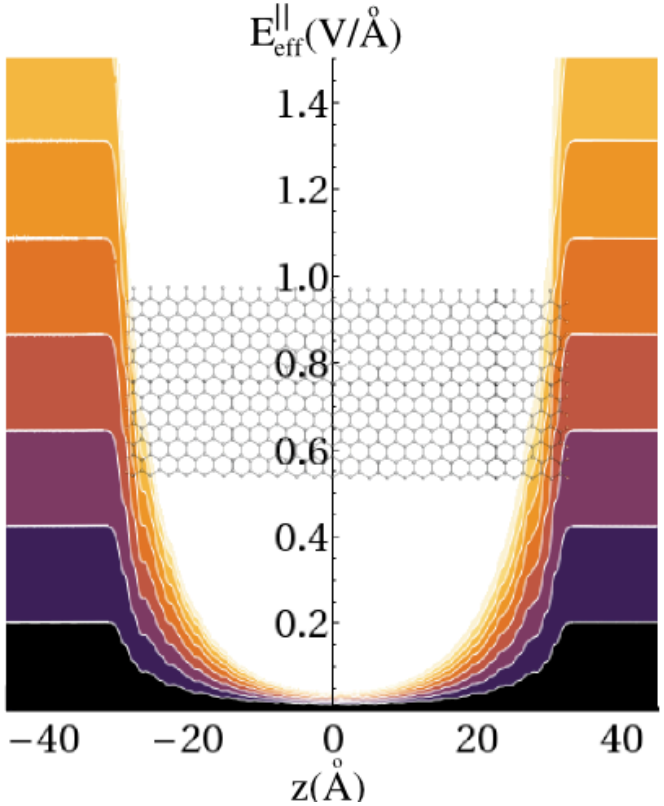
Electric Field Dependence of the Effective Dielectric Constant (in-plane and out-of-plane)



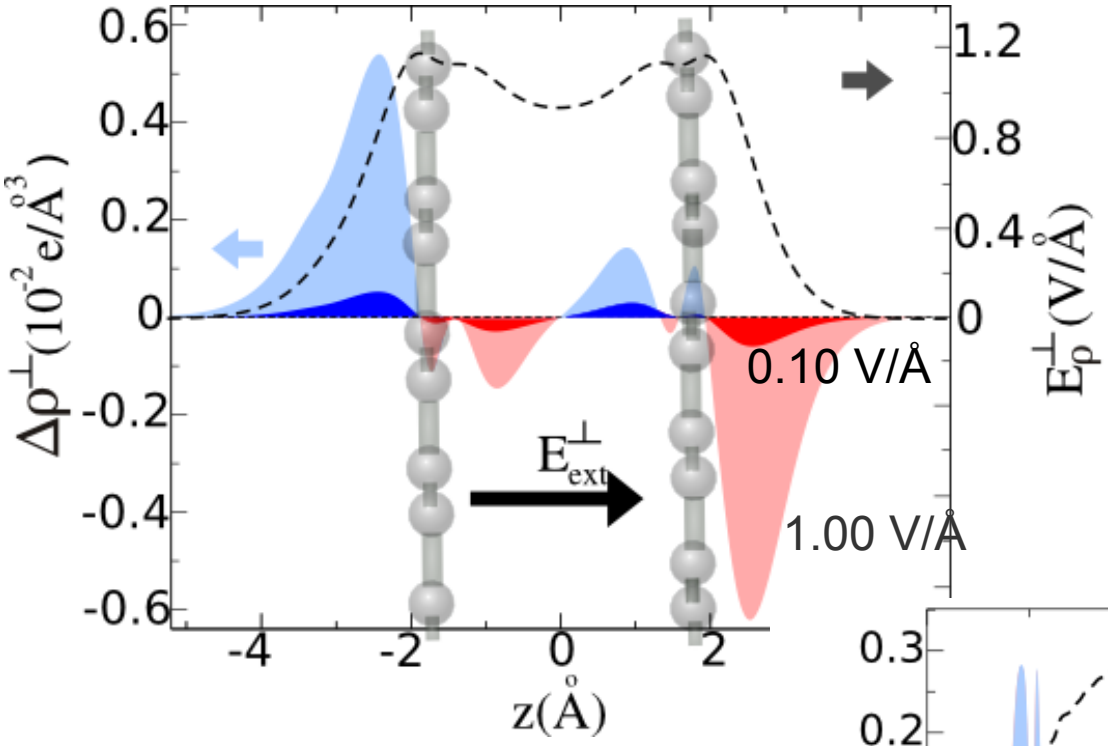
Inter-layer electric field is not constant

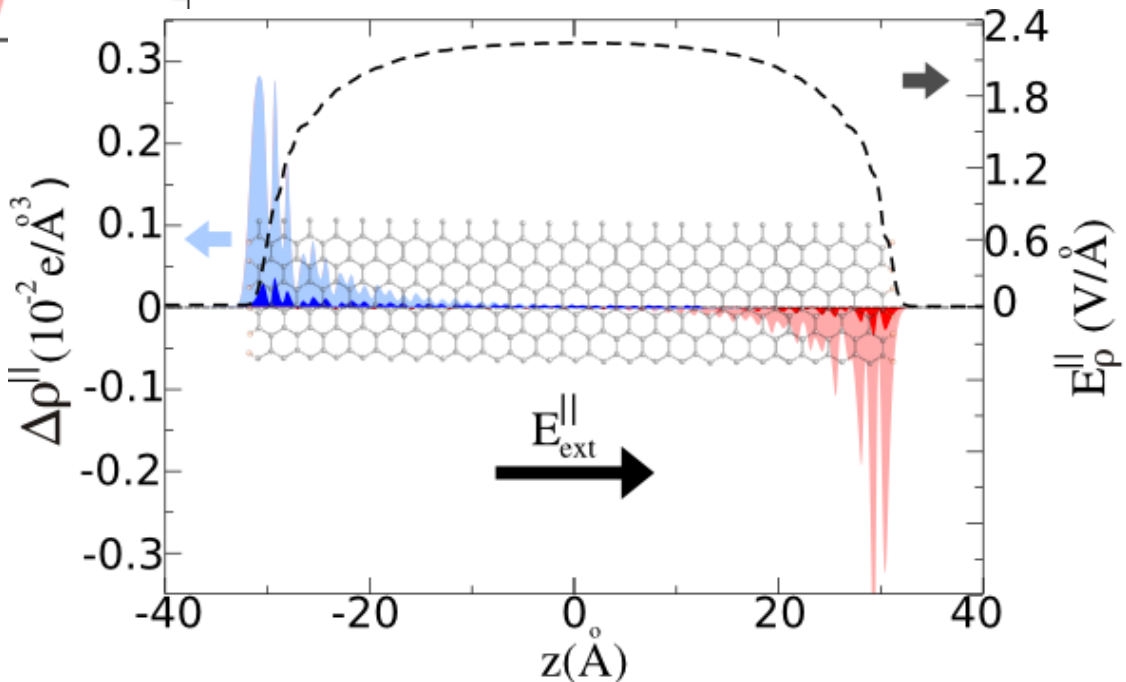
$\varepsilon_G = \mathbf{E}_{ext}/\mathbf{E}_{eff}$





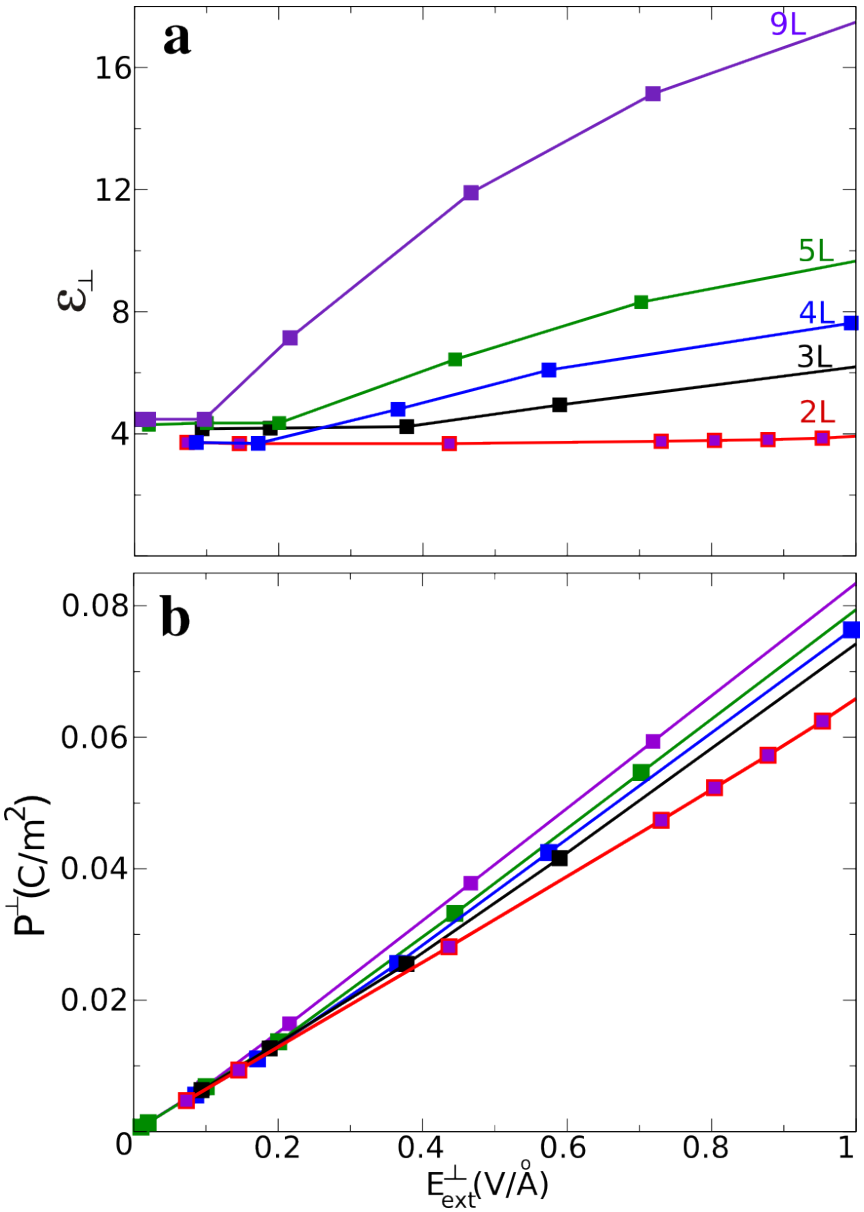
Polarization charge is field dependent

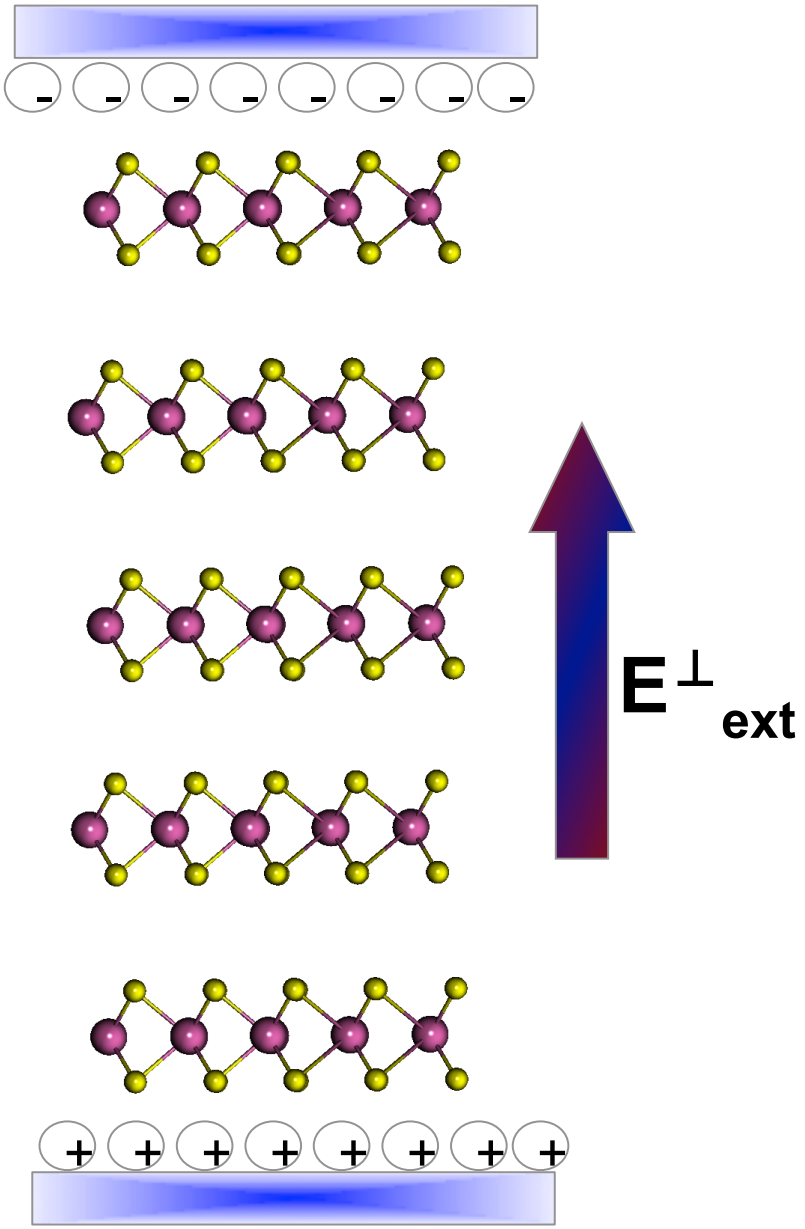




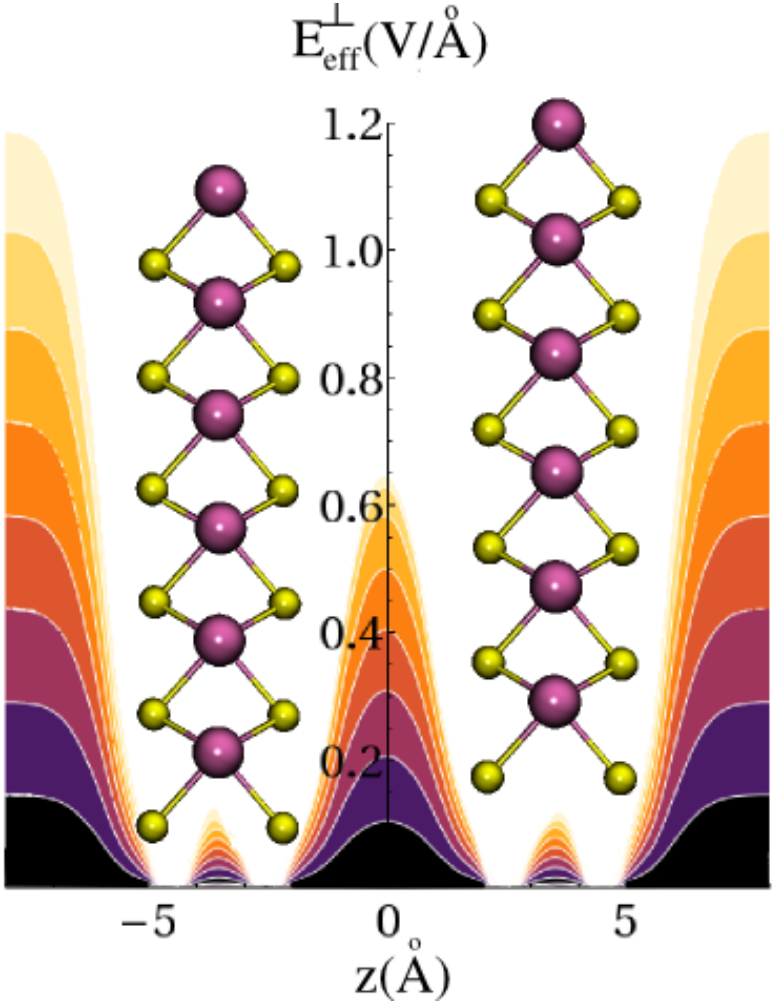
$E_{tot} = E_{ext} - E_{\rho}$

Electric-field control of the static dielectric constant in MoS_2

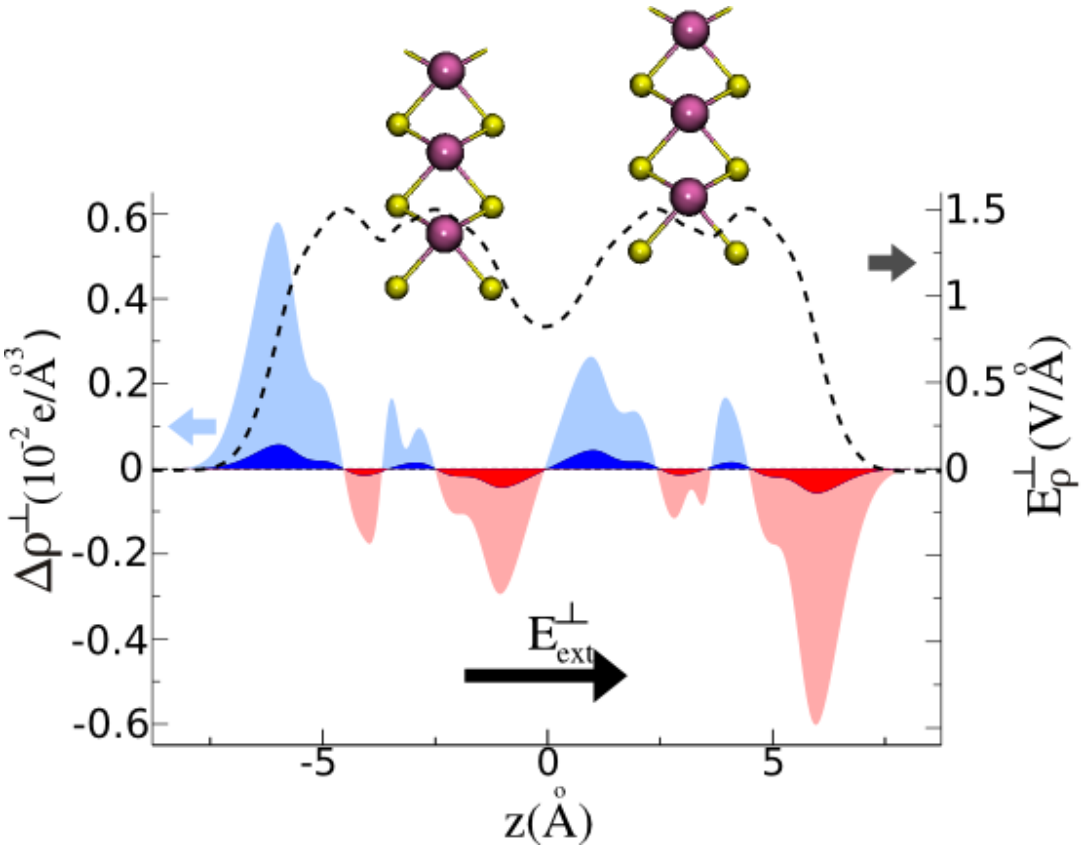




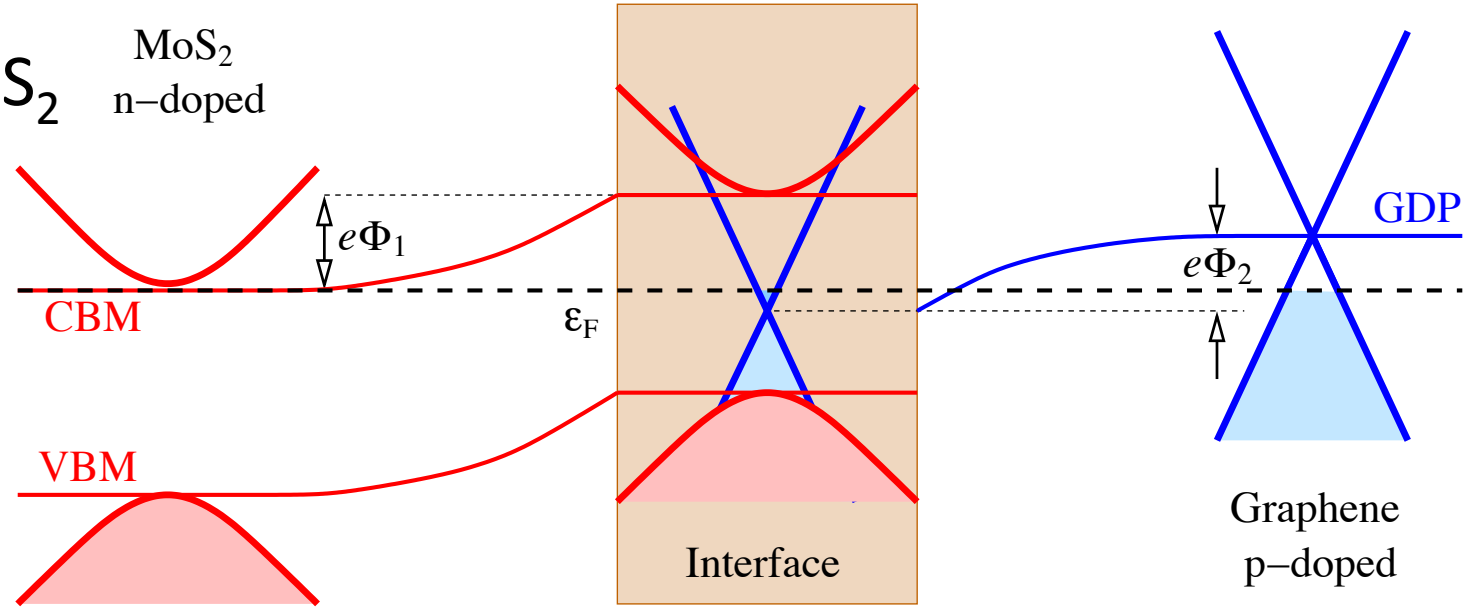
Similar behavior as in multilayer graphene

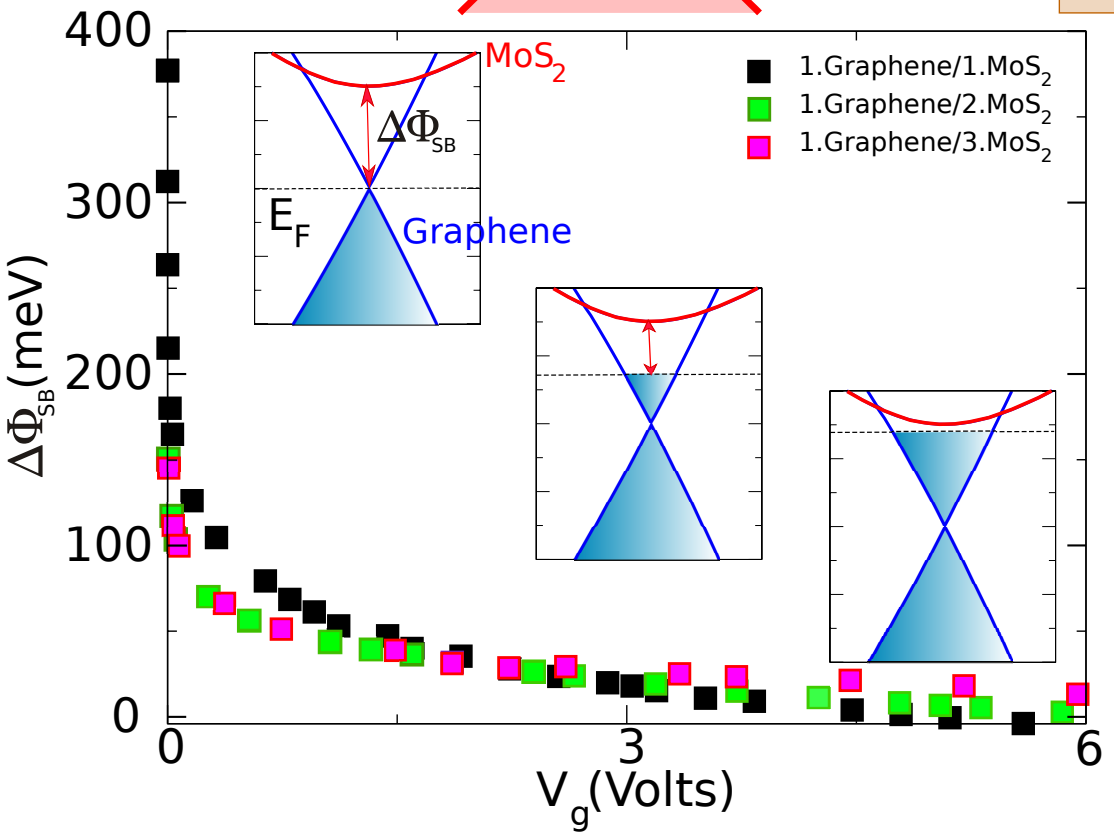


The polarization charge and the response field depend on external field



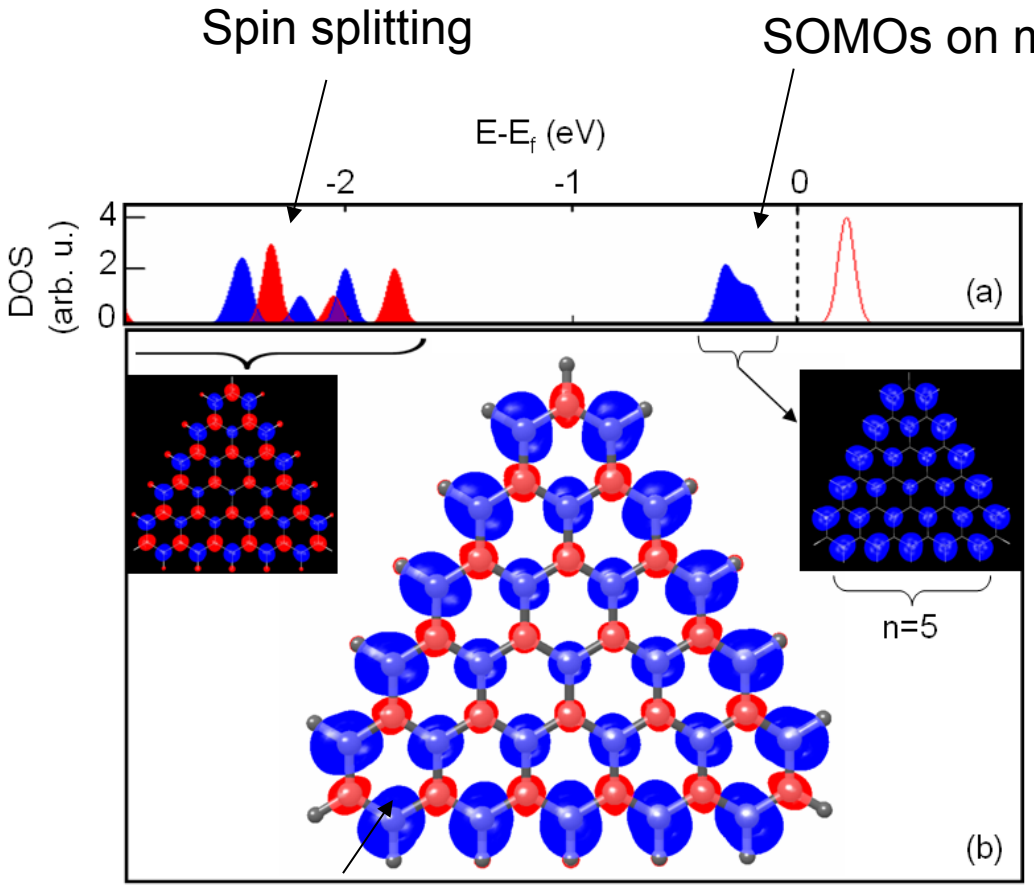
Graphene-MoS_2 devices





In collaboration with
- P. Kim (Columbia)
- T. Palacios (MIT)

Graphene Nano Flakes (GNFs) as building blocks for spintronic devices

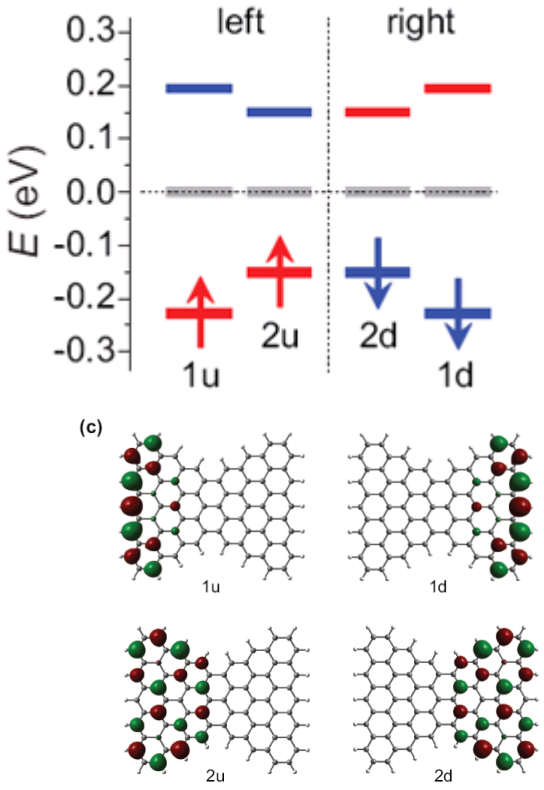


Net spin increases with GNF size

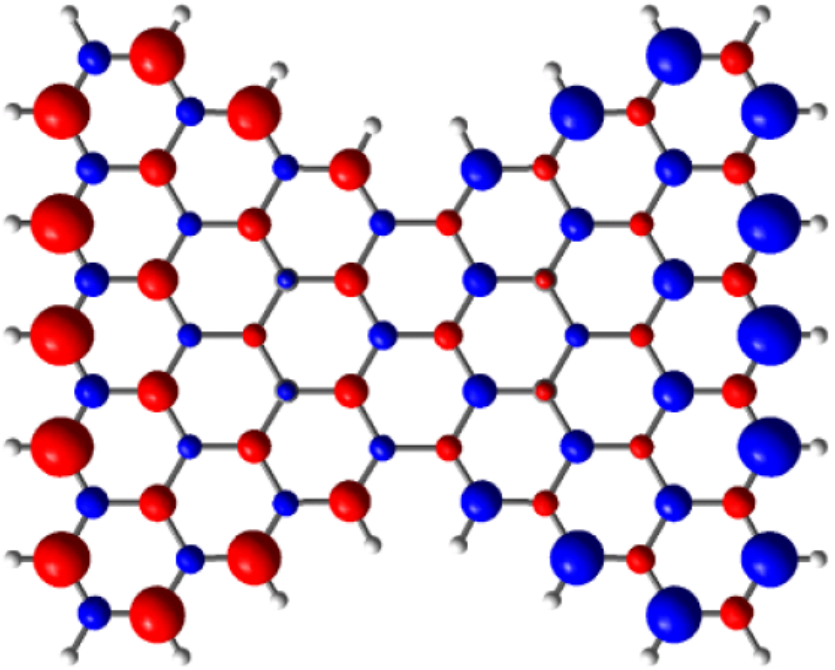
$[\rho_u(r) - \rho_d(r)]/2$ =0.0025/Å^3

Wang, *et al*. Nano Lett. 8, 241(2008).

Spin orbitals in bowtie GNFs



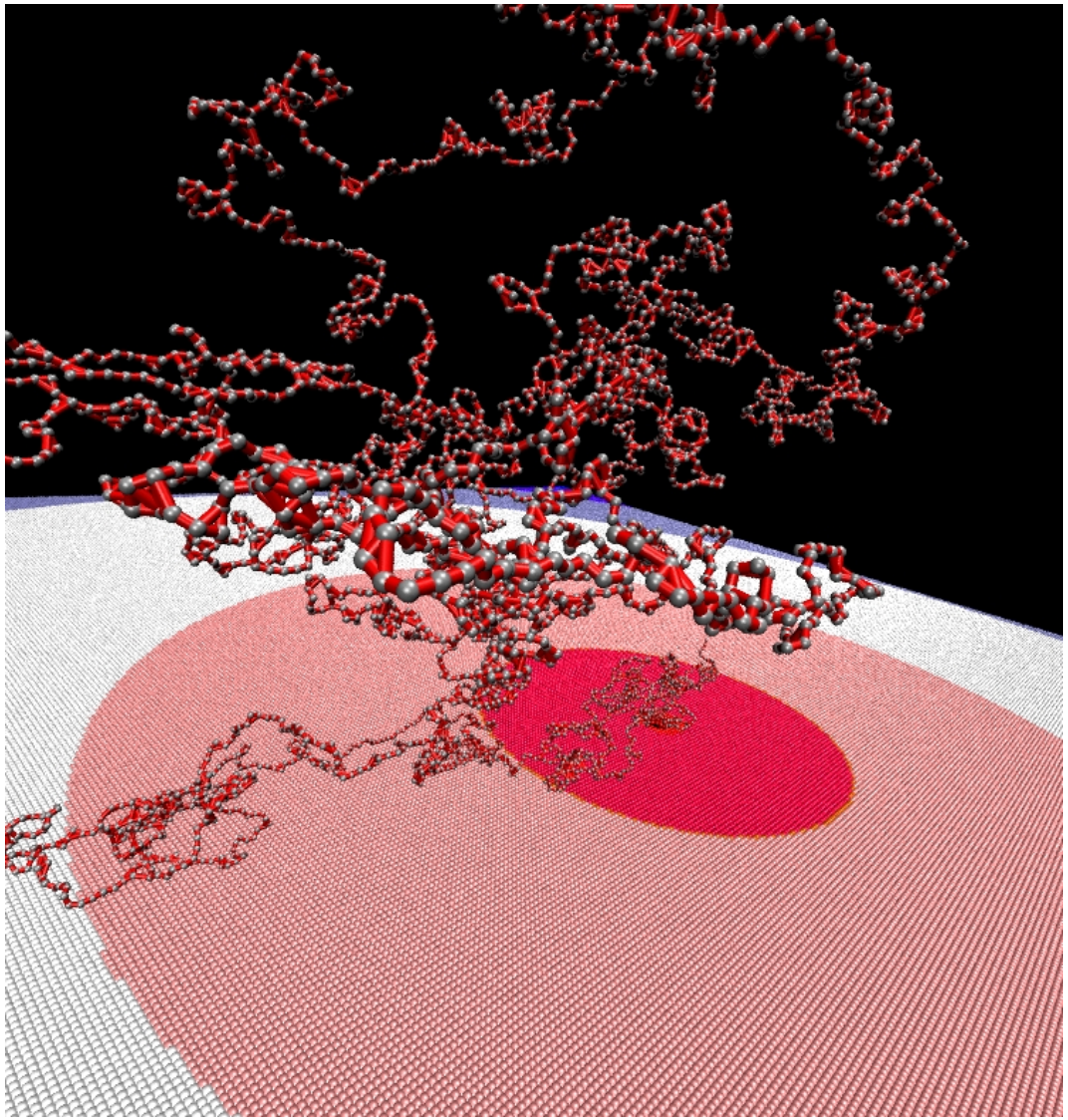
Frustration on both sub-lattices



Depends sensitively on shape

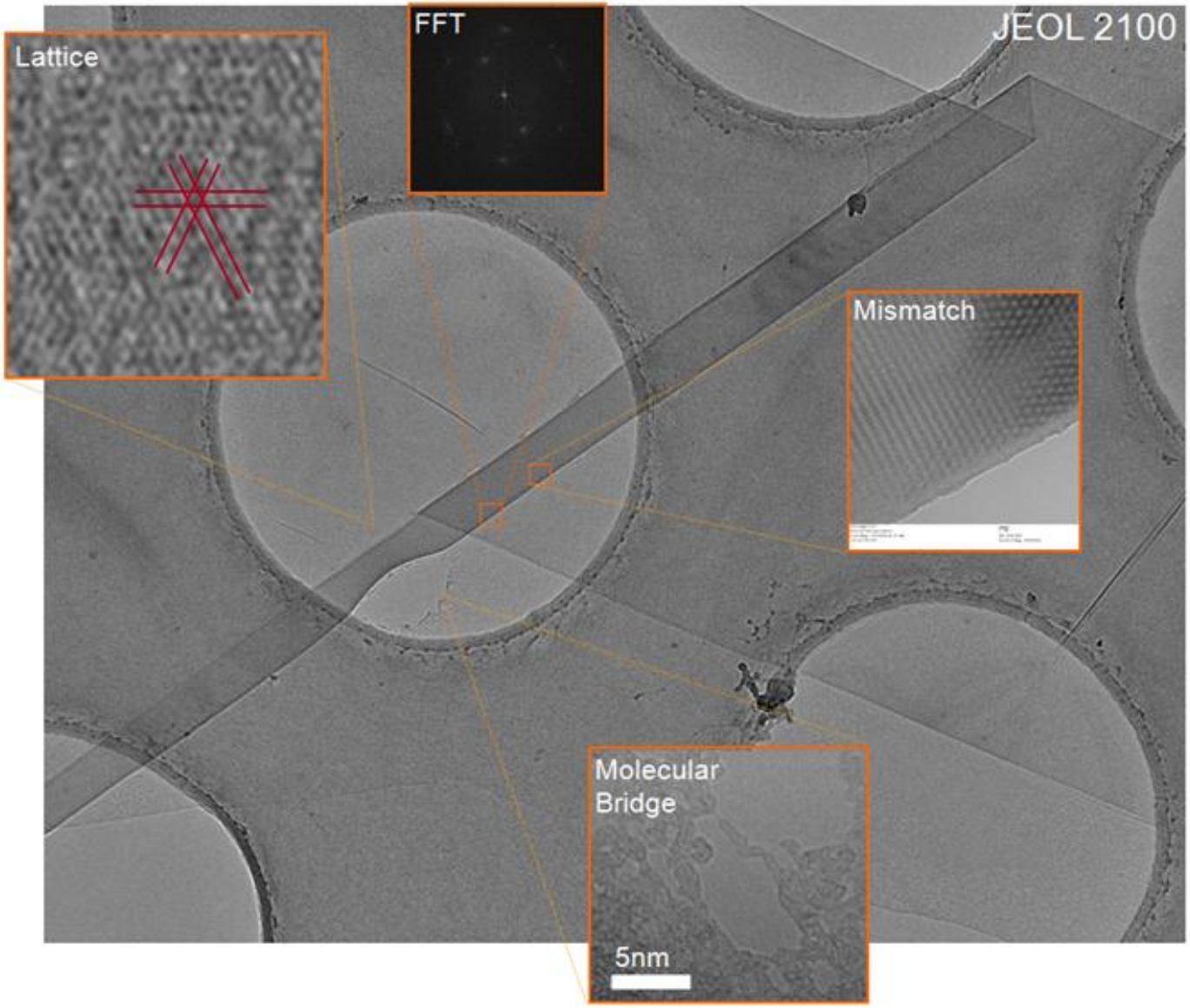
How can one “carve out” such features (e.g. flakes, pores) in graphene?

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



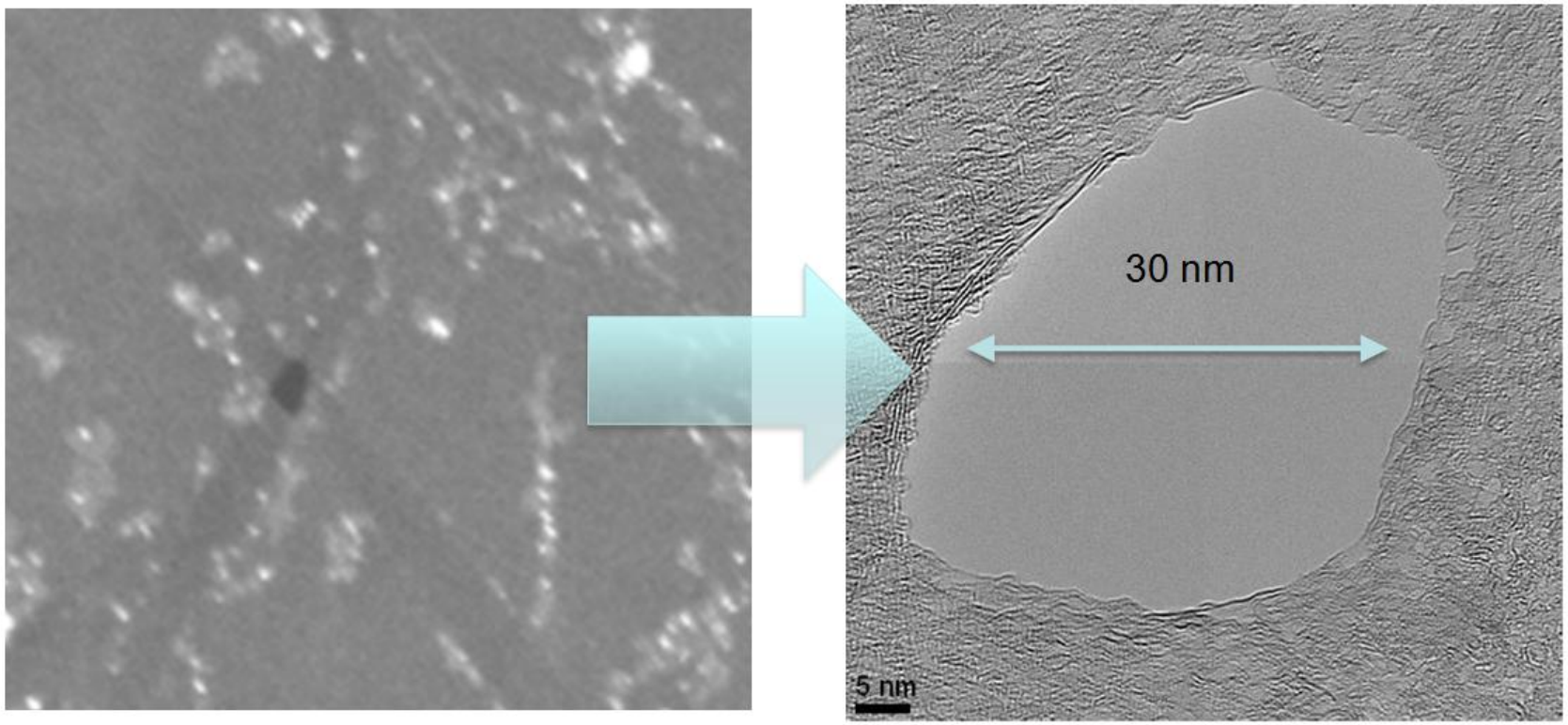
Need precise control of pore size

Sculpting suspended graphene



Images obtained at the Berkeley National Lab's STEM facility
(by W.L. Wang)

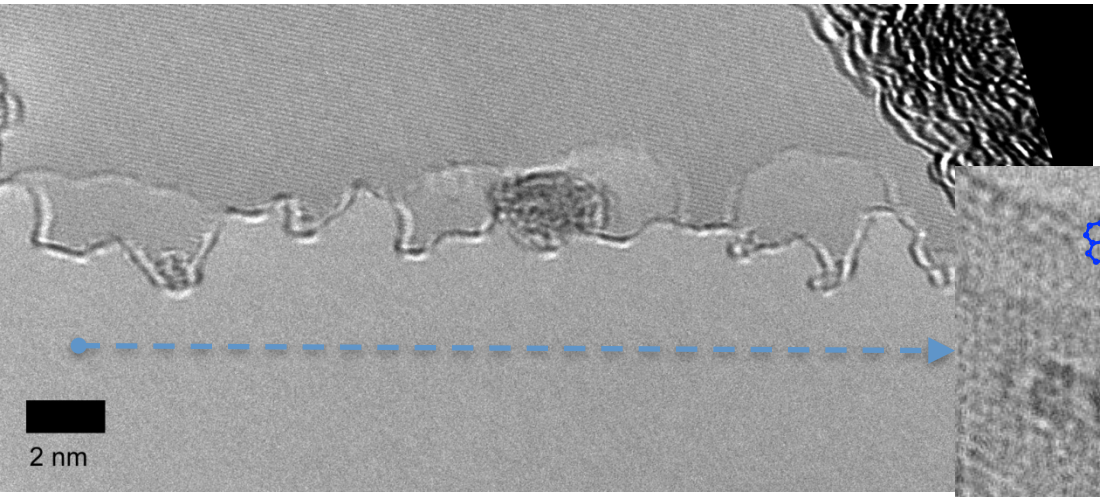
Punching nanopore with STEM

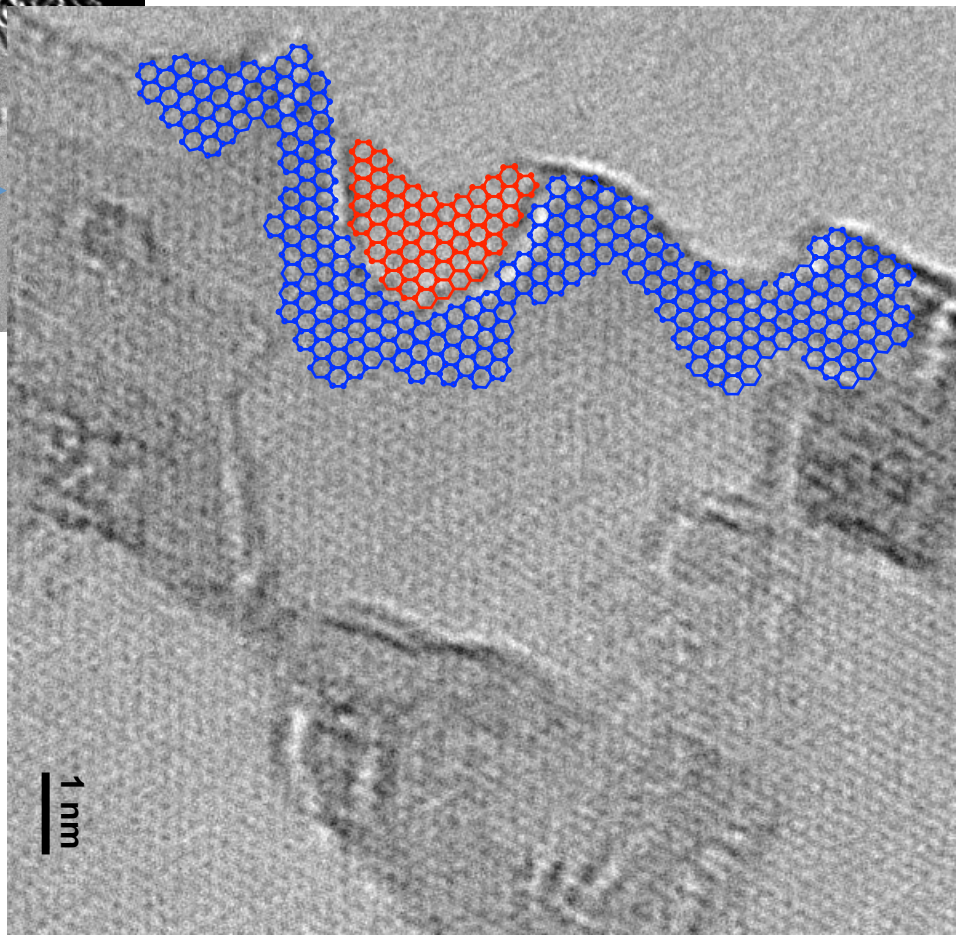


ADF Cs STEM Image at 200 KV

Imaging at 80 KV
Cs TEM Image

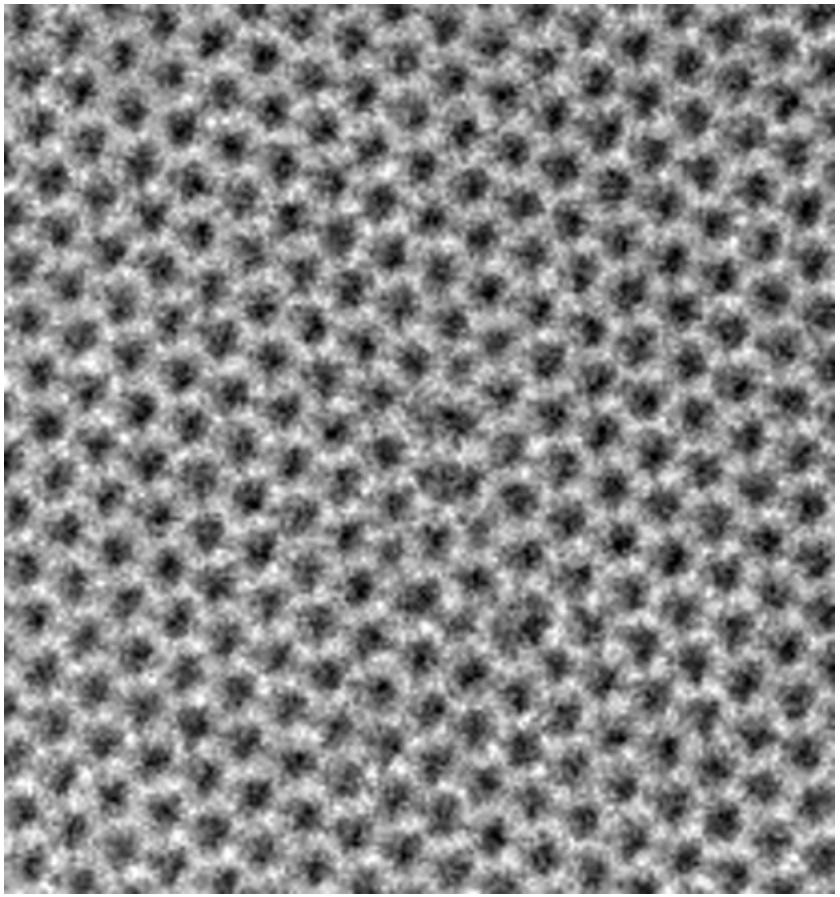
Cutting graphene edges

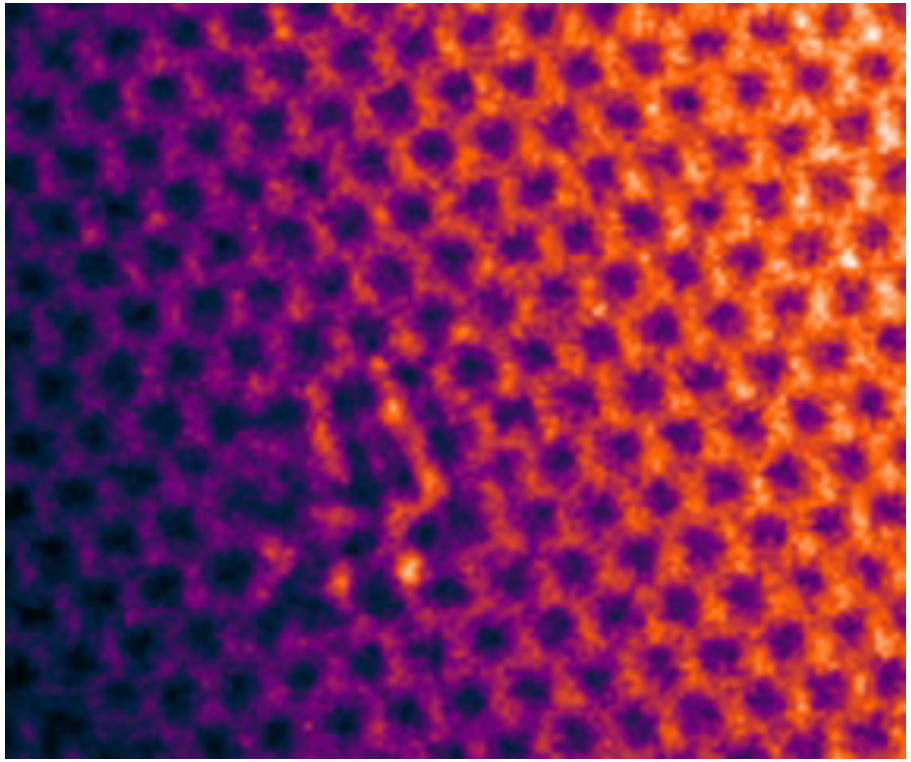


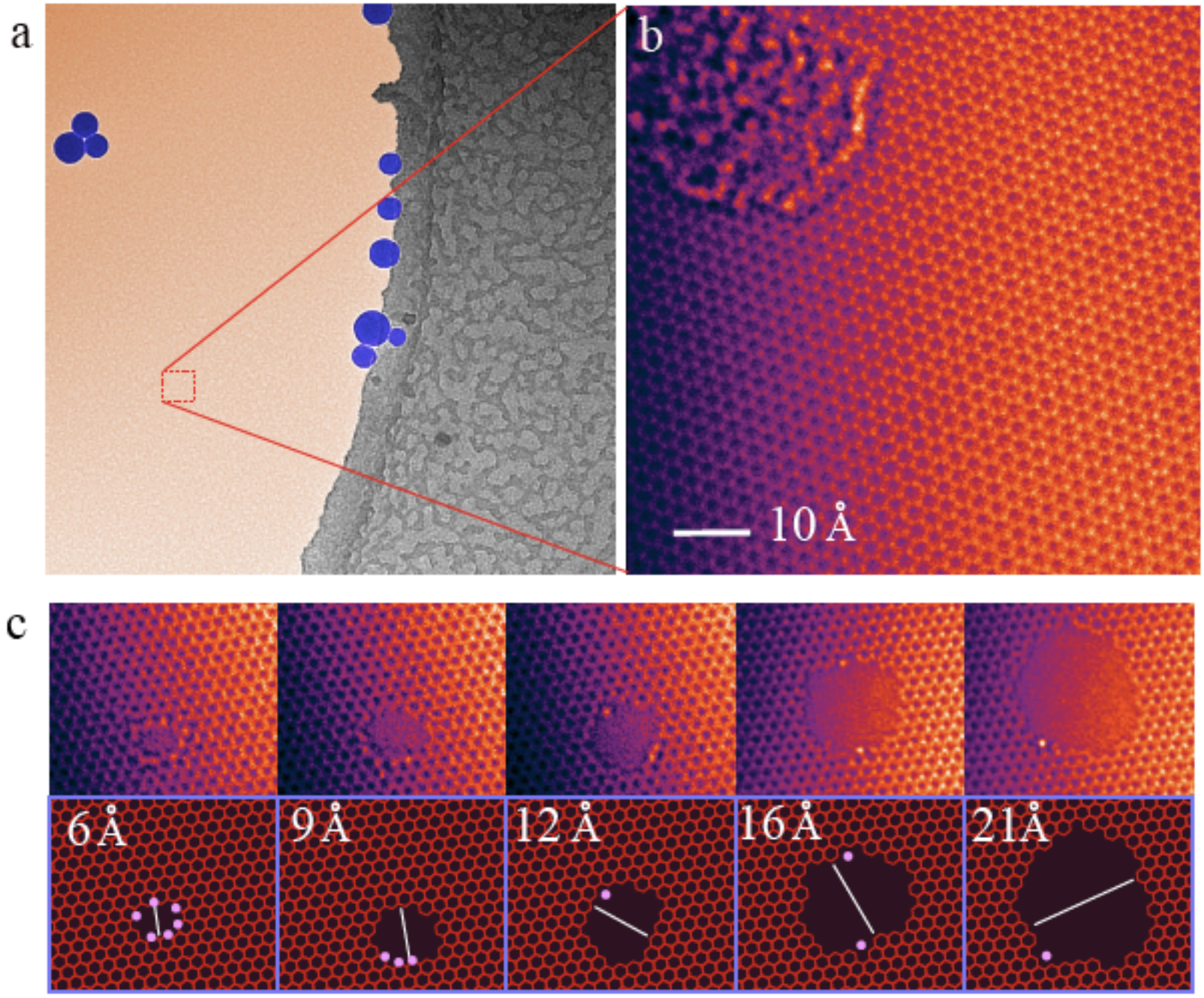


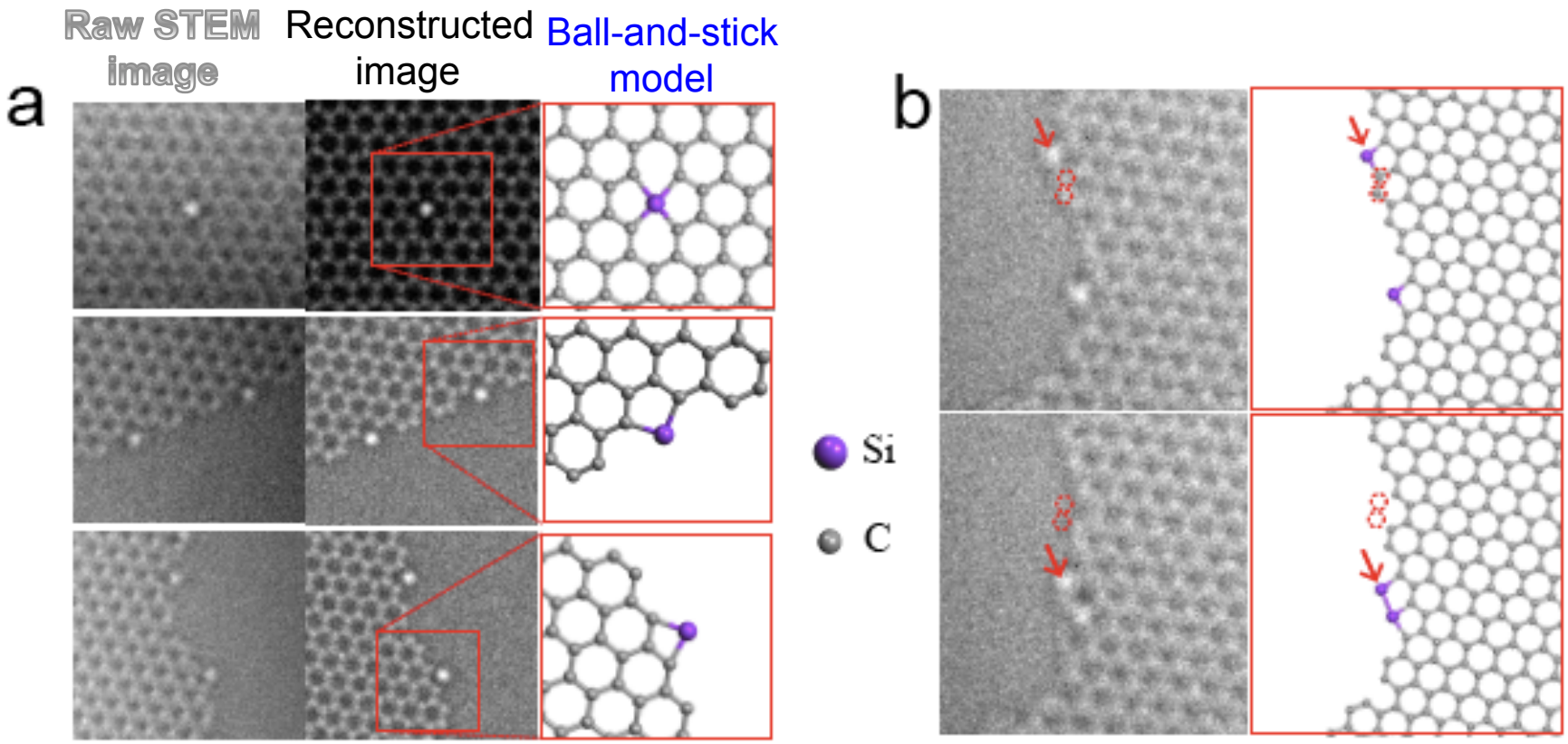
An atomic-scale chisel for sculpting graphene

By Wei Li Wang
Expts. carried out at LBNL's NCEM



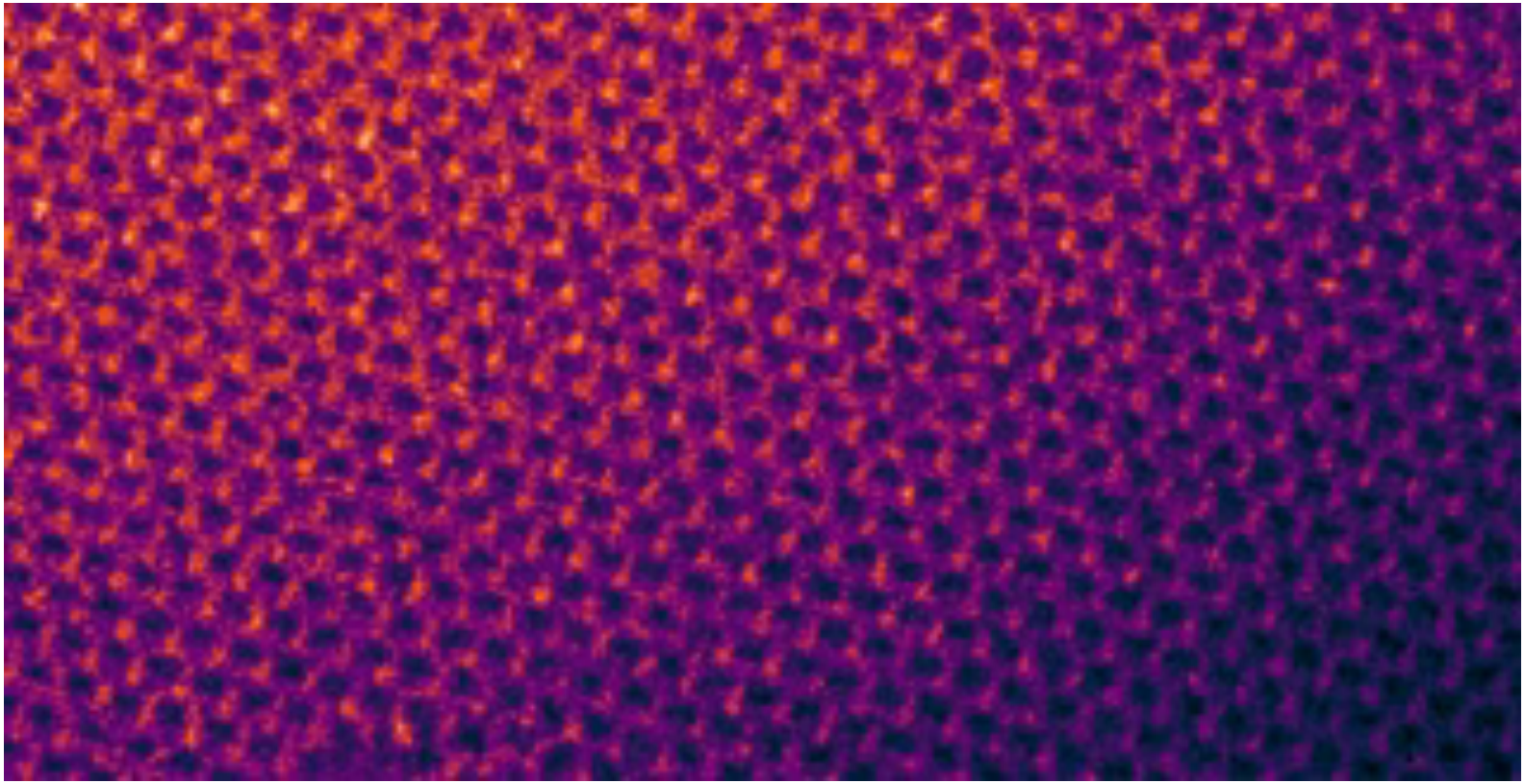


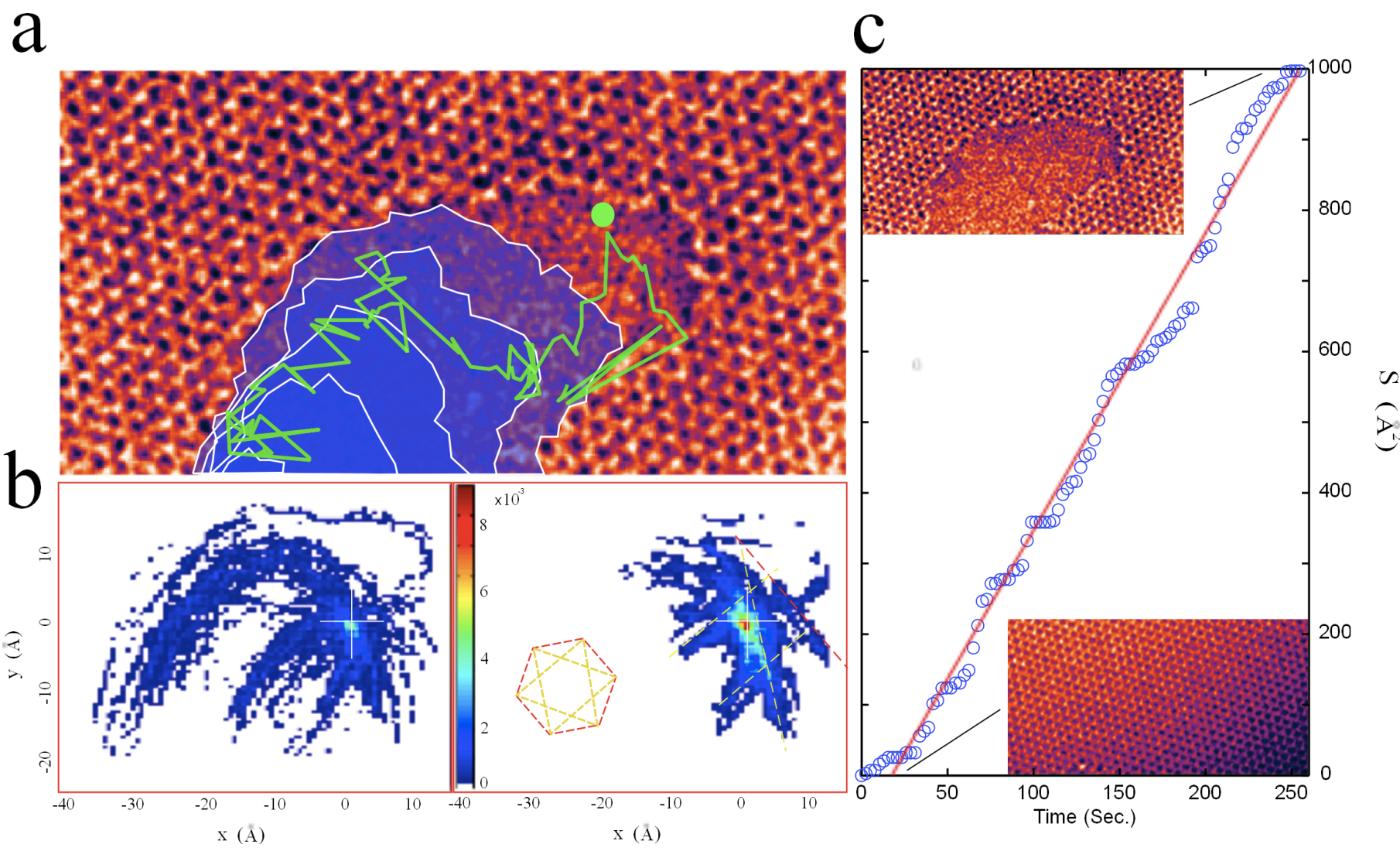

a
b
10 Å
c
6 Å
9 Å
12 Å
16 Å
21 Å



Equilibrium configurations

Action on edges





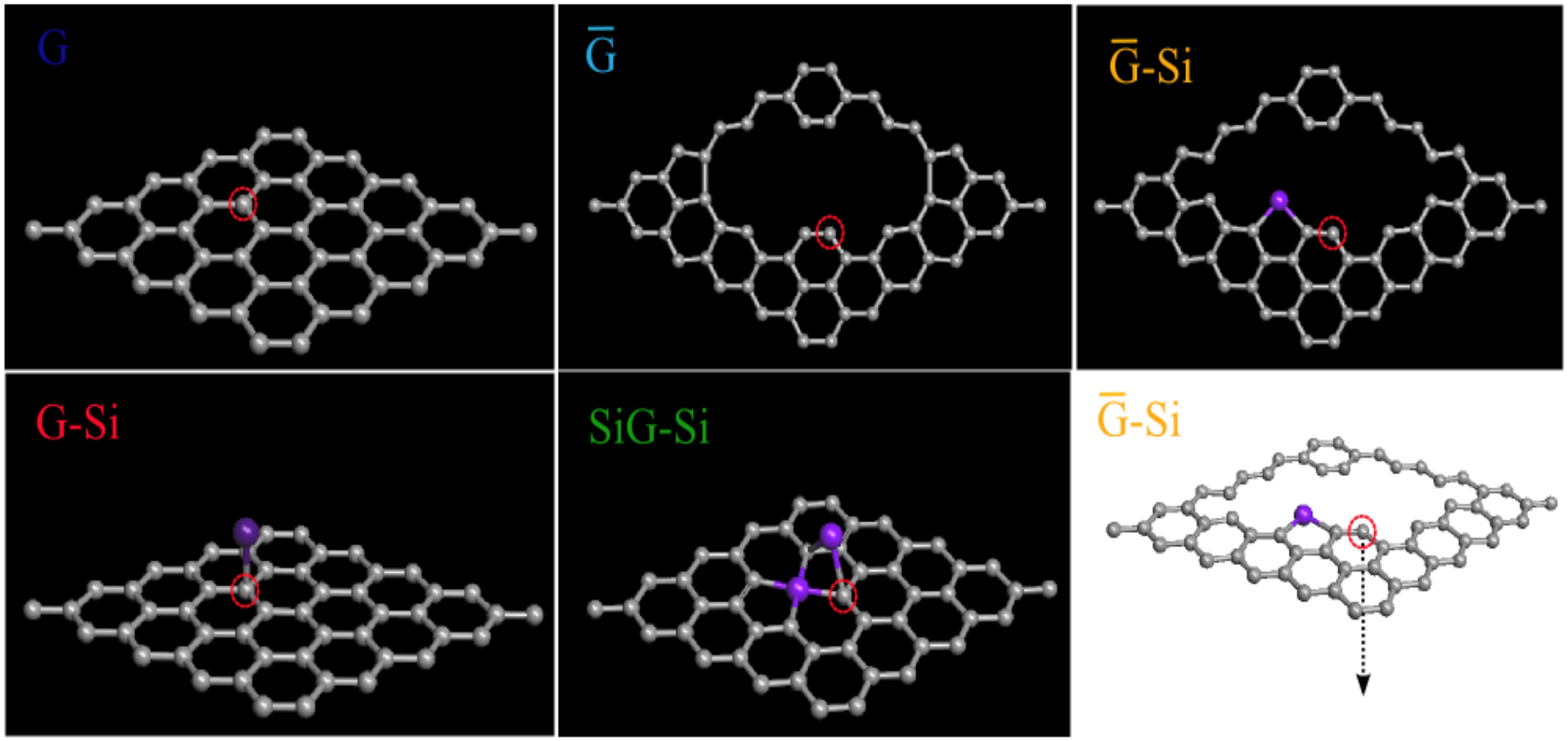
$\mathbf{a} = \mathbf{r}_p - \mathbf{r}_{Si}$

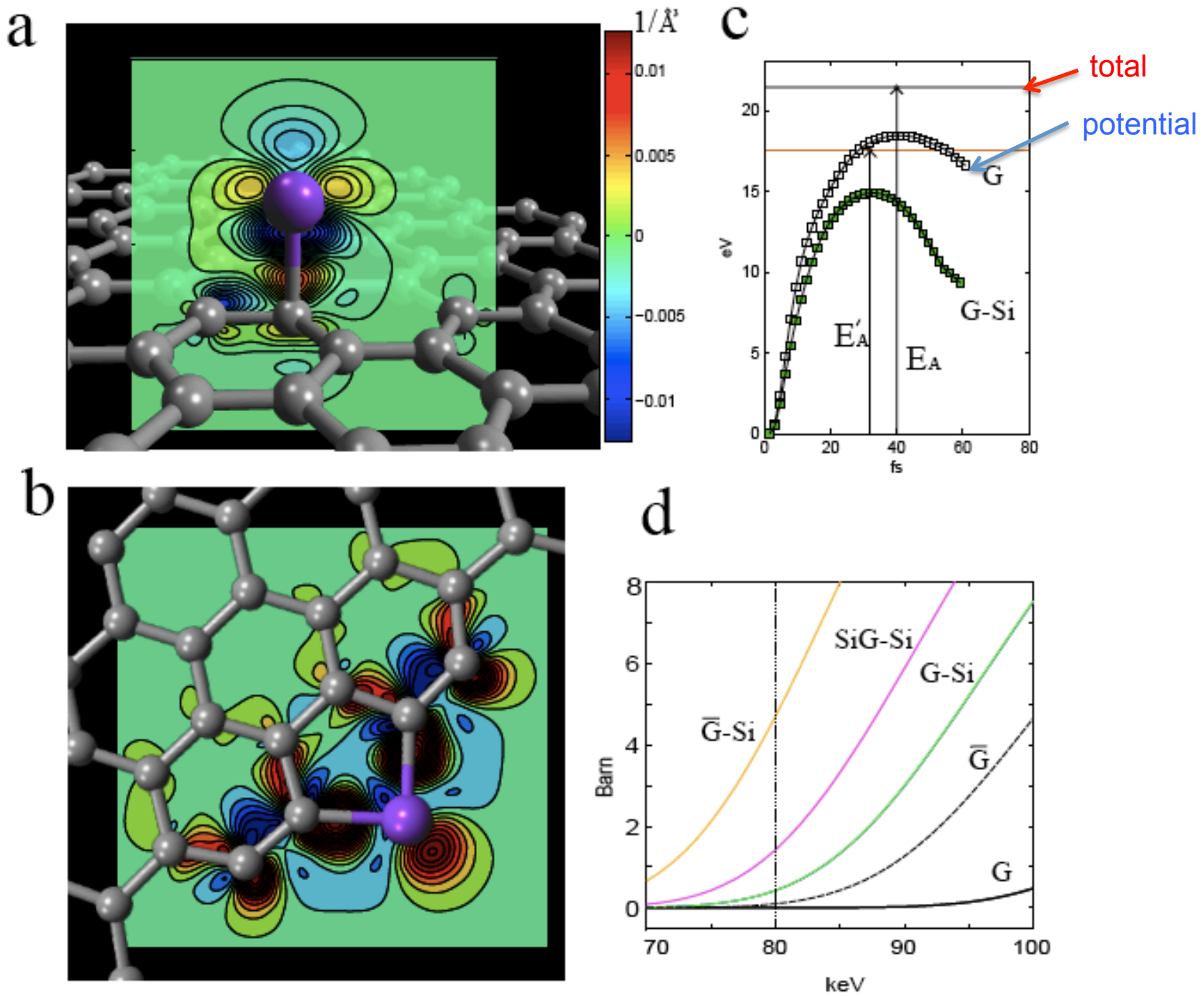
edge atom

$\mathbf{b} = \mathbf{r}_m - \mathbf{r}_{Si}$

removed atom

Simulation of C atom removal from G and $\overline{G}$ (edges) with and without Si impurities




a
1/Å³
0.01
0.005
0
−0.005
−0.01
b
c
total
potential
G
G-Si
E′A
EA
eV
fs
0
5
10
15
20
0
20
40
60
80
d
SiG-Si
G-Si
G
G-Si
G
Barn
keV
0
2
4
6
8
70
80
90
100

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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