Magnetoelectric coupling, screening and electronic states in graphene- and molybdene-based layered nanostructures

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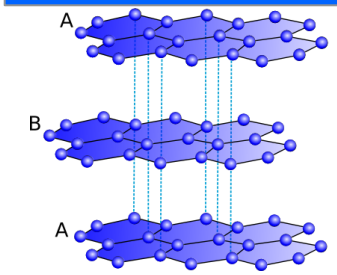
9th International Conference on Nanosciences & Nanotechnologies
3-6 July 2012, Thessaloniki, Greece

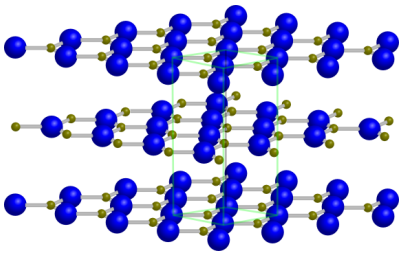
(also attended NN06, NN08, NN09)

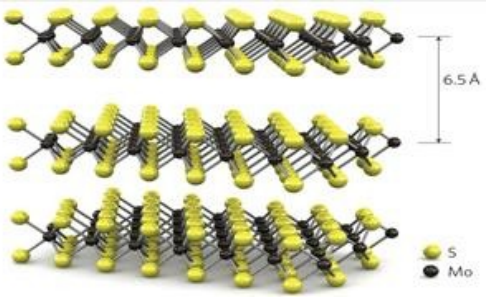
Graphene-multilayers

h-BN

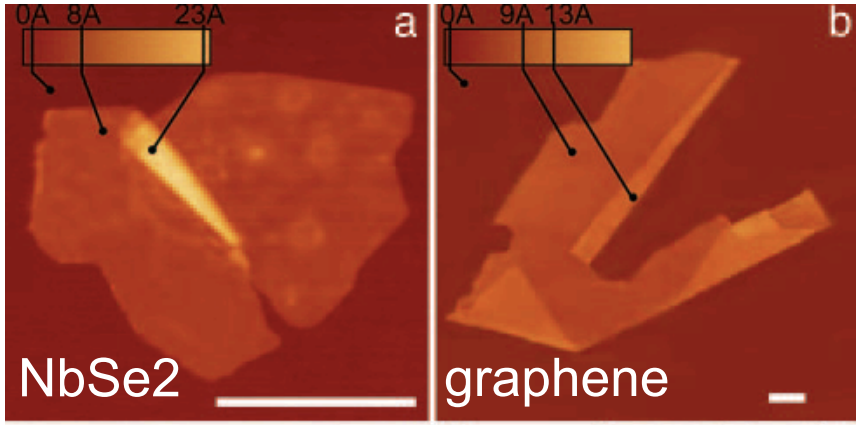
Metal dichalcogenide
(WS_2, TiS_2, ZrS_2, $MoSe_2$, MoS_2, ...)

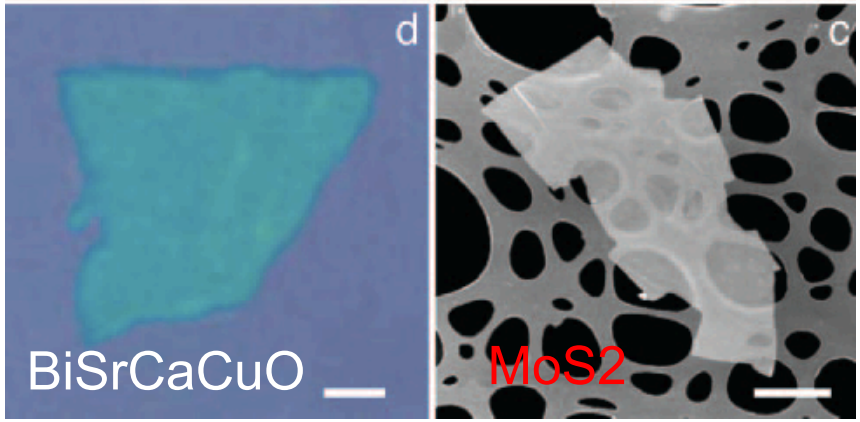




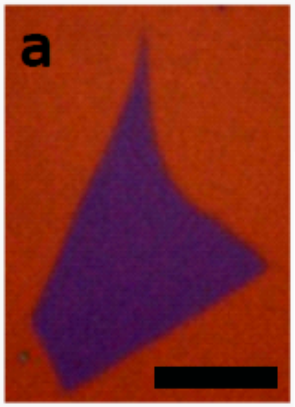


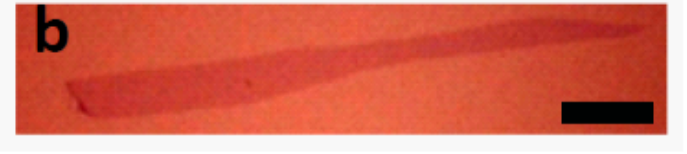
E_{gap} 0.0 eV 5.0 eV 1.7 eV

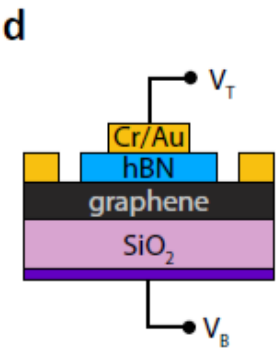


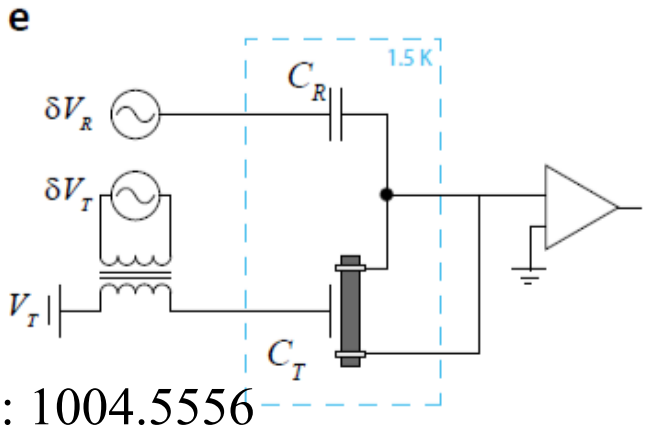


PNAS, **102**, 10451 (2005)









arXiv: 1004.5556

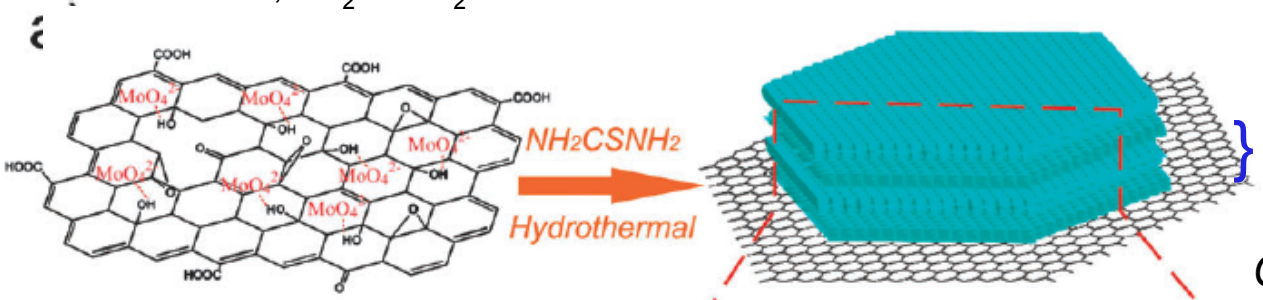
Graphene-MoS_2 interface: Experiments I

Starting materials

Sodium molybdate ($Na_2MoO_4.2H_2O$),
graphene oxide (GO)
NaOH, NH_2CSNH_2

Products

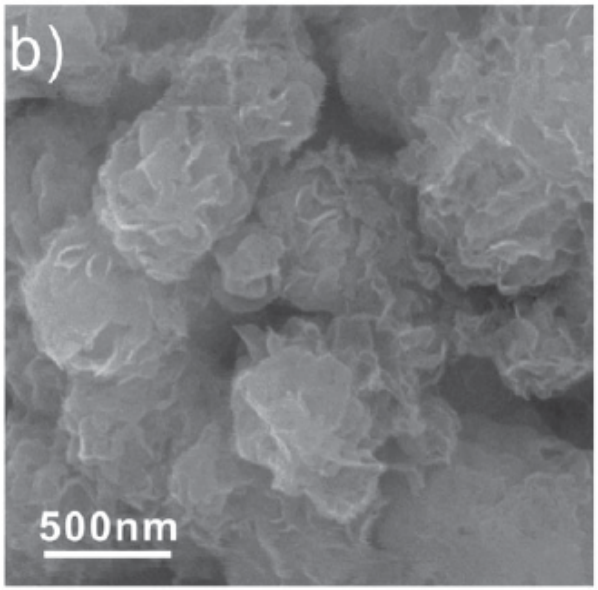
G/MoS_2 composites



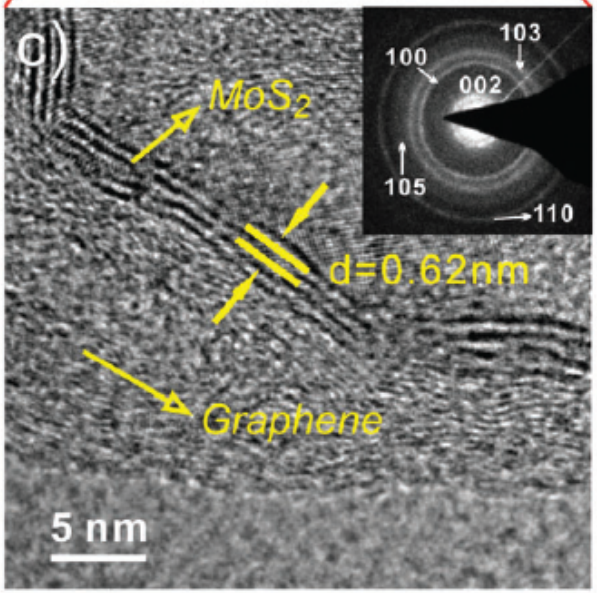
} 4-5 layers

Chem. Commun. (2011), **47**, 4252
ACS Nano, (2011), **5**, 4720

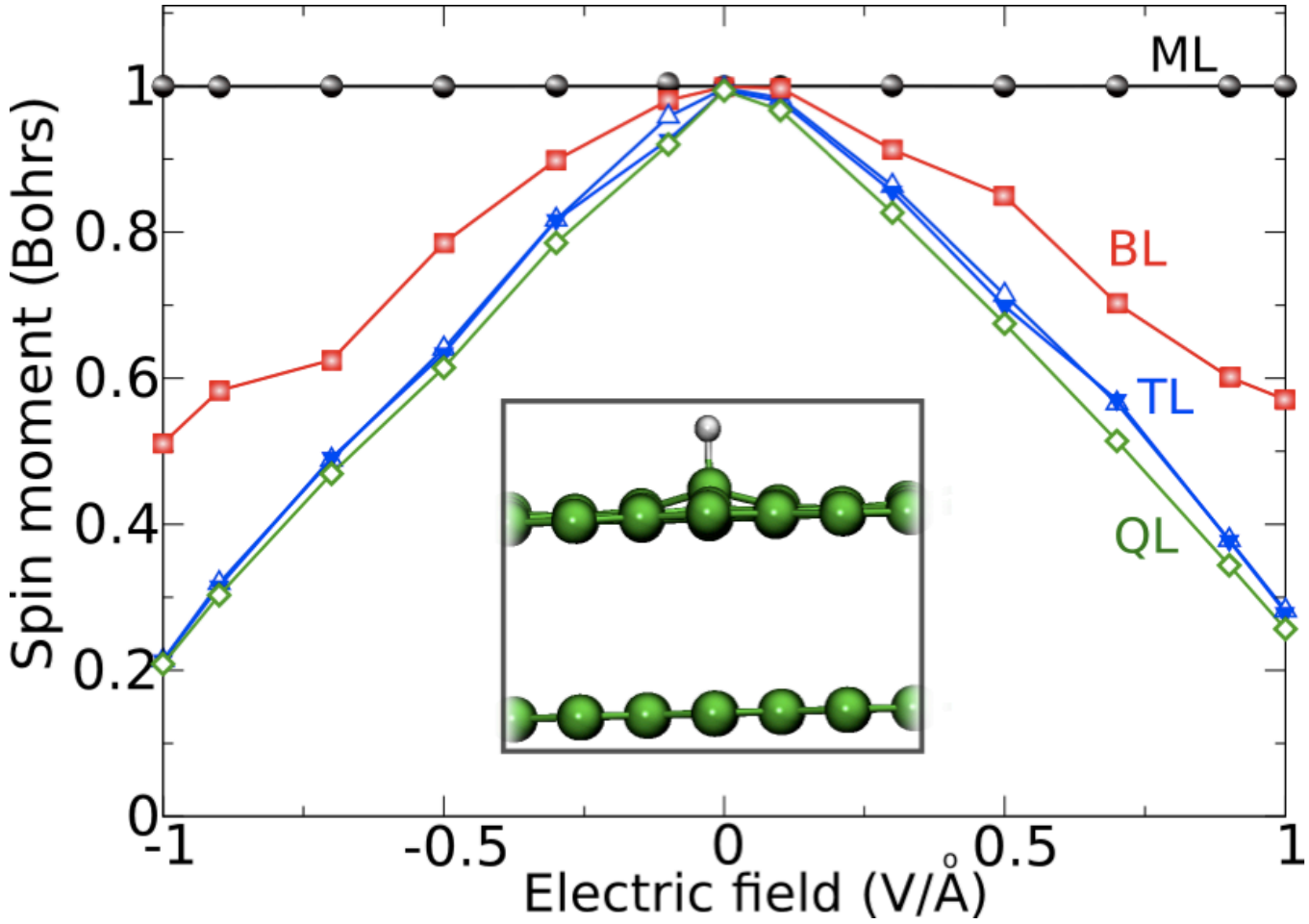
SEM (G/MoS_2 composites)



HRTEM

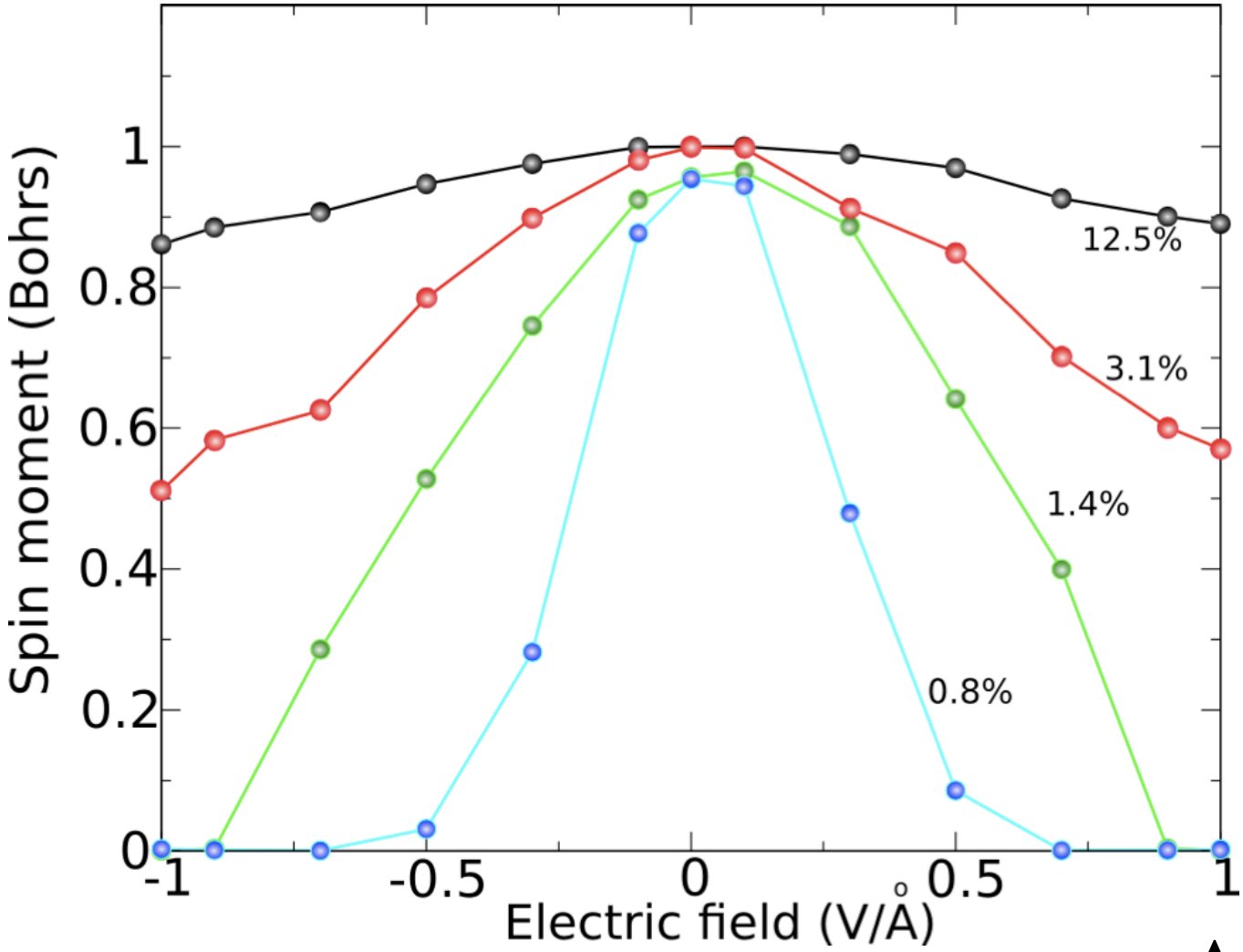


Magnetoelectric Effect in Covalently Functionalized Few-Layer Graphene



H concentration: 3.1%

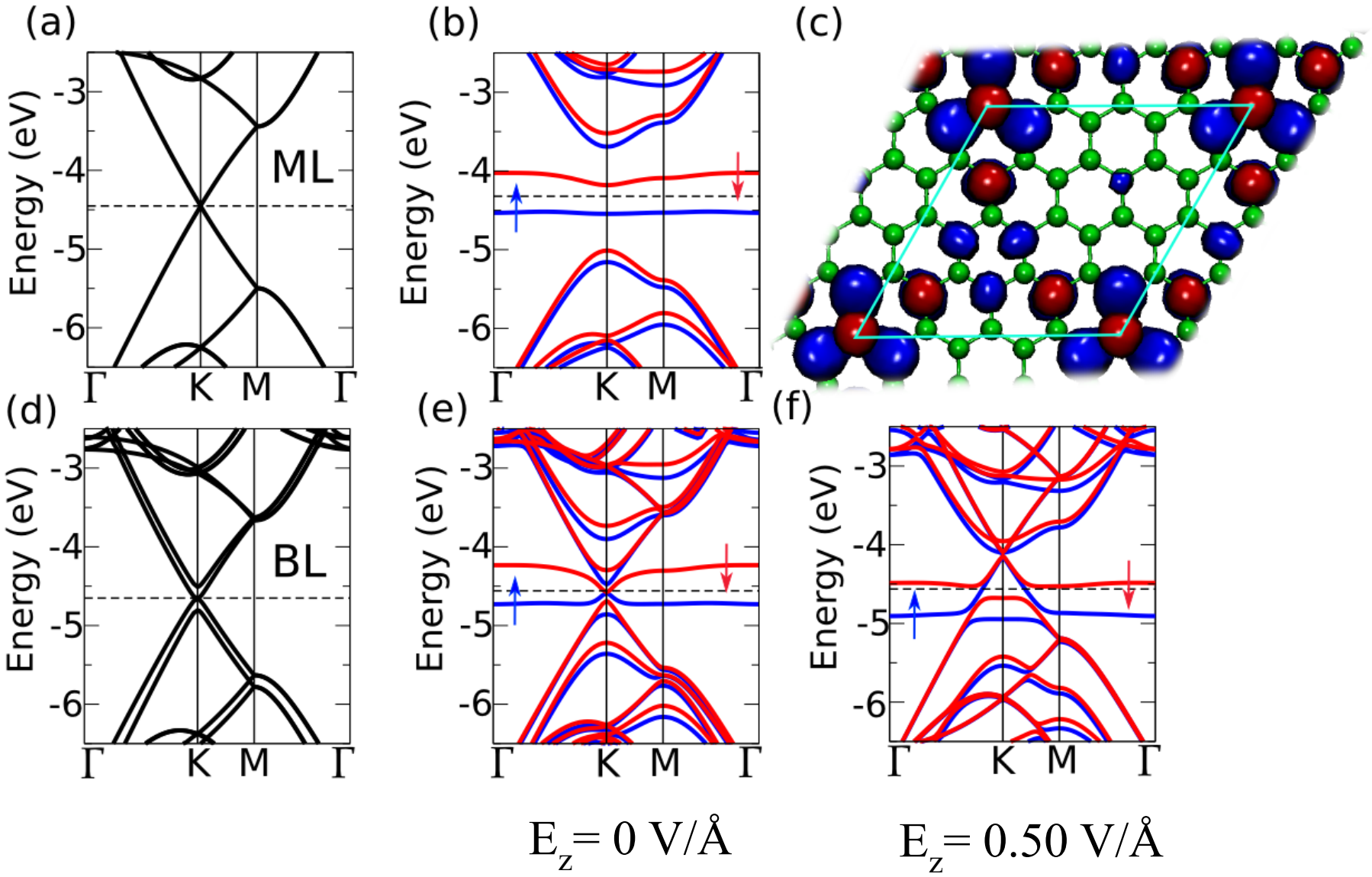
Impurity concentration plays a significant role

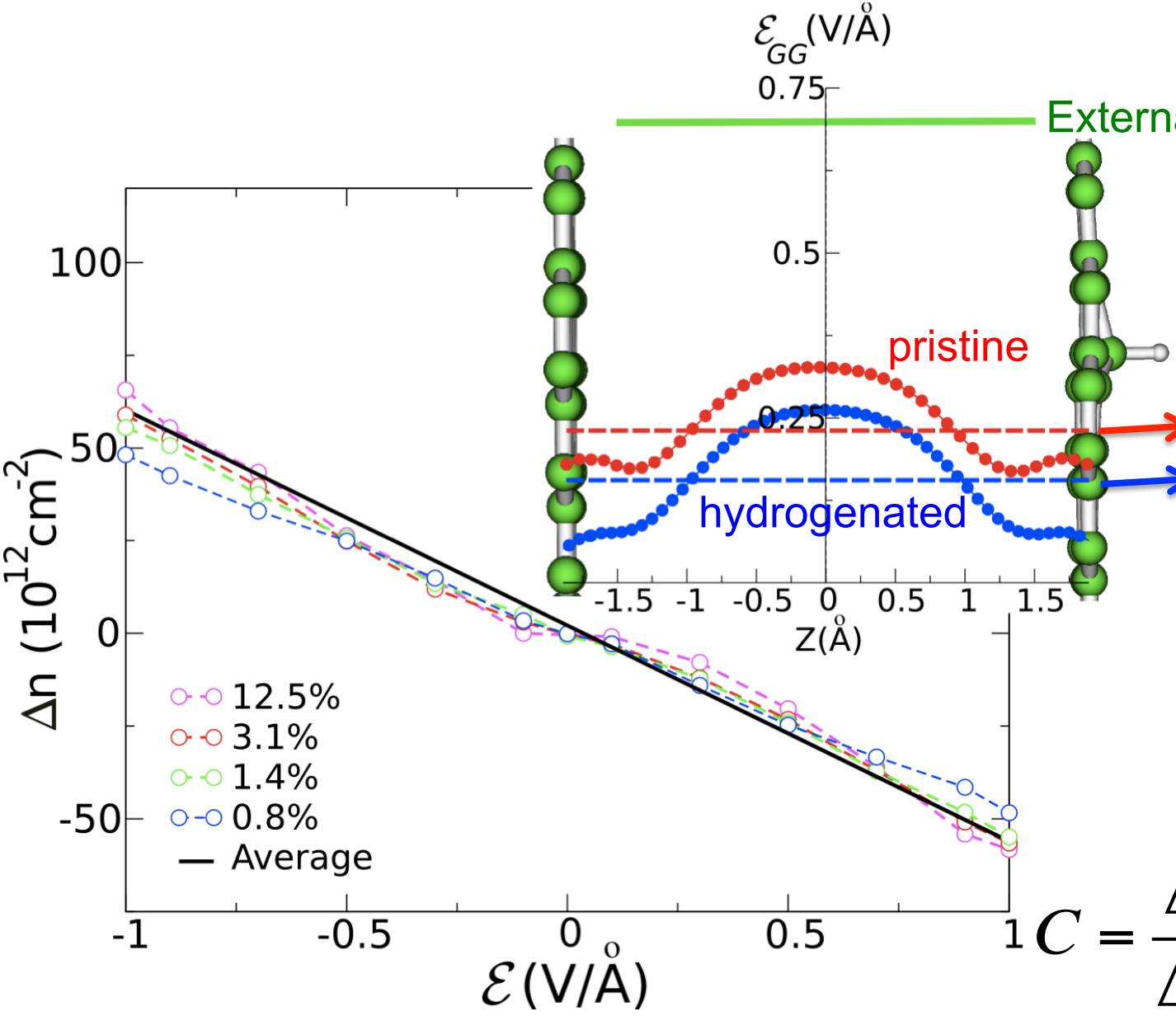


Magnetoelectric coefficient: $\alpha = \mu_0 \frac{\Delta S}{\Delta E}$

~3 times larger that those at ferromagnetic films: Fe (001), Ni(001) and Co(001)

Interplay of defect-level and electric field on the electronic structure





$\varepsilon_0 \approx 3.0$

$\varepsilon_H \approx 4.5$

Capacitance:

$$C = \frac{\Delta n}{\Delta V}, \quad \Delta V = d\frac{E}{\varepsilon}$$

C_0= 5.4 μF/cm^2

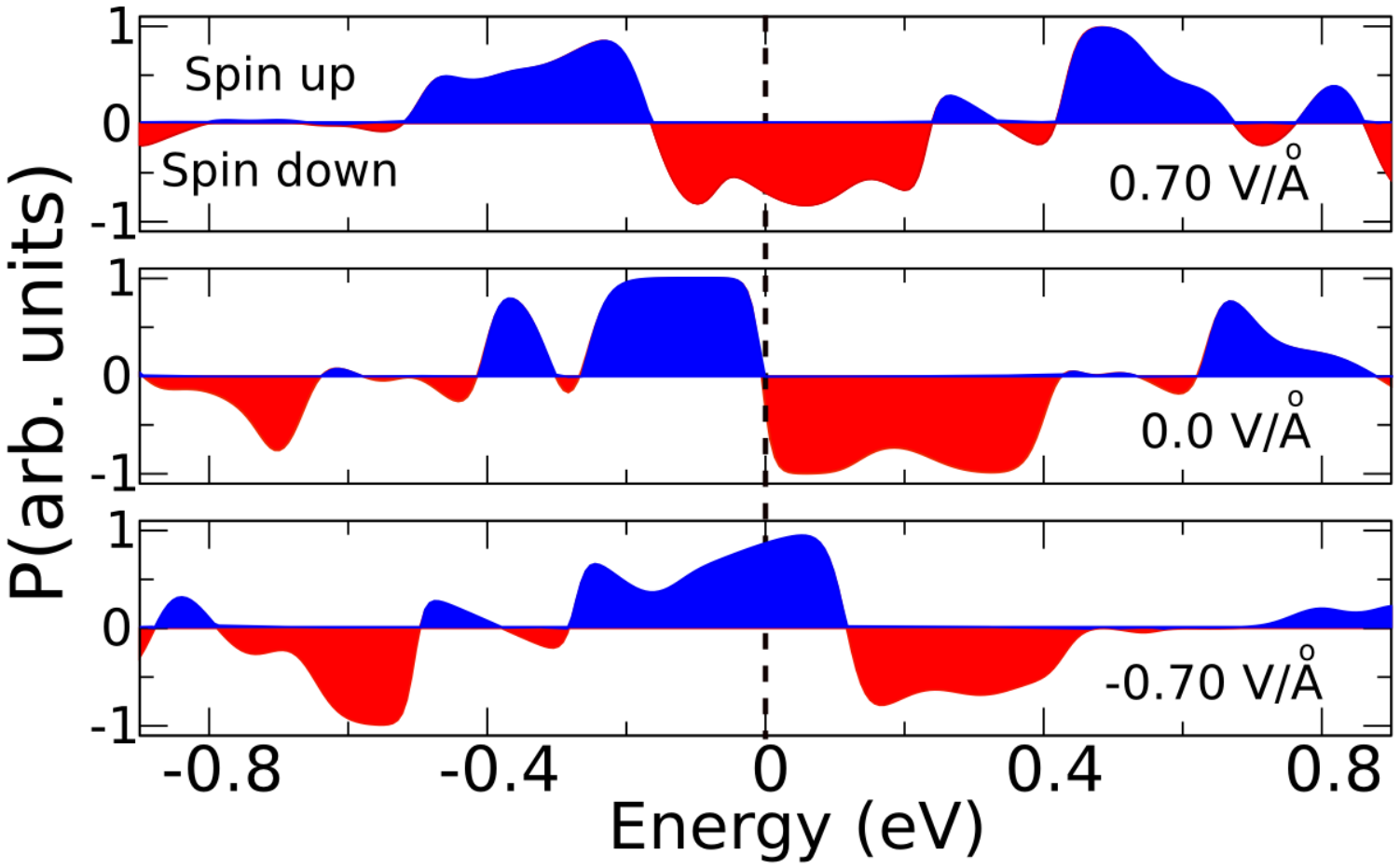
C_H= 10.1 μF/cm^2

Experiments :

C_0=6.8-7.4 μF/cm^2

PRL 076601 (2012), PRB 201408 (2012)

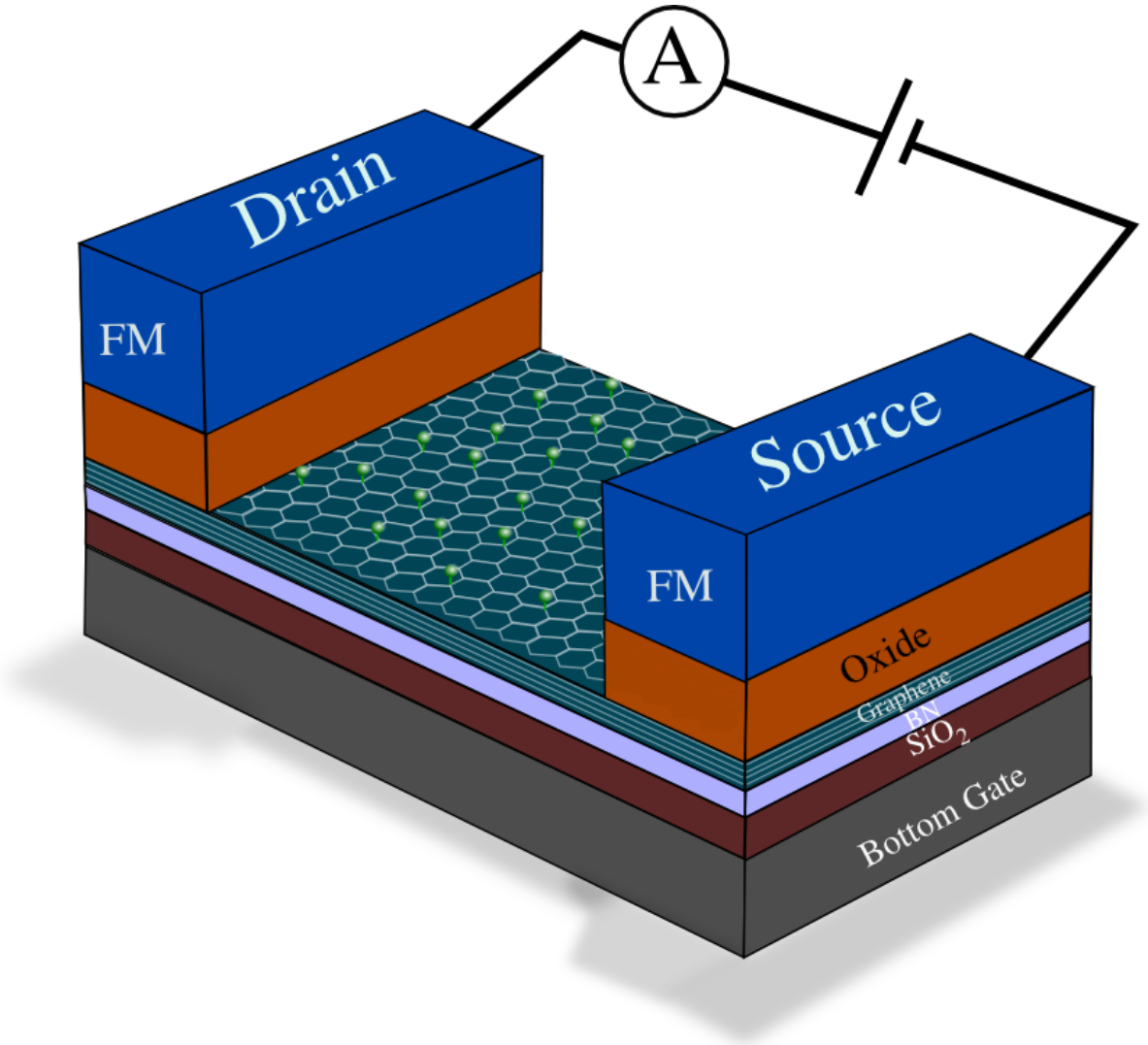
Doping-induced half-metallic behavior: graphene bilayer



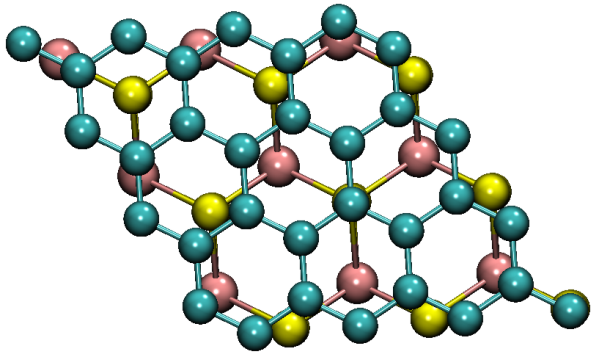
$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

Selection of the spin-channel with an electric bias

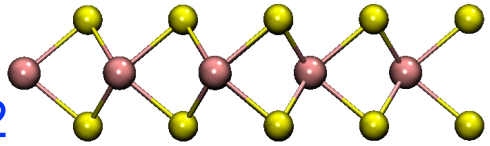
Proposal of an experimental setup to check our predictions



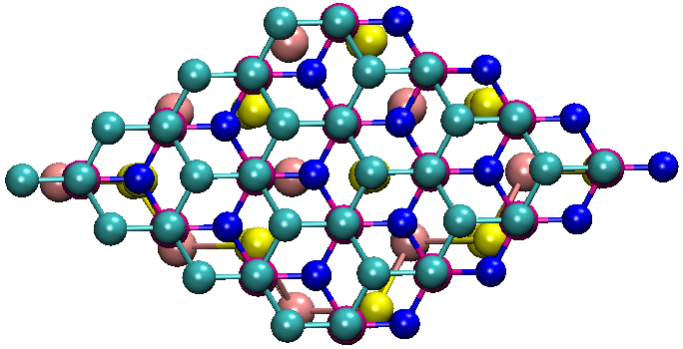
Work in progress:



G



MoS_2



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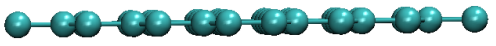
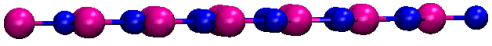
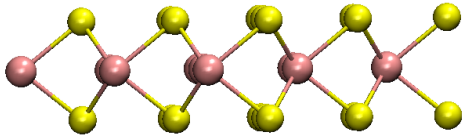
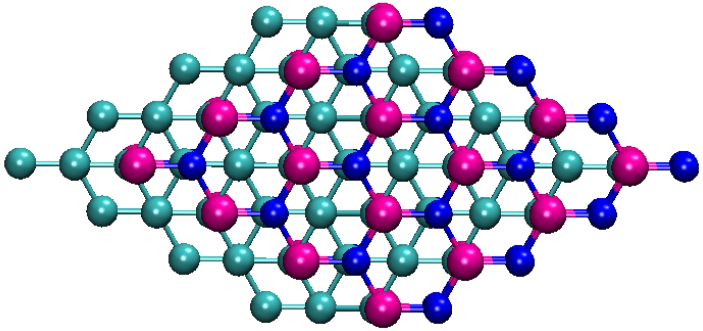


h-BN



MoS_2





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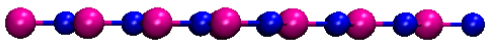

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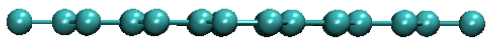

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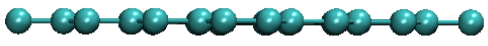
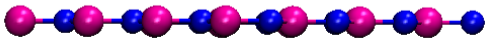
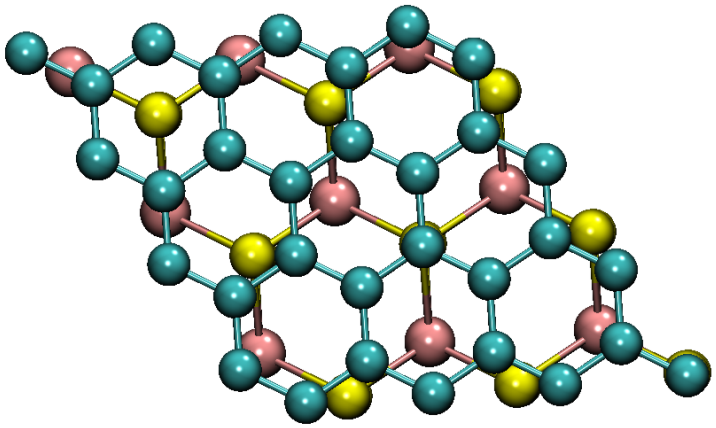


h-BN



Graphene-MoS_2 Interface: interaction



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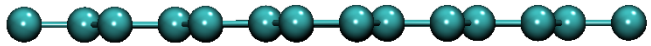
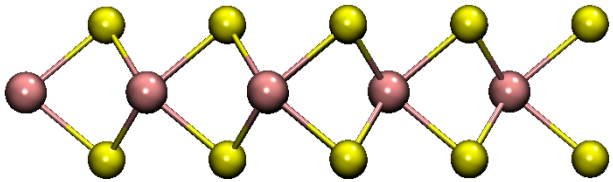


MoS_2

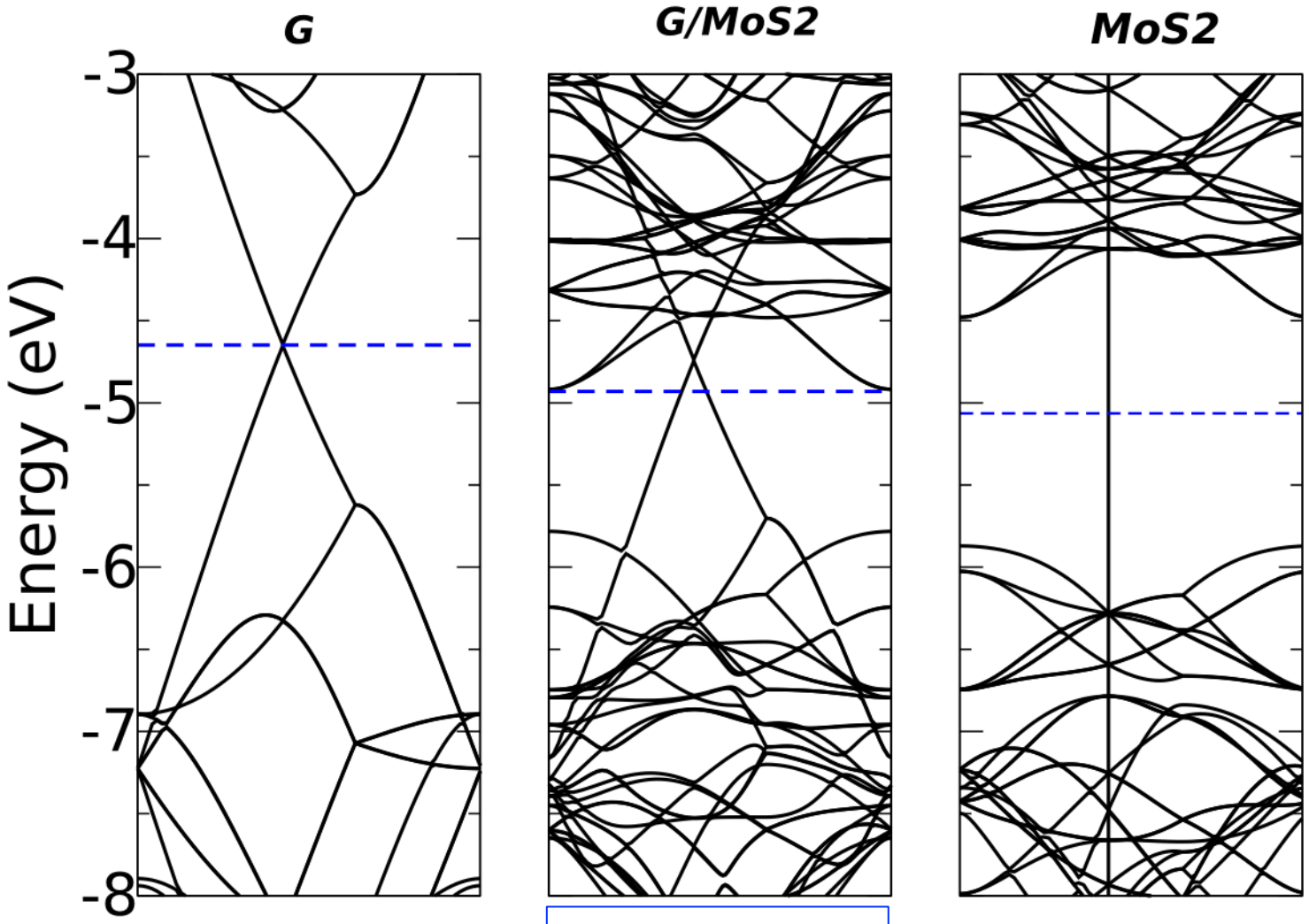


Including vdW's interaction:
E_B ~ 35 meV/C

	Graphite	BN	MoS_2
a [Å]	2.47 (2.46)[a]	2.51 (2.50)[b]	3.23 (3.160)[c]
c [Å]	7.52 (6.70)[d]	7.26 (6.66)[b]	12.6 (12.29)[c]
E_0 [meV/atom]	24 (35 ± 10)[e]	26	60
B_0 [GPa]	12 (~ 33)[a]	11	39
C_{33} [GPa]	13 (37–41)[a]	11	49

PRL (2003), **91**, 126402

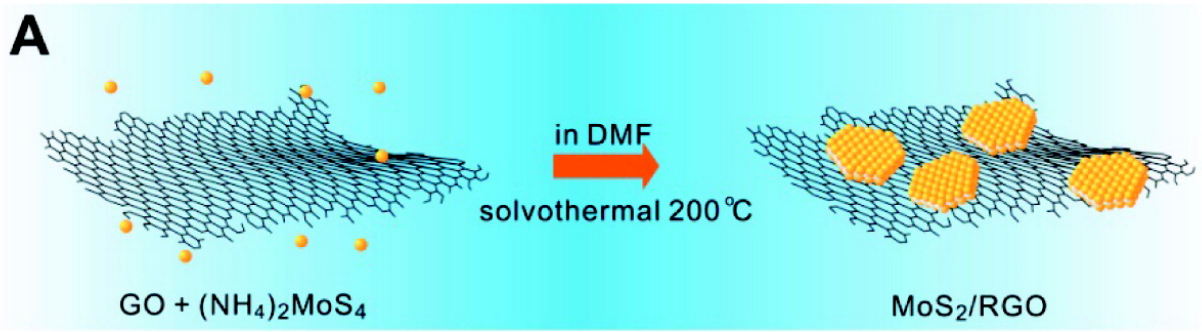
Graphene-MoS_2 Interface: band structure

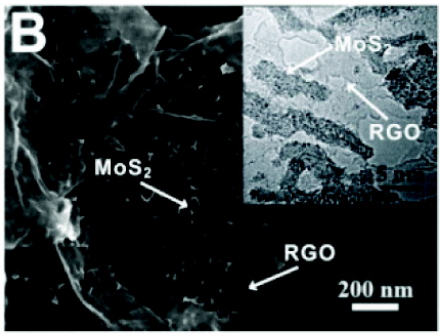


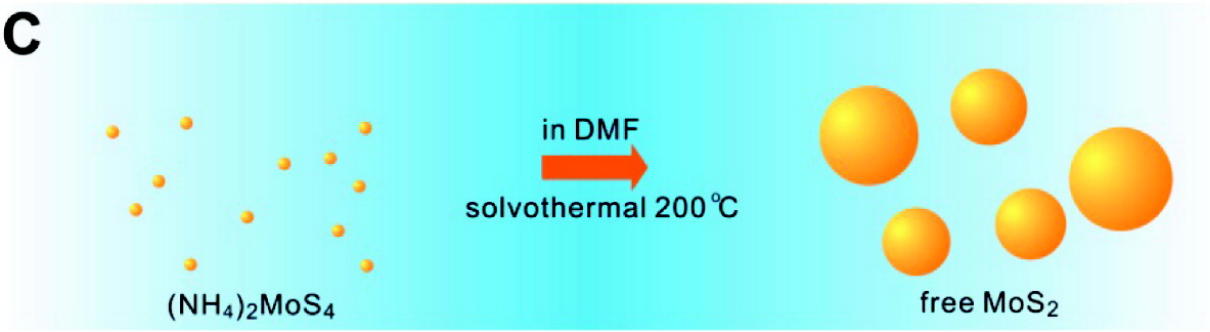
MoS_2 bands modified by strain

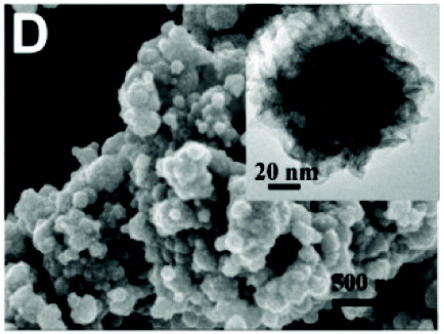
Small charge-transfer from G to MoS_2 (0.1 e)

Graphene-MoS_2 interface: Experiments II





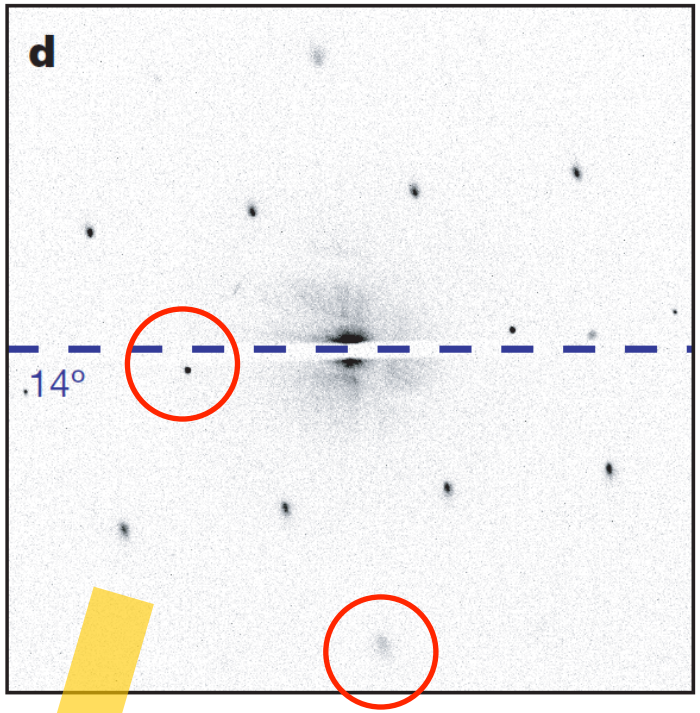


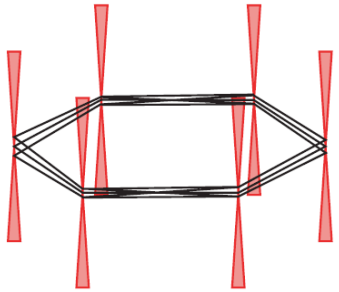


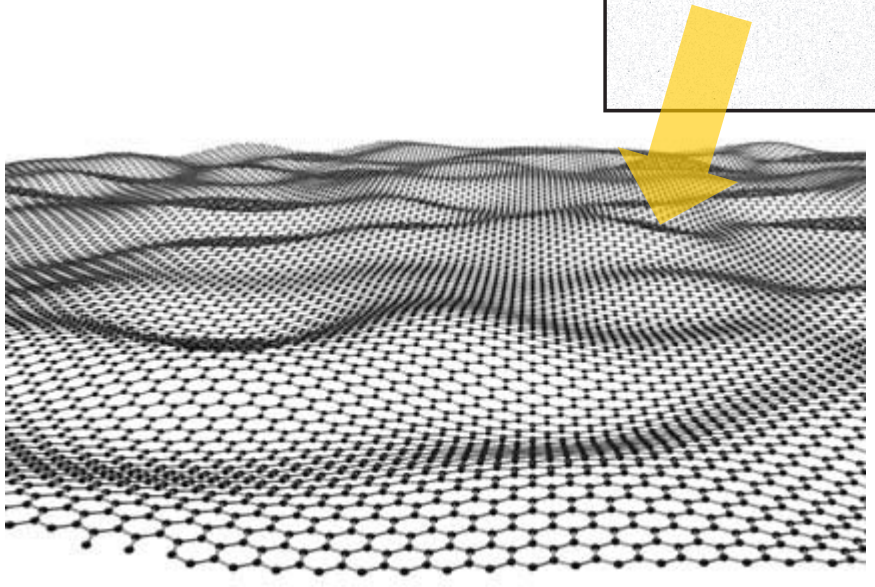
Selective growth of MoS_2 on top of GO

JACS (2011), **133**, 7296.

Intrinsic ripples in graphene

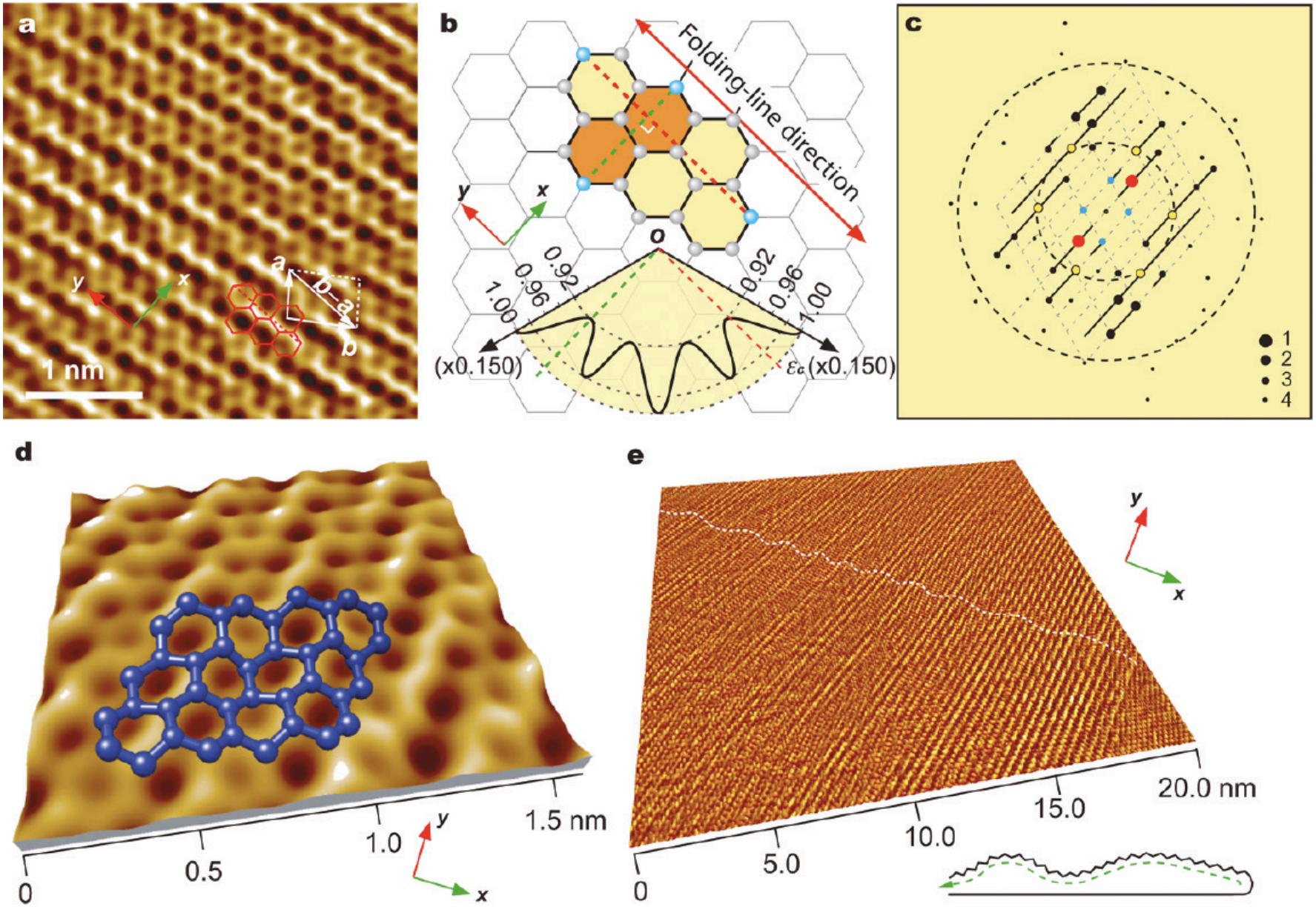






Meyer, J. C. et al. Nature **446**, 60-63, 2007.

Mermin, N. D. Phys. Rev. **176**, 250–254, 1968.
Nelson, D. R., Piran, T. & Weinberg, *World Scientific*, Singapore, 2004.

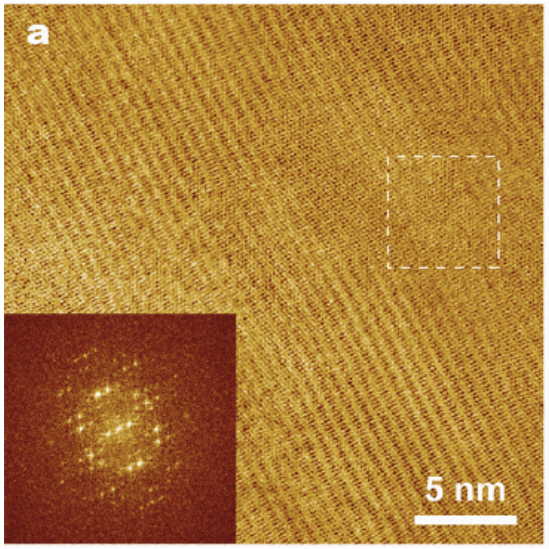


Graphene Structures at an Extreme Degree of Buckling

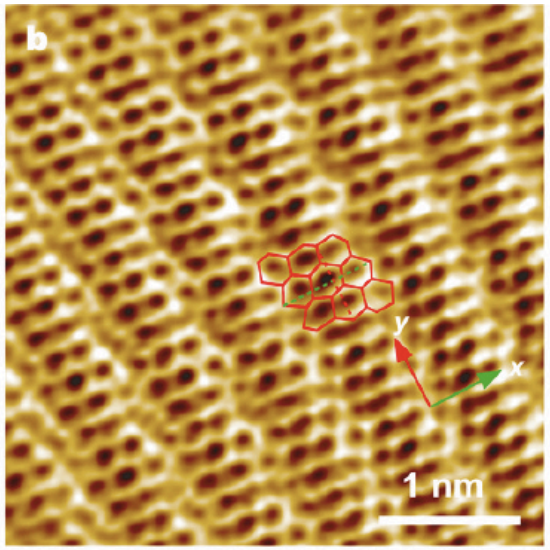
Youdong Mao, Wei L. Wang, Dongguang Wei, Efthimios Kaxiras, and Joseph G. Sodroski

ACS NANO, **5**, 1395–1400 (2011)

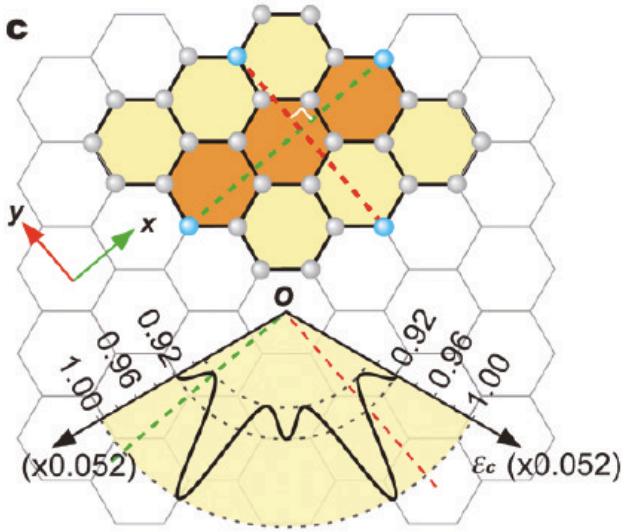
TEM

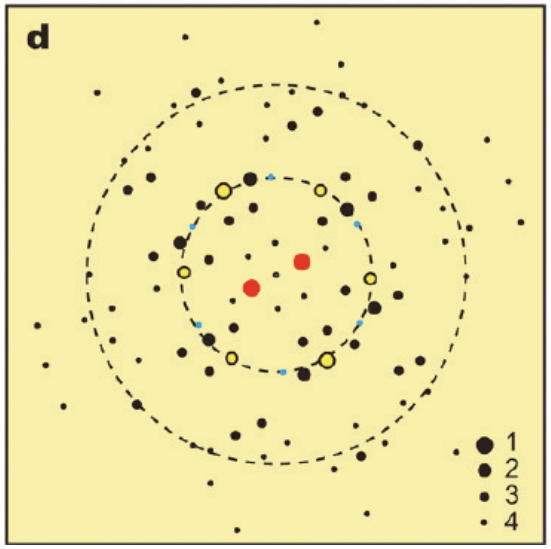


TEM

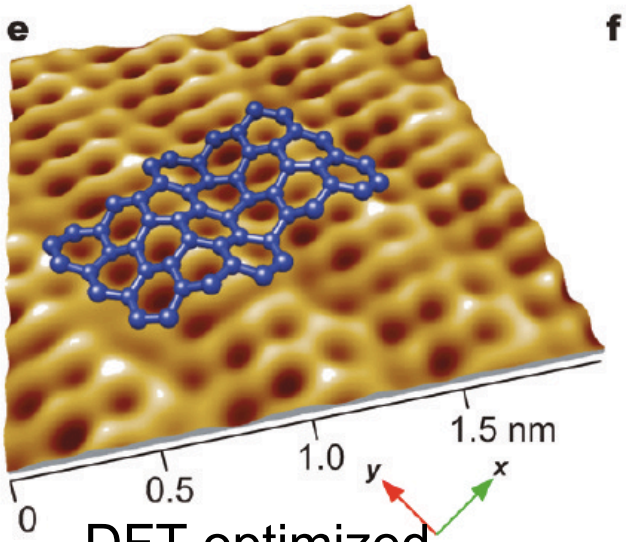


Atomic model

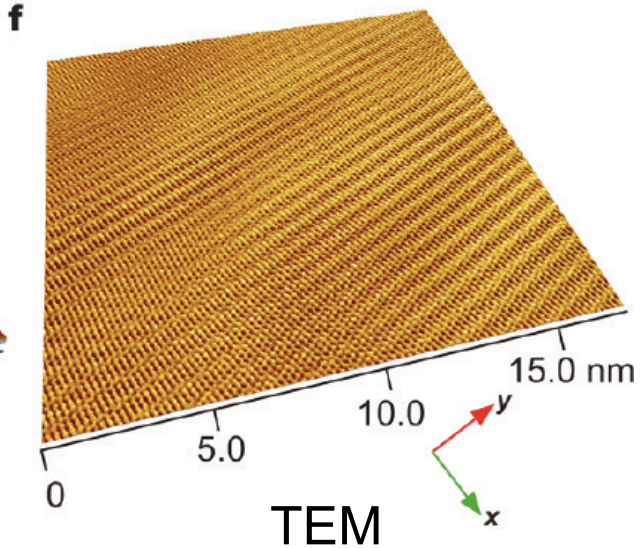




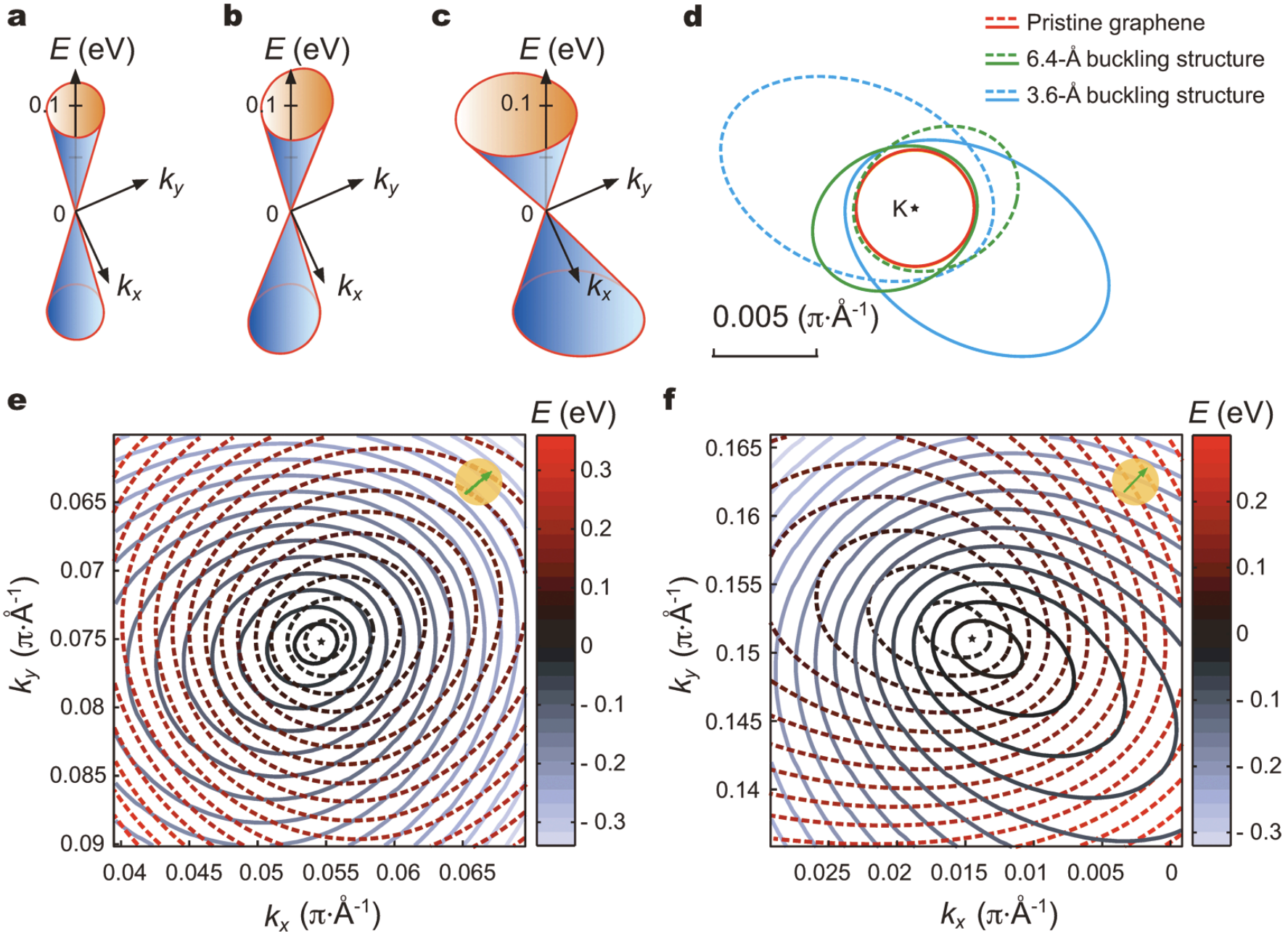
Fourier spectrum



DFT-optimized structure



TEM


a
b
c
d
e
f
E (eV)
0.1
0
k_y
k_x
Pristine graphene
6.4-Å buckling structure
3.6-Å buckling structure
K
0.005 (π·Å^{-1})
0.3
0.2
0.1
0
- 0.1
- 0.2
- 0.3
0.065
0.07
0.075
0.08
0.085
0.09
0.04
0.045
0.05
0.055
0.06
0.065
k_y (π·Å^{-1})
k_x (π·Å^{-1})
0.165
0.16
0.155
0.15
0.145
0.14
0.025
0.02
0.015
0.01
0.005
0

Direct imaging in real space of aperiodic rippling

Why

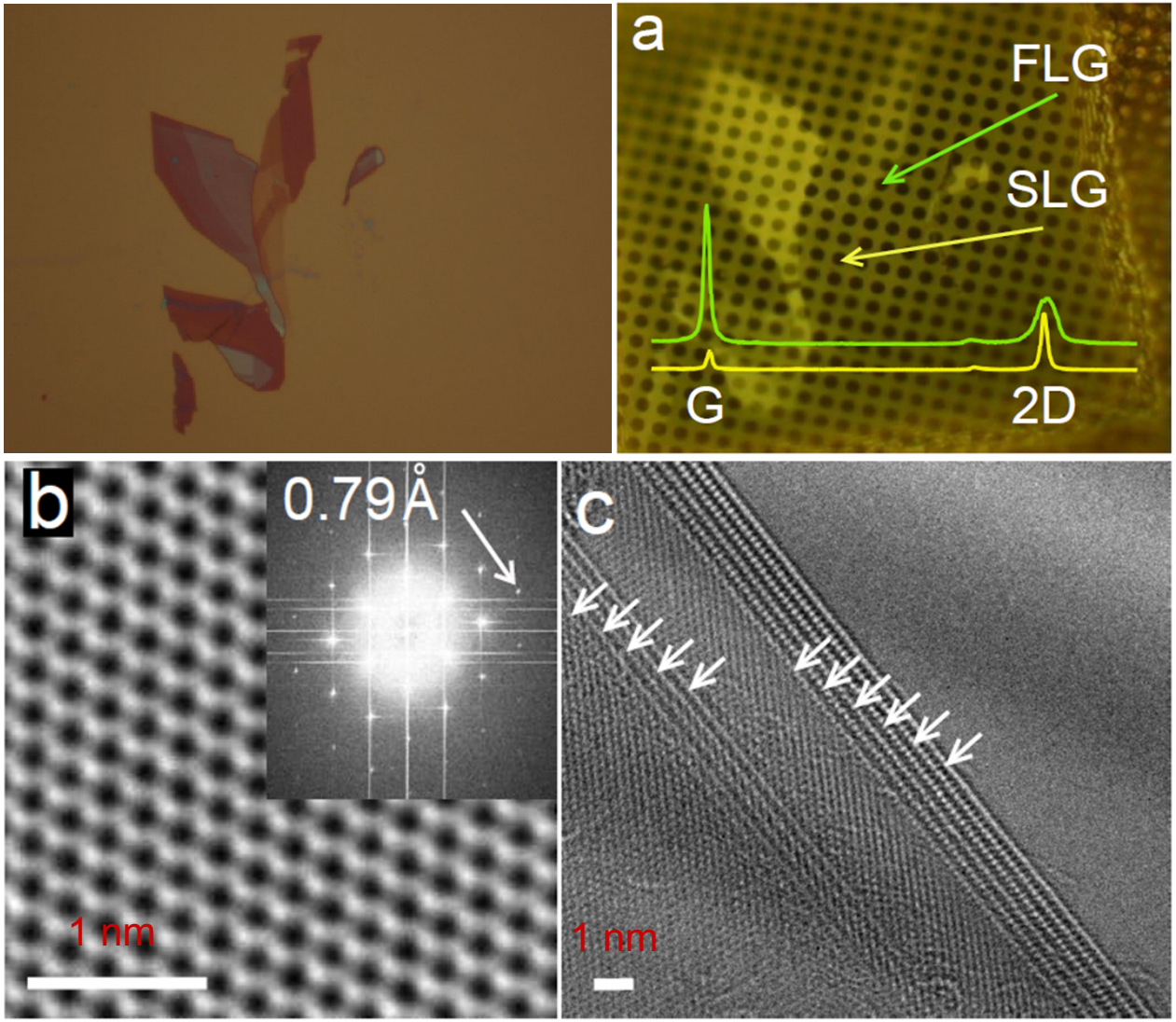
- Ripple topography including amplitude and wavelength
- Dynamic properties

How

- Convergent beam electron diffraction
- Bond length variations
- Thicker samples

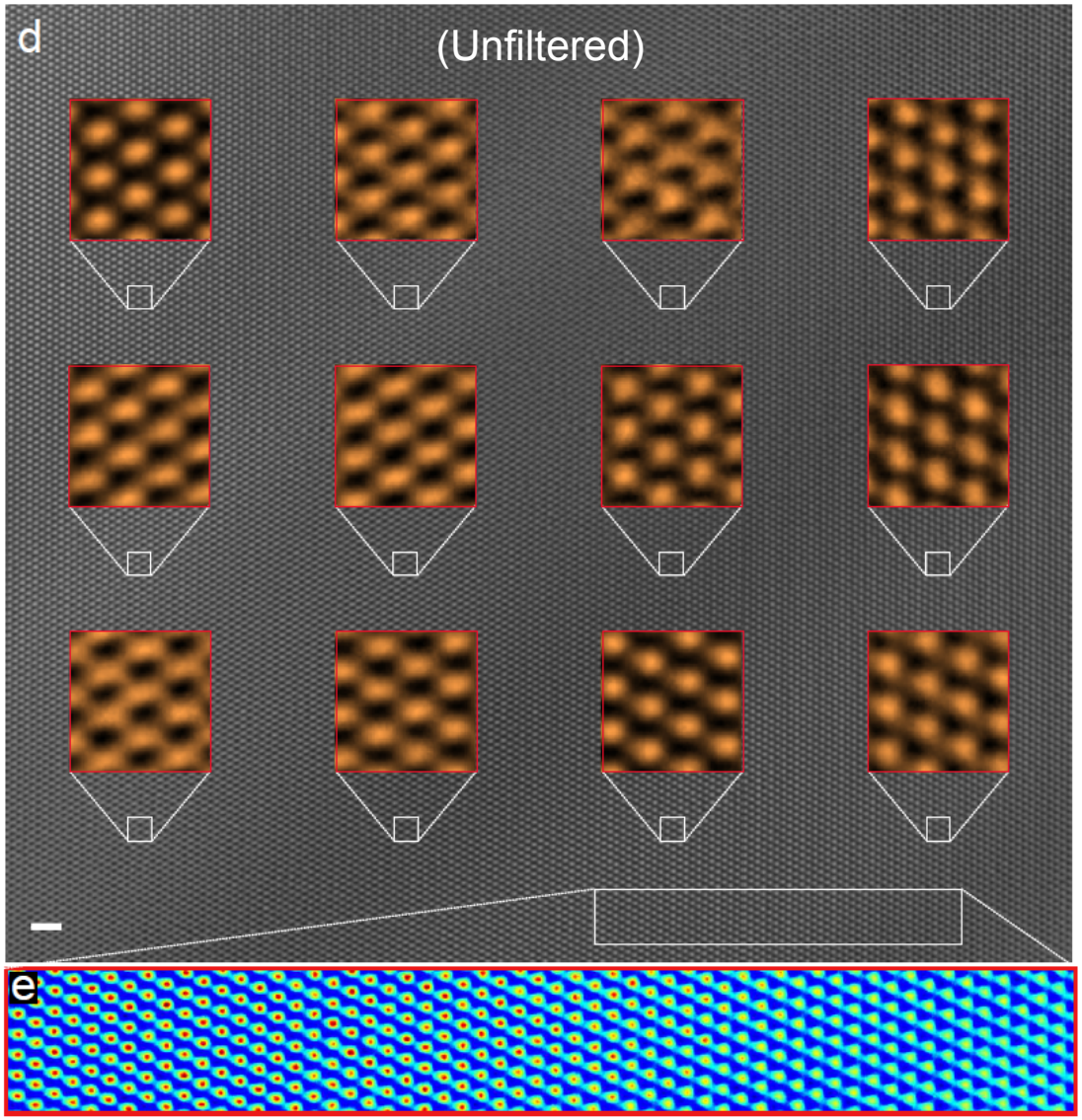
Meyer, J. C. *et al*. Nature **446**, 2007
Bangert, U. *et al*. Phys Status Solidi A **206**,1117-1122, 2009

Imaging graphene samples

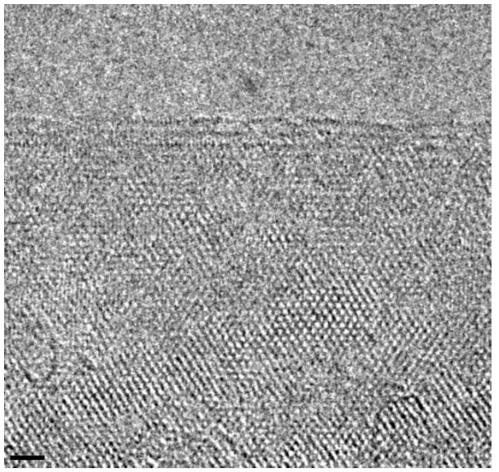


Libra MC 200-80
- Monochromated
- Aberration Corrected
- Operated at 80 kV

Ripples in real space



FEI Titan, 300 kV



Meyer, J. C. *et al*.
Nature **446**, 2007.

Calculate total potential with a transferable core correction

DFT:

- Pseudopotential : wrong core
- All electron: too expensive
- Pseudopotential + core correction

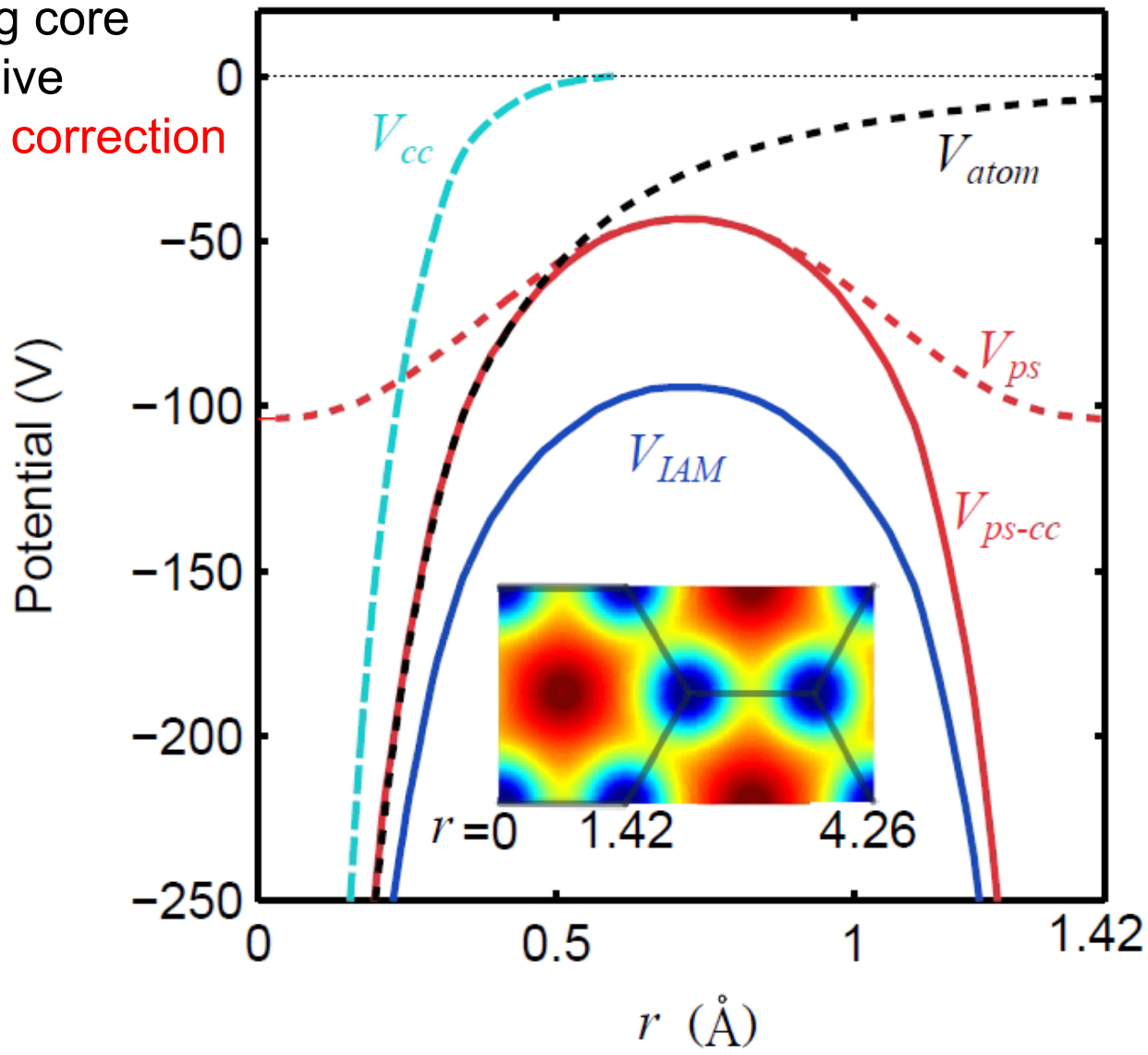
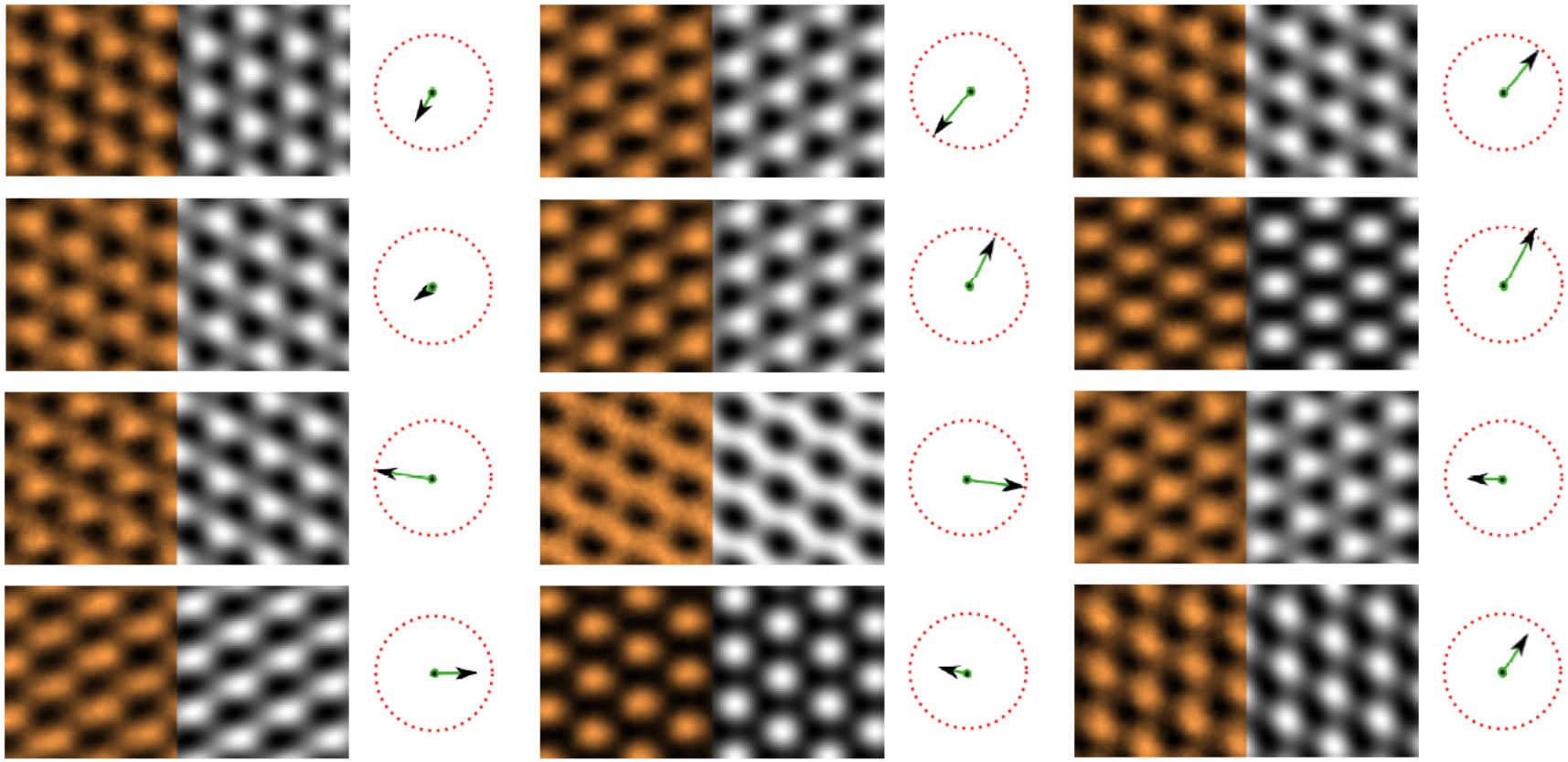


Image matching

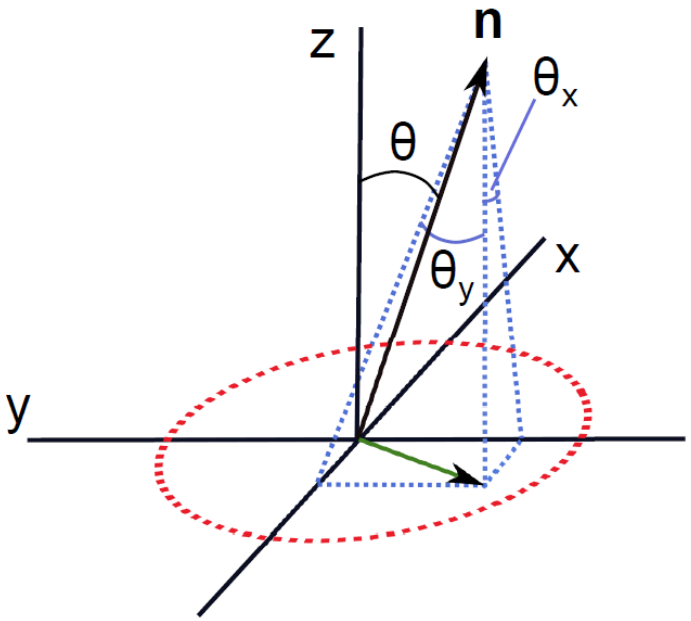


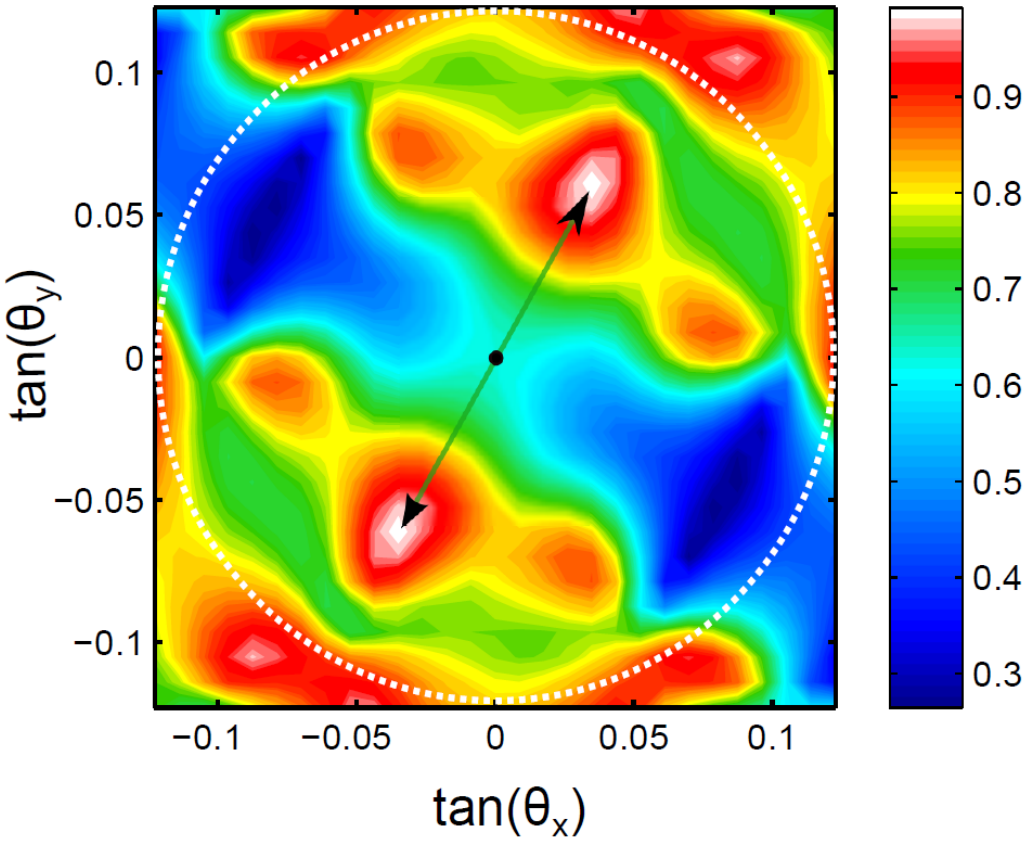
Matching based on a normalized cross-correlation functional:

$$C(f_{exp}, f_{sim}) = \frac{\sum_{xy}(f_{exp}(x,y) - \overline{f}_{exp})(f_{sim}(x,y) - \overline{f}_{sim})}{\sqrt{\sum_{xy}(f_{exp}(x,y) - \overline{f}_{exp})^2 \sum_{xy}(f_{sim}(x,y) - \overline{f}_{sim})^2}}$$

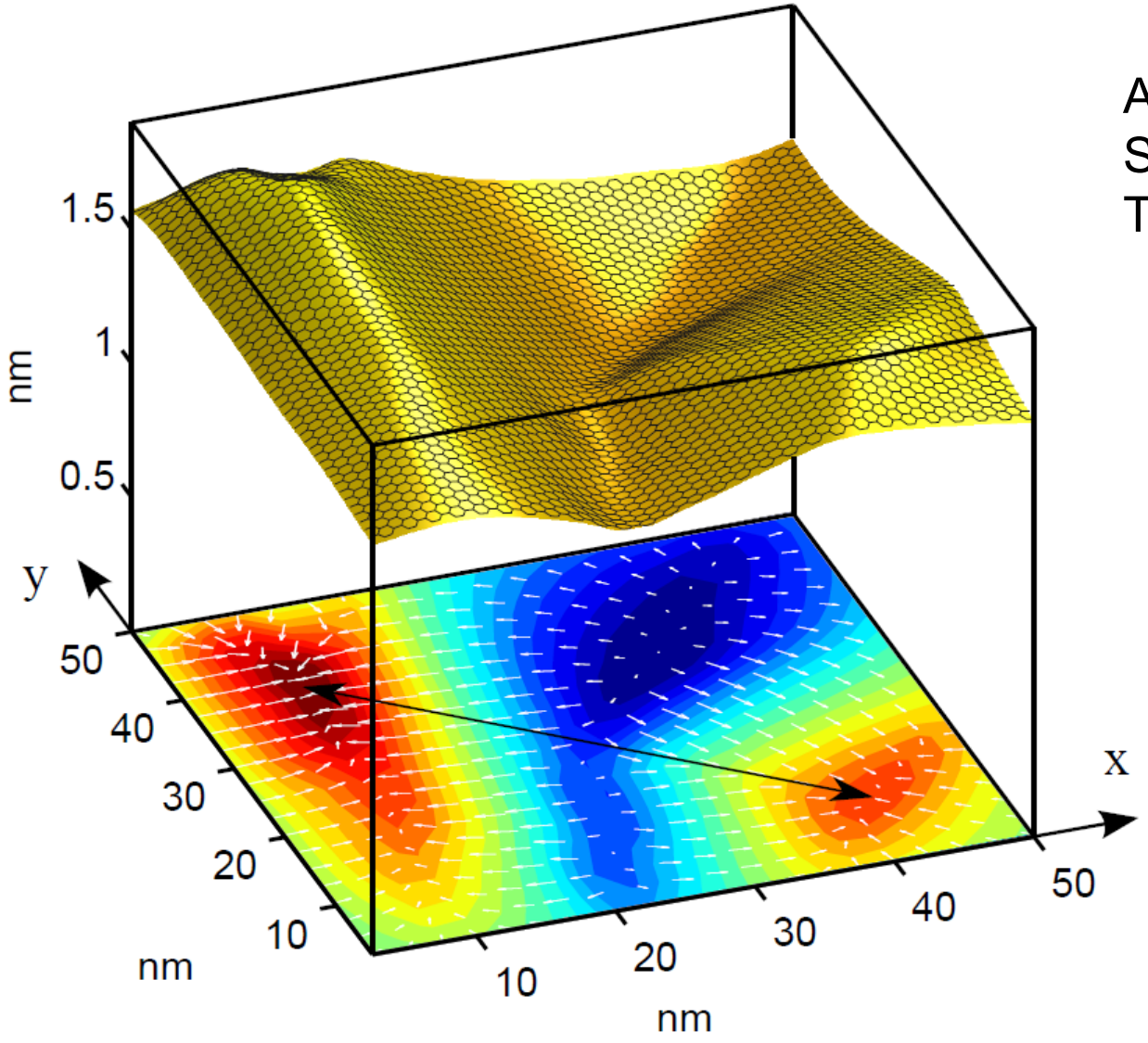
Kirkland, E. J. *Advanced computing in electron microscopy* (Springer, 2010).

Ambiguity: inversion symmetry





Topography Reconstruction



Amplitude: 0.5 nm
Std. dev.: 0.13 nm
Typical width: 45 nm

NanoLetters (2012)
Accepted

Experiment:

- Dr. Wei Li Wang (Harvard Physics & SEAS)
- Prof. Robert Westervelt (Harvard Physics & SEAS)
- Dr. David Bell (Harvard, CNS)
- Dr. Wei Yi (Harvard, now HP lab)
- Sagar Bhandari (Harvard, SEAS)

Theory:

- Dr. Wei Li Wang (Harvard Physics & SEAS)
- Dr. Elton Gomes dos Santos (Harvard SEAS)