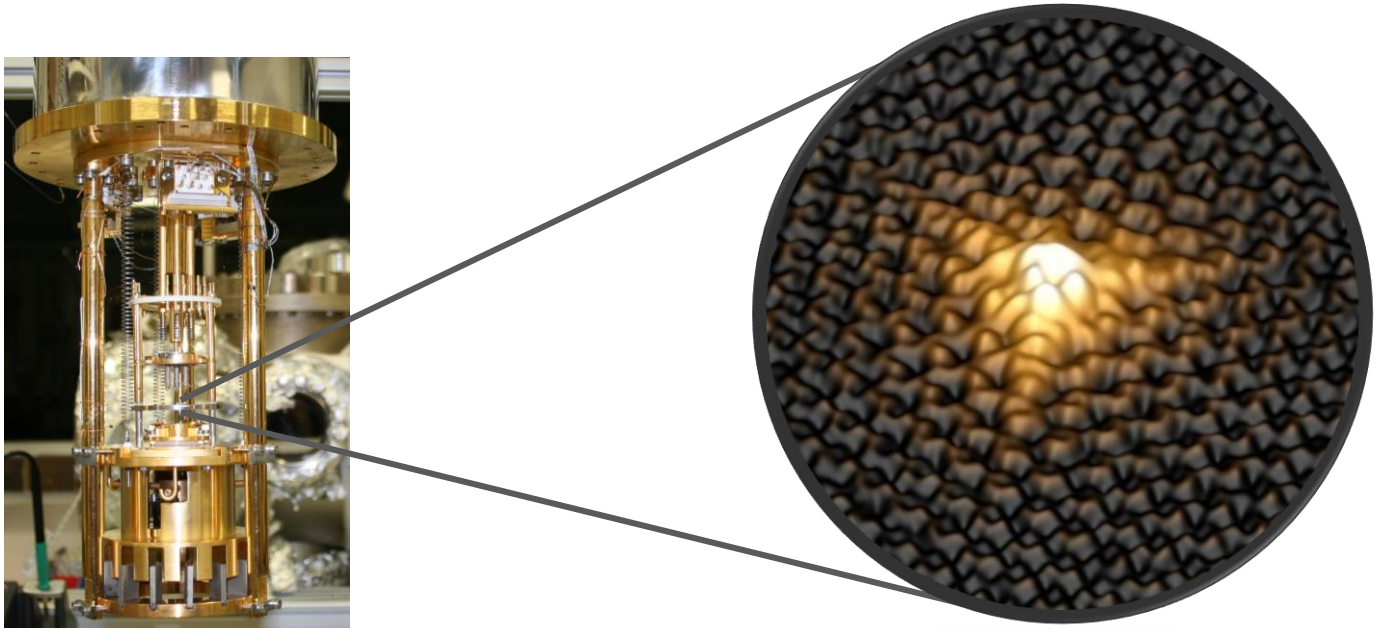
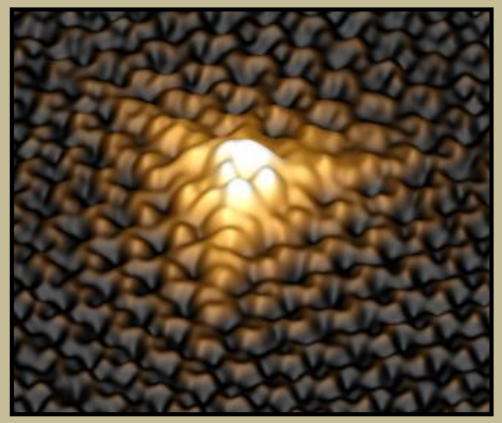
Point defects as a source of local magnetic moments on graphene layers



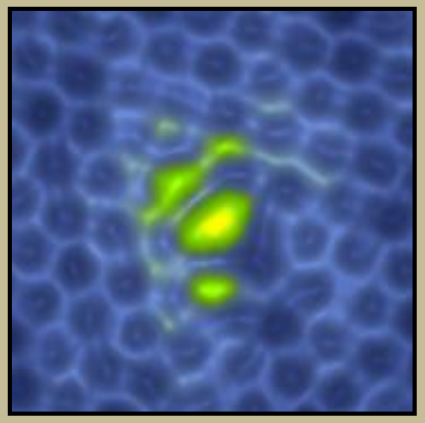
ivan.brihuega@uam.es
www.ivanbrihuega.com

Evora, *October2014*

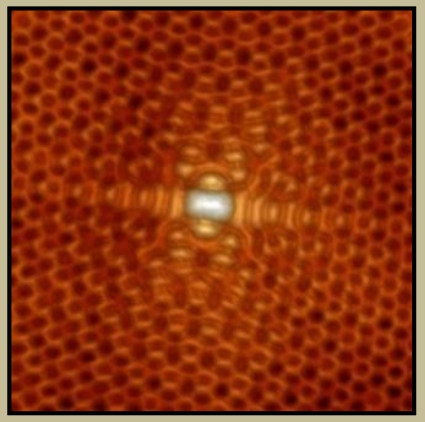
Point defects in graphene systems



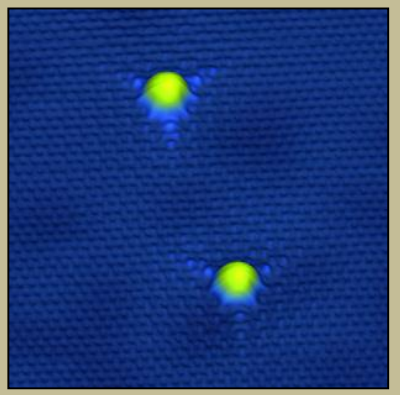
Vacancy on HOPG



Vacancy on G/Pt(111)

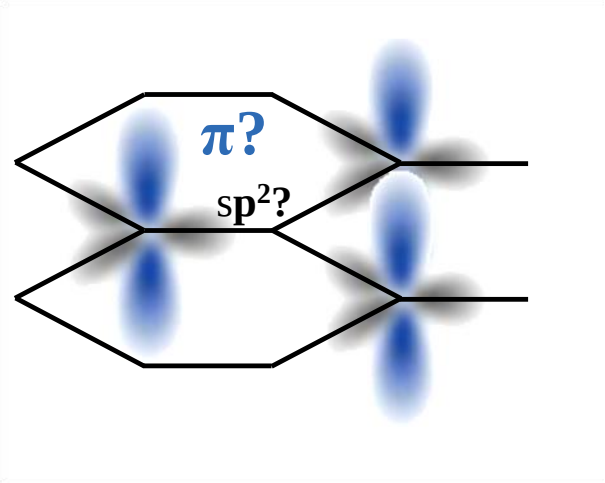


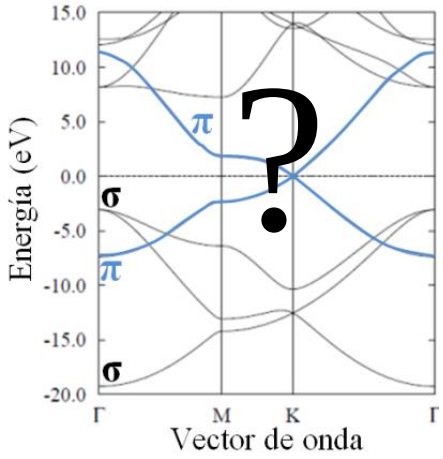
Divacancy

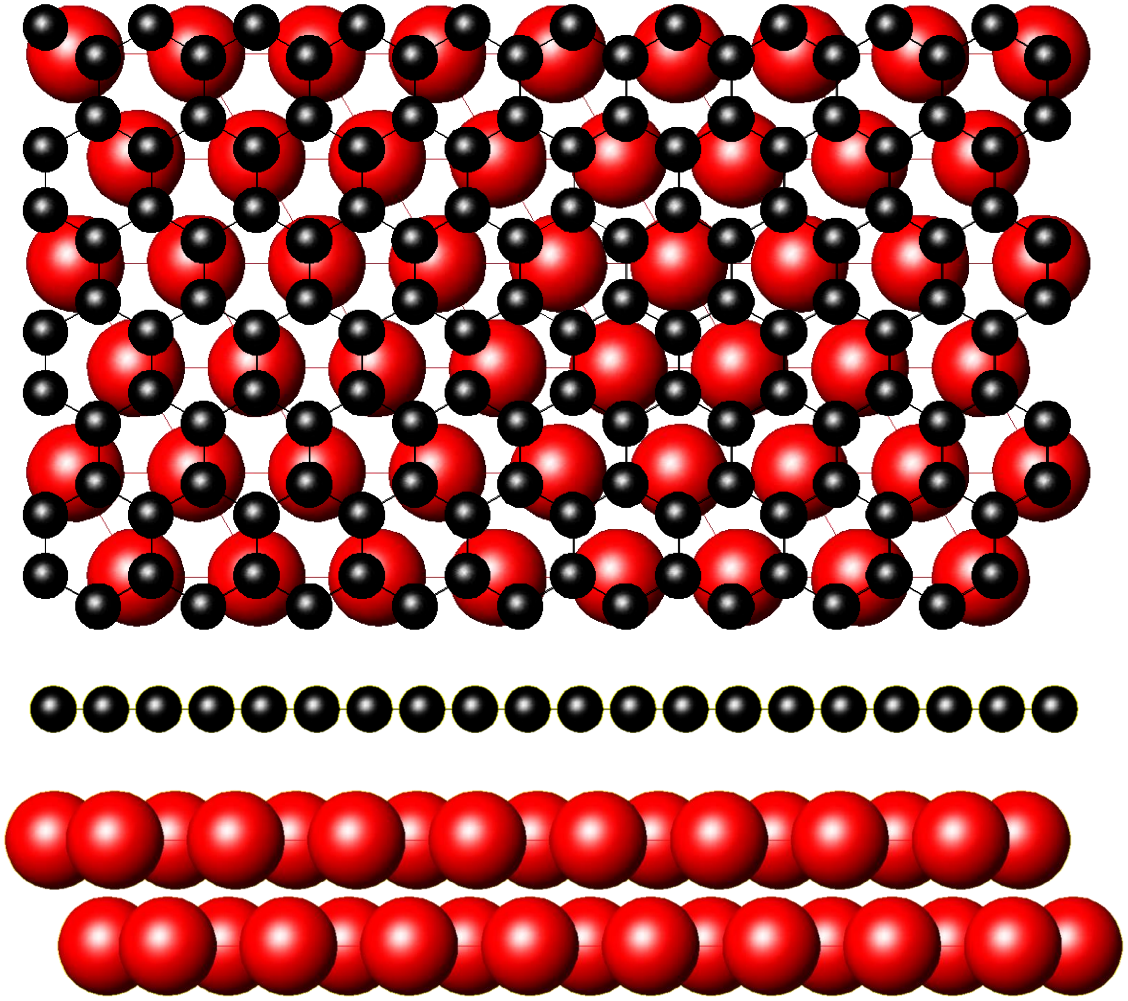


Atomic Hydrogen

Motivation





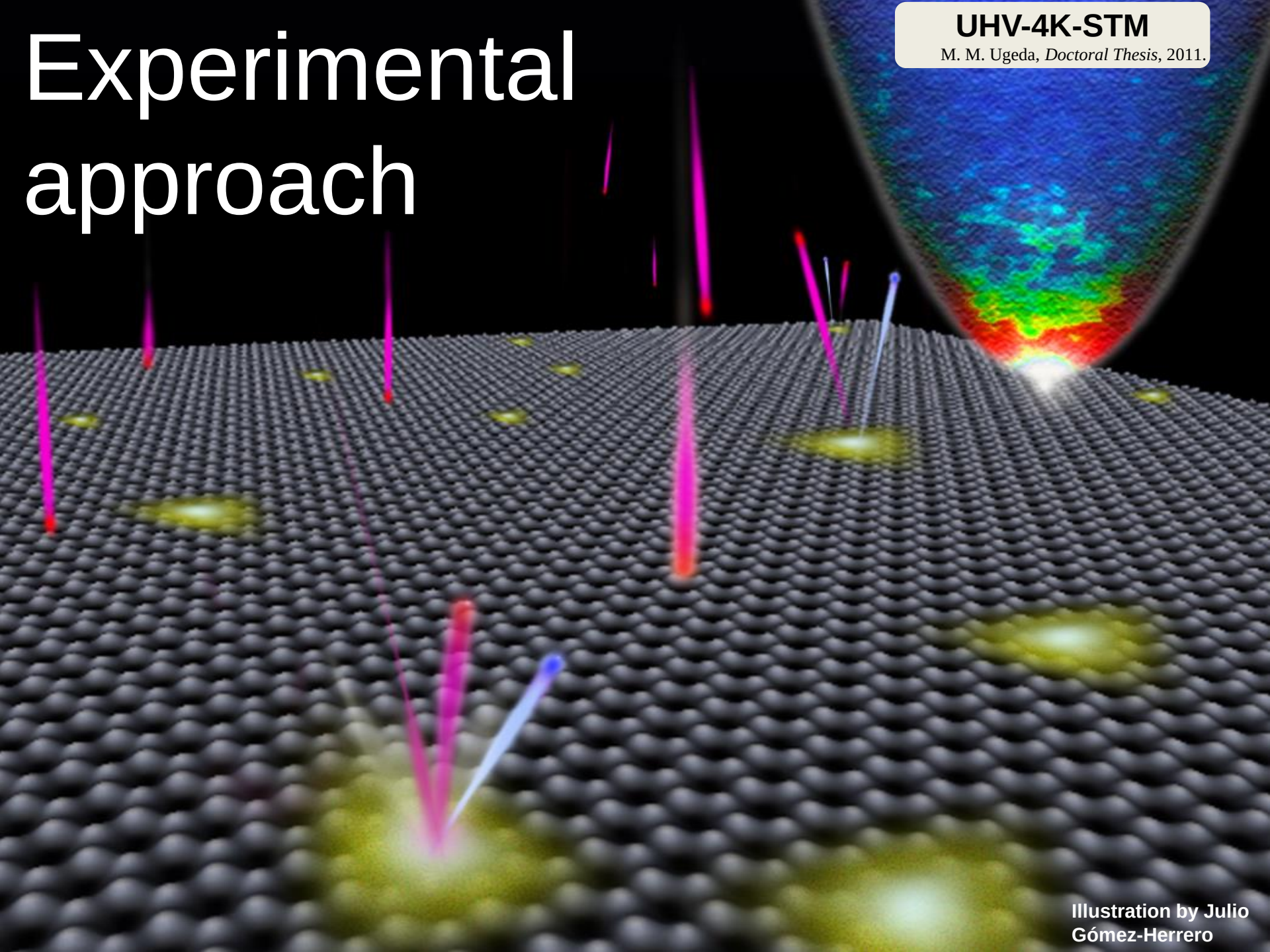


Single atomic vacancies in graphene weakly coupled to the substrate: HOPG surface

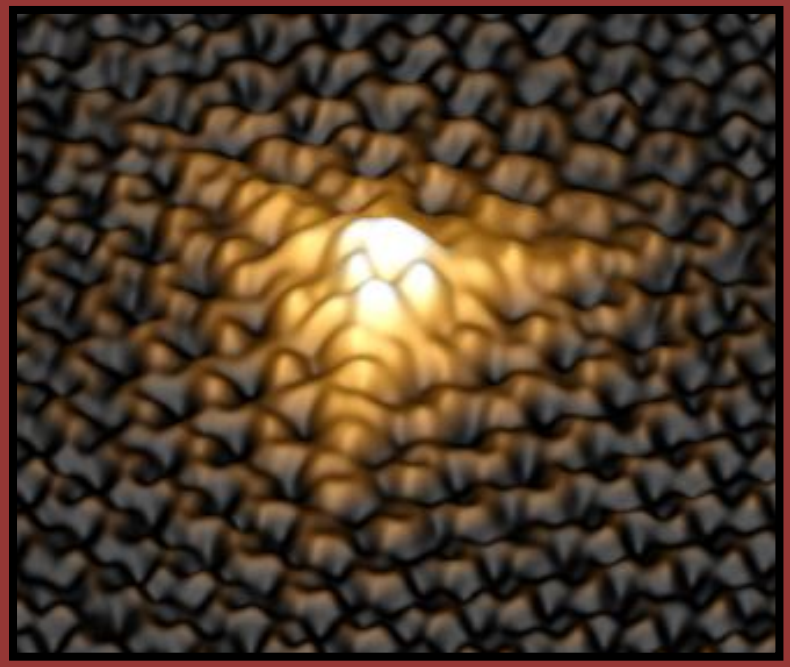
Other structural point defects in graphene: Divacancies

Single atomic vacancies in graphene weakly coupled to a metallic substrate: G/Pt(111)

Experimental approach



Single Carbon Vacancies on HOPG surfaces



Theory support from:

F. Guinea

CSIC

UAM UNIVERSIDAD AUTONOMA DE MADRID

Experiments:

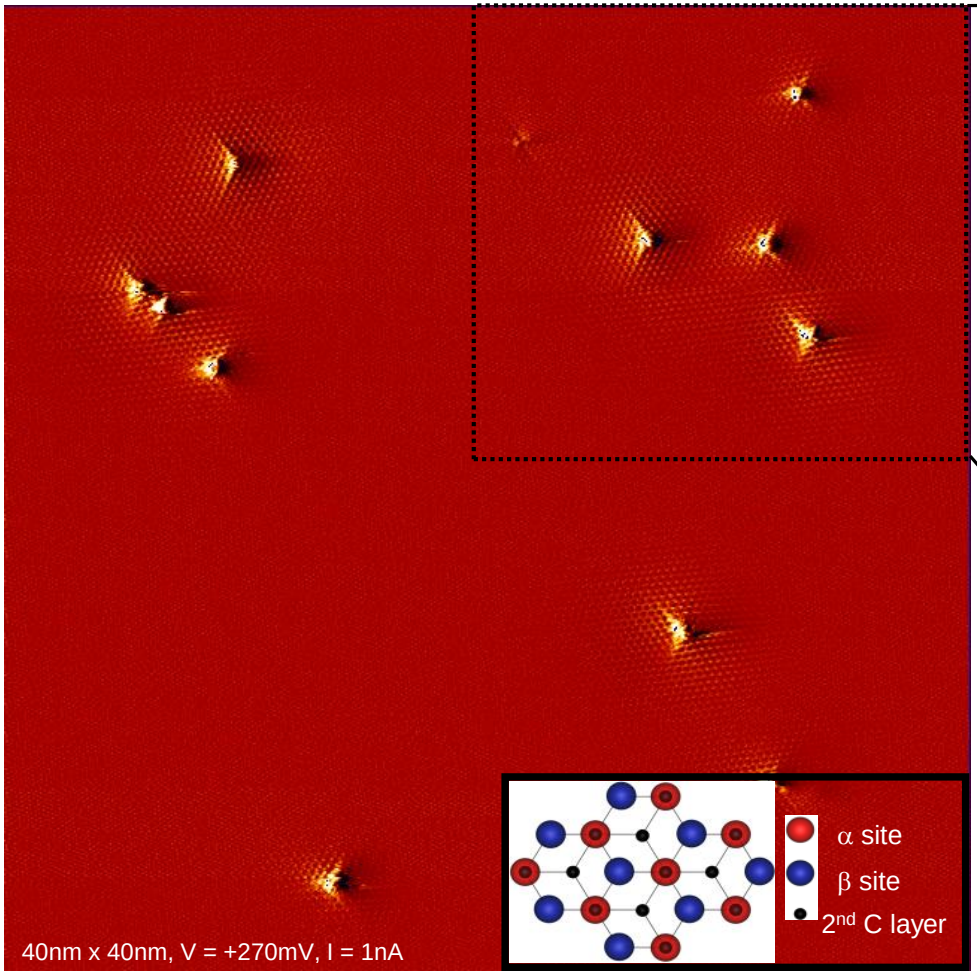
M. M. Ugeda

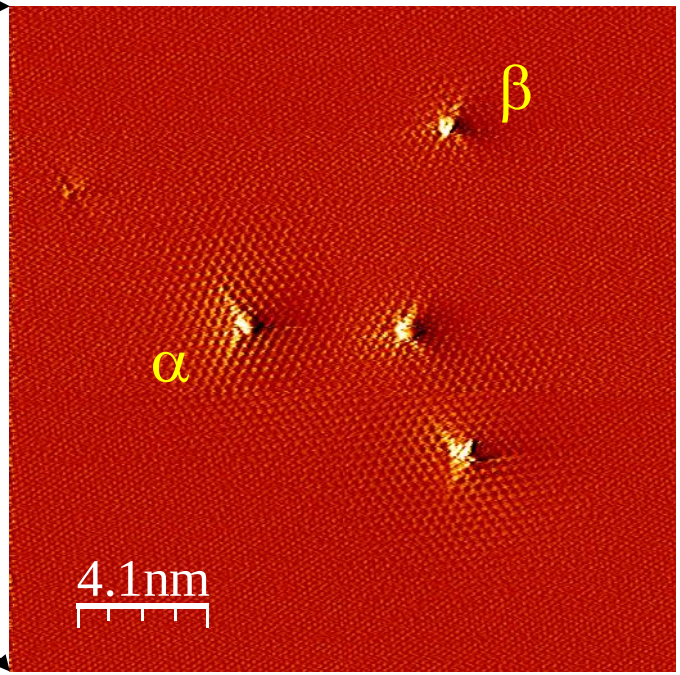
J.M. Gómez-Rodríguez

I. Brihuega

Vacancies on HOPG

✓ Creation of single vacancies by Ar^+ irradiation at RT





Some standard irradiation parameters

Ion energy = 140eV

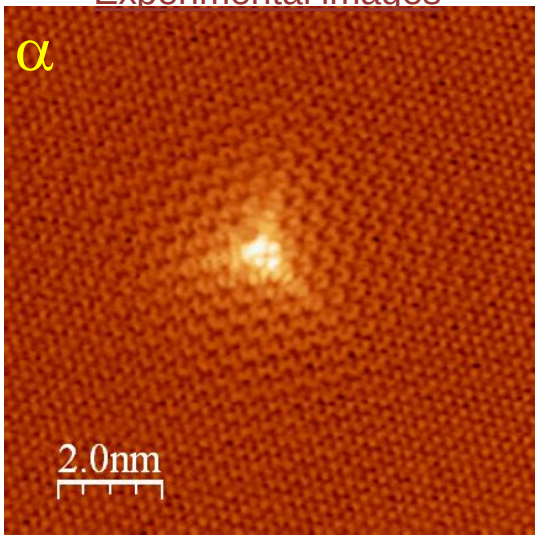
Flux = 0.3 μA

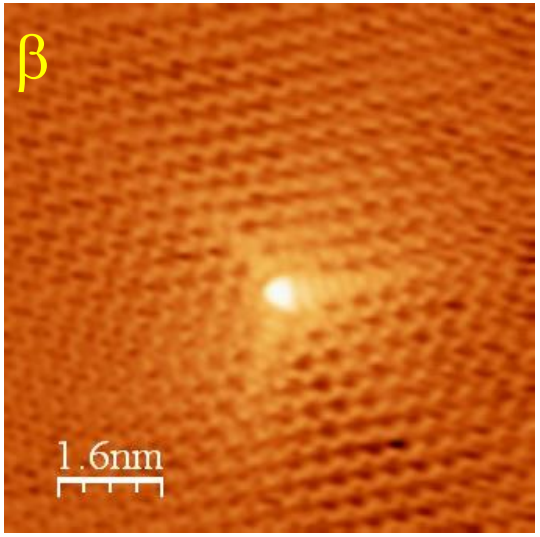
Time = 10s

Density of vacancies ~ $3 \cdot 10^{11}$ cm^{-2}

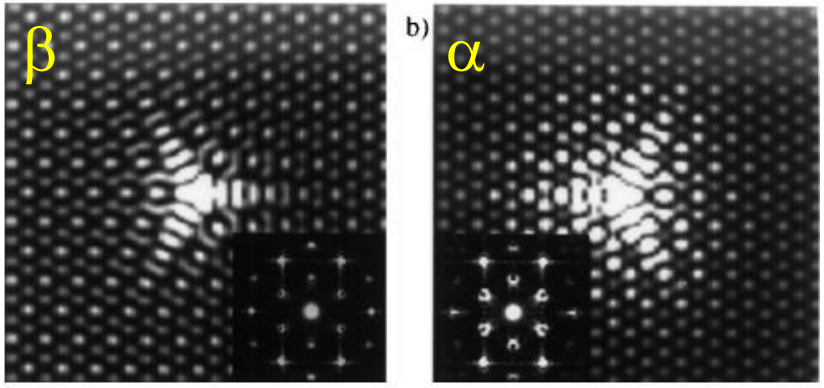
Vacancies on HOPG

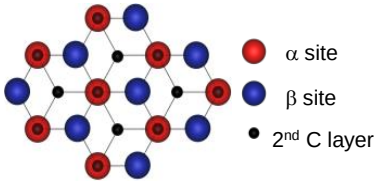
Experimental images





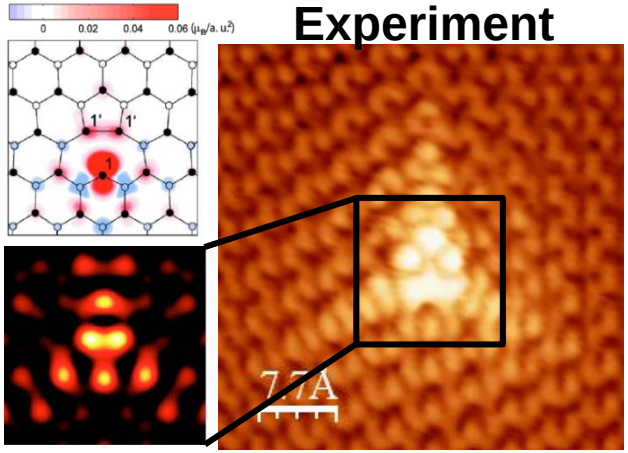
✓ tight-binding model of monovacancies in GRAPHITE

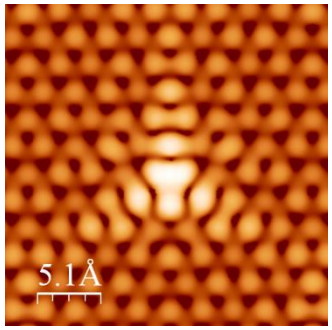




Kelly.K et al, Surf. Science 416 L1085 (1998)

✓ DFT simulations of vacancies in GRAPHENE

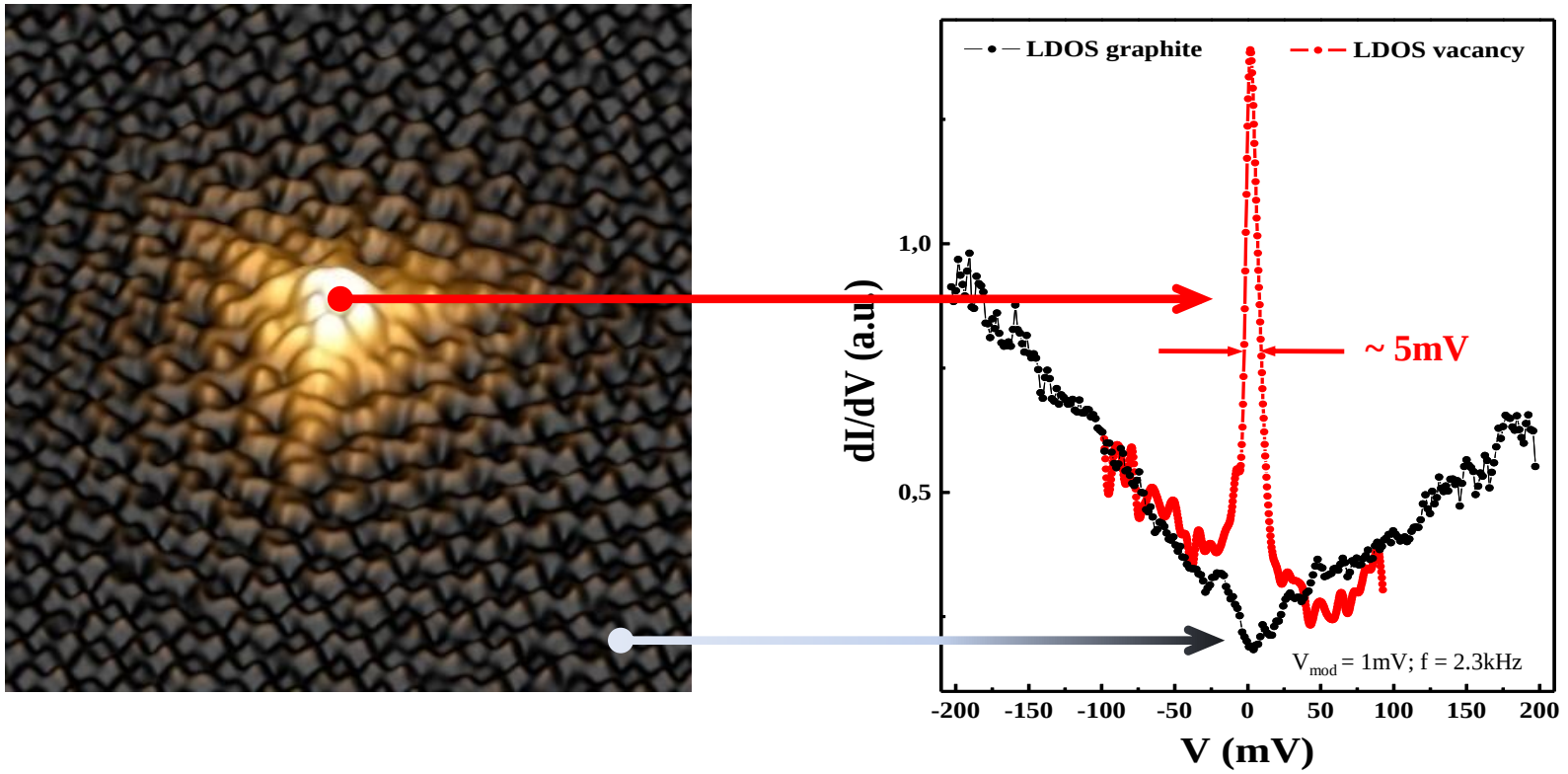




F. Yndurain

O. Yazyev et al, PRB. B. 75, 125408 (2007)

Tunneling Spectroscopy



✓Sharp resonance peak around E_F of FWHM ~ 5mV on the vacancies

✓In agreement with theoretical expectations for graphene*

✓Fundamental implications due to the existence of the resonance:

- Formation of a magnetic moment. The e^-- e^- interaction and the localization at E_F allow the polarization of the state.
- Strong reduction of the electronic mobility (T. Stauber, PRB 76, 205423 (2007))

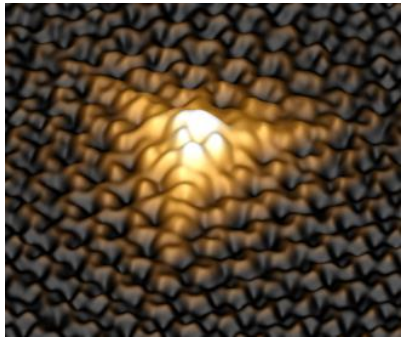
•P. O. Lehtinen *et al*, Phys. Rev. Lett. 93, 187202 (2004)

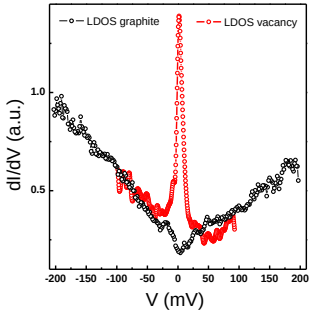
•V. M. Pereira *et al*, Phys. Rev. Lett. 96, 036801 (2006)

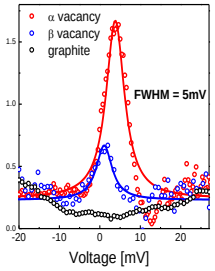
•O. Y. Yazyev, Phys. Rev. Lett. 101, 037203 (2008)

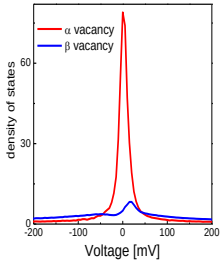
Carbon vacancies in graphene systems

HOPG







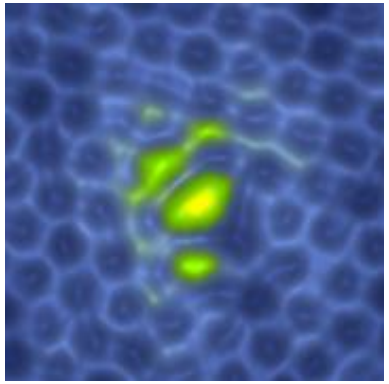


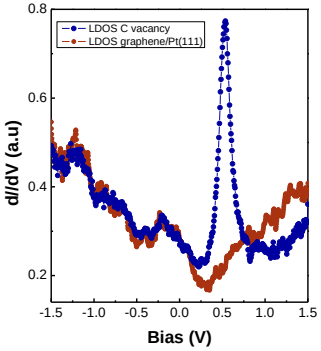
✓Expected ferrimagnetic ground state with $T_c(n_v)$

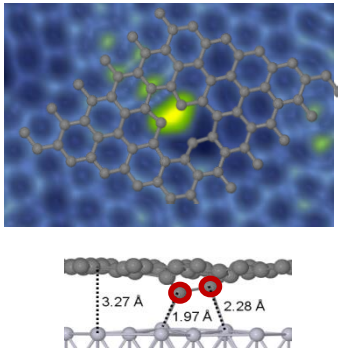
M. M. Ugeda *et al*, **PRL 104**, 096804 (2010)

Physical Review Focus

G/Pt(111)



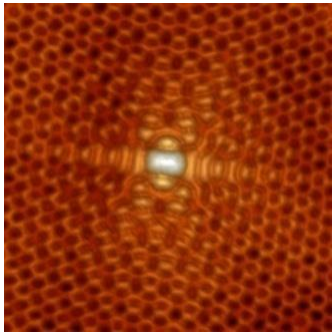


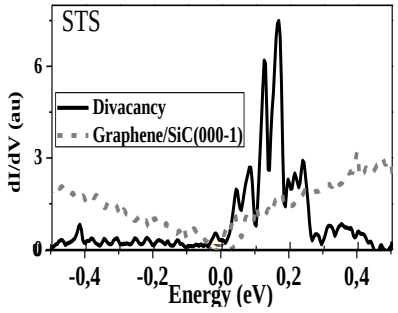


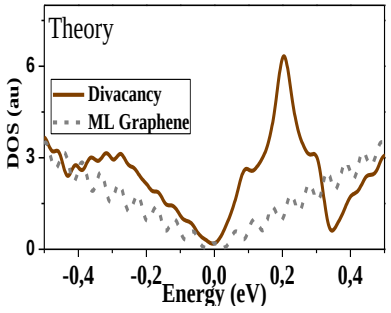
✓ Graphene interaction with the metal strongly increases due to vacancies

M. M. Ugeda *et al*, **PRL 107** 116803 (2011)

Divacancy







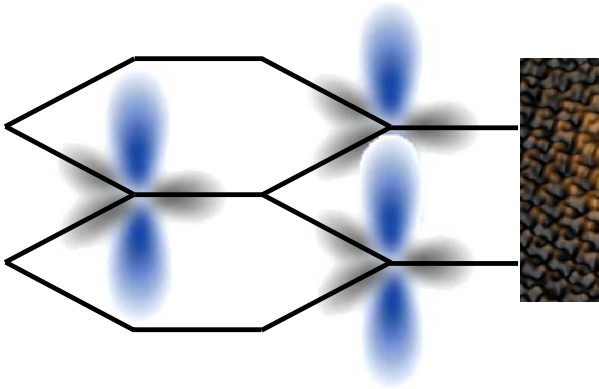
✓ Non-magnetic, key defects for transport properties

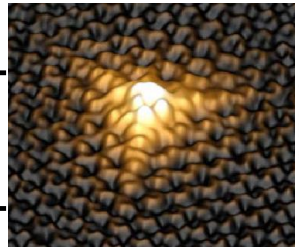
M.M. Ugeda *et al*, **PRB,85**, 121402 (R) (2012)

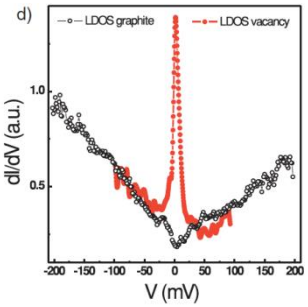
RAPID

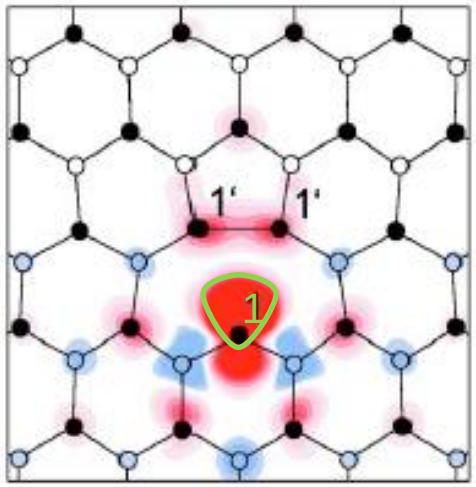
Magnetism in graphene: just remove a p_z orbital

Single vacancy



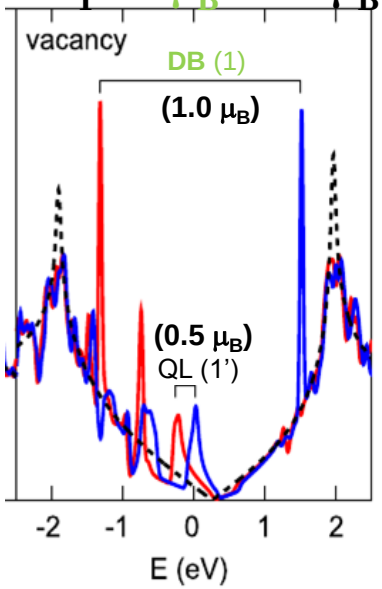




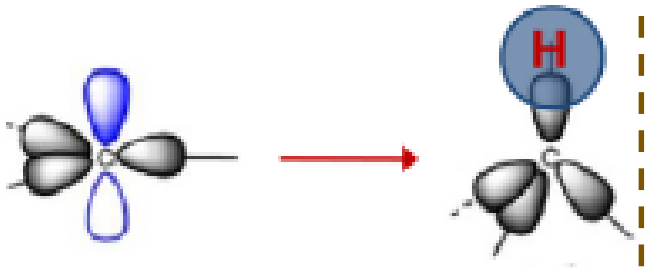


O. Yazyev et al, Phys. Rev. B. 75, 125408 (2007)

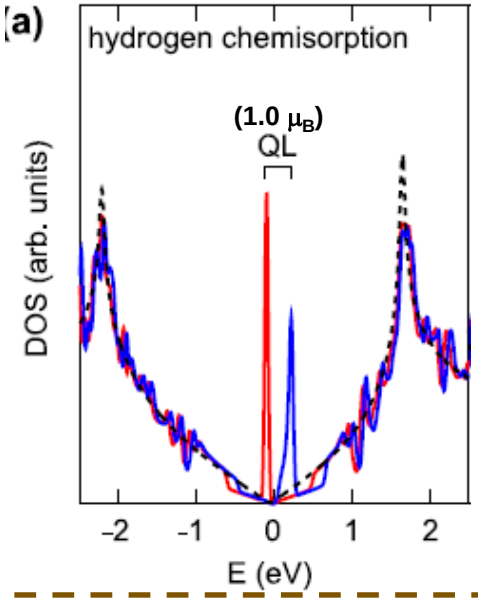
$m_T \approx 1\mu_B + 0.5\mu_B$



Atomic Hydrogen



$m_T = m_\pi = 1\mu_B$



nice review: O. Yazyev, **Rep. Prog. Phys. 73** 056501 (2010)

Atomic Hydrogen on SiC(000-1)

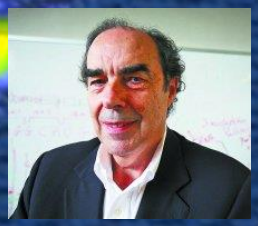
Theory support from:

UNIVERSIDAD AUTONOMA DE MADRID


J.J. Palacios


M. Moaied


C. Salgado


Félix Yndurain

Experiments:

H. González-Herrero

M.M. Ugeda

J.M. Gómez-Rodríguez

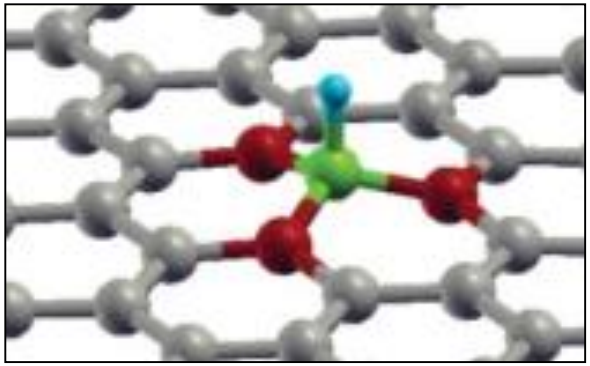
Pierre Mallet

Jean-Yves Veuillen

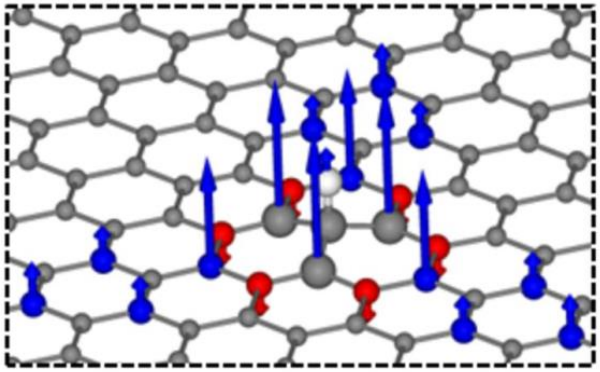
I. Brihuega

Atomic Hydrogen on Monolayer Graphene

Relaxed Atomic structure

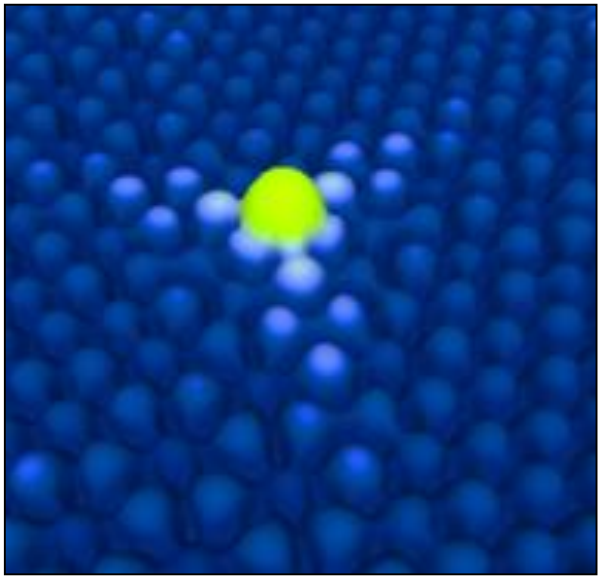


Calculated spin density

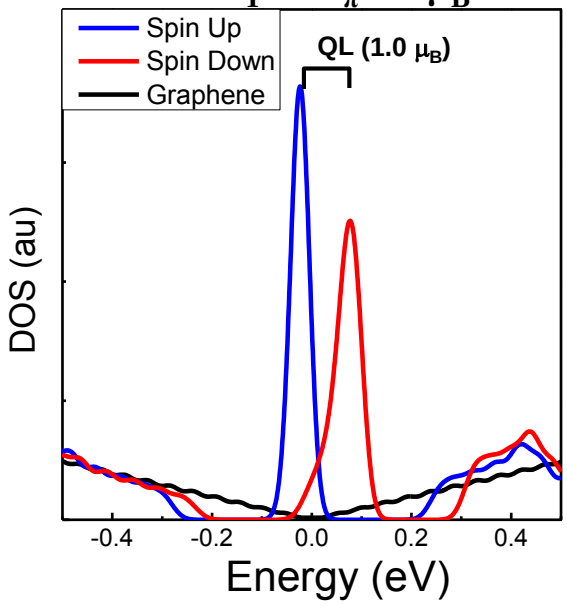


- Magnetic moment = $1\mu_B$
- spin density located on the opposite triangular sublattice.

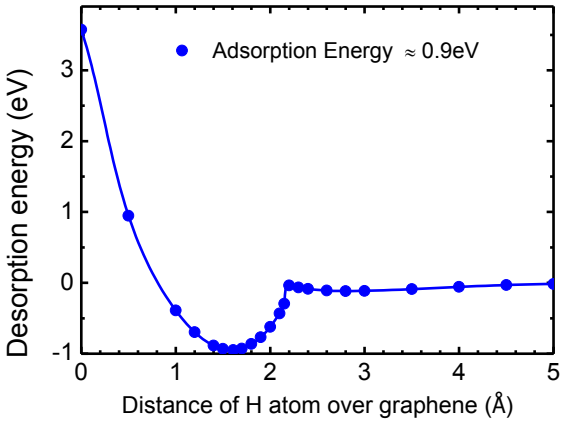
Simulated STM image (Tersoff-Hamann)



$\mathbf{m_T = m_\pi = 1\mu_B}$



H chemisorbs on Graphene



DFT calculations: M. Moaied, J.J Palacios, Felix Yndurain

- Spin Polarized – DFT SIESTA code // (DZP) basis set.