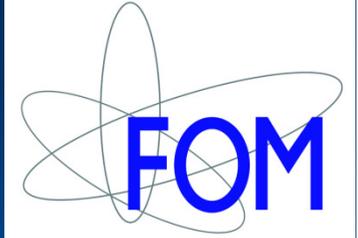


Radboud Universiteit Nijmegen



# *Theory of carbon-based magnetism*

Mikhail Katsnelson

Theory of Condensed Matter  
Institute for Molecules and Materials  
RU

# Outline

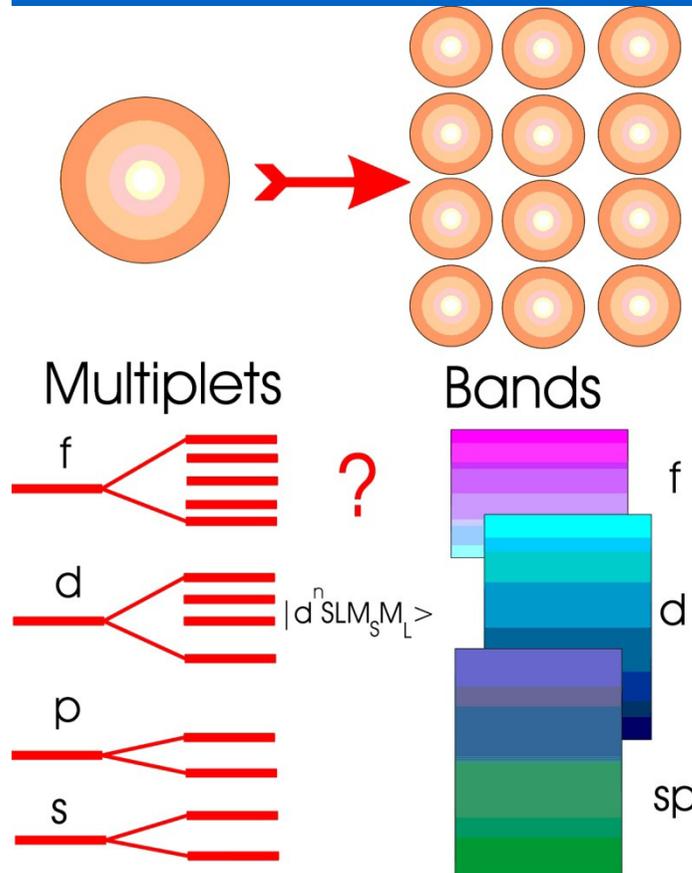
- *sp* magnetism in general: why it is interesting?
- Defect-induced magnetism in graphene: Lieb theorem, midgap states, and all that
- Zigzag edges, grain boundaries, carbon foam, defected fullerenes...
- Noncollinear magnetism in  $C_2H$  and  $C_2F$
- Electron-electron interactions in graphene from first principles
- Effective Hubbard model for carbon materials



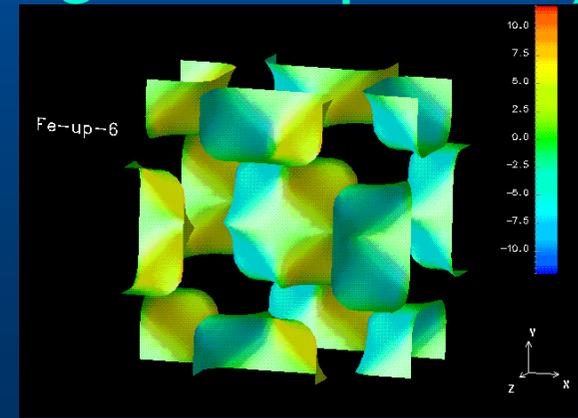
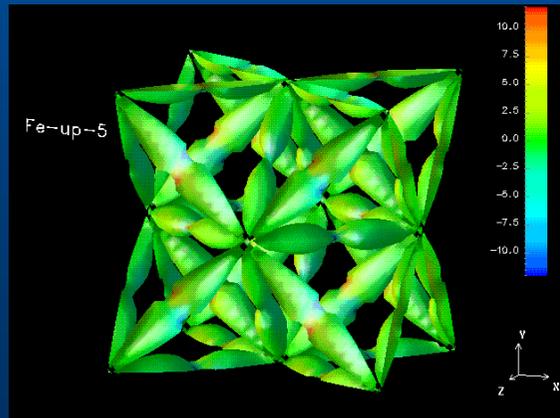
# Problem: coexistence of localized and itinerant behavior

Local magnetic moments do exist above  $T_C$  (Curie-Weiss law, spectroscopy, neutrons...)

d electrons are itinerant (FS, chemical bonding, transport...)



Iron, majority spin FS



4f electrons are normally pure localized but not 3d

# Magnetism of *sp* electrons in narrow impurity bands: Model considerations

D.M.Edwards & MIK, JPCM 18, 7209 (2006)

**Motivation: “semi-reproducible” magnetism  
in carbon systems,  $\text{CaB}_6$ , etc.: defect-related**

**Theoretically: any essential difference with  
Fe, Co, Ni itinerant-electron magnetism?  
Yes!!! Possible way to high Curie temps.**

# Two main differences

## Standard itinerant-electron ferromagnets:

- Strong suppression of Stoner parameter by correlation renormalizations (Kanamori)
- $T_C$  is determined by spin waves rather than Stoner excitations

If Fe would be Stoner magnet it would have  $T_C \approx 4000 \text{ K}$  (in reality  $1043 \text{ K}$ )

*sp*-electron itinerant electron FMs are Stoner magnets and thus can have much higher  $T_C$  than usual dilute magnetic semiconductors

# Stoner criterion

$$I_{\text{eff}} N(E_{\text{F}}) > 1$$

$N(E_{\text{F}})$  is the density of one-electron states

$I_{\text{eff}}$  is an on-site interaction parameter

**Equation for the Curie temperature:**

$$I_{\text{eff}} \int dE \left( -\frac{\partial f}{\partial E} \right) N(E) = 1$$

**$f(E)$  Fermi function**

**Rectangular band, width  $W_{\text{imp}}$ :**

$$k_{\text{B}} T_{\text{c}} = W_{\text{imp}} / \left[ 4 \tanh^{-1} \left( W_{\text{imp}} / I_{\text{eff}} n_{\text{imp}} \right) \right]$$

$$k_{\text{B}} T_{\text{c}} < I_{\text{eff}} n_{\text{imp}} / 4$$

**Stoner parameter  $\approx 1\text{eV}$   
Room-temperature FM:**

$$n_{\text{imp}} > 0.01$$

# Kanamori renormalization

**T-matrix:  $I_{eff} \approx I / [1 + \text{const } I/W]$**

**Usually (Fe, Co, Ni...) Stoner criterion satisfies at the border  $I_{eff} N(E_F) \approx 1.2$ .**

**Impurity bands: T-matrix renormalization can be unusually small due to spectral weight transfer effects**

# General theory of T-matrix renormalization

## Hamiltonian

$$H = H_t + H_U$$

$$H_t = \sum_{\lambda\lambda'\sigma} t_{\lambda\lambda'} c_{\lambda\sigma}^\dagger c_{\lambda'\sigma}$$

$$H_U = \frac{1}{2} \sum_{\{\lambda_i\}\sigma\sigma'} \langle \lambda_1\lambda_2 | v | \lambda'_1\lambda'_2 \rangle c_{\lambda_1\sigma}^\dagger c_{\lambda_2\sigma'}^\dagger c_{\lambda'_2\sigma'} c_{\lambda'_1\sigma}$$

## Equation for T-matrix

$$\begin{aligned} \langle 13 | T^{\sigma\sigma'}(i\Omega) | 24 \rangle &= \langle 13 | v | 24 \rangle - \frac{1}{\beta} \sum_{\omega} \sum_{5678} \langle 13 | v | 57 \rangle G_{56}^{\sigma}(i\omega) \\ &\times G_{78}^{\sigma'}(i\Omega - i\omega) \langle 68 | T^{\sigma\sigma'}(i\Omega) | 24 \rangle, \end{aligned}$$

$\omega = (2n + 1)\pi k_B T$  are the Matsubara frequencies

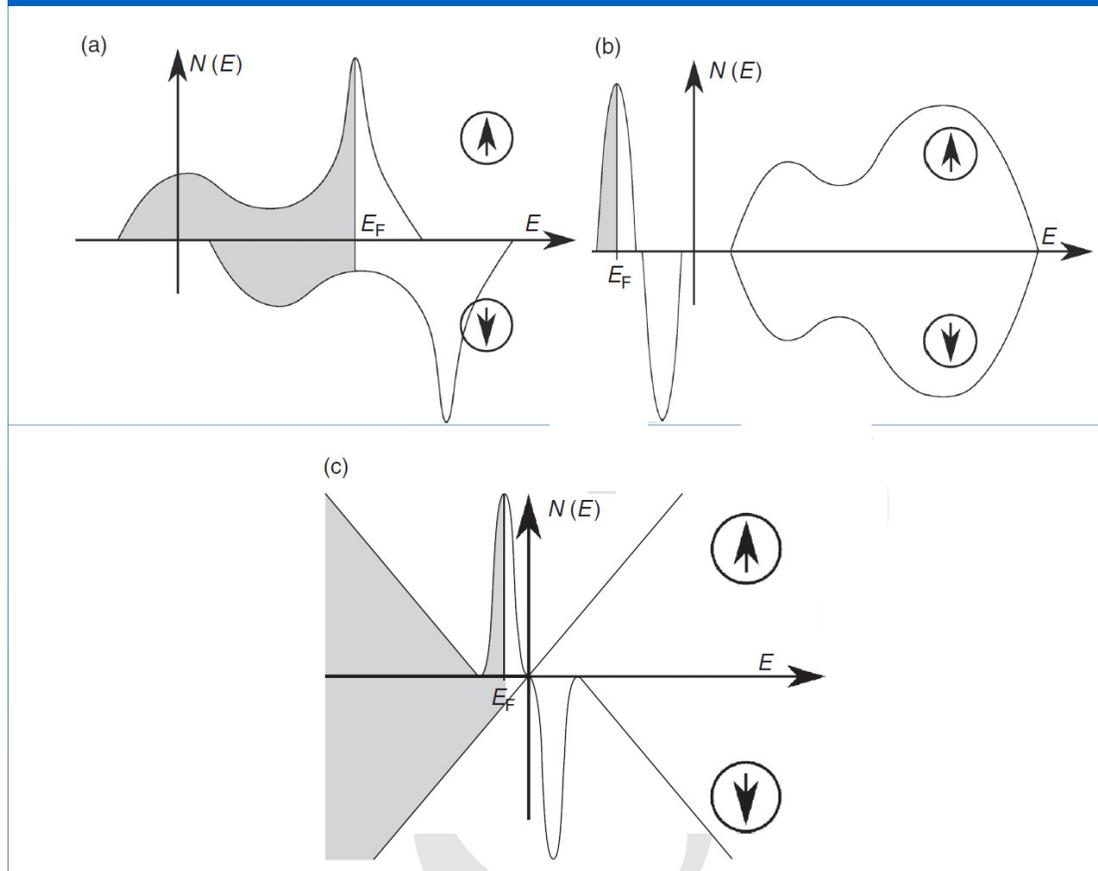
# General theory of T-matrix renormalization II

**Spectral representation:**  $G_{56}^{\sigma}(i\omega) = \int_{-\infty}^{\infty} dx \frac{\rho_{56}(x)}{i\omega - x}$

**On-site (Hubbard) interaction)**

$$\langle 13 | T(E) | 24 \rangle = \langle 13 | v | 24 \rangle + \sum_{5678} \langle 13 | v | 57 \rangle \langle 57 | P(E) | 68 \rangle \langle 68 | T(E) | 24 \rangle$$
$$\langle 57 | P(E) | 68 \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{1 - f(x) - f(y)}{E - x - y} \rho_{56}(x) \rho_{78}(y)$$

# Conventional itinerant-electron FM vs impurity-band FM



One-band FM, weak polarization

Broad main band (region I)

Impurity band (region II)

Fig. 12.1. A sketch of the electronic structures for various types of itinerant-electron ferromagnet: (a) the conventional case; (b) and (c) defect-induced half-metallic ferromagnetism in semiconductors and in graphene, respectively.

# FM in impurity bands

$$\int_{\text{I}} \int_{\text{I}} \frac{dx dy}{x+y} \rho(x) \rho(y) \sim \frac{1}{W} Z_{\text{band}}^2,$$

$$\int_{\text{II}} \int_{\text{II}} \frac{dx dy}{x+y} \rho(x) \rho(y) \sim \frac{1}{W_{\text{imp}}} Z_{\text{imp}}^2,$$

$$\int_{\text{I}} \int_{\text{II}} \frac{dx dy}{x+y} \rho(x) \rho(y) \sim \frac{1}{W} \ln \left( \frac{W}{W_{\text{imp}}} \right) Z_{\text{band}} Z_{\text{imp}}$$

$$Z_{\text{imp}} = \int_{\text{II}} dx \rho(x),$$

$$Z_{\text{band}} = \int_{\text{I}} dx \rho(x) = 1 - Z_{\text{imp}}$$

**Shallow impurities:**

**$Z_{\text{imp}} \ll 1$**

**which suppress  
suppression of /**

# Magnon stiffness constant in impurity – band FM

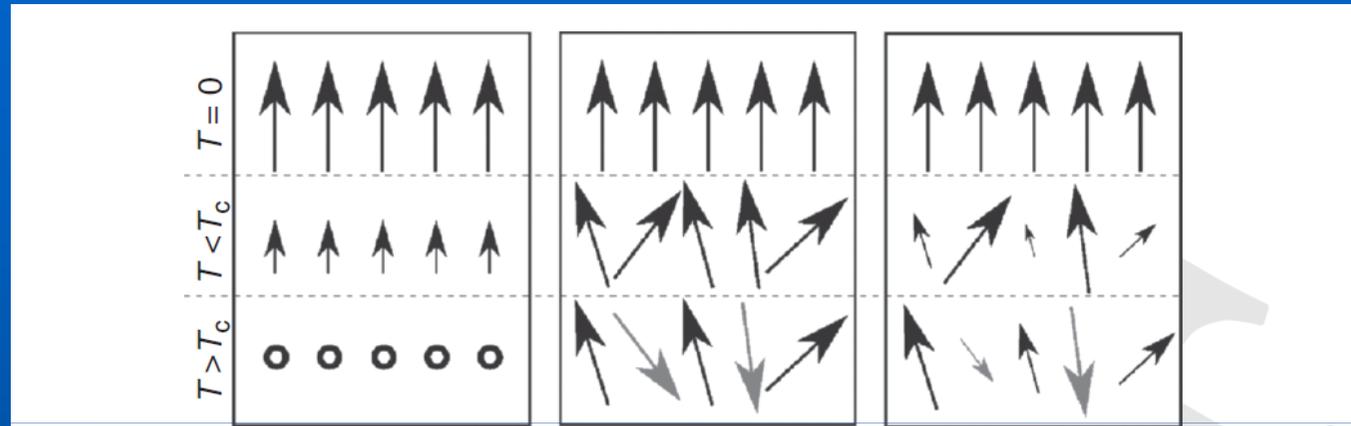


Fig. 12.3. The temperature evolution of ferromagnetic states in the Stoner model (left panel), in the Heisenberg model (middle panel) and in real itinerant-electron ferromagnets (right panel).

## Exchange integrals through local rotations

$$c_{im} \rightarrow U(\theta_i, \varphi_i) c_{im}$$

where

$$U(\theta, \varphi) = \begin{pmatrix} \cos \theta/2 & \sin \theta/2 \exp(-i\varphi) \\ -\sin \theta/2 \exp(i\varphi) & \cos \theta/2 \end{pmatrix}$$

$$\theta_i = \text{const} \text{ and } \varphi_i = \mathbf{q} \cdot \mathbf{R}_i$$

# Magnon stiffness constant in impurity – band FM II

$$\delta H = \sum_{ij} Tr_{L\sigma} [t_{ij} c_i^+ (U_i^+ U_j - 1) c_j] = \delta_1 H + \delta_2 H$$

$$\delta_1 H = \sin^2 \frac{\theta}{2} \sum_k Tr_{L\sigma} [(t(\mathbf{k}+\mathbf{q}) - t(\mathbf{k})) c_{\mathbf{k}}^+ c_{\mathbf{k}}]$$

$$\delta_2 H = \frac{1}{2} \sin \theta \sum_{ij} Tr_L [t_{ij} c_{i\downarrow}^+ c_{j\uparrow}] (\exp(i\mathbf{q}\mathbf{R}_i) - \exp(i\mathbf{q}\mathbf{R}_j))$$

**Perturbation theory up to  $\theta^2$  with local self-energy (the only approximation)**

# Magnon stiffness constant in impurity – band FM *III*

$$D = \frac{1}{6\pi(n_{\uparrow} - n_{\downarrow})} \text{Im} \int_{-\infty}^{E_F} dE \sum_{\mathbf{k}} \left[ G_{\mathbf{k}}^{\uparrow}(E) - G_{\mathbf{k}}^{\downarrow}(E) \right]^2 |\nabla_{\mathbf{k}} \epsilon(\mathbf{k})|^2$$

**RPA value of the stiffness constant:**

$$D_0 = -\frac{R^2}{6(n_{\uparrow} - n_{\downarrow})} \langle H_0 \rangle = \frac{1}{12} R^2 W$$

**Estimation for simplest model, NN hopping**

$$D = D_0 + D_1 \simeq \frac{1}{9} \frac{\hbar^2}{2m^*} = \frac{1}{9} D_0$$

no smallness  
in electron  
concentration!

Magnon energies are higher than the Fermi energy of electrons!

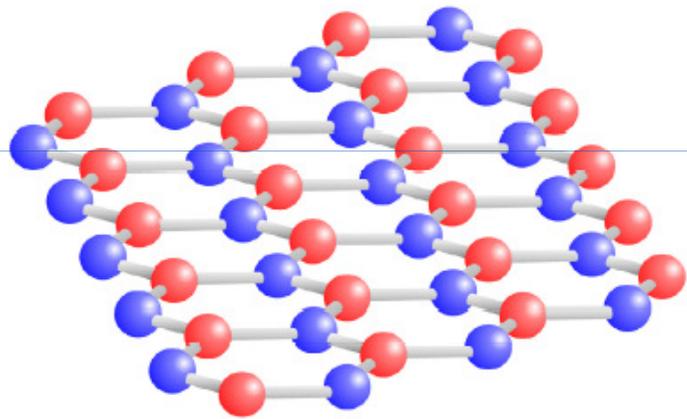
- normal itinerant- electron magnets: easier to rotate spins than to change their length
- *sp*-magnets: Stoner magnets (after 70 years of existence of the Stoner model a region of applicability was found)

# Vacancies and other $sp^3$ defects

Lieb theorem: Hubbard model for bipartite lattice

$$\hat{H} = \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\hat{t}_{AA} = \hat{t}_{BB} = 0 \quad \text{NN approx.}$$



Two equivalent sublattices, A and B (pseudospin)



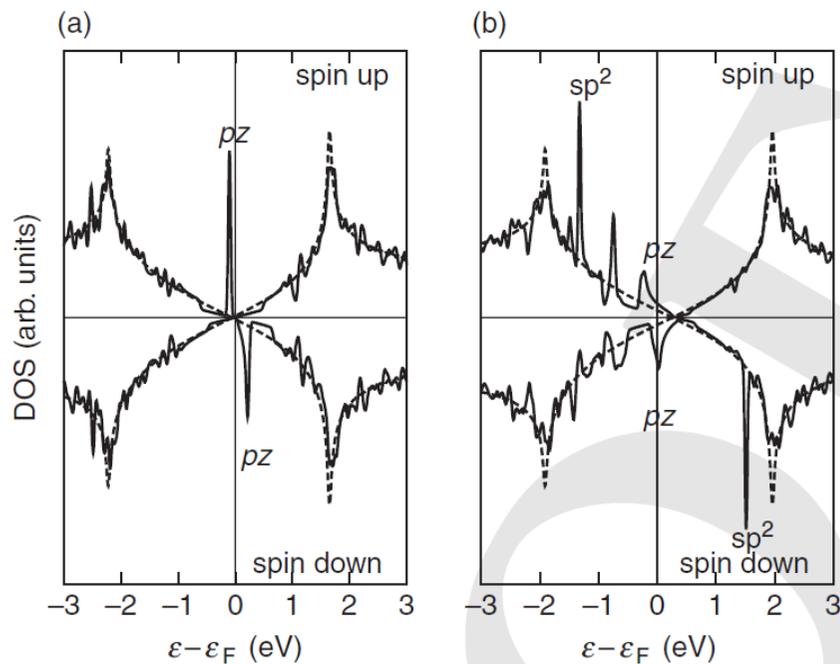
$N_A$  and  $N_B$

Number of sites in sublattices

The ground state spin:  $S = \frac{N_B - N_A}{2}$  Lieb, PRL 1989

# Vacancies and other $sp^3$ defects II

- Mid-gap states lead to (local) spin polarization
  - FM exchange in the same sublattice, AFM between A and B
- Hydrogen and other  $sp^3$  defects act very similar to vacancies



(a) H adatom  
(b) Vacancy

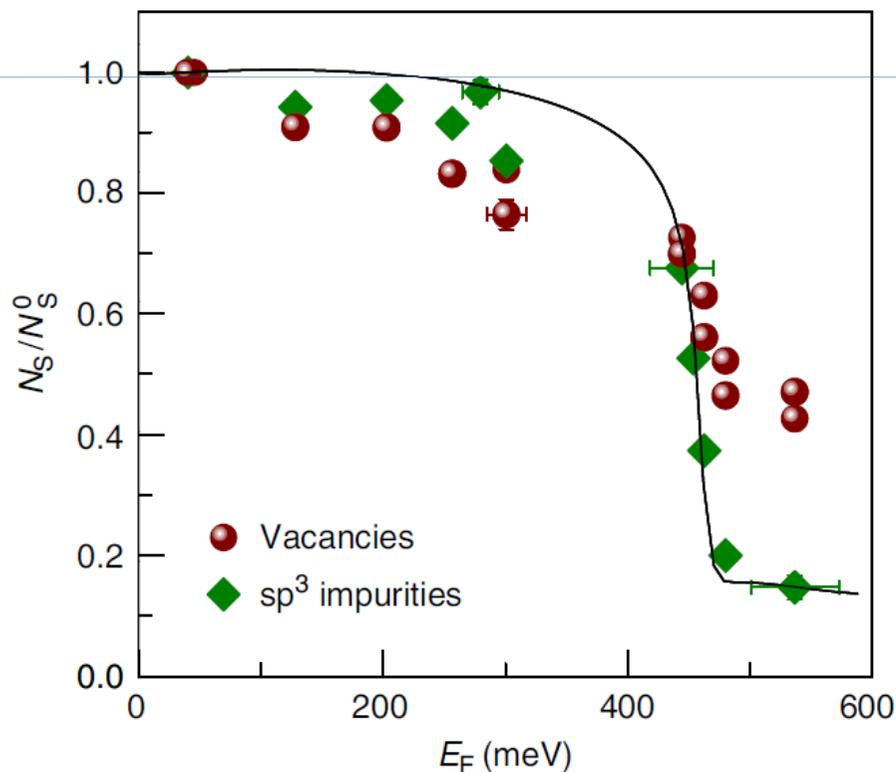
Yazyev & Helm, PRB 2007

# Vacancies and other $sp^3$ defects III

Dual origin of defect magnetism in graphene and its reversible switching by molecular doping

R.R Nair<sup>1</sup>, I-L Tsai<sup>1</sup>, M. Sepioni<sup>1</sup>, O. Lehtinen<sup>2</sup>, J. Keinonen<sup>2</sup>, A.V Krasheninnikov<sup>2,3</sup>, A.H Castro Neto<sup>4</sup>, M.I Katsnelson<sup>5</sup>, A.K Geim<sup>1</sup> & I.V Grigorieva<sup>1</sup>

NATURE COMMUNICATIONS | 4:2010 | DOI: 10.1038/ncomms3010



Vacancies: two types of LMM:  $\pi$  (midgap states) and  $\sigma$  (dangling bonds); admolecules: only  $\pi$

No signs of magnetic order!!!

# Polymerized fullerenes

A very controversial issue (experimentally)

D.W. Boukhvalov & MIK, EPJ B 68, 529 (2009)

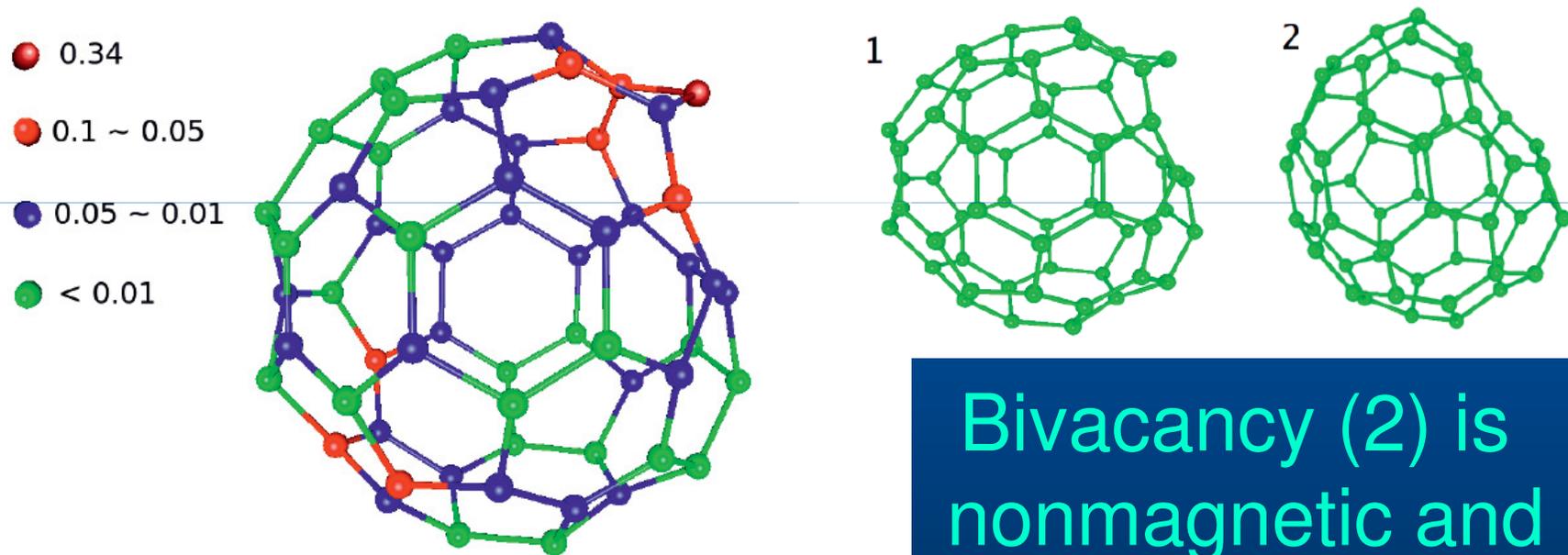


Fig. 4. (Color online) Distribution of magnetic moments in  $\mu_B$  on  $C_{60}$  sphere with single vacancy in rhombohedral phase.

Single vacancy is magnetic

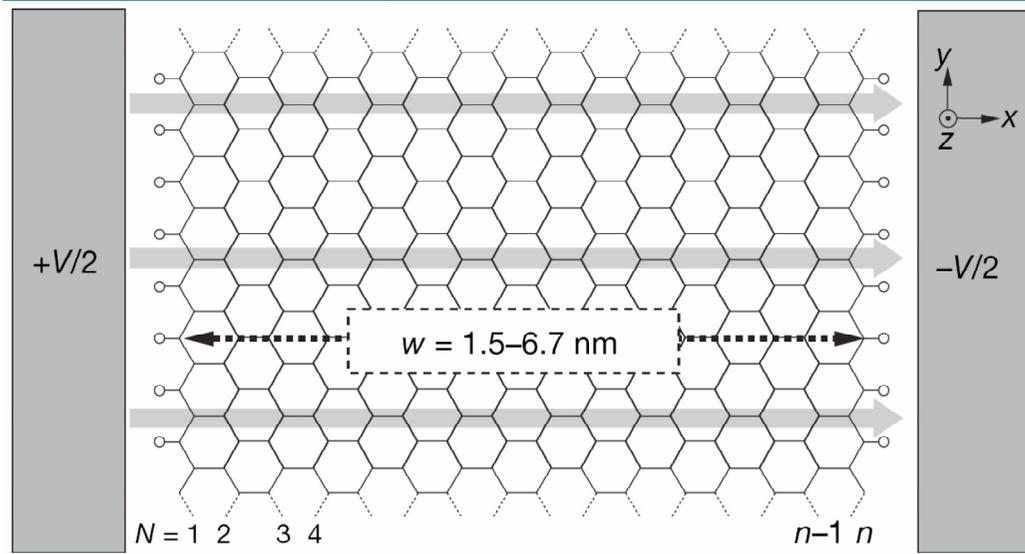
Bivacancy (2) is nonmagnetic and more favourable (2 eV per atom lower)

# Magnetism at zigzag edges

## Half-metallic graphene nanoribbons

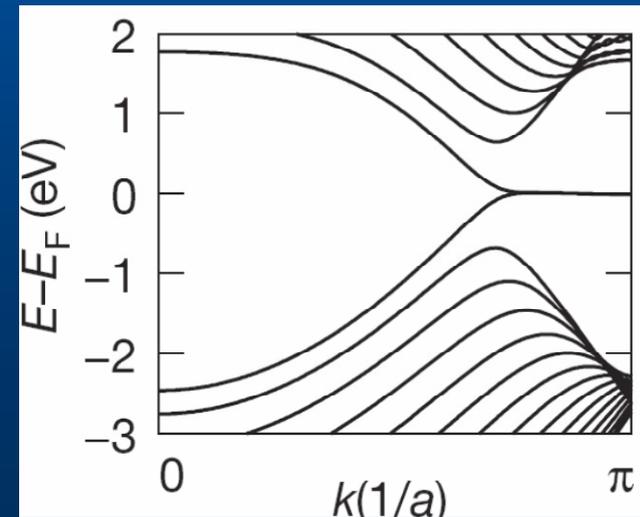
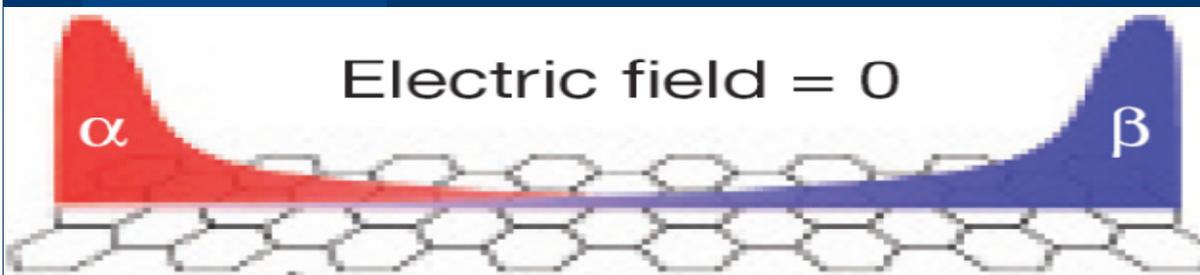
Young-Woo Son<sup>1,2</sup>, Marvin L. Cohen<sup>1,2</sup> & Steven G. Louie<sup>1,2</sup>

Nature 444, 347 (2006)



Zigzag edges: midgap states in nonmagnetic case (true in a generic case as well)

Spin polarization arises



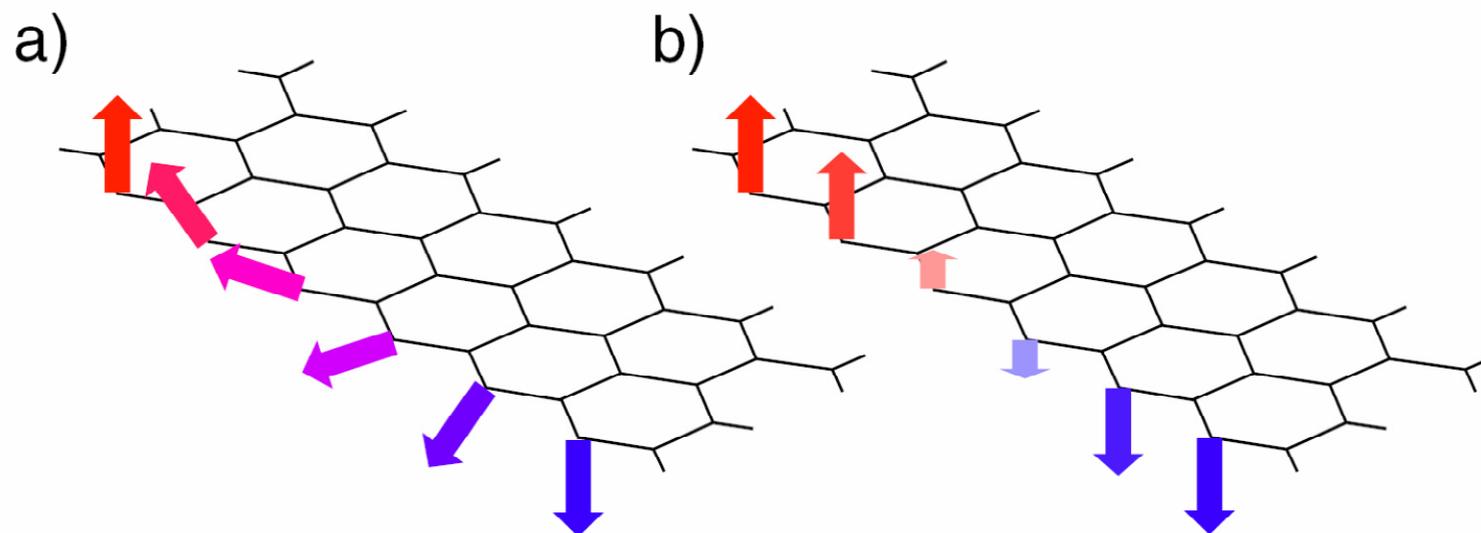
# Magnetism at zigzag edges II

1D systems: no magnetic ordering at finite T

Exchange interactions and finite-T magnetism

Yazyev & MIK PRL 100, 047209 (2008)

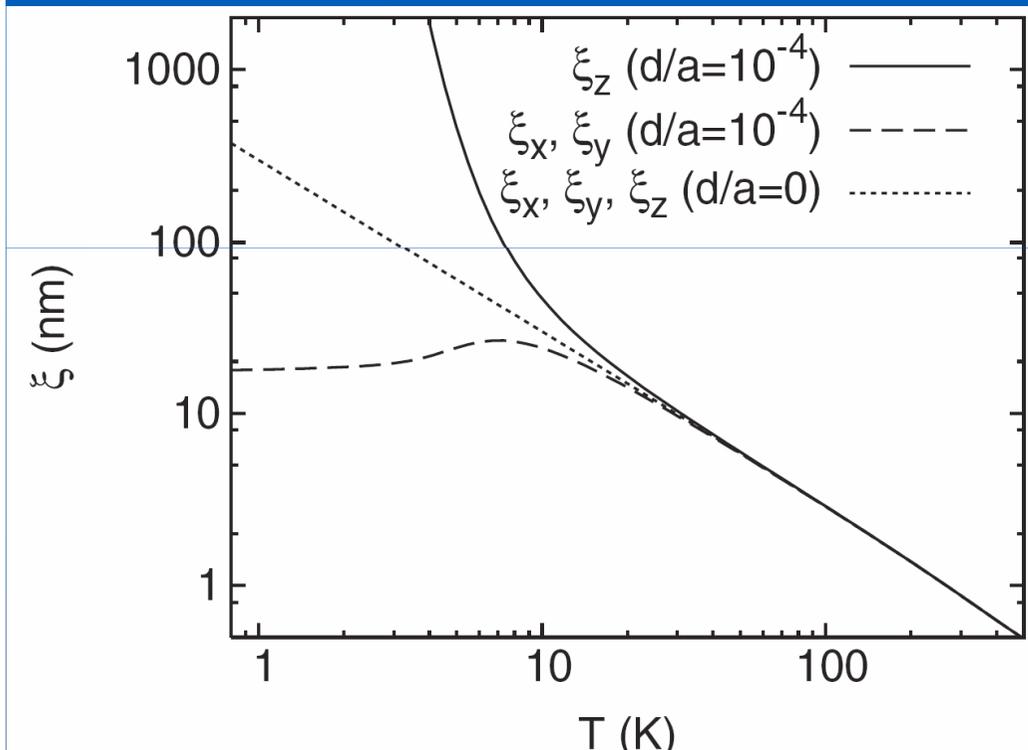
Energies of transverse (a) and longitudinal (b) configurations, DFT-SIESTA calculations



# Magnetism at zigzag edges III

A very high spin stiffness constant

$$D = 2100 \text{ meV } \text{\AA}^2$$



@ RT:  
Superparamagnetism  
Enhancement factor 8

Low temperatures:  
spin coherence at  
0.1  $\mu\text{m}$

FIG. 3. Correlation lengths of magnetization vector components orthogonal ( $\xi_z$ ) and parallel ( $\xi_x, \xi_y$ ) to the graphene plane as a function of temperature  $T$  for weakly anisotropic ( $d/a = 10^{-4}$ ) and isotropic ( $d/a = 0$ ) Heisenberg models.

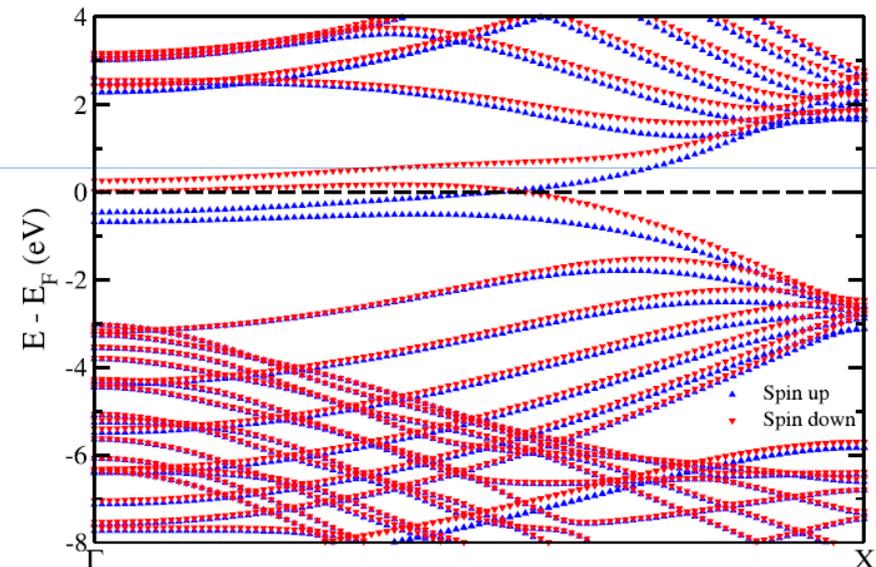
# Magnetism at zigzag edges IV

Bhandary, Eriksson, Sanyal & MIK, PRB 82, 165405 (2010)

Double-hydrogenated zigzag edges in nanoribbons: still ferromagnetic!

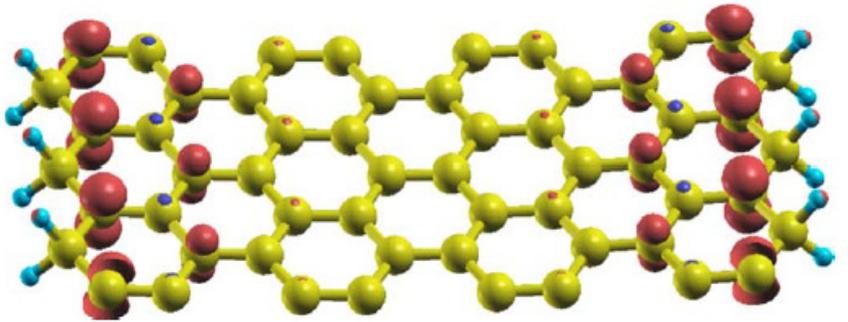
TABLE I. Difference in total energies between the nonmagnetic and ferromagnetic states ( $\Delta E$ ) and the corresponding magnetic moments in the ferromagnetic state. The energy differences and total magnetic moments are quoted for the unit cell whereas the edge moment is for one C atom at the edge.

Width (rows)	$\Delta E$ (meV)	Total moment ( $\mu_B$ )	Edge moment ( $\mu_B$ )
8	1.63	1.04	0.34
10	5.3	1.23	0.38
15	4.9	1.29	0.39
20	3.81	1.3	0.39



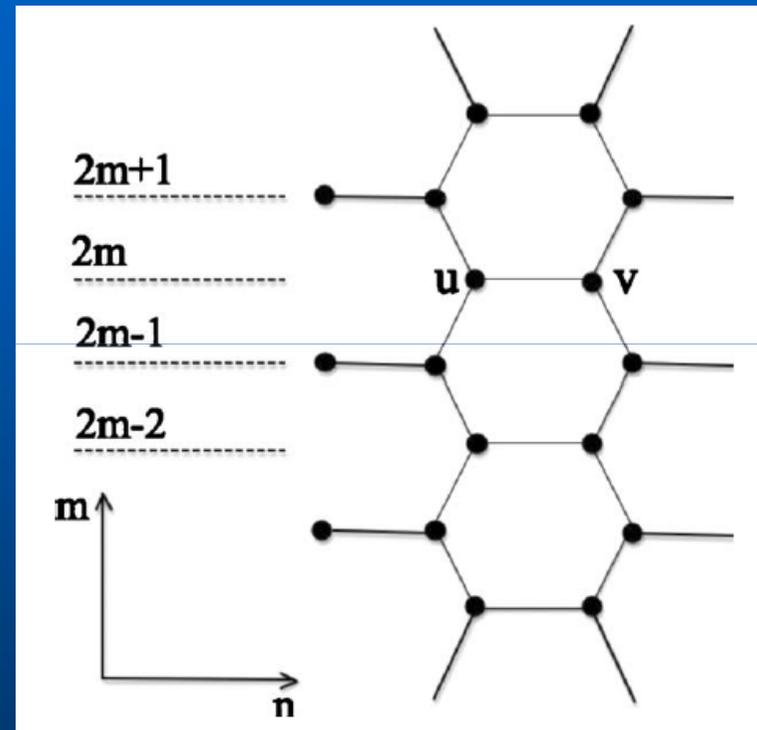
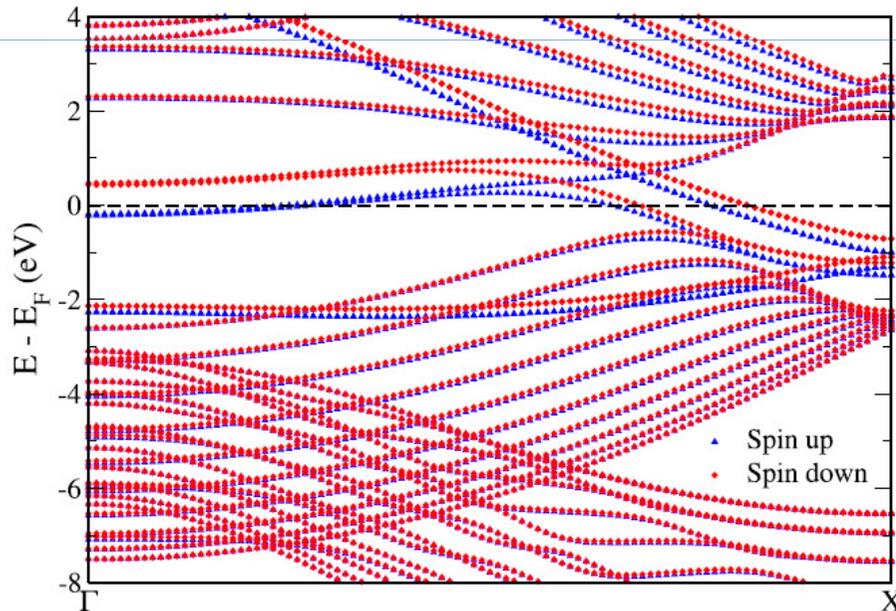
Despite the absence of dangling bonds...

# Magnetism at zigzag edges V



The model: just cut off double-hydrogenated carbon atoms

## Magnetization density

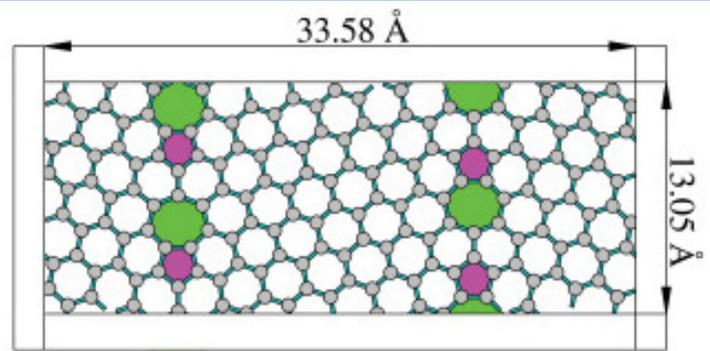


Zero-energy mode appears!

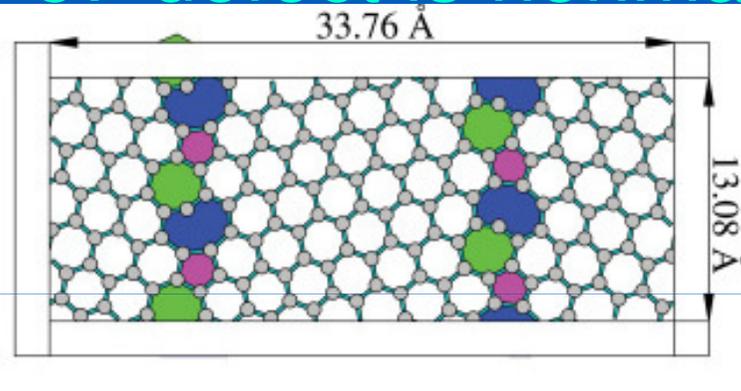
Spin-polarized bands in carbon-terminated nanoribbons

# Dangling bonds in grain boundaries

Akhukov, Fasolino, Gornostyrev & MIK, PR B 85, 115407 (2012)

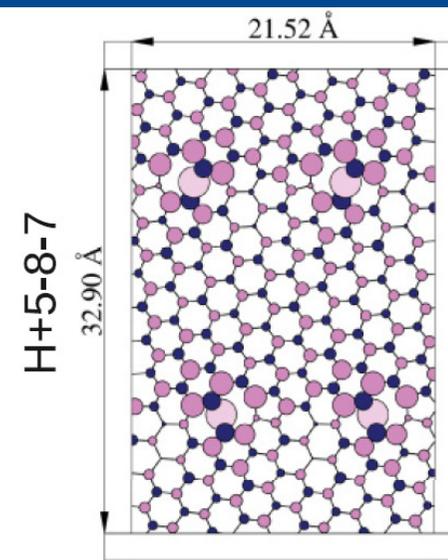
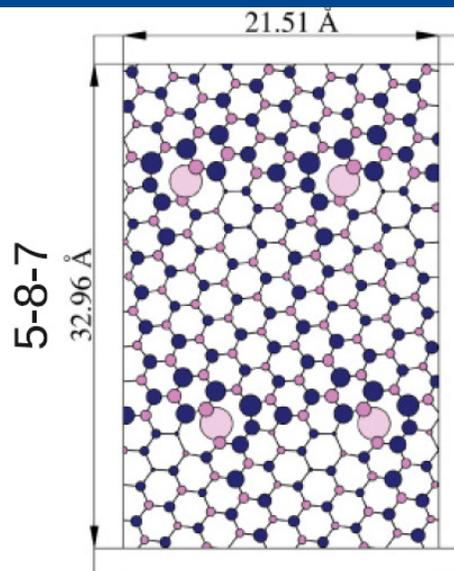
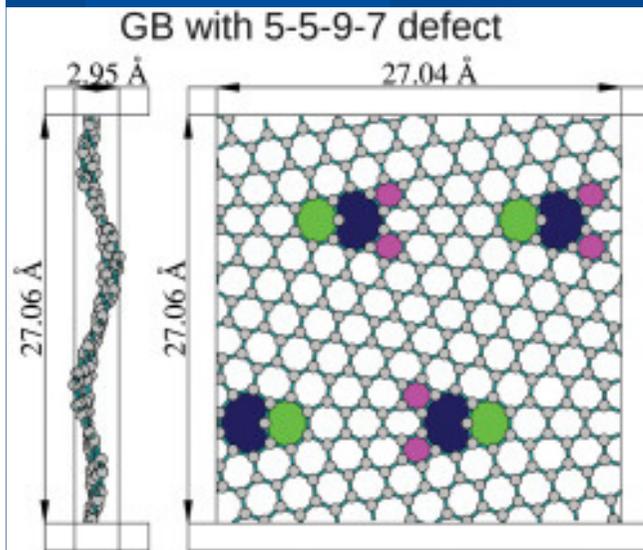


57 defect is nonmagnetic



587  
Magnetic  
and typical

And more...

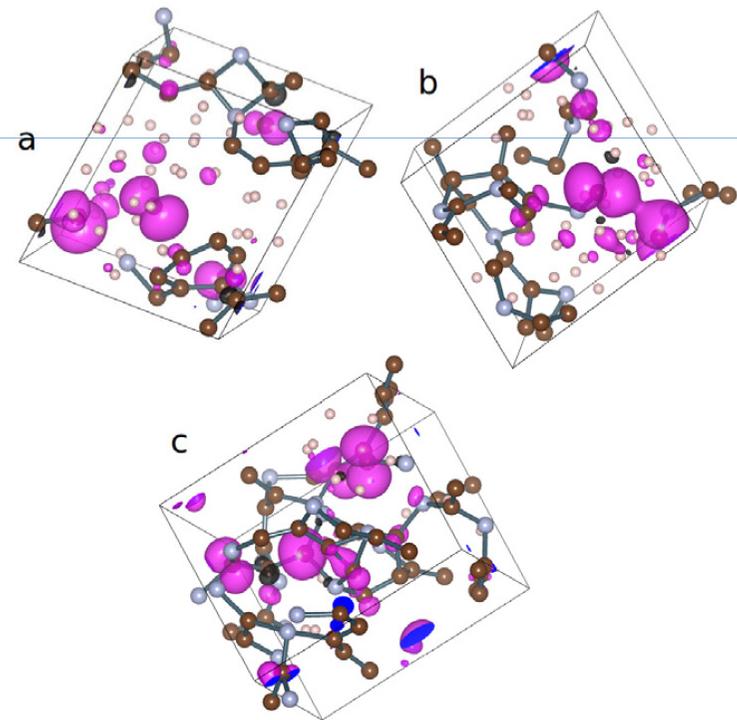
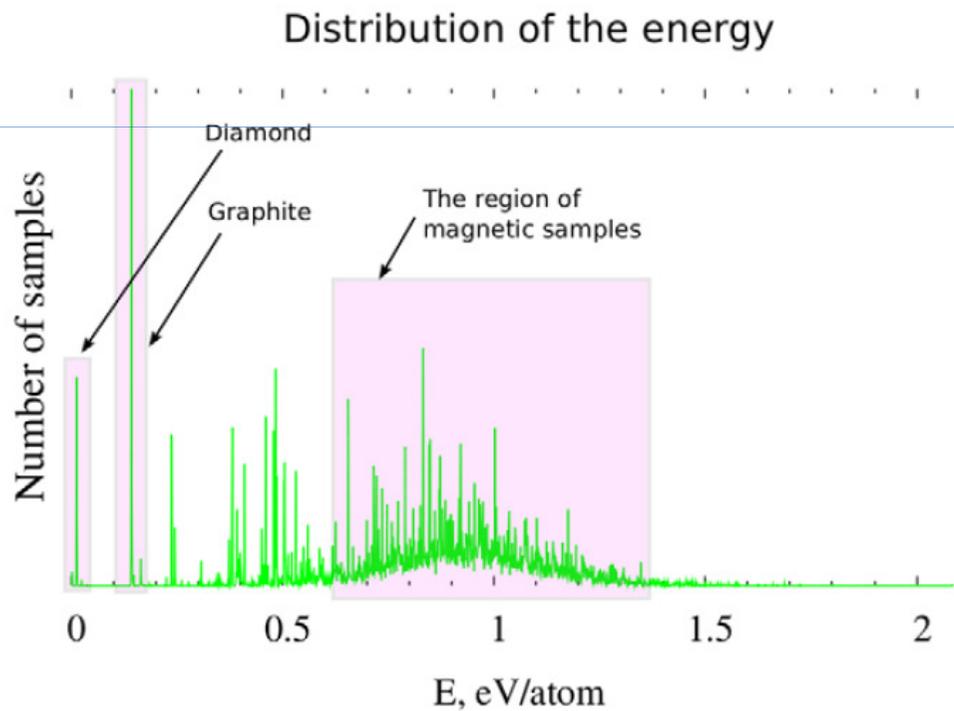


Spin  
density

# Carbon foams

Akhukov, MIK & Fasolino, J. Phys.: Cond. Mat. 25, 255301 (2013)

24,000 configurations; about 1% have magnetic moments



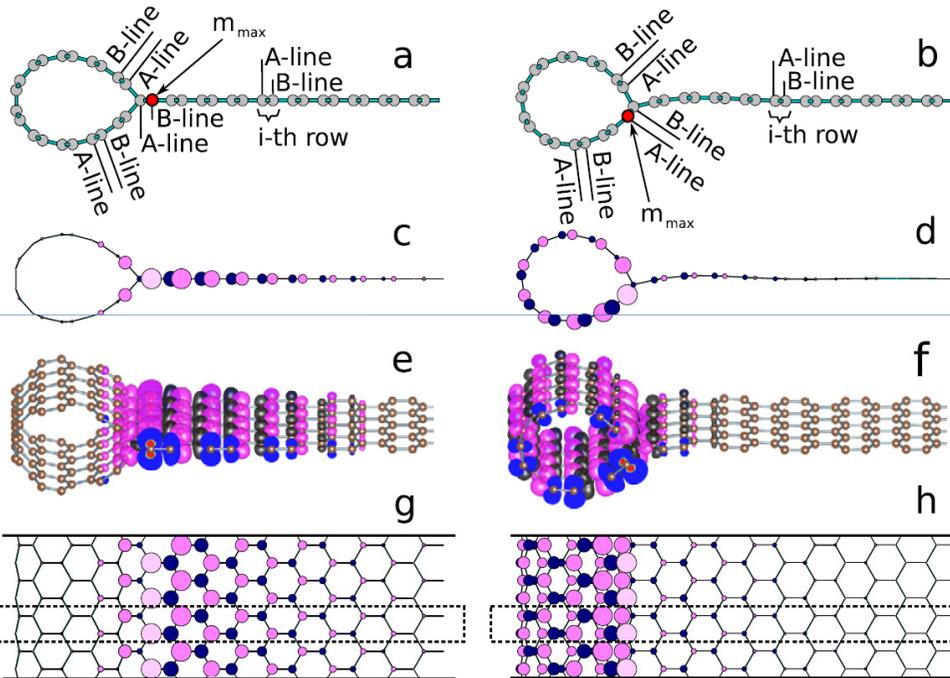
# Nanotube-terminated nanoribbons

Akhukov, Yuan, Fasolino & MIK, New J. Phys. 14, 123012 (2012)

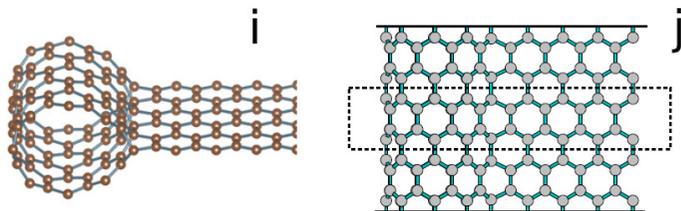
## Edges with armchair nanotube

symmetric

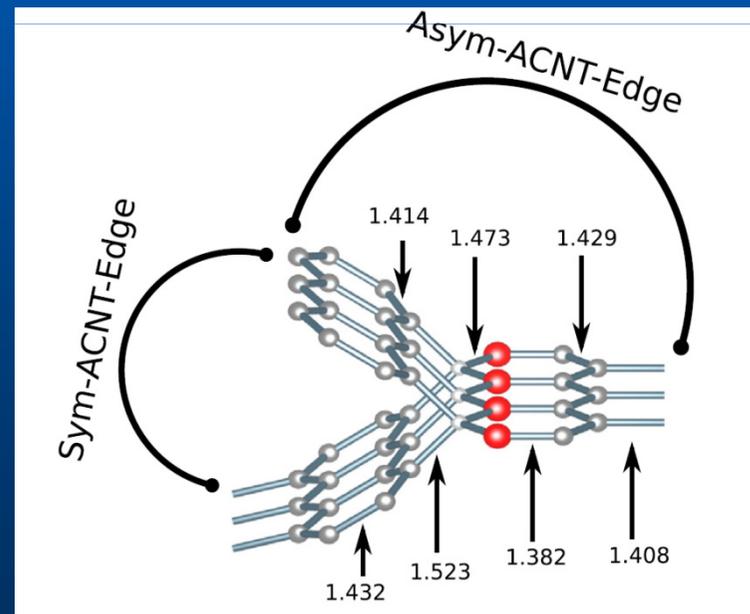
asymmetric



## Edges with zigzag nanotube



**Figure 1.** (a)–(h) Structure and spin density for symmetric (left) and asymmetric (right) AC nanotube terminated edges. (a), (b) Atomic structure; (c), (d) side, (e), (f) three-dimensional (3D) and (g), (h) top view of schematic spin representation. The box with a dashed line in (g), (h) indicates half of the unit cell in the density functional theory (DFT) calculation. For the symmetric case, the contribution to the magnetic moment from atoms belonging to the A- and B-sublattices are  $m_A = 0.958\mu_B$  and  $m_B = -0.217\mu_B$  (per half unit cell), and for the asymmetric case  $m_A = 1.048\mu_B$  and  $m_B = -0.300\mu_B$ . The maximum of the magnetic moment is located on the atom indicated by the arrow with the value  $m_{\max} = 0.379\mu_B$  in both the symmetric and asymmetric cases. (i), (j) 3D and top view of AC nanoribbons terminated by ZZ nanotubes. The box with a dashed line in (j) indicates half of the unit cell in the DFT calculation.



red = magnetic;  $sp^2$ - $sp^3$  bonds

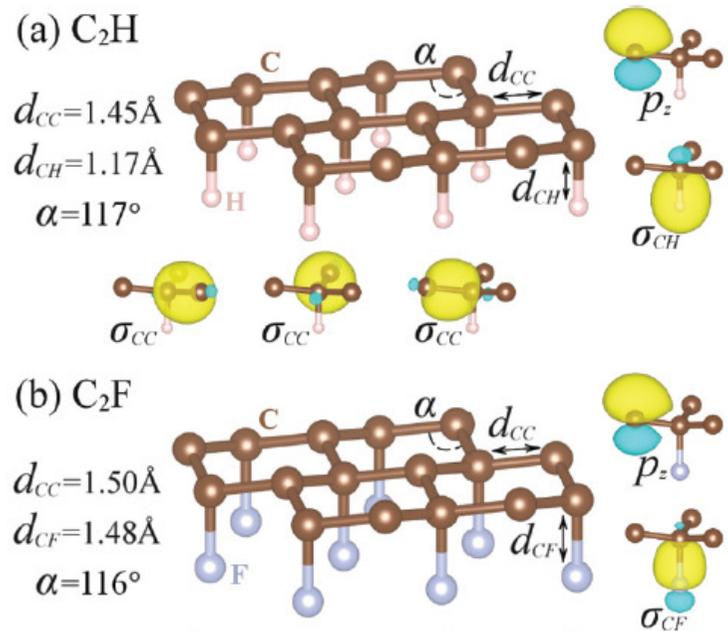
# Exchange interactions in concentrated systems

PHYSICAL REVIEW B 88, 081405(R) (2013)

## Exchange interactions and frustrated magnetism in single-side hydrogenated and fluorinated graphene

A. N. Rudenko,<sup>1,\*</sup> F. J. Keil,<sup>1</sup> M. I. Katsnelson,<sup>2</sup> and A. I. Lichtenstein<sup>3</sup>

Two-side fluorinated or hydrogenated graphene is nonmagnetic. Single-side: claim for FM



Structure,  
orbitals,  
nonmagnetic  
bands

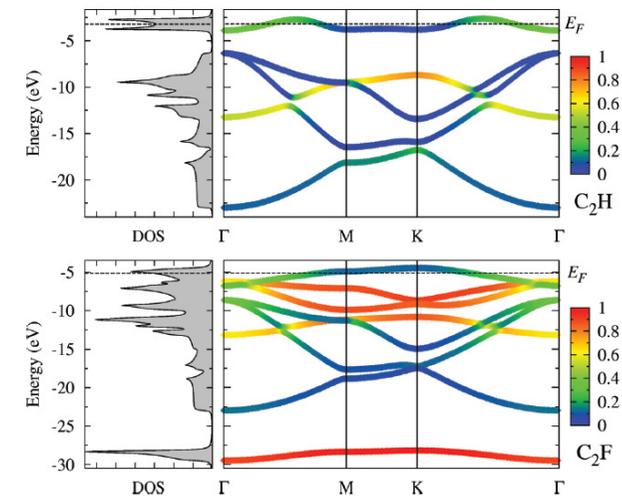


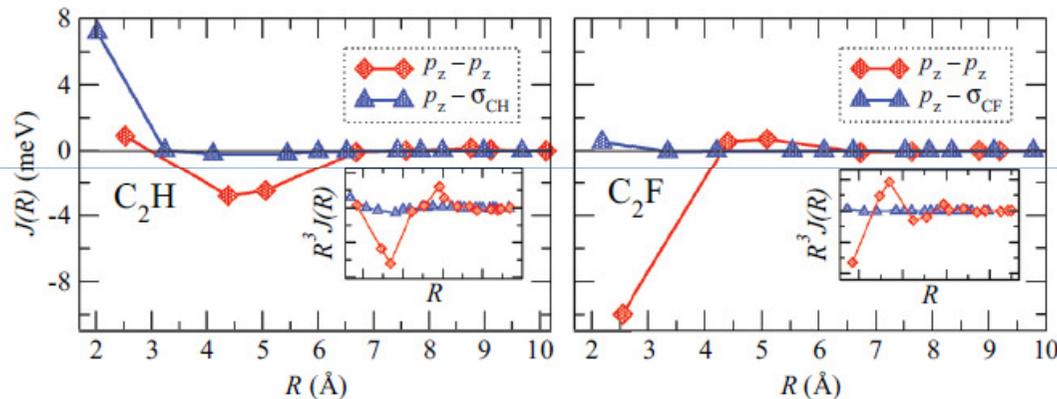
FIG. 2. (Color online) Band structure and density of states (DOS) for  $C_2H$  and  $C_2F$  obtained from non-spin-polarized calculations. Contributions from the impurity orbitals ( $s$  for H and  $sp$  for F) are shown by color.

# Single-side C<sub>2</sub>F and C<sub>2</sub>H

Mapping on classical Heisenberg model (A. Lichtenstein & MIK)

$$H = - \sum_{i \neq j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j$$

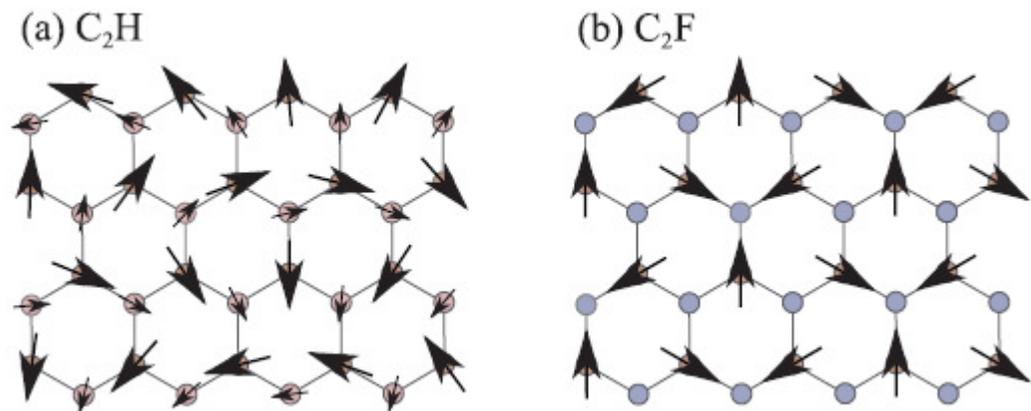
$$J_{ij}^{\alpha\beta} = \frac{1}{4\pi} \int_{-\infty}^{E_F} d\varepsilon \operatorname{Im} [\Delta_{\alpha} G_{ij}^{\alpha\beta\downarrow}(\varepsilon) \Delta_{\beta} G_{ji}^{\beta\alpha\uparrow}(\varepsilon)]$$



Well-localized  
magnetic moments

Quantum effects:  
Quantum spin liquid?!

FIG. 5. (Color online) Spin structures corresponding to a classical ground state for (a) C<sub>2</sub>H (incommensurate spin spiral) and (b) C<sub>2</sub>F (120° Néel state).

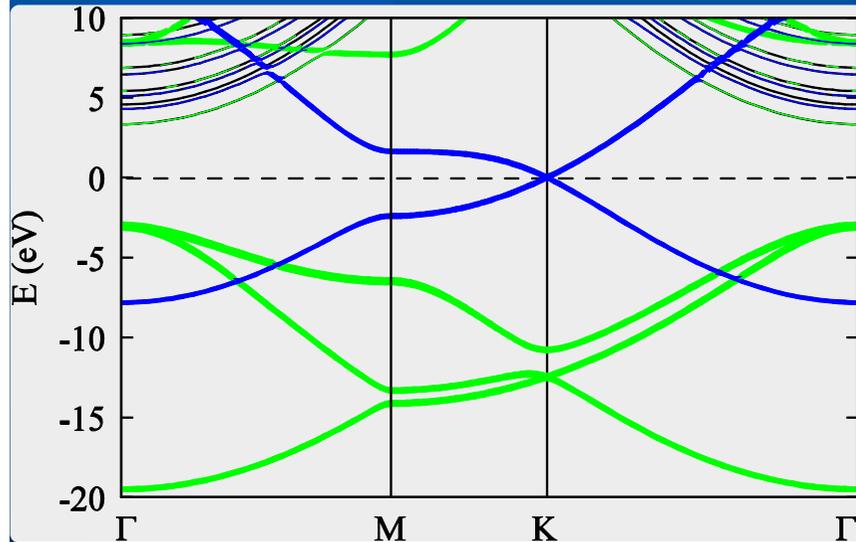


# Strength of Coulomb interactions in graphene

Wehling, Şaşıoğlu, Friedrich, Lichtenstein, MIK & Blügel, PRL106, 236805 (2011)

## Generalized Hubbard model for $\pi$ -bands only

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U_{00} \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{1}{2} \sum_{i \neq j, \sigma, \sigma'} U_{ij} n_{i,\sigma} n_{j,\sigma'}$$



$\pi$  bands (blue) crossing Fermi level

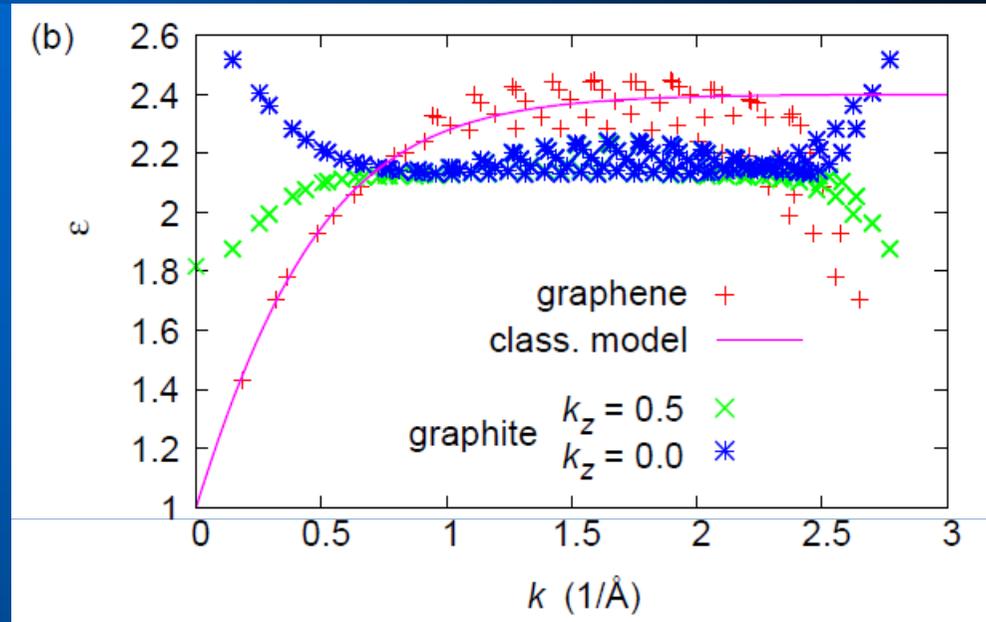
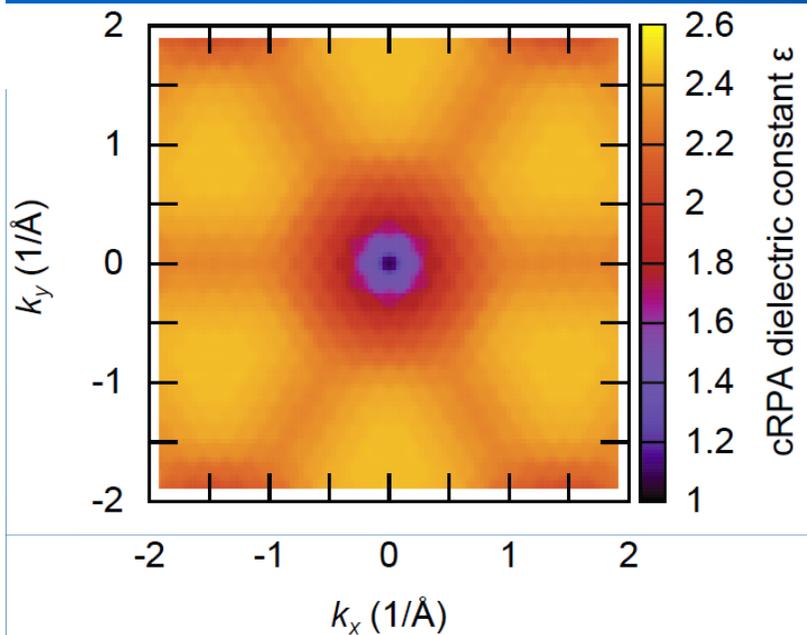
$\sigma$  bands (green) at higher energies

All electrons **except**  $\pi$  contribute to screening of the Coulomb interactions (**constrained RPA**)

$$P(\mathbf{r}, \mathbf{r}'; \omega) = \sum_i^{\text{occ}} \sum_j^{\text{unocc}} \psi_i(\mathbf{r}) \psi_i^*(\mathbf{r}') \psi_j^*(\mathbf{r}) \psi_j(\mathbf{r}') \times \left\{ \frac{1}{\omega - \varepsilon_j + \varepsilon_i + i0^+} - \frac{1}{\omega + \varepsilon_j - \varepsilon_i - i0^+} \right\}$$

Polarization function

# Strength of Coulomb interactions in graphene II



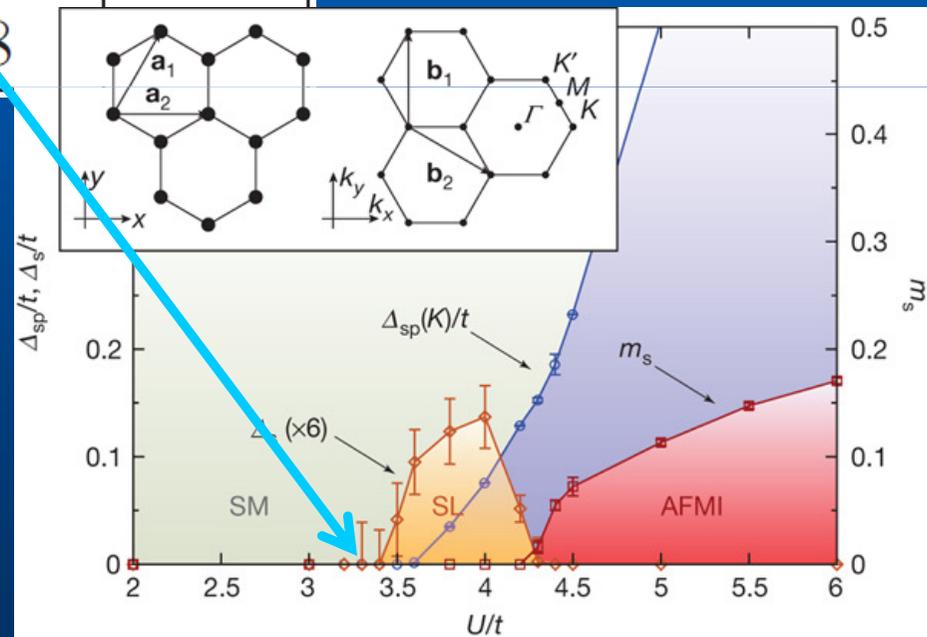
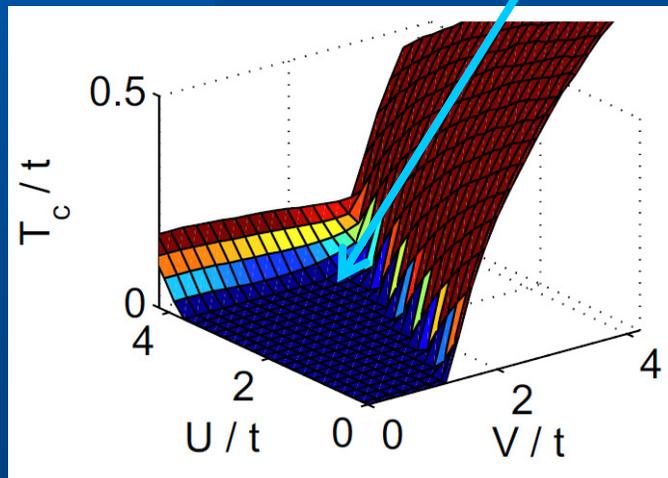
## Graphene vs graphite

Static cRPA dielectric function of graphene in momentum space

	graphene		graphite	
	bare	cRPA	bare	cRPA
$U_{00}^A$ (eV)	17.0	9.3	17.5	8.0
$U_{00}^B$ (eV)	17.0	9.3	17.7	8.1
$U_{01}$ (eV)	8.5	5.5	8.6	3.9

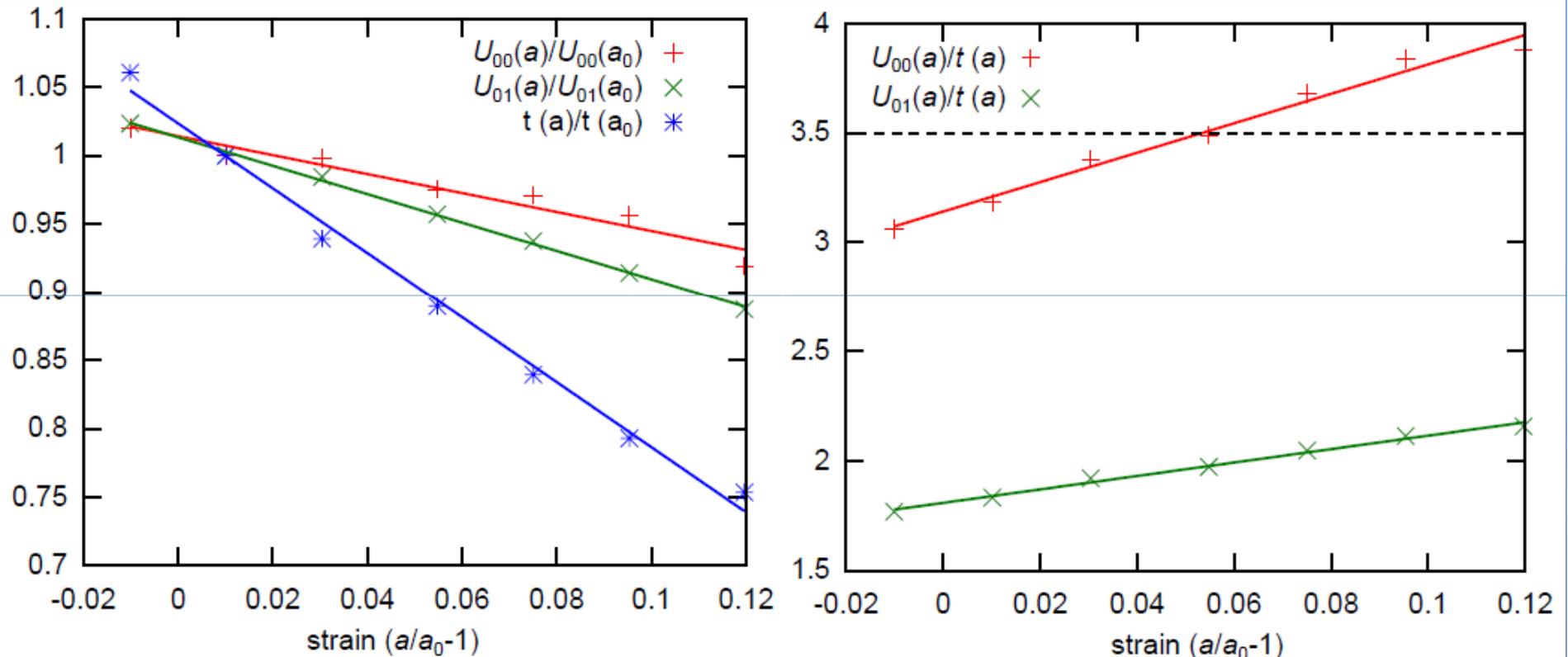
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Honercamp, PRL 100, 146404 (2008) Z. Y. Meng et al., Nature 464, 847 (2010)

# Effect of strain on Coulomb interactions in graphene



Coulomb interaction  $U_{ij}$  and hopping parameters  $t$  as function of lattice constant  $a$ .

The equilibrium lattice constant is  $a_0 = 2.47\text{\AA}$ .

# Semimetal-insulator phase transition

M. Ulybyshev, P. Buividovich, MIK & M. Polikarpov, PRL111, 056801 (2013)

Lattice QMC simulations; Hubbard-Stratonovich transformation:

18 by 18 sites,  
20 time slices,  
 $T = 0.5$  eV

(should be improved  
in future!)

$$\exp\left(-\frac{\delta}{2} \sum_{x,y} \hat{q}_x V_{xy} \hat{q}_y\right) \cong \int \mathcal{D}\varphi_x \exp\left(-\frac{\delta}{2} \sum_{x,y} \varphi_x V_{xy}^{-1} \varphi_y - i\delta \sum_x \varphi_x \hat{q}_x\right),$$

$$\text{Tr} e^{-\beta \hat{H}} = \int \mathcal{D}\varphi_{x,n} \mathcal{D}\psi_{x,n} \mathcal{D}\eta_{x,n} \mathcal{D}\bar{\psi}_{x,n} \mathcal{D}\eta_{x,n} e^{-S[\varphi_{x,n}] - \sum_{x,y,n,n'} (\bar{\eta}_{x,n} \bar{M}_{x,y,n,n'} \eta_{y,n'} + \bar{\psi}_{x,n} M_{x,y,n,n'} \psi_{y,n'})},$$

$$\text{Tr} e^{-\beta \hat{H}} \cong \int \mathcal{D}\varphi_{x,n} e^{-S[\varphi_{x,n}]} |\det(M[\varphi_{x,n}])|^2$$

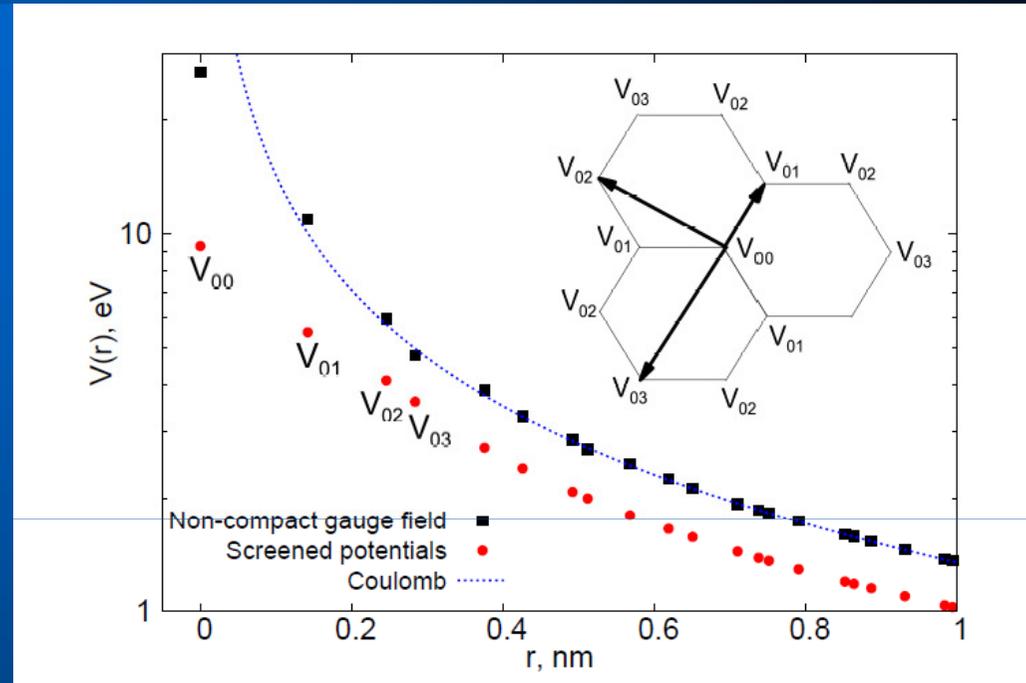
Neutrality point:  $\mu = 0$

No sign problem (e-h symmetry)!

$$S[\varphi_{x,n}] = \frac{\delta}{2} \sum_{x,y,n} \varphi_{x,n} V_{xy}^{-1} \varphi_{y,n}$$

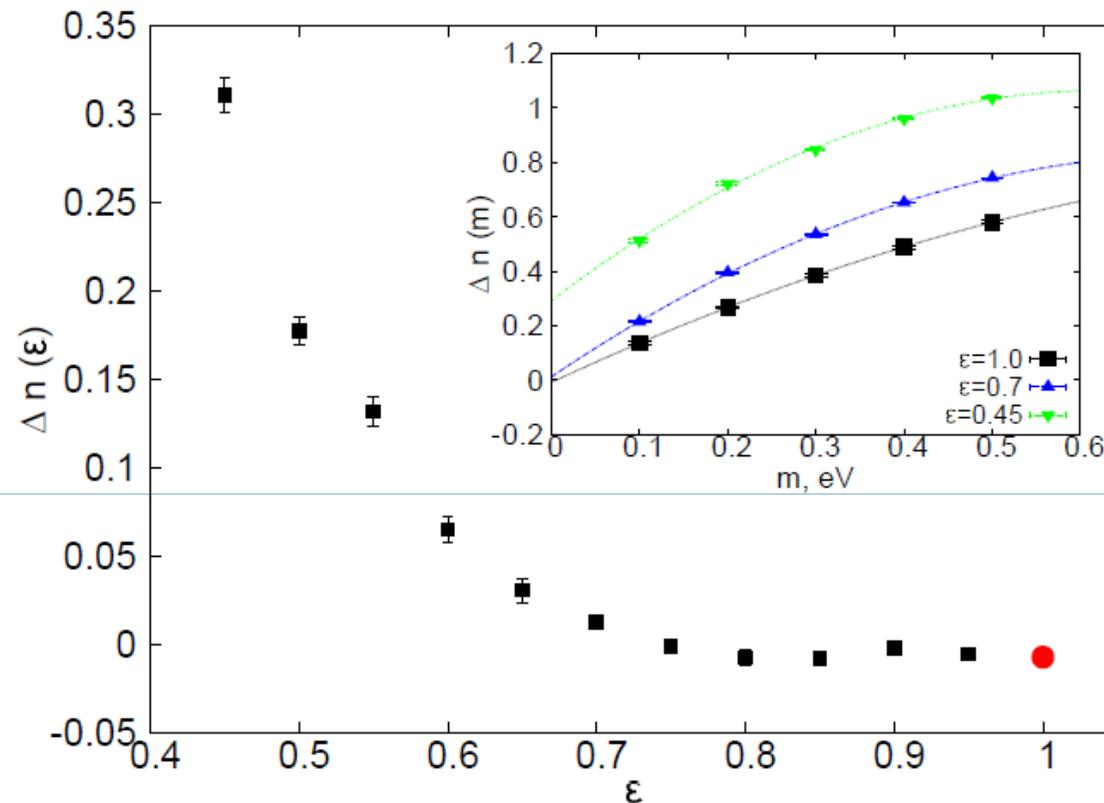
# *Semimetal-insulator phase transition II*

The effect of screening by  $\sigma$ -bonds is essential. At our distances a factor 1.4



- (1) Introduce the mass term  $m$
- (2) Chiral condensate  $\Delta n$ , difference in occupation number between A and B sublattices
- (3) Introduce external dielectric constant (due to substrate)  $\epsilon$

# Semimetal-insulator phase transition III



We are on semimetal side (screening by  $\sigma$  bonds is crucial) but not too far from the transition point  $\epsilon \approx 0.7$

Exciton fluctuations may be important

FIG. 2: The dependence of the chiral condensate (11) on  $\epsilon$  and on  $m$  (in the inset) for the  $18 \times 18$  lattice with  $N_t = 20$  and  $\delta = 0.1 \text{ eV}^{-1}$ . For  $\epsilon = 1.0$  we show the results obtained on the  $24 \times 24$  lattice with  $N_t = 40$ ,  $\delta = 0.05 \text{ eV}^{-1}$ .

# Effective Hubbard model for graphene

Schüler, Rösner, Wehling, Lichtenstein & MIK, PRL 111, 036601 (2013)

Long-range Coulomb interaction is crucially important for graphene but not everywhere, e.g., for magnetism effective Hubbard model should be OK. How to build it?

We have:

$$H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{\substack{i \neq j \\ \sigma, \sigma'}} V_{ij} n_{i\sigma} n_{j\sigma'}$$

We want:

$$H^* = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U^* \sum_i n_{i\uparrow} n_{i\downarrow}$$

# Effective Hubbard model for graphene II

The idea: Feynman-Peirels-Bogoliubov variational principle

$$\tilde{\Phi}[\rho^*] = \Phi^* + \langle H - H^* \rangle^*$$

$$\Phi^* = -\frac{1}{\beta} \ln Z^*$$

$$\rho^* = 1/Z^* e^{-\beta H^*}$$

$$Z^* = \text{Tr} \{ e^{-\beta H^*} \}$$

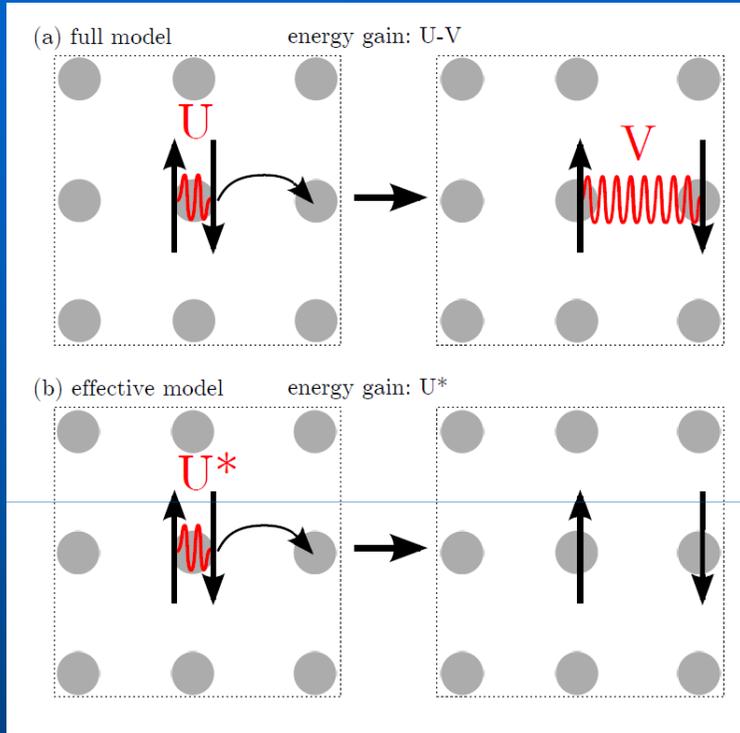
$\langle \dots \rangle^*$  denotes the Gibbs average over the trial system

$$\partial_{U^*} \tilde{\Phi}[U^*] = 0$$

$$U^* = U + \frac{1}{2} \sum_{\substack{i \neq j \\ \sigma, \sigma'}} V_{ij} \frac{\partial_{U^*} \langle n_{i\sigma} n_{j\sigma'} \rangle^*}{\sum_l \partial_{U^*} \langle n_{l\uparrow} n_{l\downarrow} \rangle^*}$$

The calculations are done by lattice QMC

# Effective Hubbard model for graphene III



For translationally invariant system:

$$U^* = U - \bar{V}$$

$$\bar{V} = - \sum_{\substack{j \neq 0 \\ \sigma'}} V_{0j} \frac{\partial_{U^*} \langle n_{0\uparrow} n_{j\sigma'} \rangle^*}{\partial_{U^*} \langle n_{0\uparrow} n_{0\downarrow} \rangle^*}$$

Number of particle conservation

$$\sum_{j\sigma} \langle n_{0\uparrow} n_{j\sigma} \rangle^* = N/2$$

$$\partial_{U^*} \langle n_{0\uparrow} n_{0\downarrow} \rangle^* = - \sum_{j \neq 0, \sigma} \partial_{U^*} \langle n_{0\uparrow} n_{j\sigma} \rangle^*$$

A naive estimation:

$$U^* = U - V_{01}$$

turns out to be amazingly good

# Effective Hubbard model for graphene IV

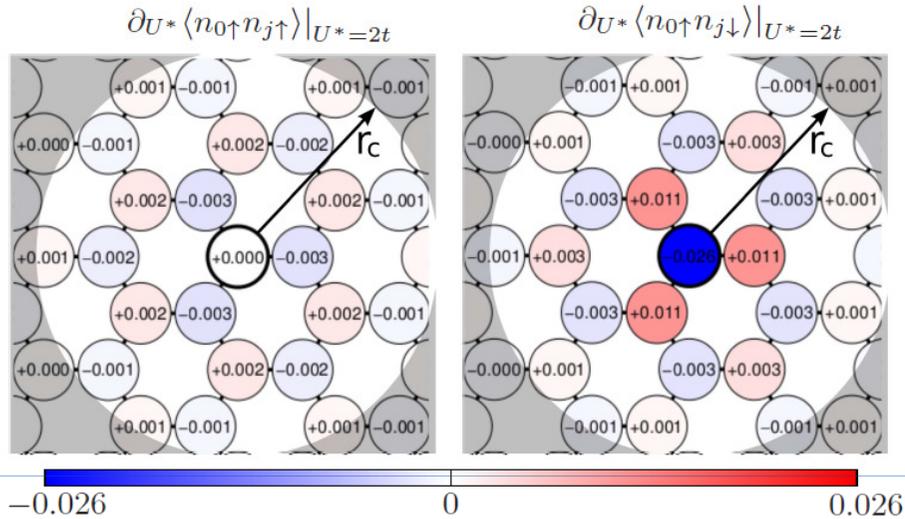


Figure 2. (Color online) Derivatives of the correlation functions  $\langle n_{0\uparrow} n_{j\sigma} \rangle$  with respect to  $U^*$  for graphene (16x16 unit cells) calculated with DQMC for inverse temperature  $\beta = 9t$  and  $U = 2t$ . Each circle corresponds to one carbon atom. The shaded area depicts the region of nearly vanishing derivatives. The cutoff radius is  $r_c$ . The thick drawn circles indicate the lattice site with index  $i = 0$ .

Decrease of effective  $U$   
roughly by a factor of 2

Calculations for benzene,  
graphene and silicene

Table I. First three rows: Coulomb matrix elements obtained with cRPA ( $t_{\text{graphene}} = 2.80$  eV,  $t_{\text{silicene}} = 1.14$  eV,  $t_{\text{benzene}} = 2.54$  eV). Last three rows: Effective local Coulomb matrix elements with and without the approximation that electrons are only displaced to next neighbors and the factor by which the local Coulomb interaction is decreased.

	Graphene	Silicene	Benzene
$U/t$	3.63	4.19	3.96
$(V_{01}, V_{02})/t$	2.03, 1.45	2.31, 1.72	2.83, 2.01
$(V_{03}, V_{04})/t$	1.32, 1.14	1.55, 1.42	1.80
$U^*/t$	$1.6 \pm 0.2$	$2.0 \pm 0.3$	1.2
$(U - V_{01})/t$	1.6	1.9	1.1
$U^*/U$	$0.45 \pm 0.05$	$0.46 \pm 0.05$	0.3

# Conclusions

- sp electron magnetic semiconductors can be better than conventional – if one finds FM...
- local magnetic moments is not a problem but FM is; even when one has strong exchange it is not necessarily FM
- very unclear situation for magnetism at the edges (beyond the talk)
- for theoretical studies one can use Hubbard model with first-principles Hubbard parameter; Intersite Coulomb interaction decrease it roughly by a factor of 2

# Main collaborators

M.Akhukov, A.Fasolino, A.Rudenko (Nijmegen)  
A.Geim, I.Grigorieva, K.Novoselov (Manchester)  
D.Edwards (Imperial, London)  
O. Yazyev (Lausanne)  
A.Lichtenstein (Hamburg)  
T.Webling (Bremen)  
M.Polikarpov (Moscow)  
D.Boukhvalov (Seoul)  
O.Eriksson (Uppsala)

MANY THANKS!