FACULTY OF PHYSICS UNIVERSITY OF WARSAW

E-MRS Spring Meeting,
Lille, 27 May 2014

ICMM

Doping induced Rashba spin splitting in graphene

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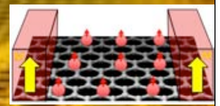
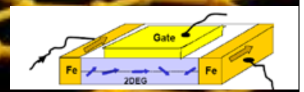
Motivation: Graphene hope for future electronic & spintronic devices

- The first material to demonstrate *room temperature spin transport*



- *Very long spin lifetime owing to extremely small spin-orbit coupling*
- *Too small spin splitting not favorable for spin FET*



The basis principle of the spin Field Effekt Transisor

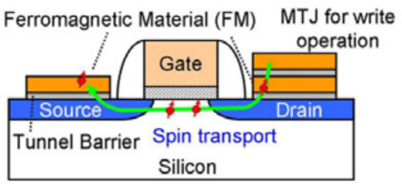


Diagram of Toshiba's spintronics-based MOS field-effect transistor

- Tuning of the spin lifetime by the gate

➡ Motivation: How to improve functionality of spin FET based on graphene ?

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Possibility to modify spin-orbit coupling in graphene layers

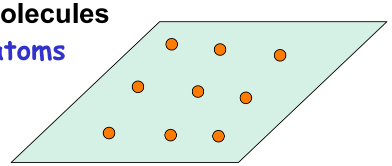
- Substrate can influence the spin splitting dramatically

This talk:

- On purpose modification of spin-orbit coupling

➡ Decoration of graphene with atoms or molecules

Here: Ge & Sn ad-atoms



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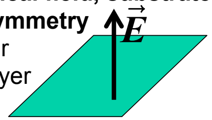
Nature of the spin-orbit coupling in graphene

- ***Intrinsic*** **spin-orbit coupling of carbon atoms (smaller in graphene than in diamond)**
- ***Extrinsic (Rashba)*** **spin-orbit coupling induced by an external factor (e.g., electrical field, substrate ad-atoms) that diminishes the symmetry**



Field perpendicular to the graphene layer

$\lambda_R \sim E$

For model treatment of S-O in graphene:

$$H_{eff} = \lambda_{so}\sigma_z\tau_z s_z + \lambda_R(\sigma_x\tau_z s_y - \sigma_y s_x)$$

Strength of the *intrinsic* & extrinsic spin-orbit coupling

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Spin-orbit coupling in semiconducting structures

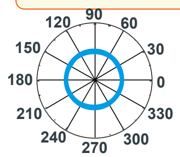
$$\hat{H} = \frac{\hbar^2 \vec{k}^2}{2m^*} + \frac{\hbar}{2}\vec{\sigma}\cdot\vec{B}_{eff}(\vec{k})$$

$$\vec{B}_{eff}(\vec{k}_{||}) = \alpha_{SIA}\vec{k}_{||}\times\vec{n} + \alpha_{BIA}\vec{\Omega}(\vec{k}_{||})$$

Structure Inversion Asymmetry (Rashba) — **Bulk Inversion Asymmetry**

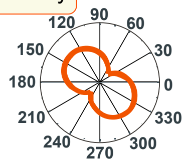
Rashba term requires uniaxial symmetry

BIA



BIA + SIA

C.b.b. spin splitting



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Method: Density Functional Theory (DFT) with relativistic effects included

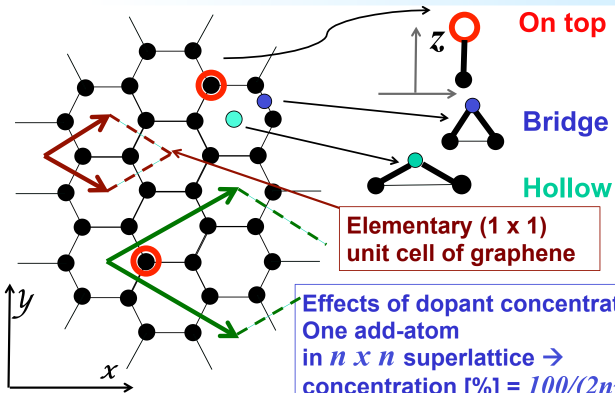
- $E[\rho] = \int d\vec{r}\, \upsilon_{ext}(\vec{r})\rho(\vec{r}) + T_S[\rho] + U[\rho] + E_x[\rho] + E_c[\rho]$
- Generalized Gradient Approximation (GGA) to the exchange & correlation $E_{xc}^{GGA}[\rho] = \int d\vec{r} f_{xc}(\rho(\vec{r}), \nabla\rho(\vec{r}))$
- $\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + \upsilon_{ext}(\vec{r}) + \upsilon_H(\vec{r}) + \upsilon_x(\vec{r}) + \upsilon_c(\vec{r})\right]\varphi_i(\vec{r}) = \varepsilon_i\varphi_i(\vec{r})$
- **Relativistic effects, spin-orbit coupling included, are taken into account through relativistic pseudopotentials** (used also to account for electron - ion interaction)

$$\rho(\vec{r}) = \sum_{i=1}^{N}\varphi^*_i(\vec{r})\varphi_i(\vec{r})$$

Codes used:

- *VASP*
- *Our own*

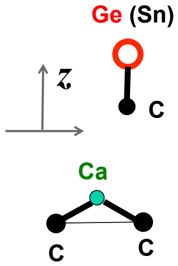
Geometry of the decorated graphene



Effects of dopant concentration: One add-atom in *n x n* superlattice → concentration [%] = $100/(2n^2)$

Full optimization of geometry performed

RESULTS: equilibrium positions of ad-atoms



Structure	Position	z in Å
1x1 Ge	TOP	3.602
2x2 Ge	TOP	2.156
4x4 Ge	TOP	2.156
1x1 Sn	TOP	3.822
2x2 Sn	TOP	2.621
4x4 Sn	TOP	2.401
1x1 Ca	HOLLOW	2.083
2x2 Ca	HOLLOW	2.205

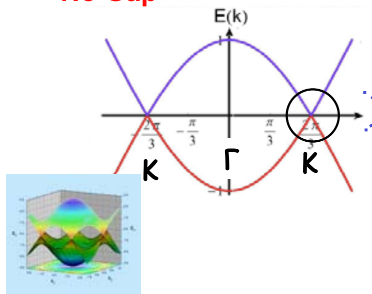
RESULTS: spin splitting in pristine graphene

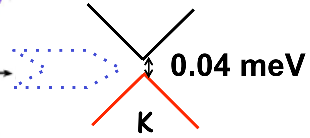
No Spin-Orbit

No Gap

Spin-Orbit (Intrinsic)

Very Tiny Gap





Double degeneracy of bands remains

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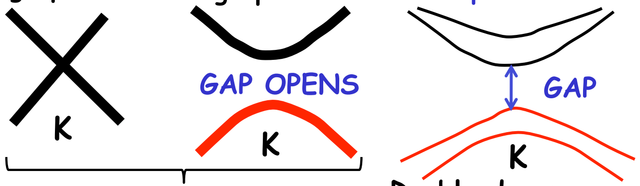
RESULTS: spin splitting of the decorated graphene

Qualitative description of the band structure around K

Pristine graphene | Decorated graphene | Decorated Graphene + SO



Doubly degenerated bands

Double degeneracy of bands removed

- Considerable spin splitting of bands'
- Difficult to distinguish between intrinsic and extrinsic spin-orbit couplings

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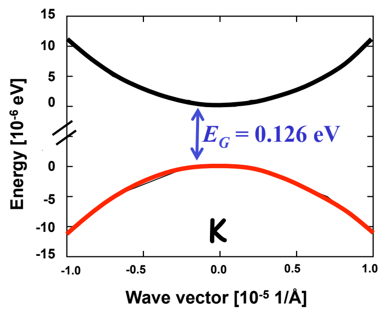
RESULTS: valence & conduction band around K point in 2x2 GR + Ge



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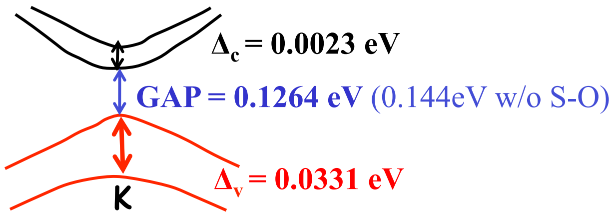
RESULTS: spin splitting in Ge decorated graphene

1Ge in 2x2 graphene (Ge concentration = 12.5%)



- **Spin splitting caused by spin-orbit coupling reaches values characteristic for 'normal' semiconductors**
- **E_G, Δ_c, and Δ_v diminish with smaller Ge concentration**

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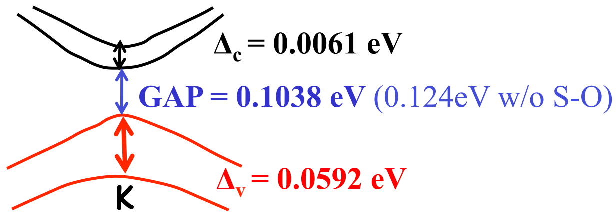
RESULTS: spin splitting in Sn decorated graphene

1Sn in 2x2 graphene (Sn concentration = 12.5%)



- **Spin splitting in Sn decorated graphene are generally larger than in Ge decorated structures**
- **As in the case of Ge, E_G, Δ_c, and Δ_v diminish with smaller Sn concentration**

Summary & Outlook

- *Ab initio* calculations clearly demonstrate that the spin splitting of bands in graphene can be modified by decorating the layers with heavier atoms.

- Furthes studies of the electronic structure of graphene with various decorating atoms (Pb) and molecules.
- Modeling of the growth process (chemical reactions) that could lead to effective incorporation of adatoms.

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Thank you !

Acknowledgements

SiCMAT Project, European Founds for Regional Development (Contract No. UDA-POIG.01.03.01-14-155/09).

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