TECHNISCHE UNIVERSITÄT DRESDEN

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Fakultät Maschinenwesen, Institut für Werkstoffwissenschaft, Professur Materialwissenschaft und Nanotechnik

Graphene edge magnetism for spintronics applications: Dream or Reality?

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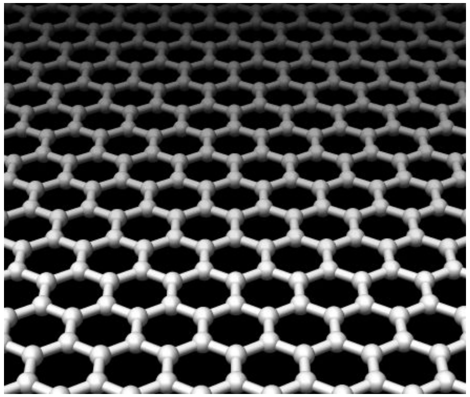
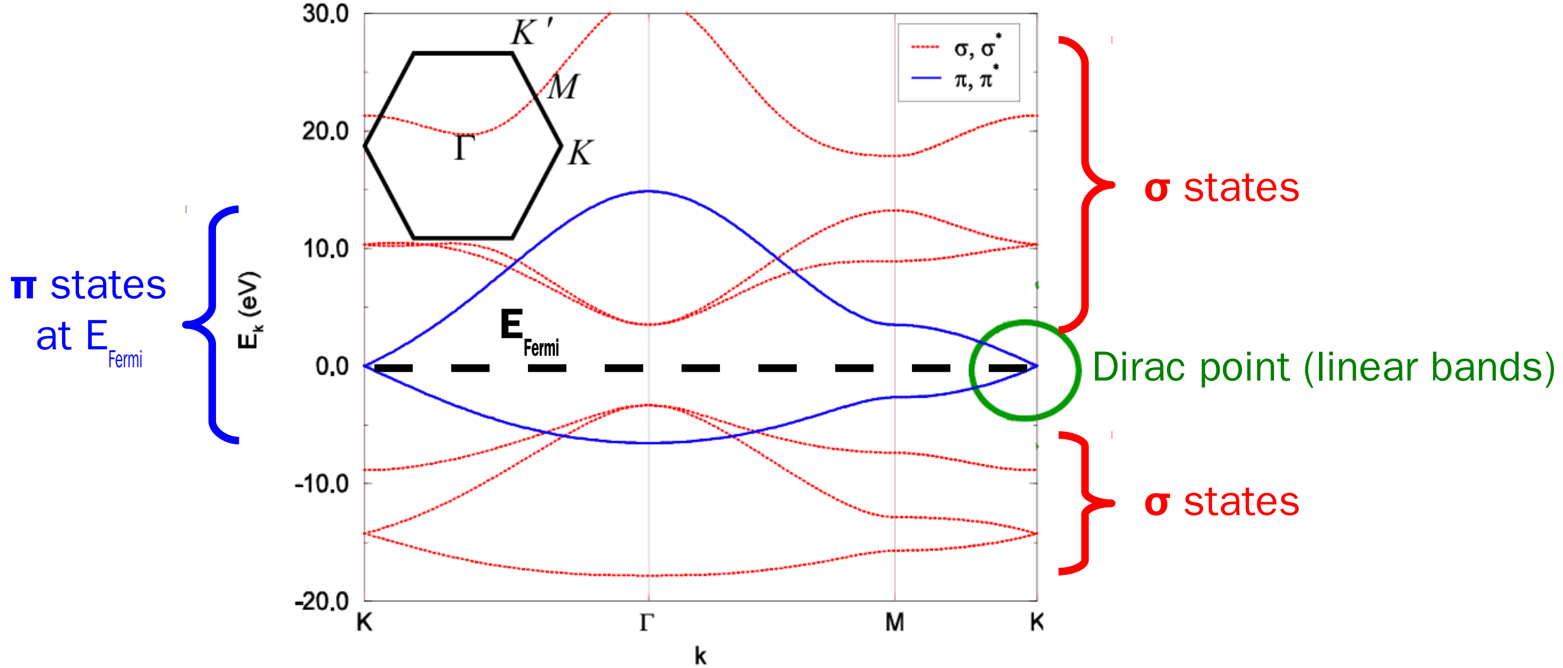
Introduction

Graphene



- single atomic layer of carbon with hexagonal structure
- Ideal 2D system
- Electronic structure:
  sp^2 = **π** states (out of plane)
  + **σ** states (in plane)

band structure of graphene

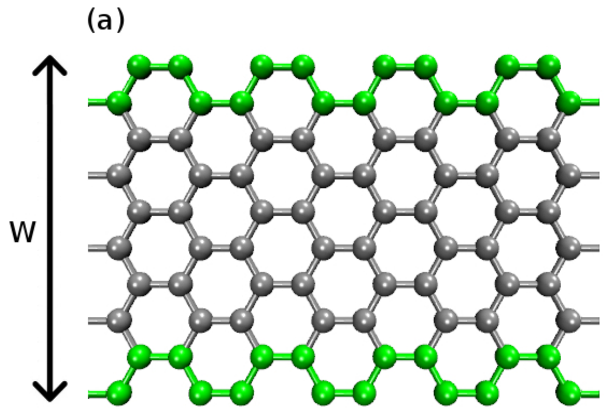


Introduction

Graphene nanoribbons (GNRs)

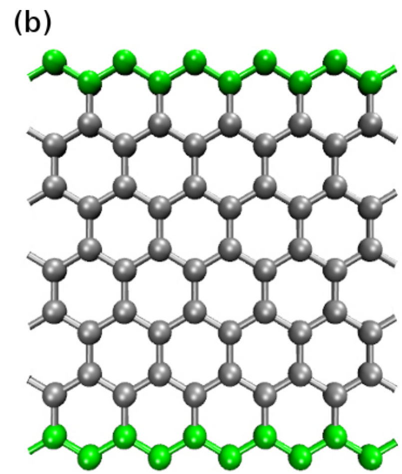
- a graphene nanobibbon (GNR) is a graphene strip of finite width W and infinite length
- 1D system
- can be fabricated in the lab (since 2007)

armchair GNR (AGNR)



- semiconducting

zigzag GNR (ZGNR)



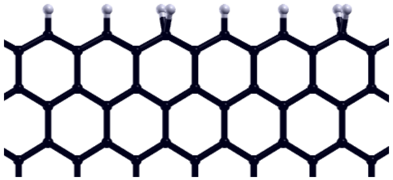
- System has magnetic **edge states**
- antiferromagnetic semiconductor

?

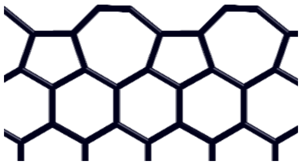
Results

Overview

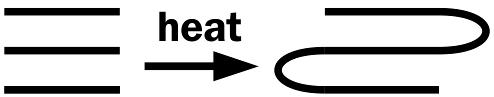
1. magnetic **edge states** are unlikely to exist



edge passivation

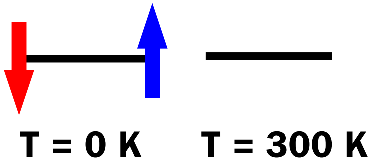


edge reconstruction



edge closure

2. Even if they exist, the **edge magnetism** is not stable at room temperature



not stable at
room temperature

J. Kunstmann, C. Özdogan, A. Quandt, H. Fehske, Phys. Rev. B **83**, 045414 (2011).

Methods

- Method: Density Functional Theory (DFT)
  Exchange-correlation: GGA (PW91)
  Basis set: PAW (pseudopotentials + plane waves)
  Code: VASP

- **edge energy** = enthalpy of the virtual reaction

$$\text{graphene} + N_{\mathrm{H}}/2\ \mathrm{H}_2 \longrightarrow \mathrm{ZGNR}$$

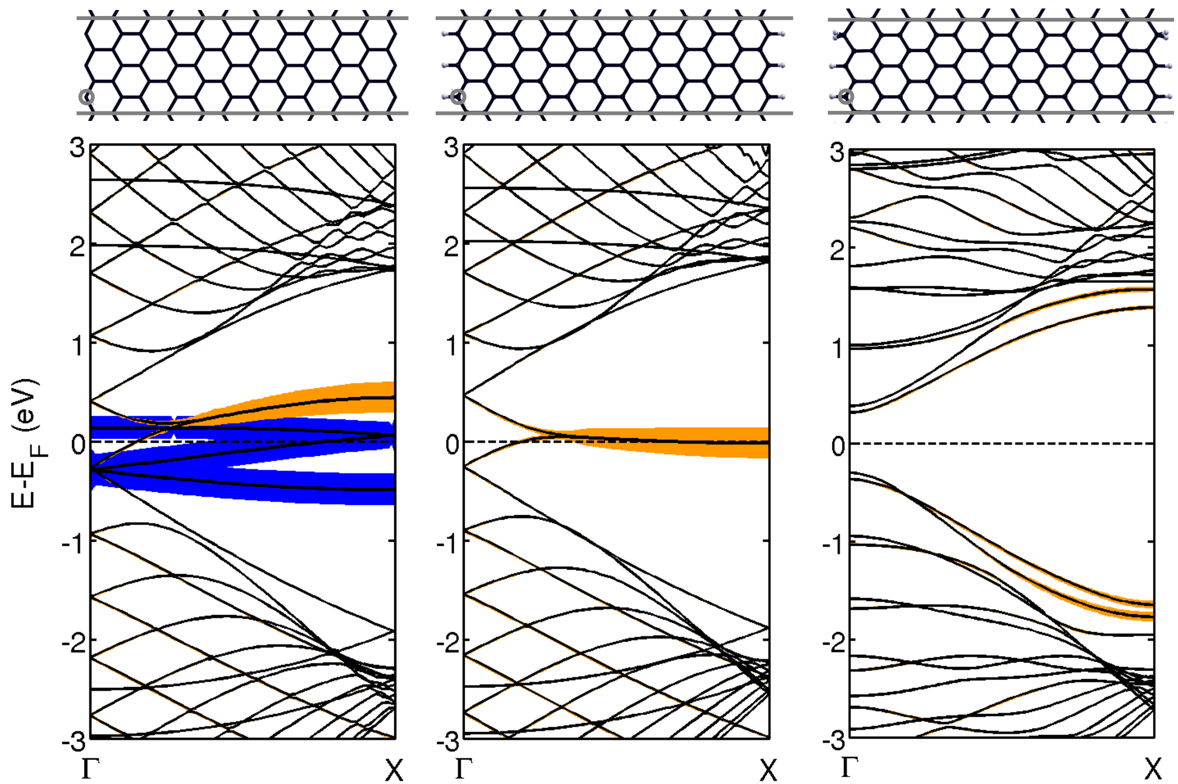
$$E_{\mathrm{edge}}^{\mathrm{at}} = (E_{\mathrm{tot}}^{\mathrm{ZGNR}} - N_{\mathrm{C}} E_{\mathrm{coh}}^{\mathrm{graphene}} - N_{\mathrm{H}} E_{\mathrm{coh}}^{\mathrm{H}_2})/N_{\mathrm{C}}^{\mathrm{edge}}$$

1. Stability of graphene edge states

1. Stability of graphene edge states

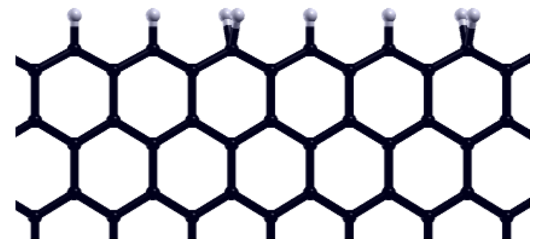
Edge passivation

unpassivated | hydrogen passivated | passivated with z_{211} edge



$E_{\mathrm{edge}}^{\mathrm{at}}$ = 3.00 eV/at. = 0.28 eV/at. = 0.08 eV/at.

z_{211} edge



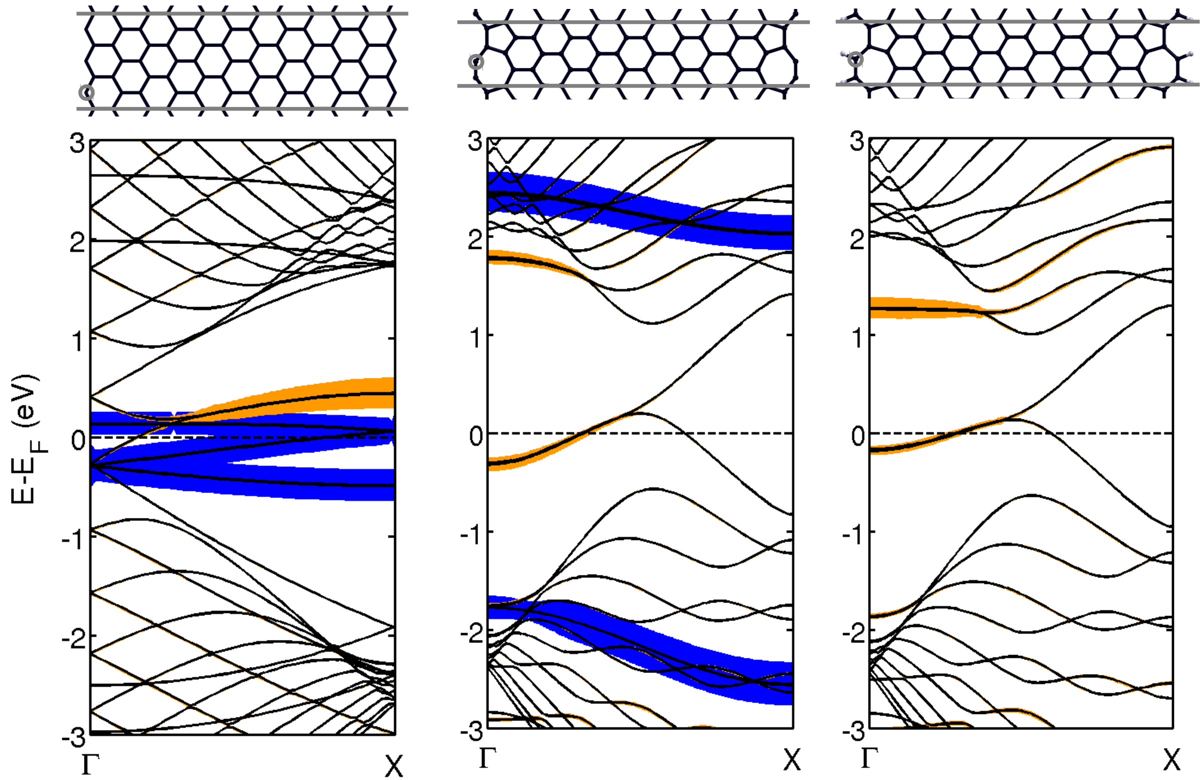
Wassmann, PRL **101**, 096402 (2008).

- z_{211} edge is the most stable edge that is known
- semiconducting
- no edge states
- non-magnetic

1. Stability of graphene edge states

Edge reconstruction

unpassivated	5-7 edge reconstruction	5-7 edge reconstruction + H passivation



$E_{\mathrm{edge}}^{\mathrm{at}}$ = 3.00 eV/at. = 2.39 eV/at. = 0.87 eV/at.

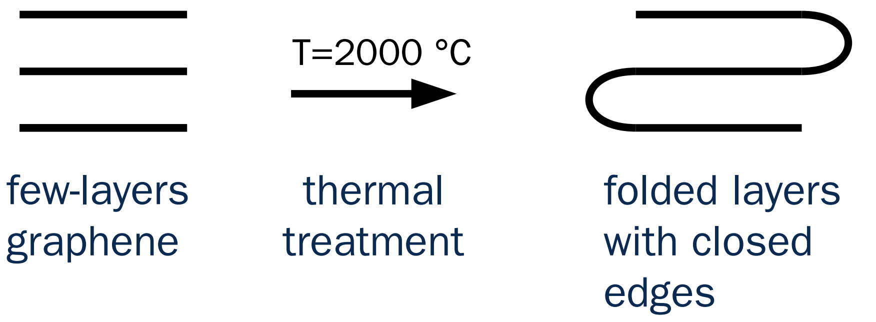
5-7 edge reconstruction

Koskinen, PRL **101**, 115502 (2008).

- only moderate stability of the 5-7 edge reconstruction
- edge states but no flat bands
- metallic
- non-magnetic
- experimentally observed
  Koskinen, PRB **90**, 073401 (2009).

1. Stability of graphene edge states

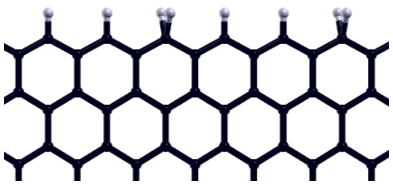
Edge closure



- no edges / edge states / edge magnetism
- experimentally observed
  Liu, Suenaga, Harris, Iijima, PRL **102**, 015501 (2009).

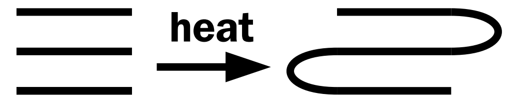
1. Stability of graphene edge states

Resume



edge passivation

edge reconstruction



edge closure

- in real graphene systems the edges are likely to be passivated, reconstructed, or closed
  → no / very little magnetic edge states
- magnetic **edge states** are unlikely to exist

2. Stability of graphene edge magnetism

1. Stability of graphene edge magnetism

Stable magnets

- Magnetic DFT calculations can find different magnetic states of one system
  - NM - non-magnetic
  - FM – ferromagnetic
  - AFM – antiferromagnetic
  - other
- Different magnetic states are compared via the **magnetic stabilization energy**

$$\Delta E_{\mathrm{mag}} = (E_{\mathrm{tot}} - E_{\mathrm{tot}}^{\mathrm{GS}})/N_{\mathrm{MA}},$$

System	State	ΔE_{mag} (meV/at)	$T_c^{\max}$ (K)	T_c (K)
Fe	NM FM	395 0	4585	1043
NiO	NM FM AFM	244 237 0	2745	525

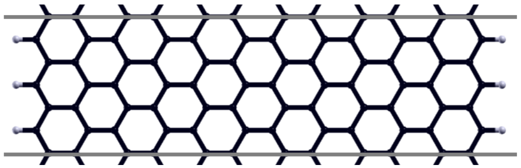
- upper bound for the **critical temperature** $T_c^{\max}$ is

$$\Delta E_{\mathrm{mag}}^{\mathrm{GS+1}} = \mathrm{k} T_c^{\max}$$

1. Stability of graphene edge magnetism

Ideal zigzag graphene nanoribbons

- let's assume that ideal zigzag graphene nanoribbons (ZGNRs) can be made

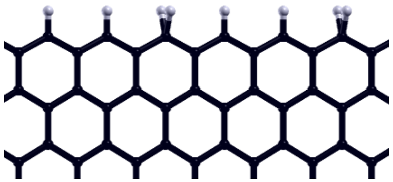


System	State	ΔE_{mag} (meV/at)	T_c^{max} (K)
10-ZGNR+H	NM FM AFM	27 6 0	70
12-ZGNR+H	NM FM AFM	29 4 0	46

- No stable magnetism at room temperature
  → no spintronics applications of edge magnetism

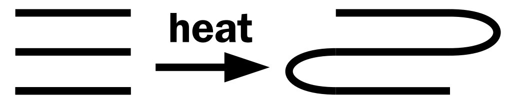
Summary

1. magnetic **edge states** are unlikely to exist



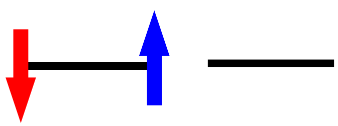
edge passivation

edge reconstruction



edge closure

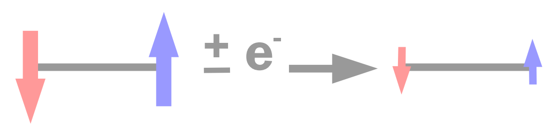
2. Even if they exist, the **edge magnetism** is not stable at room temperature



T = 0 K T = 300 K

not stable at room temperature

edge defects



charge doping

J. Kunstmann, C. Özdogan, A. Quandt, H. Fehske, Phys. Rev. B **83**, 045414 (2011).

Thanks for your attention

DFG

support is appreciated
(SPP 1459)

»Wissen schafft Brücken.«