Graphene edge magnetism for spintronics applications: Dream or Reality?

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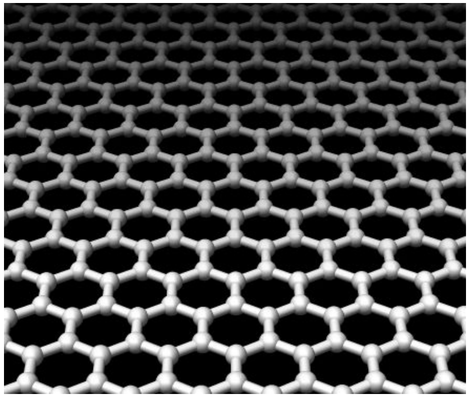
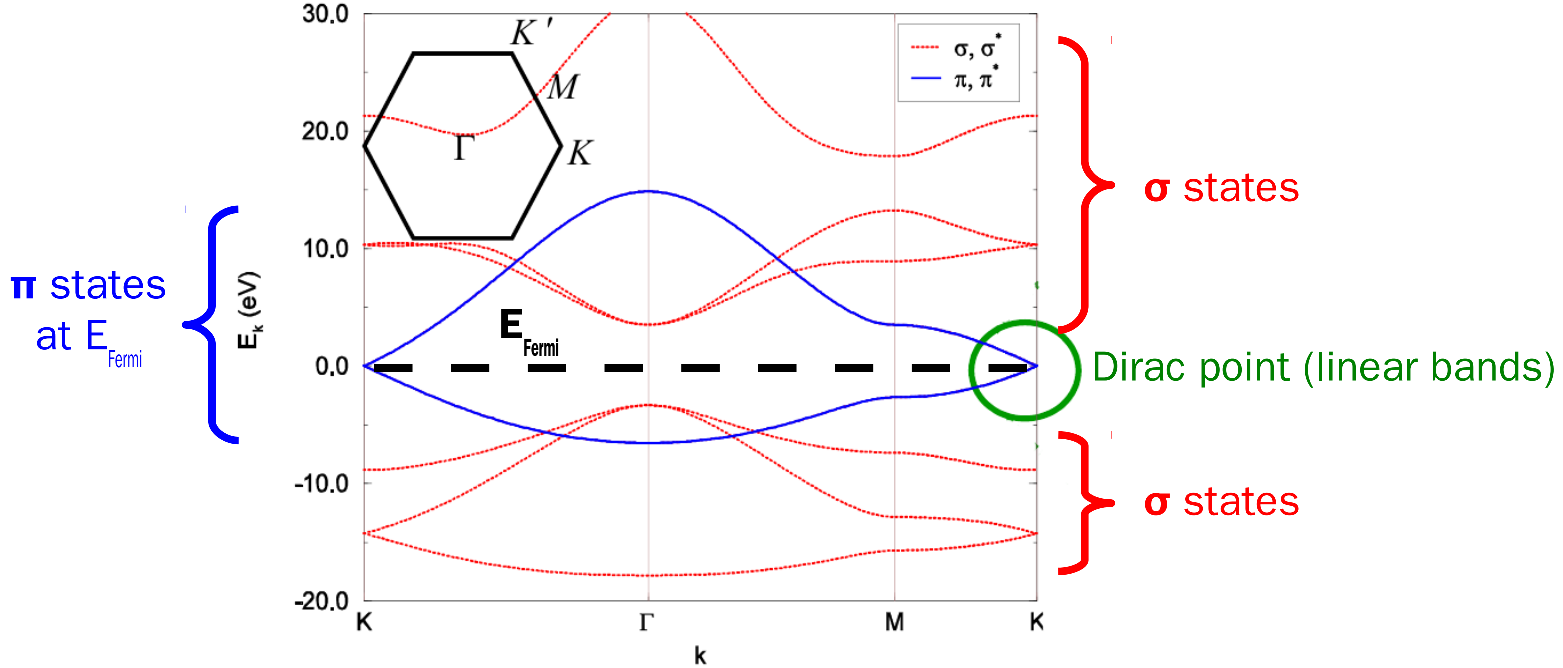
Introduction

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

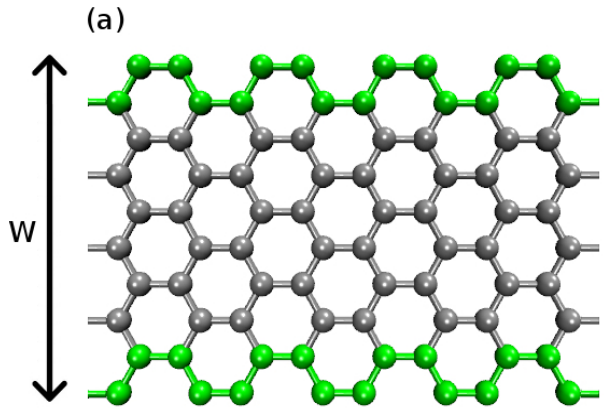


Introduction

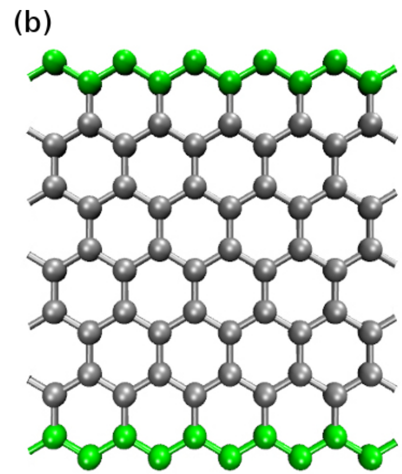
Graphene nanoribbons (GNRs)

- 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)



zigzag GNR (ZGNR)



- semiconducting

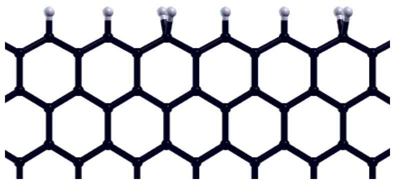
- System has magnetic **edge states**
- antiferromagnetic semiconductor

?

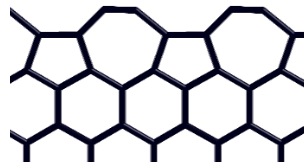
Results

Overview

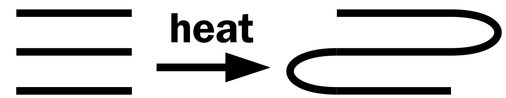
1. magnetic **edge states** are unlikely to exist



edge passivation

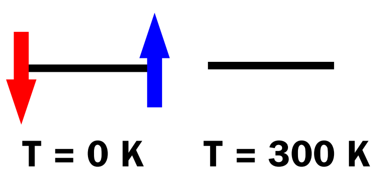


edge reconstruction



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

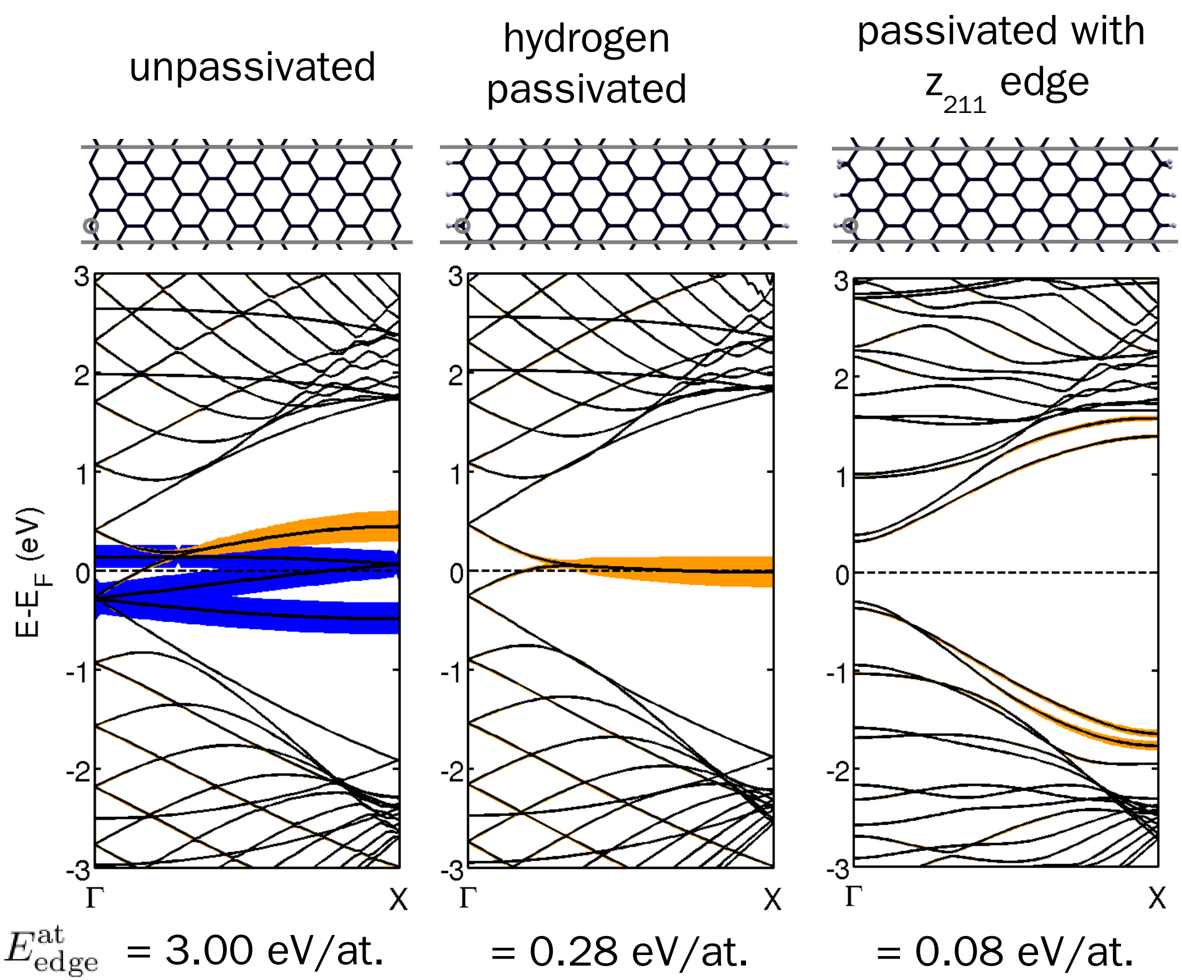
$$\text{graphene} + N_{\text{H}}/2\ \text{H}_2 \longrightarrow \text{ZGNR}$$

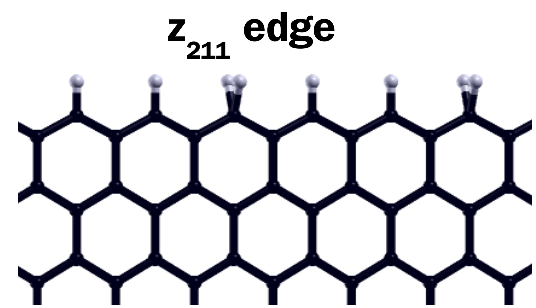
$$E_{\text{edge}}^{\text{at}} = (E_{\text{tot}}^{\text{ZGNR}} - N_{\text{C}} E_{\text{coh}}^{\text{graphene}} - N_{\text{H}} E_{\text{coh}}^{\text{H}_2})/N_{\text{C}}^{\text{edge}}$$

1. Stability of graphene edge states

1. Stability of graphene edge states

Edge passivation





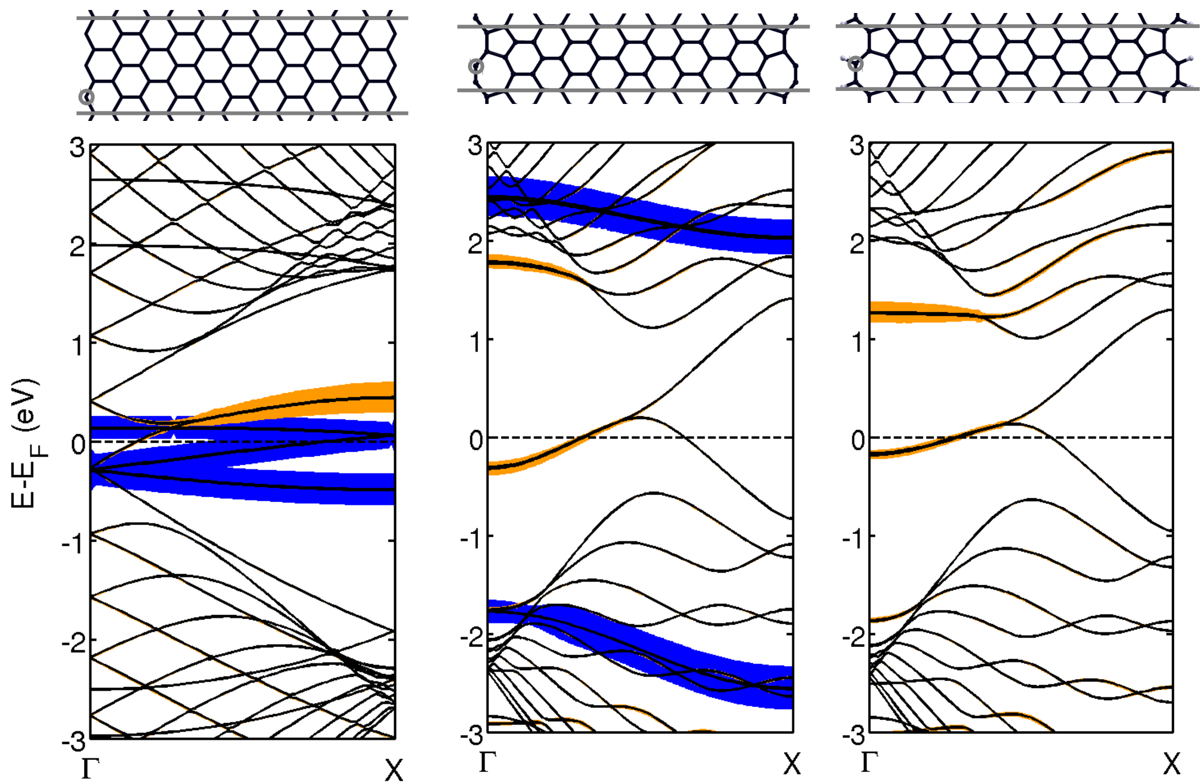
Wassmann, PRL **101**, 096402 (2008).

- 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^{at}_{edge} = 3.00 eV/at. = 2.39 eV/at. = 0.87 eV/at.

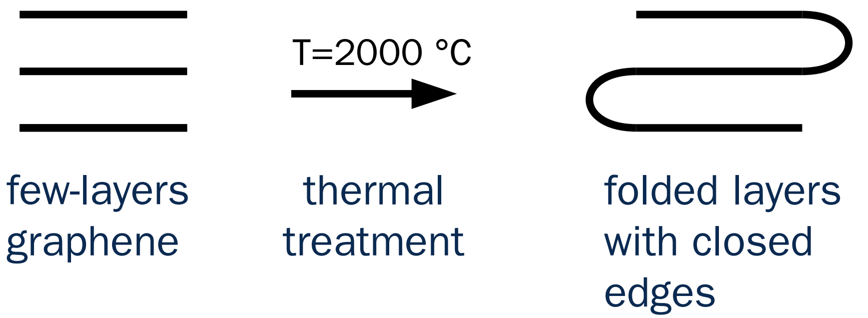
5-7 edge reconstruction

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

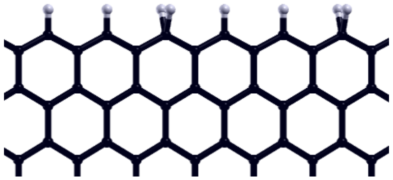
Edge closure



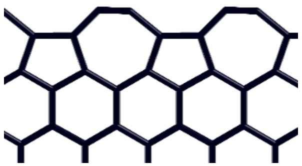
- no edges / edge states / edge magnetism
- experimentally observed
  Liu, Suenaga, Harris, Iijima, PRL **102**, 015501 (2009).

1. Stability of graphene edge states

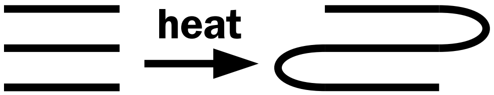
Resume



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	395	4585	1043
	FM	0		
NiO	NM	244	2745	525
	FM	237		
	AFM	0		

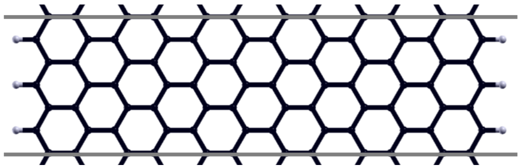
- upper bound for the **critical temperature** $T_c^{\max}$ is

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

1. Stability of graphene edge magnetism

Ideal zigzag graphene nanoribbons

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

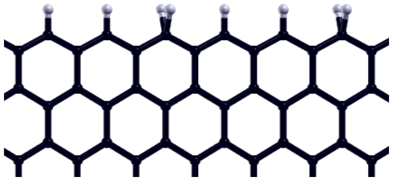


System	State	ΔE_{mag} (meV/at)	T_c^{max} (K)
10-ZGNR+H	NM	27	**70**
	FM	6	
	AFM	0	
12-ZGNR+H	NM	29	**46**
	FM	4	
	AFM	0	

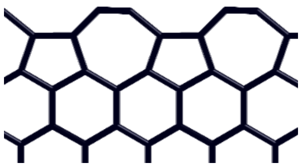
- No stable magnetism at room temperature
  → no spintronics applications of edge magnetism

Summary

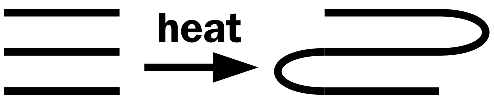
1. magnetic **edge states** are unlikely to exist



edge passivation

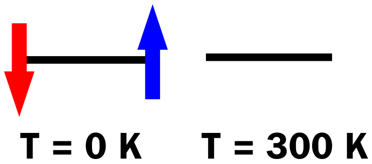


edge reconstruction

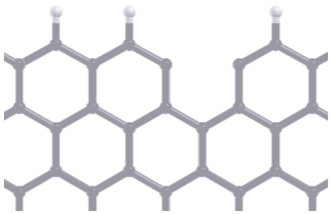


edge closure

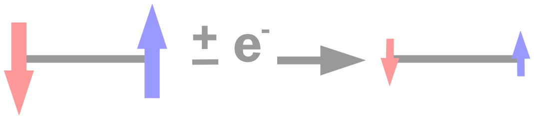
2. Even if they exist, the **edge magnetism** is not stable at room temperature



not stable at
room temperature



edge defects



charge doping

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Thanks for your attention

DFG

support is appreciated
(SPP 1459)

»Wissen schafft Brücken.«