Spin Scattering in Edge-free Graphene Quantum Dots

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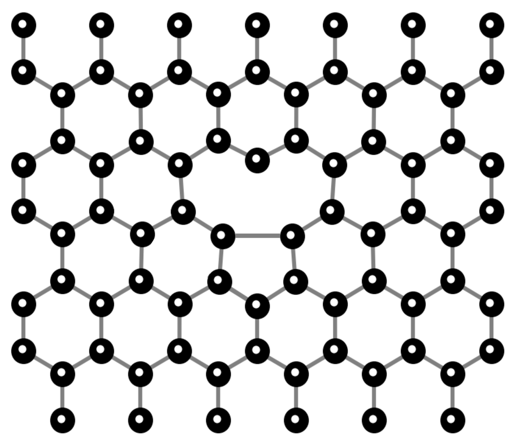
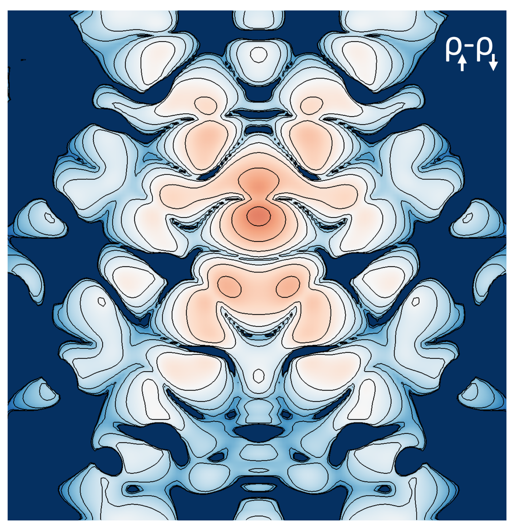
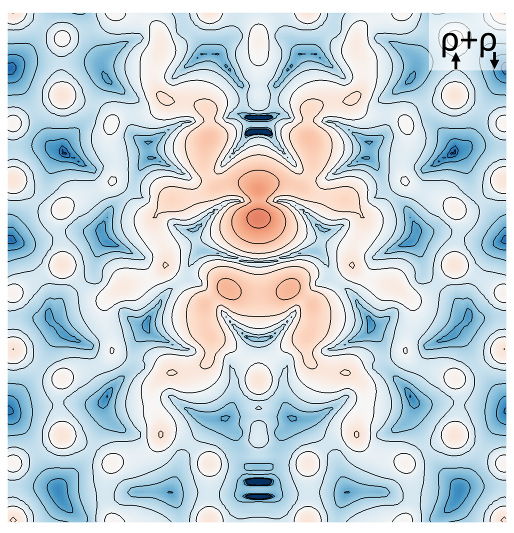
Novel spintronic applications require appropriate host materials. Due to its small spin-orbit, negligible hyper fine interaction and high mobility graphene has the potential to replace current state-of-the-art host materials (GaAs, [1]). However, measurements find spin life times that are up to three orders of magnitude lower than expected, calling into question the current understanding of spin scattering in graphene nano devices. Recent studies show that the formation of magnetic impurities from intrinsic single vacancy defects could resolve this discrepancy. We study the influence of single vacancy defects in large scale tight binding simulations with defect parametrization extracted from densitiy functional theory. Our simulations encompass both multi-defect scattering for electronic transport as well as manipulation of spin states in smoothly confined quantum dots.

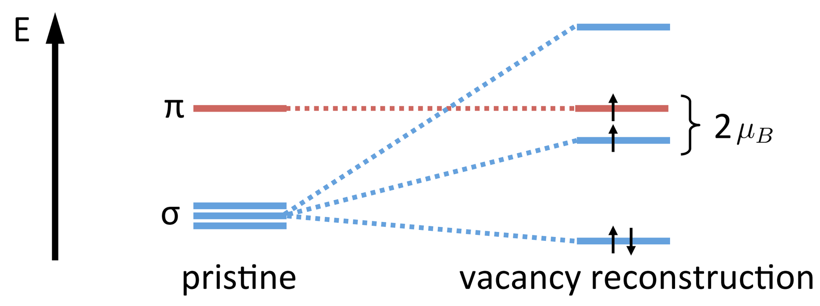
Single Vacancy Defect Parametrization [2,7,8]



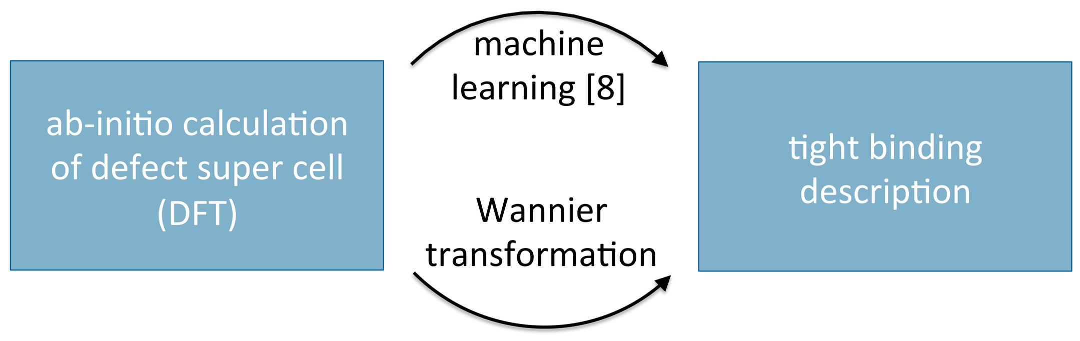


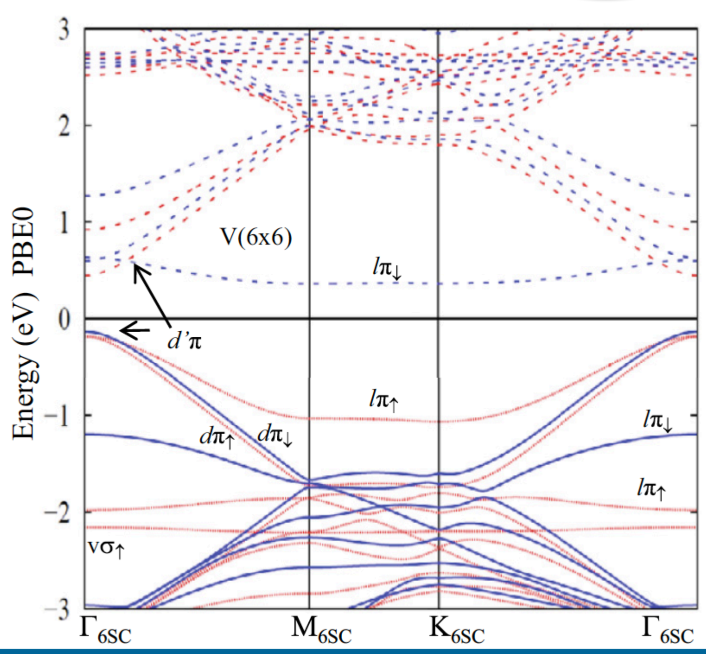


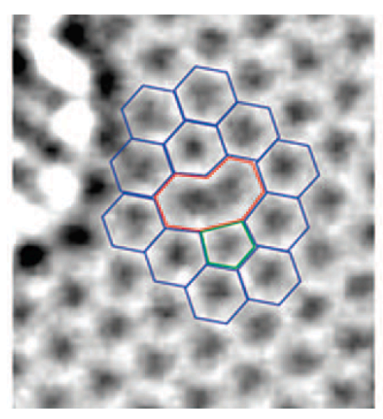
- occurs naturally & can be created via ion bombardment
- single carbon site vacant ⟶ dangling bond introduces a localized magnetic moment [2]



- planar Jahn-Teller distortion (formation energy ~7.5eV) [7]

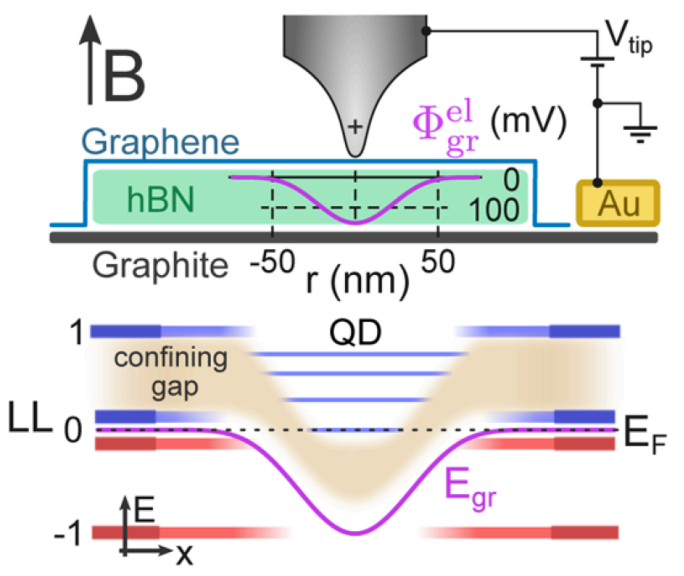


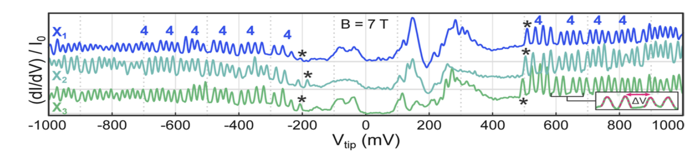


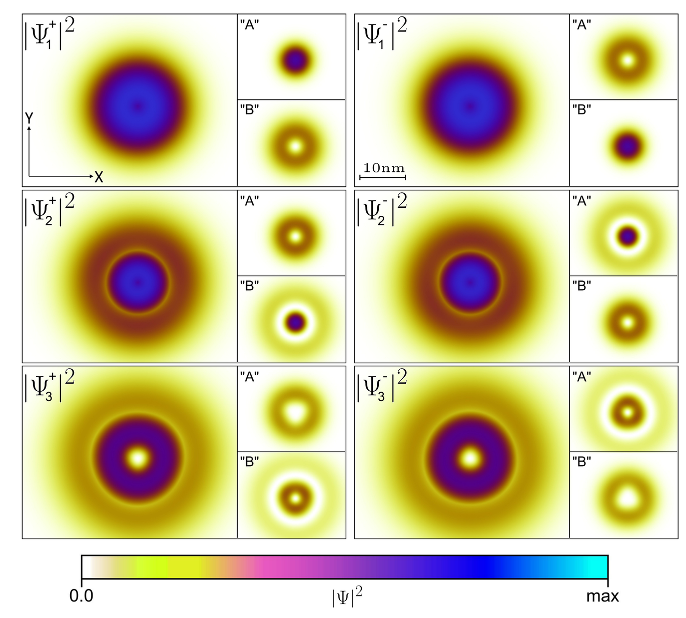


Smoothly Confined GQDs [5,6]

- single layer graphene in homogeneous magnetic field
- scanning tunneling microscopy (STM) tip induces potential dip and localizes state within Landau gaps
- experimentally resolvable charging events [5]



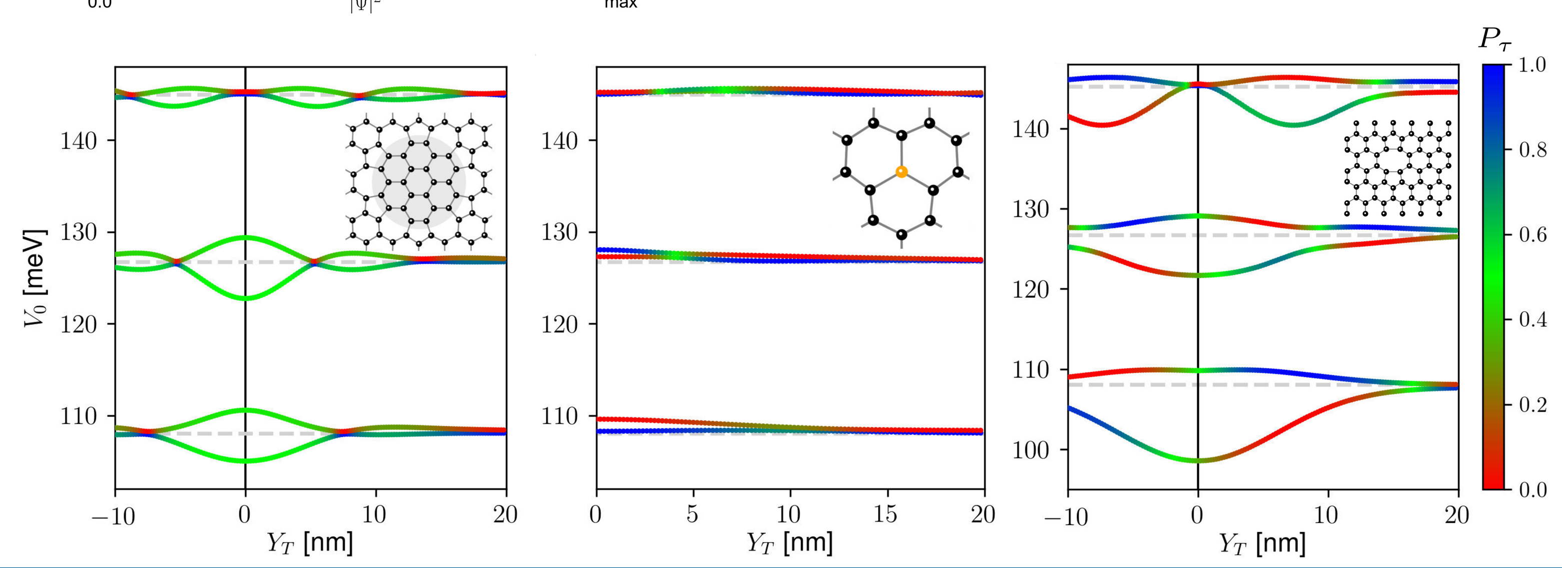




- absence of edge disorder ⟶ intact valley quantum number & well ordered level spectrum

$$|\psi_j^+\rangle = \begin{pmatrix} |\phi_{|j|-1}\rangle \\ |\phi_{|j|}\rangle \end{pmatrix}, \quad |\psi_j^-\rangle = \begin{pmatrix} |\phi_{|j|}\rangle \\ |\phi_{|j|-1}\rangle \end{pmatrix}$$

- controlled breaking of valley DOF through nearby lattice defects [6]
- dynamical change of tip-defect distance allows for controlled state transitions



Spin Transport & Manipulation in Graphene [3,4]

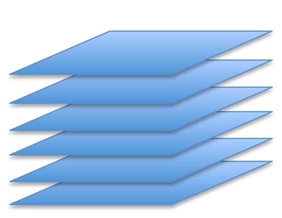
- large-scale electronic transport simulations spanning the spin space of the itinerant electron as well as several local defect spins

$$|\Psi_c\rangle \otimes |\sigma_c\rangle \otimes |\sigma_{D1}\rangle \otimes |\sigma_{D2}\rangle \otimes \ldots$$

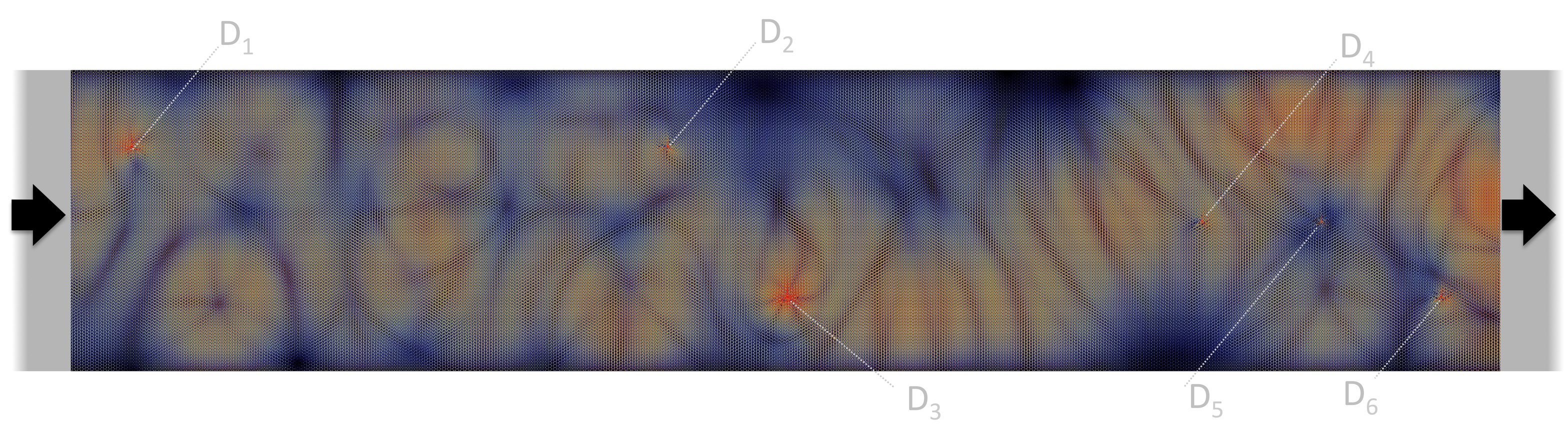
- local spins are indirectly coupled via exchange interaction with the conduction electron

$$V_{CD} \approx J\vec{S}_C \cdot \vec{S}_D$$

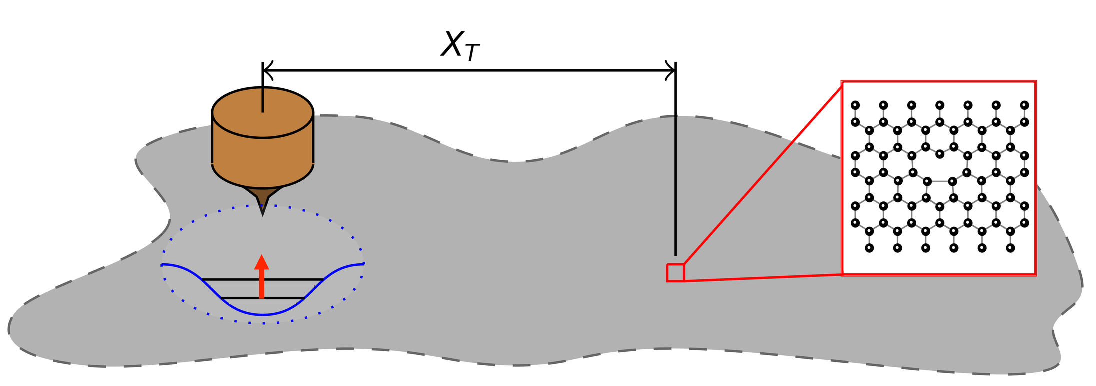
- full spin space in „layered" TB description

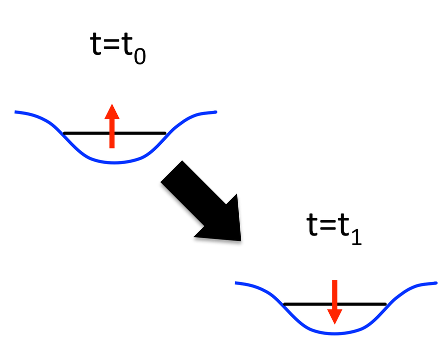


$$\begin{bmatrix} H_{\Uparrow\Uparrow} & & & \\ & H_{\Uparrow\Downarrow} & V_{CD} & \\ & V_{CD} & H_{\Uparrow\Downarrow} & \\ & & & H_{\Downarrow\Uparrow} & V_{CD} \\ & & & V_{CD} & H_{\Downarrow\Uparrow} \\ & & & & & H_{\Downarrow\Downarrow} \end{bmatrix}$$



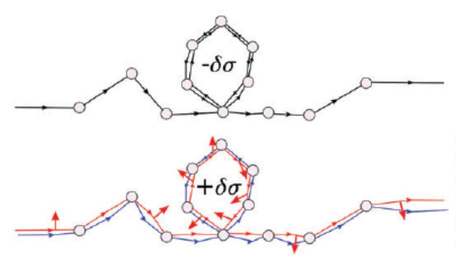
- manipulation of spins confined in GQDs via nearby single vacancies
- quantum mechanical time evolution of dynamically induced GQD
- controlled spin flips?





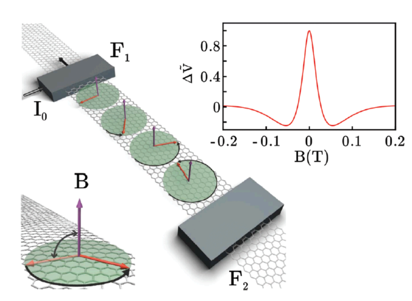
- compare to experimental results for spin relaxation time and length τ_s & λ_s
- extracted from various complementary experimental methods

weak localization / weak anti-localization



... infering time scales of relaxation processes from quantum mechanical conductance corrections due to interference effects in closed scattering paths.

Hanle precession in lateral spin valves



... precession of spin-polarized charge current gives rise to quantifiable dephasing by means of non-local voltage measurements.

References & Collaborators

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[3] Garcia et. al. , Chem. Soc. Rev. **47** 3359 (2018)
[4] Kochan et. al. , PRL **112** 116602 (2014)
[5] Freitag et. al. , Nano Lett. **16**, 5798 (2016)
[6] Schattauer et. al. , Phys. Rev. B **102** 155430 (2020)
[7] Meyer et. al., Nano Lett. **8** 3582 (2018)
[8] Schattauer et. al., (in preparation)

ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

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