SPINTRONICS AT THE INTERFACE

Zeila Zanolli

RWTH Aachen University, Theoretical Solid State Physics, D-52056 Aachen, Germany
and European Theoretical Spectroscopy Facility (ETSF)

E-mail: zanolli@physik.rwth-aachen.de

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show [1] that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and $BaMnO_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones (~300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.
Spin Orbit Coupling calculations reveal that the influence of graphene on the substrate is even more radical and is able to change the direction of the easy axis with respect to the bare $BaMnO_3$ surface. We predict a Rashba-like splitting of the electronic bands near the K point, leading to non-trivial topological insulating properties and Quantum Anomalous Hall conductivity [2].
Going further, we investigate spin dynamics at finite temperature using a Monte Carlo approach with exchange coupling parameters fitted from first principles. We find that graphene strongly affects the magnetic properties of the substrate, well beyond the interface layer, and induces a softening of the Mn magnetization [2].

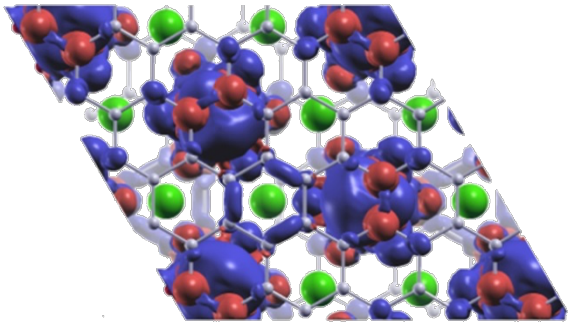

Figure 1: Spin density ($\rho\uparrow - \rho\downarrow$) of the graphene-$BaMnO_3$ interface (top view). Blue and red indicate positive and negative sign isodensities. Spin polarization is induced in the pristine C network from the underlying Mn atoms [from Ref. 1].

[1] Z. Zanolli, Sci. Rep., 6 (2016) 31346
[2] Z. Zanolli, G. Bihlmayer, Ph. Mavropoulos, C. Niu, M. J. Verstraete, S. Blügel, *submitted* 2018

Funding:
Marie-Curie Intra European Fellowship (PIEF-Ga-2011-300036)
Deutsche Forschungsgemeinschaft (ZA 780/3-1).

Computational resources:
PRACE-3IP (FP7 RI-312763, resource Lindgren based in Sweden at KTH),
PRACE DECI-13 (13DECI0197, Archer, UK),
PRACE DECI-14 (14DECI0040, Beskow, SE)
JARA-HPC projects: jara0088, JIAS16, JHPC39 (resource JURECA at FZJ)