Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Spin-orbit coupling in fluorinated graphene[1] SUSANNE IRMER, TOBIAS FRANK, SEBASTIAN PUTZ, MARTIN GMITRA, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — We theoretically study spin-orbit coupling effects of fluorine chemisorbed on graphene. Both dense and dilute limit reveal a giant local enhancement of spin-orbit coupling by a factor of 1000 in the vicinity of the adatom—spin-orbit strength of about 10 meV. We present results of fully converged first-principles calculations and analyze them by a tight-binding Hamiltonian based on symmetry arguments. Our work covers different limits of fluorine concentration from dense to intermediate to dilute coverage. We find that fluorine's native spin-orbit coupling exceeds the effect of the sp^3 distortion of the lattice. Moreover, we identify fluorine as a weak resonant scatterer giving rise to resonant signatures in the band structure off the Dirac point by about 0.3 eV. Our findings are important for studies on relaxation and transport. Details can be found in the following manuscript: http://arxiv.org/abs/1411.0016

[1]This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

Susanne Irmer
University of Regensburg

Date submitted: 11 Nov 2014 Electronic form version 1.4