

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Tight-binding description of spin-orbit coupling in graphene due to adatoms**<sup>1</sup> SUSANNE IRMER, DENIS KOCHAN, KLAUS ZOLLNER, MARTIN GMITRA, TOBIAS FRANK, JAROSLAV FABIAN, University of Regensburg — We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH<sub>3</sub> [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsics, Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models. [1] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013). [2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015). [3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

<sup>1</sup>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: 06 Nov 2015

Electronic form version 1.4