

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms**<sup>1</sup> MARTIN GMITRA, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

<sup>1</sup>This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570

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Date submitted: 09 Nov 2012

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