Spin-orbit coupling enhancement in graphene due to hydrogenation

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Spin-orbit coupling is an essential ingredient for magnetoanisotropies, spin relaxation, as well as for recently emerged topological quantum spin Hall phenomena. The intricate history of spin-orbit coupling in graphene have brought revival investigations of its essentials [1]. It has now been established that spin-orbit coupling of the itinerant electrons in graphene comes from hybridized $2p_z$ and $3d$ orbitals forming π bands [1, 2]. The coupling splits the bands at the K point of about 24 μeV [1]. Our first-principles and tight-binding analyses [3] show that the intrinsic spin-orbit coupling in bilayer, trilayer and multilayers of graphene – all the way to graphite – have the same origin derived from the physics of graphene. When graphene is placed in a transverse external electric field, mixing of the $\sigma - \pi$ states is allowed and bands are further split by the Rashba effect. The calculated splitting is about 10 μeV in field of 1 V/nm [1].

When hydrogen is absorbed on graphene, it covalently bonds to a carbon atom and modifies the trigonal sp^2 structure towards the tetragonal sp^3 one. The $\sigma - \pi$ mixing is responsible for the enhancement of the intrinsic spin-orbit coupling as reported in buckled graphene [1]. In the talk we will present 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 FLEUR code [4]. The covalent bond between the hydrogen and carbon atoms locally deforms the graphene sheet, 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. Based on group theoretical principles we derive effective tight-binding Hamiltonian models and identify dominant contributions to the spin-orbit coupling that comes from breaking of pseudospin inversion symmetry. The calculated spin-orbit coupling induced splittings on the band structure and the emerging spin patterns of the electronic states well agree with first-principles calculations.

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