

Abstract Submitted
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Theory of hydrogen induced giant spin-orbit coupling in graphene¹ MARTIN GMITRA, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — Adatoms seem for now the most perspective way of increasing and controlling spin-orbit coupling in graphene. Hydrogen in particular is a role representative, as it gives both lattice deformation and covalent bonding, both contributing towards sigma-pi hybridization needed for the increase of the spin-orbit coupling around K. To establish the relevant physics of the H induced spin-orbit coupling in graphene, we have performed systematic calculations of hydrogenated graphene. We found that the magnitude of the coupling is of the order of meVs, exactly what is needed to explain the experimental data on spin relaxation. Doing both first-principles calculations and tight-binding modeling we calculate the spin-orbit splittings and introduce an effective hopping model that can be used in realistic investigations.

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