Local tight-binding description of magnetism and spin-orbit coupling in defective graphene

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Similarities between the behavior of itinerant electrons in graphene and massless relativistic particles have caused much excitement not only about the opportunity to observe new physical phenomena in a solid-state material but also about the realization of brand-new applications. Spintronics is one of those promising field of applications. Ultra-high electrons mobilities and long spin lifetimes enable efficient spin propagation over unprecedented length scales [1-4].

On the one hand, low-energy carriers in graphene have weak spin-orbit coupling (SOC) as is desirable for long spin lifetimes. The energy gap arising from the intrinsic SOC is estimated to be about 25 μeV only, and spin relaxation times of several microsecond are predicted [5,6]. On the other hand, despite recent advances, experiments consistently report shorter spin lifetimes [1-3,7,8]. The elucidation of these discrepancies is very important in order to enable future applications of graphene for spin processing and it would contribute to the elaboration of a unified picture of spin relaxation in graphene based nanostructures.

Potential culprits for the enhanced spin relaxation are adatoms, structural defects such as ripples or sustrate induced effects. For example, it has been demonstrated that adatoms locally increase the spin-orbit coupling owing to the sp^3 character of the chemical bond [9,10]. In this work, we focus on the local description of the spin-orbit structure of defective graphene in the dilute limit. At first, the magnetic structure and spin-orbit coupling induced by hydrogen adatoms and monovacancies are investigated using first-principles techniques. Then, an optimal representation of the low-energy eigenstates in terms of localized support functions is derived. The respective quality of various tight-binding representations is assessed by comparison with the first-principles results. We believe that the quality of the model Hamiltonian is crucial for a reliable description of spin transport and relaxation in mesoscopic systems. Hence, the extraction of the tight-binding parameters is discussed in some details.

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