Magnetism and spin-orbit coupling in defective graphene from first-principles

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Abstract

Owing to the weak spin-orbit coupling, vanishing hyperfine interaction and ultra-high mobilities of its low-energy carriers, graphene is a promising material for spin channel applications. However, while theory predicts spin lifetimes of ~1 μs [1,2], experiments consistently report much shorter values [3-7]. 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 unifed picture of spin relaxation in graphene based nanostructures. Potential culprits for the enhanced spin relaxation are adatoms, structural defects such as ripples or substrate induced effects. As an example, it has been recently shown that a small amount of covalently bonded hydrogen atoms is sufficient to increase the spin-orbit interaction of graphene by several orders of magnitude [8,9].

In this work, we investigate the magnetic structure and spin-orbit interaction induced by structural point defects (i.e. vacancies and Stone-Wales) and light adatoms by means of first-principles methods. We first detail the impact of the defects on the spin-orbit coupling strength both in the dense and dilute limits. As some defects such as vacancies and H-adatoms come with local magnetic moments, we then investigate the interplay between spin-orbit and exchange couplings, unravelling a rather large effect not easily explained by phenomenological models. Eventually, the spin-textures for in-plane and out-plane magnetic configurations are computed and the magnetic anisotropy of defective graphene is discussed.

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