Inducing magnetism in graphene in a view of spintronics

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Graphene has emerged as one of the most promising material for developing "beyond CMOS" nanoelectronics [1]. It is very attractive for spin electronics (spintronics) [2] since long spin lifetimes are expected within this material due to its intrinsic weak spin-orbit coupling. Inducing magnetism in graphene, however, remains one of the most challenging problems for its applications to spintronics. Magnetic states in graphene can be induced using magnetic substrates, e.g. transition metals Co and Ni [3]. For instance, interesting perpendicular magnetic anisotropy properties of Co/graphene interfaces have been reported [4]. However, growing on conducting substrates limits graphene applications for electronic devices. Alternative possibilities are to use magnetic insulating material EuO as a substrate [5] or to explore shape induced magnetism in graphene nanomesh structures [6,7] inspired by recent reports on possibility of inducing localized spin polarization and magnetic moments at one-dimensional zigzag edges in graphene nanoribbons [8]. Here we present first principles investigations of both substrate and shape induced magnetism and report promising potential for producing high spin polarization and exchange splitting values [7].

Our calculations were performed using Vienna Ab-Initio Simulation Package (VASP) which is based on density functional theory with generalized gradient approximation for exchange correlation and projector augmented wave based pseudopotentials [9]. All calculations have been performed to ensure the Hellman-Feynman forces acting on carbon atoms to be less than 10-3 eV/Å.

First, magnetic properties in graphene nanomesh structures (GNM) will be presented. For pure GNM, non-spin-polarized states are found stable in armchair-type edges while antiferromagnetic states are found stable for balanced zigzag edge structures. Furthermore, an unbalanced edge structure shows stable ferrimagnetic state giving rise to a net magnetic moment up to 4 uB per 6 x 6 unit cell. We also found the gap opening in the balanced zigzag edge GNMs which may reach up to 0.40 eV. For hydrogen terminated GNM, we found that the ground state strongly depend both on the hole size and shape. For instance, a large net magnetic moment (~2.15μ_B and ~3.62μ_B) is induced in the ground state for GNM with pentagon and trianglular shaped holes shown in Fig. 1(h) and (c), respectively. At the same time, the ground state is found to be paramagnetic for GNM with rhombic and 6-ring shaped holes represented in Fig. 1(f) and (e). Interestingly, the net magnetic moment for GNM with intermediate between trianglular and rhombic shaped holes is equal to 1.04μ_B (Fig. 1(g)) providing that it scales between two end case values of 2.15μ_B and 0μ_B. The magnetization is found to depend strongly on GNM hole size as seen in Fig. 1 and 2. Such behavior can be explained in the framework of Lieb's theorem with a few cases, however, going beyond the latter (Fig. 2(a)). Of note, magnetic configurations get more stable compared to non-magnetic ones as the hole sizes increases as seen in Fig. 2(b). Finally, one of the most interesting results is that the exchange splitting increases as a function of Δ_{AB} and reaches the values of the order of half eV (Fig. 2(a)) which is very promising for room temperature spintronics [7].

The second part of the presentation will be devoted to possibility of inducing spin polarization in graphene by means of magnetic insulator proximity effect. Using the optimized structure of graphene on EuO, we calculated the local density of states for this system. We found that due to very strong spin polarization of EuO substrate, magnetic properties of graphene are strongly affected. The average spin polarization in graphene layer is found to be about 12%. We will also discuss an impact of magnetic insulator proximity on Dirac point properties.

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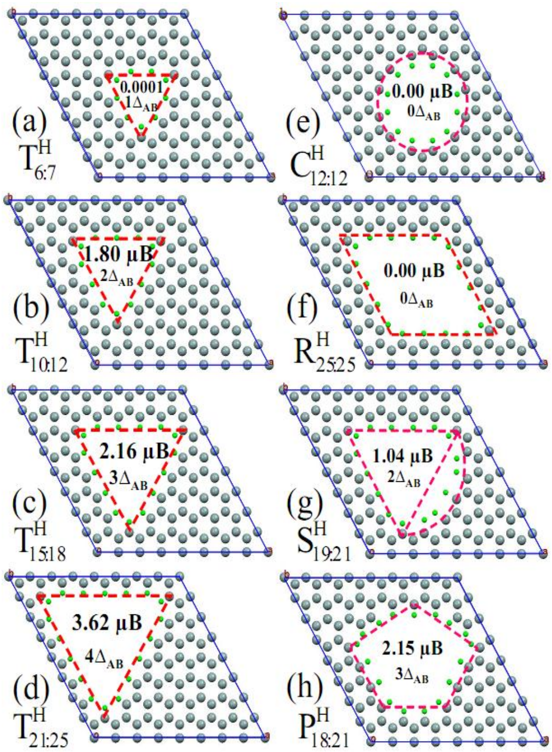

Fig. 1. *(a)-(h) H-passivated GNMs with different shapes. The corresponding net magnetic moments for each structure are also indicated.*

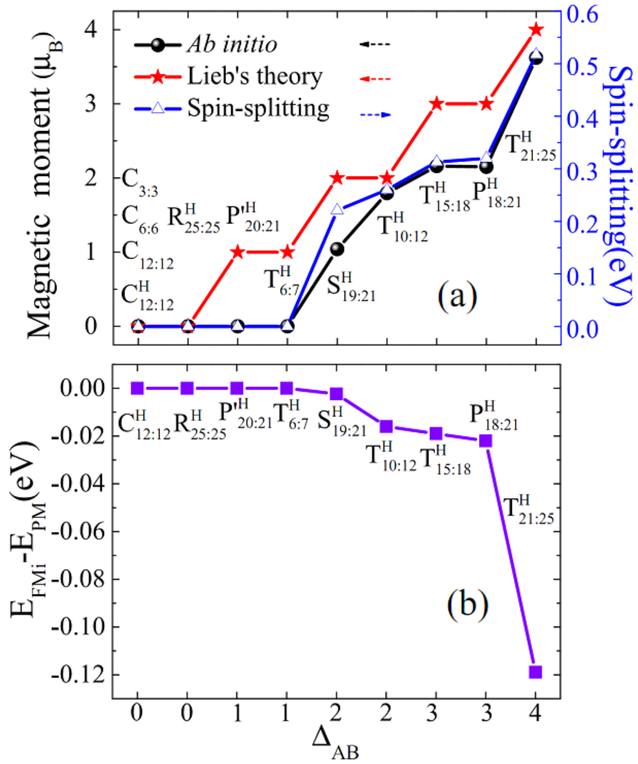

Fig. 2. *(a) Total magnetic moment (μ_B /cell) (left) and spin-splitting (right) as a function of Δ_{AB} for various GNM geometries. The result of the Lieb's theorem prediction is also given for comparison. (b) Energy difference between ferrimagnetic and paramagnetic states.*