Shape induced Magnetic Moment in Graphene Nanomesh from First-Principles

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Unique electronic properties arising from confinement of electrons in two dimensions leading to very large charge mobility make graphene to be extremely promising material for "beyond CMOS" nanoelectronics developments [1]. Furthermore, the inherently weak spin-orbit coupling allows long spin coherence times for carriers [2] making graphene also primary candidate for spin electronics (spintronics) [3]. Recent reports on possibility of inducing localized spin polarization and magnetic moments at one-dimensional zigzag edges in graphene nanoribbons open the way to novel concepts of building nanoscale spintronic devices [4]. Magnetic states in graphene can be also induced by single defects and disorder [5]. On another hand, recent reports on possibility of experimental fabrication of graphene nanomesh (GNM) gave rise to possibility of introducing of large scale patterned defects into graphene [6].

Motivated by recent reports on successful fabrication of GNM, on the one hand, and possibility of edge and defect induced spin polarization, on the other hand, we performed first-principles investigations of electronic and magnetic properties of pure and hydrogen terminated graphene nanomesh. Calculations were performed using Vienna Ab-Initio Simulation Package (VASP) which is based on density functional theory with generalized gradient approximation, for the exchange correlation potential and projector augmented wave based pseudopotentials [7]. Full structural relaxations in shape and volume have been performed to ensure the Hellman-Feynman forces acting on carbon atoms to be less than 10^{-3} eV/Å.

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) is induced in the ground state for GNM with pentagon and trianglular shaped holes shown in Fig. 1(a) and (d), 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(b) 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(c)) providing that it scales between two end case values of 2.15μ_B and 0μ_B, respectively. The magnetization is found to depend strongly on GNM hole size. Such behavior can be explained in the framework of Lieb's theorem [8].

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Figures

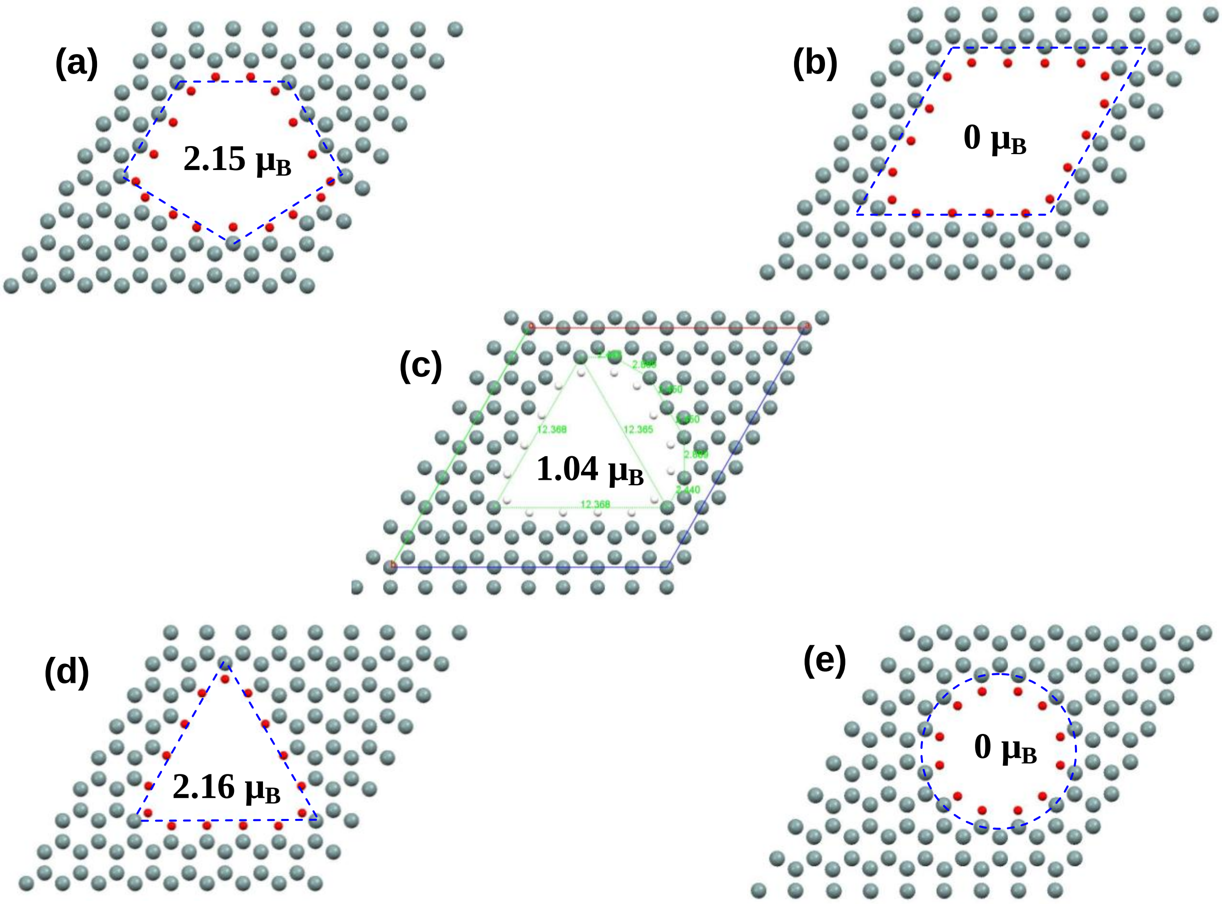

Fig.1. Total magnetic moment in the ground state for geometries for (a) pentagon, (b) rhombic, (c) triangle-to-rhomb intermediate, (d) triangle and (e) 3-ring H-terminated GNMs.