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Effects of shape and edge-passivation on magnetic moments in graphene nanomesh by first-principles investigation HONGXIN YANG, MAIRBEK CHSHIEV, SPINTEC, UMR-8191, CEA-INAC/CNRS/UJF-Grenoble 1/Grenoble-INP, Grenoble, France, SPINTEC TEAM — First-principles calculations of electronic and magnetic properties of pure and H-terminated graphene nanomesh (GNM) are presented. We found stable antiferromagnetic and nonmagnetic ground state for GNM with balanced zigzag and armchair-type edge structures, respectively. At the same time, a band gap opening in the balanced zigzag edge GNMs which can reach up to 0.40 eV is also found. Interestingly, GNM with unbalanced edge structure shows stable ferrimagnetic state giving rise to a net moment up to 4 Bohr magnetons per unit cell, and the exchange energy between ferrimagnetic state and paramagnetic state is larger than 1 eV per unit cell providing potential for high Curie temperature in this material. Furthermore, we found that the ground states for H-terminated GNM strongly depend on the hole symmetry: large spin polarization ground state is found for GNMs with triangle and pentagon hole shapes, while for GNMs with parallelogram and hexagon shaped holes the ground states are paramagnetic. Finally, we found that the magnetization of the GNM structure is strongly affected by the hole size: the larger hole size attains large moments, while small one may even kill all the moments.

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