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Correlated magnetic states in domain and grain boundaries in graphene[1] RICARDO W. NUNES, SIMONE S. ALEXANDRE, U. F. Minas Gerais - Brazil, ALINE D. LUCIO, U. F. Lavras - Brazil, ANTONIO H. CASTRO NETO, Graphene Research Centre and Physics Dept. National Univ. Singapore and Physics Dept. Boston Univ. — Ab initio calculations indicate that while the electronic states introduced by grain boundaries in graphene are only partially confined to the defect core, a domain boundary introduces states near the Fermi level that are very strongly confined to the core of the defect, and that display a ferromagnetic ground state. The domain boundary is fully immersed within the graphene matrix, hence this magnetic state is protected from reconstruction effects that have hampered experimental detection in the case of ribbon edge states. Furthermore, our calculations suggest that charge transfer between one-dimensional extended defects and the bulk in graphene is short ranged for both grain and domain boundaries. http://arxiv.org/abs/1109.6923

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