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Spin-Strain Phase Diagram of Defective Graphene

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Graphene can sustain elastic deformations as large as 20 %, and it is typically under a strain of several percent when deposited on surfaces [1]. However, there are not many experimental conditions under which layers of graphene remain strictly planar. Strong rippling of this kind can be induced by adsorbates [2] and defects [3] such as that recently discovered for OH impurities [4]. Understanding the interaction between defect-induced deformations and ripples is one of the main challenges now faced in the study of the electronic structure of graphene. By theoretical calculations, it has been shown that substitutional doping [5] and the presence of defects [6] in graphene, and in graphitic materials in general, produce magnetism that is of interest in the potential use of these materials in spintronics. In experiments, the irradiation [6] and ion bombardment [7] of carbon-based materials create vacancies which indeed are linked with magnetic signals. The vacancies [8] and edges [9] present in graphene layers have been the focus of detailed theoretical studies. Although there have been both studies of the changes in the electronic structure induced by rippling and studies of defects in graphene, to our knowledge there have been no studies of the magnetism of rippled graphene. Such a study is of particular interest when considered alongside the effect of strain on the structural and electronic properties of graphene.

Using calculations on defective graphene from first principles, we herein consider the dependence of the properties of the monovacancy of graphene under isotropic strain, with a particular focus on spin moments [10]. At zero strain, the vacancy shows a spin moment of 1.5 Bohr magnetons that increases to 2 Bohr magnetons when the graphene is in tension. The changes are more dramatic under compression, in that the vacancy becomes non-magnetic when graphene is compressed more than 2 %. This transition is linked to changes in the atomic structure that occurs around vacancies, and is associated with the formation of ripples. For compressions slightly greater than 3 %, this rippling leads to the formation of a heavily reconstructed vacancy structure that consists of two deformed hexagons and pentagons. Our results suggest that any defect-induced magnetism that occurs in graphene can be controlled by applying a strain, or some other mechanical deformations.

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Figures

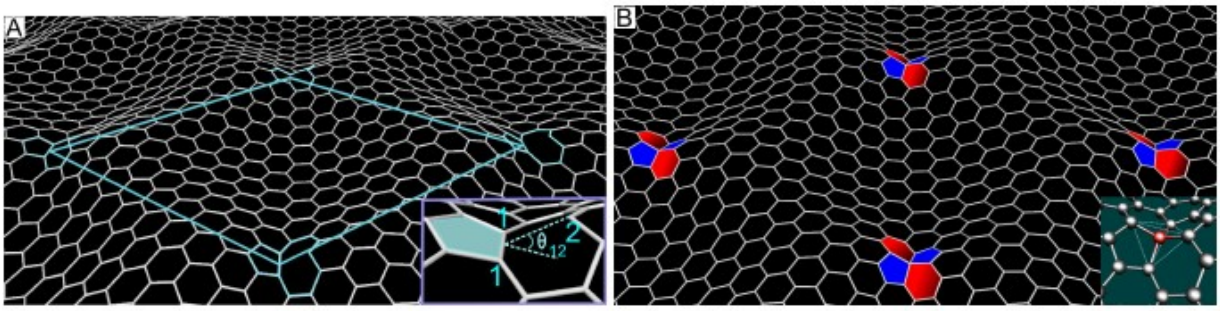

Figure caption: (A) Graphene with vacancies under an isotropic compression of 1.2%. As an example we use the 10x10 unit cell (highlighted). The inset shows the geometry of the vacancies and the atomic labels. The local bending at the vacancies is described by the angle theta between the pentagon and the plane defined by three C atoms around the vacancy, i.e. two equivalent atoms labeled 1 and a third atom labeled 2. Note the rippling of graphene sheets with vacancies at the saddle points. (B) A different vacancy structure for a compression slightly under 3%. It has two distorted hexagons and pentagons, while the central C atom shows strong sp_3 hybridization.