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Interplay of Defects, Magnetism, Ripples and Strain in Graphene[1] ELTON J.G. SANTOS, Department of Physics and School of Enginnering and Applied Sciences, Harvard University. 17 Oxford Street, Cambridge 02138, MA, ANDRES AYUELA, DANIEL SANCHEZ-PORTAL, Centro de Fisica de Materiales MFC, CSIC-UPV/EHU and Donostia International Physics Center. Paseo Manuel de Lardizabal 4/5, San Sebastian, 20018,Spain — We present a comprehensive study based on first-principles calculations about the interplay of four important ingredients on the electronic structure of graphene: defects + magnetism + ripples + strain. So far they have not been taken into account simultaneously in a set of ab initio calculations. Furthermore, we focus on the strain dependence of the properties of carbon monovacancies, with special attention to magnetic spin moments. We demonstrated that such defects show a very rich structural and spin phase-diagram with many spin solutions as function of strain. At zero strain the vacancy shows a spin moment of 1.5 Bohrs that increases up to 2 Bohrs with stretching. Changes are more dramatic under compression: the vacancy becomes non-magnetic under a compression larger than 2%. This transition is linked to the structural modifications associated with the formation of ripples in the graphene layer. Our results suggest that such interplay could have important implications for the design of future spintronics devices based on graphene derivatives, as for example a spin-strain switch based on vacancies.

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