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Electronic and Structural Properties of Vacancies and Hydrogen Adsorbates on Trilayer Graphene MARCOS MENEZES, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro — Using ab initio calculations, we study the electronic and structural properties of vacancies and hydrogen adsorbates on trilayer graphene. Those defects are found to share similar low-energy electronic features, since they both remove a p_z electron from the honeycomb lattice and induce a defect level near the Fermi energy. However, a vacancy also leaves unpaired σ electrons on the lattice, which lead to important structural differences and also contribute to magnetism. We explore both ABA and ABC stackings and compare properties such as formation energies, magnetic moments, spin density and the local density of states (LDOS) of the defect levels. These properties show a strong sensitivity to the layer in which the defect is placed and smaller sensitivities to sublattice placing and stacking type. Finally, for the ABC trilayer, we also study how these states behave in the presence of an external electrical field, which opens a tunable gap in the band structure of the non-defective system. The p_z defect states show a strong hybridization with band states as the field increases, with reduction and eventually loss of magnetization, and a non-magnetic, midgap-like state is found when the defect is at the middle layer.

Marcos Menezes
Universidade Federal do Rio de Janeiro

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