

Abstract Submitted  
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**Hyperfine interaction in hydrogenated graphene** NOEL GARCIA, International Iberian Laboratory (INL), MANUEL MELLE, Centro ALGORITMI, Universidade do Minho, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Laboratory (INL) — We study the hyperfine interaction of Hydrogen chemisorbed in graphene nanostructures with a gap in their spectrum, such as islands and ribbons. Chemisorption of Hydrogen on graphene results in a bound in-gap state that hosts a single electron localized around the adatom. Using both density functional theory and a four-orbital tight-binding model we study the hyperfine interaction between the hydrogen nuclear spin and the conduction electrons in graphene. We find that the strength of the hyperfine interaction decreases for larger nanostructures for which the energy gap is smaller. We then compare the results of the hyperfine interaction for large nanostructures with those of graphene 2D crystal with a periodic arrangement of chemisorbed Hydrogen atoms, obtaining very similar results. The magnitude of the hyperfine interaction is about 150 MHz, in line with that of Si:P. We acknowledge financial support by Marie-Curie-ITN 607904-SPINOGRAPH.

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