Hyperfine interaction in hydrogenated graphene

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Abstract
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 mainly in the first neighbours around the adatom[1]. 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 as the energy gap gets is smaller. We then compare the results of the hyperfine interaction for large nanostructures, obtaining very similar results. The magnitude of the hyperfine interaction is about 150 MHz, in line with that of Si:P[2,3].
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References
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Figures