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Title: A DFT study of Cu nanoparticles adsorbed on defective graphene

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Madrid, 18 January 2017

Highlights

- 1- We have found that Cu-nanoparticles supported on graphene may be a promising electrode material for borohydride fuel cell.
- 2- We show that Cu_n/graphene interaction is rather local and size independent.

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3- We show that the bigger Cu-nanoparticles can be strongly anchored to defects in graphene, while keeping their gas-phase properties.

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