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Some Relaxed Equilibrium Configurations for a Few Hydrogen Atoms Inside a Unit Graphene Cell of Variable Volume JUAN SALVADOR ARELLANO, Fisica Atomica y Molecular Aplicada, UAM-A, Mexico, D.F. — A set of hydrogen atoms (1 to 9) are considered to be inside a graphene cell with parameters a = 4.6117 and c = 5 or 10 a.u. The carbon coordinates are frozen, but hydrogen atoms are relaxed to find favorable configurations with local minimal energy. The fhi98md-LDA code has been used to do the calculations. For some sets of hydrogen atoms it has been obtained two possible configurations. The configurations are analyzed with the DOE (USA Department of Energy) criteria, respect to the characteristics that a material must meet to be considered as a good candidate to store hydrogen. Some of these criteria, for example the gravimetric density and the hydrogen volumetric concentration are discussed in particular. Higher values than 6.5 weight % and 65 kg/m^3, of stored hydrogen required by the DOE are obtained for some of the studied graphene cells.

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