

# Decoration of Graphene with metals atoms for hydrogen storage

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Hydrogen storage is important in many applications such as the development of hydrogen fuel-cell powered vehicles.[1,2,3] One of the main challenges in developing this technology is a compact, safe, and affordable storage system. A desirable system is capable of storing hydrogen with high gravimetric and volumetric densities at near room temperature and ambient pressure.[4,5,6] Recently, carbon nanomaterials with high specific area have been widely studied for hydrogen storage.

However, for carbon in any form, the interaction with hydrogen is through weak van der Waals forces with low binding energies for storage at ambient conditions.[7,8,9] Many studies have been devoted to functionalizing the surface of carbon nanostructures with transition metals to improve the binding energy. Due to the high cohesive energy, transition metals tend to cluster on the surface of the carbon nanostructures and it is difficult to achieve uniformly-coated monolayers of transition metal atoms experimentally.

The binding energies of hydrogen molecules on a AGNR (armchair graphene nanoribbons) Oxygen passivated and decorated with Ca or Mg or Ti atoms were explored using density functional theory simulations based on generalized gradient approximation method. Calcium is considered as a decorating metal superior to transition metals due to its small cohesive energy and the capability of holding multiple hydrogen atoms. Up to four hydrogen molecules have been attached to Ca/Mg/Ti atoms. The binding energy of the hydrogen have been observed to be approx.  $-0.17\text{eV}/\text{H}_2$ . An increase of the adsorption energy by a factor of more than three from approx.  $0.17\text{eV}/\text{H}_2$  vs  $0.05\text{eV}/\text{H}_2$  for “naked” nanoribbons have been observed. This could be a possible route for a 10wt.% hydrogen storage capacity.

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