# Addition of titanium as a potential catalyst for a high-capacity hydrogen storage medium (abstract only)



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# Addition of titanium as a potential catalyst for a high-capacity hydrogen storage medium

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**Abstract**

In recent years there has been increased interest in the characterization of titanium as a catalyst for high-capacity hydrogen storage materials. A first-principles study (Yildirim and Ciraci 2005 *Phys. Rev. Lett.* **94** 175501) demonstrated that a single Ti atom coated on a single-walled nanotube (SWNT) binds up to four hydrogen molecules. The bonding was claimed to be an 'unusual combination of chemisorption and physisorption'.

We report an *ab initio* study by means of the ADF program, which provides a complete insight into the donation/back-donation mechanism characterizing the bond between the Ti atom and the four $H_2$ molecules, and a full understanding of the catalytic role played by the Ti atom.

In addition, we found that the same amount of adsorbed hydrogen can be stored using benzene support for Ti in place of the SWNT, due to the dominant local contribution of the hexagonal carbon ring surrounding the Ti atom. The benzene–Ti–$H_2$ bonding is discussed on the basis of molecular orbital interaction schemes as provided by ADF.

This result advances our insight into the role of titanium as a catalyst and suggests new routes to better storage through different combinations of supports and catalysts.

 