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A.S. Shalabi, H.O. Taha, K.A. Soliman, S. Abeld Aal

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Hydrogen storage reactions on Titanium decorated carbon nanocones

Theoretical study

A.S. Shalabi [1], H.O. Taha [2], K.A. Soliman[1], S. Abeld Aal [1]

[1] Department of Chemistry, Faculty of Science, Benha University, Benha, P.O.Box 13518, Egypt.

[2] Department of Physics, Faculty of Education, Ain Shams University, Cairo, Egypt.

Abstract

Hydrogen storage reactions on Ti decorated carbon nanocones (CNC) are investigated by using the state of the art density functional theory calculations. The single Ti atom prefers to bind at the bridge site between two hexagonal rings, and can bind up to 6 hydrogen molecules with average adsorption energies of -1.73, -0.74, -0.57, -0.45, -0.42, and -0.35 eV per hydrogen molecule. No evidence for metal clustering in the ideal circumstances, and the hydrogen storage capacity