

Stoner Impurity Model in Nickel Hydride

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Abstract : The effect of hydrogen adsorption on the magnetic properties of fcc Ni has been calculated using the linear-muffin-tin-orbital formalism and using the local-density approximation for the exchange y correlation. The calculations for the ground state show that the sequential addition of hydrogen atoms is found to monotonically reduce the total magnetic moment of the Ni fcc structure, as a result of changes in the exchange-splitting parameter and in the Fermi energy. In order to physically explain the effect of magnetization reduction as the Hydrogen concentration increases, we propose a Stoner impurity model to describe the influence of H impurity on the magnetic properties of Nickel.

Keywords : electronic structure, magnetic properties, Nickel hydride, stoner model

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