عنوان مقاله:

Comparison of metal additives and Boron atom on MgH۲ absorbing-desorbing characteristics using calculated NQCCs

محل انتشار:

مجله بین المللی ابعاد نانو, دوره 6, شماره 3 (سال: 1394)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

Using ab initio calculations, the hydrogen desorption from Magnesium hydride (MgH۲) was studied. We presented the calculated nuclear quadrupole coupling constants (NQCCs) of hydrogen atom in various systems of MgH۲. The effect of interactions of some metal atoms as well as Boron atom with MgH۲ host matrix; (MgH۲+M) nanostructures (M=Al, Ti, V, Fe, Ni and B); were studied and ۲H-NQCCs were calculated. From results, introduction of B decreased ۲H-NQCC and consequently trend of decrease of charge density in the presence of B was observed. In the other hands introduction of B destabilized initial structure of MgH۲, But in (MgH۲+M) nanostructures(M=Al, Ti, V, Fe and Ni) the ۲H- NQCCs were larger than those of pure MgH۲ and consequently more difficult condition for hydrogen desorption were created. However at sufficiently low B concentration (Mg۱۵BH۳۲); the calculation predicted existence of stable dopant system with greater ۲H-NQCC.The electric field gradient (EFG) at the site of quadrupolar nuclei were .calculated to obtain NQCC parameters at HF/۳-۲۱G level of theory

کلمات کلیدی:

Nuclear quadrupole resonance (NQR), Magnesium hydride (MgH۲), Hydrogen desorption, ab initio calculations, ۲H-NQCC

لینک ثابت مقاله در پایگاه سیویلیکا: