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Hydroxyl group-Calcium complex for hydrogen storage media MANH CUONG NGUYEN, MOON-HYUN CHA, JISOON IHM, Department of Physics and Astronomy, Seoul National University — Using first - principles calculations based on the density functional theory, we study the hydroxyl group-Ca complex for hydrogen storage application. The Ca atom is bound to the hydroxyl group with a binding energy comparable to the cohesive energy of bulk Ca and the Ca atom can bind up to 7H₂ molecules in molecular form, which can give a very high weight percent storage. However, the average binding energy is about 0.1 eV per hydrogen molecule, which is somewhat smaller than the requirement for the room temperature application. This result shows a possibility of organic materials functionalized with hydroxyl group for hydrogen storage media at near ambient conditions. We also show that, in addition to the metal-H₂ hybridization, the polarization of H₂ molecules induced by the ionized Ca atom plays an important role in the binding of H₂ molecules to the Ca atom.

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