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Novel nanostructured materials with binding "pockets" for hydrogen storage media[1] SUNGJONG WOO, YOUNG-KYUN KWON, Dep. of Physics, Univ. of Mass. Lowell — Hydrogen storage issue is one of the key barrier to the effort to substitute the hydrogen with the conventional fossil fuel. Chemisorption using metal hybrides and physisorption using nanostructured carbon-based materials have suffered several serious problems such as low storage capacity, insufficient binding energy and poor releasing process. In order to overcome such issues, we have investigated novel nanostructured materials of low density that bear hydrogen binding "pockets", which can significantly enhance molecular hydrogen binding – physisorption – compared to carbon-based materials. Using numerical simulation based on the density functional theory, the hydrogen-molecule binding-energies of different candidate materials are calculated and optimized. With the obtained binding energies, we develop nanostructures similar to metal-oxide-framework that maximize the hydrogen capacity of the storage. The statistical properties of the structure, which is necessary to understand the process and efficiency of hydrogen release, are studied. In order to enhance the capacity even further, we synthesize the nanostructure with transition metals and the result will be discussed.

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