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Ab-initio study of hydrogen storage of Titanium-decorated organic systems with hydroxyl groups MANH CUONG NGUYEN, JISOON IHM, Department of Physics and Astronomy, Seoul National University — Using first-principles calculation, we study hydrogen storage of Titanium-decorated organic systems with hydroxyl groups, such as propane-1,3-diol. The results show that Ti atom is bound selectively to hydroxyl groups with the binding energy of 3.0 eV. The first hydrogen molecule adsorbed on Ti is dissociated and then Ti can bind three hydrogen molecules in molecular form more with the binding energy suitable for reversible processes (adsorption and desorption) in hydrogen storage at ambient temperature and pressure. Using thermodynamics, the usable number of hydrogen molecules per Ti atom is almost three due to the proper binding energy of the last three hydrogen molecules on Ti. Based on this result, we can design organic systems with hydroxyl groups to store hydrogen with the reduction of the tendency of transition metal clustering. We also explain the mechanism of multi-hydrogen molecules adsorption on Ti by generalizing the Kubas model.

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