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First principles study of hydrogen storage in non-transition metal decorated graphitic materials GYUBONG KIM, Department of Physics, Pohang Univerisity of Science and Technology, NOEJUNG PARK, Department of Applied Physics, Dankuk Univerisity, SEUNG-HOON JHI, Department of Physics, Pohang Univerisity of Science and Technology — Hydrogen has been considered an ideal material that can replace fossil-based fuels as its byproduct is simply water without emitting green house gases. Recently, transition metal (TM)- dispersed porous materials have been suggested as plausible candidates for hydrogen storages that possess optimal hydrogen binding characteristics. A serious problem in this approach is that TM atoms tend to aggregate instead of being atomistically dispersed, which results in the deterioration of hydrogen uptake. Here we study the hydrogen adsorption on non-transition metal (NTM) atoms dispersed on graphene using ab initio methods. We observe that the clustering energy of NTM atoms is much smaller than that of TM atoms, which indicates that NTM can be almost free of clustering on graphene. We also study hydrogen adsorption on those NTM atoms to find comparable storage capacity to that in TM dispersed graphene.

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