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Realizing nanographene activated by a vacancy to solve hydrogen storage problem[1] GAGUS KETUT SUNNARDIANTO, Graduate School of Engineering Science, Osaka University, ISAO MARUYAMA, Faculty of Information Engineering, Fukuoka Institute of Technology, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — We found a triply hydrogenated vacancy (V_{111}) in nanographene reduces an activation barrier of adsorption-desorption process in both ways in an equal manner from the known values for pristine graphene as well as those of other hydrogenated vacancies of graphene. This finding may give a key to overcome existing problems in the hydrogen uptake and release processes in known hydrogen storage materials, e.g. graphene and organic hydrides (OHs) in near ambient operation temperature. In this study, we used DFT-NEB simulation to estimate the barrier height, which is supported by realized real experiments. We consider a nanographene molecule (VANG) which contains V_{111} with armchair structure at the periphery. We found interesting feature in comparable values of energy barriers for both hydrogen uptake and release, where hydrogenation process is even a little bit endothermic and dehydrogenation is a little but exothermic nature. Thus, this material structure acts as "self-catalytic properties", which has an important role in reducing an energy barrier and as a trapping site for hydrogen serving a new material prevailing other hopeful candidates.

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