Finite-Temperature Dihydrogen Adsorption/Desorption Thermodynamics on Metallo-Porphyrin Incorporated Graphene: Enthalpy versus Vibration

EUI-SUP LEE, SUNG-JAE WOO, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701, MINA YOON, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A., YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701

— Gas adsorption is closely related to a variety of important physicochemical processes and technologies. Especially, hydrogen storage has been attracting much interest due to high energy density and the environmentally-friendly nature. Although a lot of theoretical studies have been carried out, the thermal vibration effect on hydrogen-sorbent interaction is relatively lacking. Here we report the thermodynamics of H\textsubscript{2} molecules adsorbed onto metallo-porphyrin-incorporated graphenes based on first-principles density-functional theory calculations. We found that the slow vibrations induced by weak binding tend to make the system more stable under finite temperature while the fast vibrations induced by strong binding disturb the adsorption. This tendency is expected to be universally found in various gas-sorbent systems.

Eni-Sup Lee
Graduate School of Nanoscience and Technology (WCU),
KAIST, Daejeon 305-701

Date submitted: 27 Nov 2012
Electronic form version 1.4