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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 environmetally-friendly nature. Although a lot of theoretical studies have been carried out, the thermal vibration effect on hydrogen-sorbent interaction is relatively laking. Here we report the thermodynamics of H_2 molecules adsorbed onto metallo-porphyrin-incoporated 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.

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

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