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Computational study on the hydrogen storage in 2-dimentional potential well using K-intercalated graphite oxide JAEHYUN BAE, JISOON IHM, Seoul National University, SEOUL NATIONAL UNIVERSITY TEAM — Here, we present a new hydrogen storage strategy based on a diffusive equilibrium of gas molecules under the external potential we show that density of a gas inside the potential well increases exponentially relative to the ambient gas by the corresponding Boltzmann factor. In this mechanism, hydrogen molecules reside in the delocalized gas form in the potential well, in contrast to the conventional storage localized to specific binding sites. As a realization of the potential well, we choose K-intercalated graphite oxide (KGO) as a scaffold material and show that a relatively uniform potential well arises in between KGO layers. The average potential well depth is much enhanced due to the induced dipole interaction by the electric field generated by K ions and functional groups. The grand canonical Monte-Carlo calculation is employed to obtain the equilibrium hydrogen molecule density in the room temperature and the simulation results are explained by the density enhancement due to the attractive potential inside the KGO layers.

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