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Molecular simulation of hydrogen storage on hydrogen storage in layered graphite oxide: effect of functional group and intercalated ion JAEHYUN BAE, JISOON IHM, Seoul Natl Univ, SEOUL NATIONAL UNIVERSITY TEAM — The adsorption of molecular hydrogen gas into layered graphite oxide (GO) has been studied using both classical grand-canonical Monte-Carlo simulations and ab initio calculations. Different from graphite, interlayer distance of graphite oxide can be varied by controlling the functional group density or introducing alkali metal ion in the synthesis process, this gives new ways of searching for efficient hydrogen storage in porous materials. Our ab initio calculations show that average hydrogen binding energy in the graphite oxide layers is enhanced due to the dipole interaction and small hybridization between hydrogen and functional groups. Introducing alkali metal inside the graphite oxide layers further increases average binding energy by 0.1eV and interlayer distance and hydrogen storage capacity increases close to 3wt% at 300K and 10MPa, similar to recent experiments. In the grand-canonical Monte-Carlo simulations, we use ab initio fitted H2-GO and H2-H2 interaction potential and simulation results are understood by equilibrium of interacting gases in the quasi 2-dimensional potential landscape inside the GO layers. Our computational results suggest the best way of synthesizing the optimal chemical and atomic structure of GO for hydrogen storage medium.

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