Li-Pillared Graphite and Metal Organic Framework as Hydrogen Storage Media

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Using quantum and atomistic simulations, we have investigated possibilities as practical hydrogen storage materials of graphite and Zn-based metal organic framework (MOF). A density-functional theory calculation indicates that a H₂ molecule is able to be stored in the interlayer space of graphite with above 0.6 nm. And it is found that Li-4THF (Tetrahydrofuran) complexes diffuse into interlayer spaces of graphite, and then make ternary Li-THF-GICs (graphite intercalation compounds) having interlayer distance of 11.8 nm. We have calculated H₂ uptake amount in the ternary Li-THF-GIC system through a grand canonical ensemble Monte-Carlo calculation (GCEMC) and studied effect of additional Li intercalation and hydrostatic compression on hydrogen storage of the compound. In the case of the Zn-based MOF, the dominant absorption sites are near metal oxide nodes rather than on aromatic organic linkers, which is good agreement with an experiment. The GCEMC also shows that the longer is the organic linker, the higher is the H₂ uptake capacity. Moreover, the additional adsorption of Li on the organic linker remarkably enhances the H₂ uptake ability of the MOF.

Figure. H₂ uptake behaviors at 77 K and 0.1 bar in (a) MOF-5 and (b) Li-added MOF-5