Direct Regeneration of Nanoconfined $LiAlH_4$ in N-functionalized Scaffold for Reversible Hydrogen Storage

조용준, Sichi Li[1], Vitalie Stavila[2], Brandon C. Wood[1], 조은선†
KAIST; [1]Material Science Division, Lawrence Livermore National Laboratory; [2]Sandia National Laboratories
(escho@kaist.ac.kr†)

$LiAlH_4$ has garnered considerable interests as a high capacity hydrogen storage material. In spite of this advantage, the inferior reversibility of $LiAlH_4$ severely hinders from taking full advantage of such high capacity. The direct regeneration of $LiAlH_4$ under pressurized hydrogen without the use of solvents has rarely been done. Here, we prepared nanoconfined $LiAlH_4$ in N-functionalized/non-functionalized mesoporous carbon scaffold via the solvent infiltration for sustainable high-performance hydrogen storage. The change of hydrogen desorption properties is studied for the nanoconfined $LiAlH_4$ to investigate an effect of carbon scaffold. $LiAlH_4$@NCMK-3 exhibits a reduction of the desorption onset temperature and the partial recovery of $LiAlH_4$. A theoretical study revealed that there is a strong Li-N interaction induced by the N-functionalities, offering the thermodynamic tuning of the nanoconfined $LiAlH_4$ system. This suggests that metastable hydrides, which have not been considered as candidates for a practical system, could also be a viable alternative for a sustainable hydrogen storage platform.