A Computational Analysis of Dehydrogenation from Organic Polycyclics for Hydrogen Storage Applications

신병수, 강정원*
고려대학교
(jwkang@korea.ac.kr*)

Liquid organic hydrogen carriers (LOHC) are potentially interesting hydrogen storage materials because of their reversible hydrogen sorption properties. A variety of different substances has been proposed recently. One of the prototypes for liquid organic hydrides was 9-ethylcarbazole proposed by Air Products. This heterocyclic compound can theoretically take up 6 moles of equivalent hydrogen (5.7 wt%). However, this capacity is much lower than the ultimate targets (7.5 wt%) set by U.S Department Of Energy (DOE) in early 2011. The amine borane based compounds, which was also promising group of potential carriers, satisfy the DOE target but these materials have an unreasonable heat of dehydrogenation. In this study, three carbazole based organic hydrogen carriers are proposed by using computational calculations. These candidates are able to meet the high theoretical hydrogen uptake capacity (> 7 wt%) as well as optimal heat of dehydrogenation (10 - 13 kcal/mol H_2). Reaction pathways are also predicted for the rate of reaction and activation energies were estimated using density functional theory (DFT).