Carbazole-based organic polycyclic compounds for hydrogen storage applications

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Liquid organic hydrogen carriers (LOHCs) such as 9-ethylcarbazole and amine-borane have been proposed as potential hydrogen storage materials. Although these existing LOHCs showed reasonable hydrogen storage properties, there still exist limits to satisfy the Department Of Energy hydrogen storage targets such as reusability, storage capacity and so on. In this study, thermodynamic evaluation and reaction mechanisms have been done to find new types of LOHCs beyond such limits by using molecular dynamics and density functional theory methodologies. It is found that 9-acetylcarbazole is a better candidate for dehydrogenation reaction compared with the group of carbazole candidates in terms of thermodynamic, kinetic standards. The present results can be used in the hydrogen fuel applications for on-board hydrogen storage systems.