A molecular modeling study of 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. These materials can store hydrogen under moderate-to-ambient conditions in liquid state so that the conventional fuel transport facilities can be used without significant modification. Furthermore, hydro/dehydrogenation reactions occur in much more reversible manner than solid type-hydrogen storage materials. Even though some candidate molecules such as 9-ethyl carbazole showed considerable hydrogen storage capacity, still there are some gaps for storage target and reusability suggested by DOE. In this study, thermodynamic evaluation and dehydrogenation reaction mechanism of carbazole-based compounds were performed to find new candidates of LOHCs beyond current storage capacity and reusability by molecular modelling and simulation technique. It was found that 9-acetylcarbazole was a more promising hydrogen storage candidate in terms of thermodynamic standards compared with the group of carbazole derivatives. These results provide an evaluation of the feasibility of proposed hydrogen storage candidate and suggest the direction of molecular design for hydrogen storage materials.