A Computational Analysis of Carbazole Type of Hydrogen Carriers for Liquid Hydrogen Storage

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Liquid organic hydrogen carriers (LOHCs) are potentially interesting hydrogen storage materials because of their reversible hydrogen sorption properties. LOHCs, which are 9-Ethylcarbazole and azaboraine, show low hydrogen capacity and slow dehydrogenation reaction, thus continuos studies for different catalysts based on hydrogen capacity are being conducted extensively. For the commercialization, there still exist limits to be overcome such as solidification at low temperatures, reusability, and etc. In this research, through molecular modeling and simulation as an explorer in the atomistic world, we aim to find and develop new types of LOHCs beyond such limits.