DFT study of carbazole derivatives dehydrogenation on Pd(111) catalyst

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The carbazole derivatives such as 9-ethylcarbazole have been studied as a potential hydrogen storage candidate. It is found that these materials can store hydrogen under moderate-to-ambient conditions in liquid state so that the transportation of hydrogen would be convenient. Besides, the reversibility of hydro/dehydrogenation is much better than the existing solid type of hydrogen storage carriers. However, the major problem for carbazole derivatives which contain ethyl and acetyl group is the cleavage between functional group and carbazole. Therefore, the hydrogen carrier must be regenerated cyclically, which lead to an increase in operational cost. In this work, the Density Functional Theory calculations are performed to understand the dehydrogenation reaction mechanism and decomposition of 9-ethy/acetylcarbazole on Pd(111). The secondary alcohol hydrogenated acetyl group distort the hydrogenated form of 9-acetylcarbazole on Pd(111), which lead to reducing activation energy. With respect to decomposition of functional group, 9-ethylcarbazole is slightly more stable than 9-acetylcarbazole. These results suggest the direction of molecular design for hydrogen storage materials.