First-principles study of a new LOHC and its dehydrogenation mechanism

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Identifying high-performance liquid organic hydrogen carriers (LOHCs) has been extensively studied. Herein, we theoretically designed a liquid organic hydrogen carrier (LOHC), 1-(3-cyclohexylpropyl)-3-ethylcyclohexane, and performed first-principles calculations to understand its dehydrogenation. The detailed dehydrogenation mechanism of this compound was investigated. Using integrated Crystal Orbital Overlap Population (ICOOP), integrated the Crystal Orbital Hamilton Population (ICOHP), and Mulliken population analysis, the dehydrogenation process was deeply understood. N-doping into LOHCs was found to be effective in reducing the dehydrogenation enthalpy. In addition, the analysis of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) was done to predict the chemical reactivity of the designed system. Interestingly, a decrease in the HOMO-LUMO energy gap was found by releasing hydrogen from LOHC.