DFT Insight into the Design of LOHC Compounds

Bhamu Kailash Chandra, Zhou Jingwen, 강성구†
울산대학교
(sgkang@mail.ulsan.ac.kr†)

The dehydrogenation process of a new compound, 1-(3-cyclohexylpropyl)-3-ethylcyclohexane as a liquid organic hydrogen carrier (LOHC) compound was explored using DFT calculations. The vibrational frequency analysis and formation energy calculations were performed to reveal the stability of this compound. Our results showed that this compound was dynamically and chemically stable. To reduce the enthalpy of dehydrogenation, different substitutions, such as N, Cl, and Br were introduced to the compound. Among them, N-doping was found to be useful for reducing the dehydrogenation enthalpy. Using mulliken population analysis, the role of N-doping on dehydrogenation was deeply investigated. Furthermore, to check the chemical reactivity, the energy gap between HOMO and LUMO was also calculated. These results will expand the list of the potential LOHC candidates.

References

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