Toward Development of Novel Liquid-Phase Hydrogen Storage Materials using Reactive Molecular Dynamics Simulation

배성진, 한상수†
KIST
(sangsoo@kist.re.kr†)

Liquid-phase hydrogen storage materials such as 3-methyl-1,2-BN-cyclopentane have an advantage of easy accessibility due to the use of the exist infrastructure. However, the unknown reaction pathway in the liquid-phase reduces the developing speed of proper materials for foreseeable future applications. To elucidate the dehydrogenation reaction pathways in liquid-phase, we developed a $ReaxFF_{CBN}$ for BN-substituted cyclo-hydrocarbon materials. The developed force field was verified by comparing with the molecular quantum calculations for primary molecules and the uni-molecular dehydrogenation reaction pathway. The relative stability of various CBN type molecules were confirmed by the intramolecular B-N bond length calculated by the radial distribution function of between B and N at 300 to 500 K. Using cook-off MD simulations, the macroscopic properties such as monomer decomposition rate or dehydrogenation rate were compared to obtain a valuable information for further modification of the CBN type molecule. We can insist that $ReaxFF_{CBN}$ can describe various kinds of CBN type molecules and be used to simulate an unknown prototype molecule in an effectively short time.