ReaxFF development for 3-methyl-1,2-BN-cyclopentane; Liquid-Phase Hydrogen Storage Material

Sung Jin Pai and Sang Soo Han*
Computational Science Research Center, Korea Institute of Science and Technology (KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Republic of Korea

Hydrogen is a promising energy source due to its cleanness (only H2O as its product) and efficiency (a maximum efficiency near 10% higher than a gasoline internal-combustion engine). However, since hydrogen has a low energy density by volume (9.17 MJ/L vs 34.2 MJ/L of gasoline), there have been many researches to store much hydrogen weight in a small volume for light duty vehicle. In 2011, Liu et al. succeeded in synthesizing a new kind of liquid-phase hydrogen storage material, named 3-methyl-1,2-BN-cyclopentane (CBN). Since then, many derivatives of it with different carbon functional groups have been suggested and the capacity has been increased slightly, but the average energy density was still yet low to apply for the vehicles. In this work, we tried to find optimum criteria for good CBN type materials using ReaxFF molecular dynamics simulation method. To perform this work, we developed a ReaxFF for CBN system, which called ReaxFFCBN, and it was proved that ReaxFFCBN can appropriately mimic the well-known primary reactions of CBN systems. Using ReaxFFCBN MD simulation, we found that as temperature increases, dimer dehydrogenation scheme dominants over monomer scheme. Furthermore, it was discovered that 6-member ring CBNs were better than 5-member rings in efficiency and stability.

E-mail: sangsoo@kist.re.kr