Design of molten metal alloy catalyst for direct pyrolysis of methane using atomistic modeling

차화웅, 함형철†
인하대학교
(ham.hyungchul@inha.ac.kr†)

Hydrogen (H_2) has played a key role as a CO_2-free energy resource for fuel cell application. Presently, commercially available H_2 is produced by steam methane reforming (SMR) process. This technique generates CO_2, which contributes to global warming. One alternative to eliminate CO_2 and also get a high value carbon is the direct pyrolysis of methane (CH_4) as presented in the equation (1).

$$CH_4(g) \rightarrow C(s) + 2H_2(g) \quad \triangle H^\circ = 74 \text{ kJ/mol} \quad (1)$$

Stable molten metal alloy catalysts formed by the dissolution of active metals (e.g., Pt, Ni, Pd) in inactive metals (e.g., In, Ga, Bi) have shown appreciable results for methane decomposition into H_2, where the insoluble carbon floats to the surface and can easily be skimmed off. However, single metal catalysts such as Ni have been deactivated by solid carbon. In the present study, we investigated the activity of Ga-based molten metal alloy catalysts using atomistic modeling; a combination of density functional theory (DFT) and Ab-initio Molecular dynamics (AIMD) simulations. With reference to pure Ga as catalyst, some Ga-X alloy catalysts showed enhanced activities. Specifically, Ga-Ni alloy catalyst, agrees with experimental values.