

Bi-based molten metal alloy catalyst for methane decomposition reaction: a DFT study

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Hydrogen (H_2) is an important chemical resource and could be used as a CO_2 -free energy carrier for many applications such as fuel cell. It is possible to produce hydrogen without CO_2 emission using methane pyrolysis. Methane (CH_4) pyrolysis transforms CH_4 into hydrogen and solid carbon which could be high value carbon.

In the previous study, molten metal alloy catalysts have shown remarkable activity for methane decomposition reaction. Also we have found that some Ga-based bimetallic molten catalysts (such as Ga-Ni) have enhanced activity for methane decomposition reaction compared to pure Ga. In an attempt to expand these results, we have performed Bi-based bimetallic molten catalysts for this reaction. Since Bi is cheaper component than Ga, this could be more efficient solvent. Additionally, some studies reported that higher activity of Bi-based catalyst for methane decomposition reaction. We investigated the activity of Bi-based molten metal alloy catalysts. We have performed a combination of density functional theory (DFT) and quantum-mechanical molecular dynamics (MD) simulation. Our research determine that Bi-Ni (27%) alloy catalyst showed improved activities.