Carbon Dioxide Conversion into Hydrocarbon Fuels on Defective Graphene-Supported Cu Nanoparticles from First Principles

임동희*, 조준호, 신동윤, Jennifer Wilcox[1], 함형철, 남석우
한국과학기술연구원; [1]Stanford University
(limkor@gmail.com*)

Copper has been widely used for CO2 conversion to hydrocarbon fuels; however, its conversion efficiency is yet to prove optimal. To modify the structural and electronic properties of copper for enhancing CO2 conversion, we suggest defective graphene-supported Cu nanoparticles, which demonstrate improved CO2 conversion through a comparison to experimental data. For this, density functional theory (DFT) studies of electrochemical reduction of carbon dioxide (CO2) into hydrocarbon fuels (CH4, CO, and HCOOH) on copper are conducted by using the Perdew, Burke and Ernzerhof (PBE) approximation described by a generalized gradient approximation (GGA). Through these investigations, we not only provide improved understanding of CO2 conversion mechanisms on both Cu and the Cu nanoparticle system, but also explain a key factor for enhanced CO2 conversion. A promising catalytic material for CO2 conversion into hydrocarbon fuels may allow for geometry flexibility upon interaction with a key intermediate of CHO*.