Hydrogen-Bonding-Mediated Enhancement in Nitrogen Electroreduction Reactions on Biomimetic Cu_xS Catalysts

김민철†
한국과학기술연구원 (KIST)
(mckim.sinfire@gmail.com†)

In this presentation, we introduce novel Cu_xS catalysts that show greatly enhanced electrochemical activity for nitrogen reduction reaction (NRR) via hydrogen-bonding between the catalysts and the reaction intermediates, and following a biomimetic NRR pathway. The electrochemical activity of various Cu_xS electrocatalysts is validated with a variety of experimental procedures. We investigate the origin of this unintuitive enhancement in NRR activity using density functional theory (DFT) simulations. Using the computational hydrogen electrode method, we compare the NRR pathway of the most promising catalyst with the reaction pathway on pure metal catalysts. The results reveal that the N-H-S hydrogen bonding immensely stabilizes the NRR intermediates on the Cu_xS surface and also enables a biomimetic NRR pathway which leads to a large drop on limiting potential for NRR. In addition, the N-H-S hydrogen bonding enables multiple pathways for NRR on the Cu_xS surface, resulting in increase of effective active-sites for the NRR, which hasn't been observed in pure-metal catalysts.