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Data-informed Discovery of high-performance cu-ligand catalysts for acetylene hydrochlorination

Abstract:

The development of mercury-free catalysts is essential for the green and sustainable production of the acetylene hydrochlorination process. Inexpensive Cu-based catalysts are promising candidates to replace toxic mercury chloride catalysts. For the development of high-performance Cu-ligand catalysts, it is essential to establish the correlation between catalyst structure and performance and to rationally design catalytic active sites. Here, through different ligand adjustments, we have constructed copper-ligand catalysts with different coordination environments. A volcano-type correlation was found between the reduction potential of Cu2+-Cu+ in the catalysts and the catalytic performance. The C≡C bond length of C2H2 was used as a descriptor within the limits of the reduction potential of Cu2+-Cu+ to screen for efficient ligands in the Cu ligand catalysts. Under the guidance of these two descriptors, a high-performance Cu-MPPO catalyst was successfully developed. The excellent activity and exceptional stability of the Cu-MPPO catalyst validated the established high-performance ligand screening model. Detailed structural characterization and DFT calculations of the designed catalysts were performed to reveal the catalyst structure-activity relationship. The results showed that the addition of MPPO modified the local microenvironment of Cu. The increase in electron density around Cu and Cl atoms led to the enhancement of HCl adsorption and the weakening of C2H2 adsorption, which inhibited carbon deposition. This work provides valuable insights and reference strategies for screening efficient ligands in copper-ligand catalysts.

Biography

Bao Wang is currently pursuing his PhD at the School of Chemical Engineering and Technology, Tianjin University under the supervision of Prof. Jinli Zhang. He received his B.S. (2017) and M.S. degree (2020) from Shihezi University. His research interests are the rational design of nanomaterials and green catalysis applications.