Structure-Activity Relationship of VO_x/TiO_2(001) Catalysts for Mercury Oxidation: A DFT Study

신동재, 한정우†
포항공과대학교
(jwhan@postech.ac.kr†)

Elemental mercury (Hg^0), mostly from coal combustion, poses a critical threat to human beings and ecosystem because it could accumulate in organisms through food chain as well as directly cause several fatal diseases to humans. Thus, many regulations around the world, including Mercury and Air Toxics Standards (MATS) in US, have been strengthened. Catalytic oxidation of Hg^0 into $HgCl_2$ is considered as an economical and practical option to control it, and SCR catalysts such as Titania-supported Vanadia (VO_x/TiO_2) has been proved to also oxidize Hg^0 to Hg^{2+}. Here, we would like to show the relationship between the coordinative environment of V in VO_x/TiO_2 and the catalytic activity to Hg^0 oxidation based on density functional theory (DFT) calculations. We mechanistically estimated the Hg^0 oxidation activity following reported mechanisms, and also investigated the effect of hydroxylation. Finally, we show temperature (T)- and pressure (p)-dependent thermodynamic stabilities of considered models by calculating Gibbs free energy of formation, suggesting (T, p) condition that the high-activity model favors.