Theoretical Study of Methane Oxidation on Pd(111) and Other Metallic Surfaces

유종석†
서울시립대학교
(jsyoo0927@gmail.com†)

DFT and microkinetic modeling (MKM) are used to study CH4 oxidation to CO, CO2, CH2O, and CH3OH on Pd(111). Our energetic analysis indicates that metallic sites are more active than O* sites for C–H activation. Our MKM analysis indicates that metallic sites produce only CO whereas O* sites produce only CH2O. When product pressures are increased, however, CO oxidation becomes dominant producing mostly CO2. We then extend the study to other surfaces utilizing scaling relations in the MKM. We find that many surfaces cannot effectively activate CH4 under mildly oxidizing conditions. Finally, the kinetics of CH4 oxidation to CO, CO2, CH2O, and CH3OH are described as functions of two descriptors, enabling identification of promising catalysts for selective production of the desired product.