Catalytic Activity of Pd-based Alloys Studied from First-Principles

함형철*
KIST 연료전지연구센터
(hchahm@kist.re.kr*)

In recent years, palladium (Pd) has been extensively studied for a possible alternative catalyst for Pt in fuel cells since Pd is less expensive and more abundant than Pt. However, Pd shows lower activity than Pt towards oxygen reduction reaction (ORR) in cathode and also exhibits poor carbon monoxide (CO) tolerance in anode. Alloying Pd with other transition metals (such as Co, Au, Ni, and Fe) has been suggested as one of promising solutions to enhance ORR activity and CO tolerance. However, a detailed understanding of the alloying effects is still lacking, despite its importance in designing and developing new and more cost effective fuel cell catalysts. This is in large part due to the difficulty of direct characterization. Alternatively, computational approaches based on quantum mechanics have emerged as a powerful and flexible means to unravel the complex alloying effects in multimetallic catalysts. Using periodic density-functional theory calculations, we have elucidated the underlying alloying principles (such as atomic arrangement, facet, local strain, ligand interaction, and effective atomic coordination number at the surface) that govern catalytic reactions occurring on Pd-based alloys.