

## The First-principles View of Nanometal Alloy Catalysts

Hyung Chul Ham<sup>1\*</sup>, Gyeong S. Hwang<sup>2</sup>

<sup>1</sup>Fuel Cell Research Center, KIST, <sup>2</sup>Department of Chemical Engineering, The University of Texas at Austin

Nanometal alloy catalysts have been found to significantly increase catalytic efficiency, compared to the monometallic counterparts. This enhancement can be attributed to various alloying effects: i) the existence of unquemixed-metal surface sites [the so called ensemble (geometric) effect]; ii) electronic state changes due to metal-metal interactions [the so called ligand (electronic) effect]; and iii) strain caused by lattice mismatch between the alloy components [the so called strain effect]. In addition, the presence of low-coordination surface atoms and preferential exposure of specific facets [(111), (100), (110)] in association with the size and shape of nanoparticle catalysts [the so called shape-size-facet effect] can be another important factor for modifying the catalytic activity. However, mechanisms underlying the alloying effect still remain unclear owing to the difficulty of direct characterization. Computational approaches, particularly the prediction using first-principles density functional theory (DFT), can be a powerful and flexible alternative for unraveling the role of alloying effects in catalysis since those can give us quantitative insights into the catalytic systems.

In this talk, I will present the underlying 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 using the first-principles calculations. This work highlights the importance of knowing how to properly tailor the surface reactivity of alloy catalysts for achieving high catalytic performance.

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