

Design of Geometric and Electronic Environments Using Metal Clusters for Highly Efficient Catalysis

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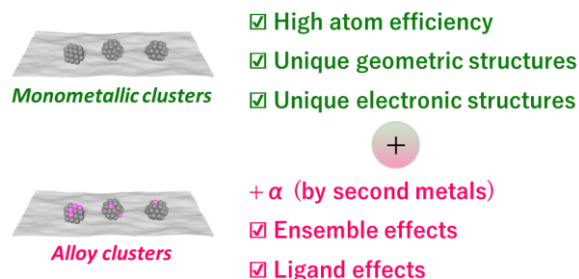
Abstract

Metal clusters have increasingly attracted attention as efficient catalysts due to their high proportion of accessible surface sites and unique geometric/electronic structures that distinguish them from both single-atoms and nanoparticles [1]. However, metal clusters possess an inherent tendency to sinter during pretreatment or reaction conditions, often irreversibly, driven by the minimization of their surface energies. Furthermore, conventional approaches often lack a deep understanding of the optimal cluster environment, hindering the rational catalyst design of high-performance catalysts.

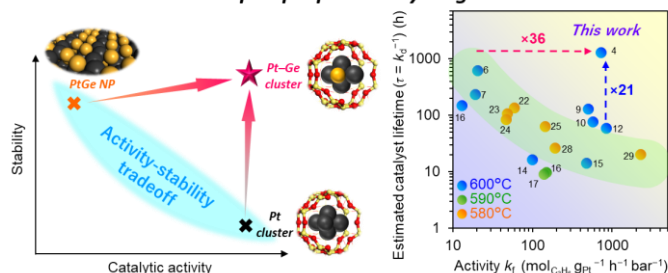
To address these challenges, we have developed synthesis strategies for small clusters and investigated catalytic performance in hydrocarbon upgrading reactions. In this presentation, we introduce the recent advancements in highly efficient catalysts for styrene hydroformylation, propane dehydrogenation, and the non-oxidative coupling of methane, and *etc.* For instance, we discovered that Rh clusters larger than 1 nm serve as optimal structures for the hydroformylation of styrene. Kinetic and theoretical analyses revealed that these Rh clusters provide a specific environment that facilitates the balanced co-adsorption of styrene, CO, and H, thereby promoting hydroformylation. In propane dehydrogenation, the synergistic effect of downsizing Pt species from the nanometric to the subnanometric regime and alloying with Ge allowed to break the activity–stability tradeoff [2]. We will discuss about the structural analysis, catalysis, and theoretical insights into hydrocarbon upgrading reactions.

Scheme I

Cluster catalysis



For example: propane dehydrogenation



References 1) Y. Nakaya and S. Furukawa, *Chem. Rev.*, 123, 5859–5947 (2023). 2) Y. Nakaya, et al., *Small*, 0, e73115 (2026).

Biography (For Plenary, Keynote, and Invited Speakers)

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Personal History:

Yuki Nakaya is currently an assistant professor in the Graduate School of Engineering at The University of Osaka. He received his B.S. (2019), M.S. (2021), and Ph.D. (2023) degrees from Hokkaido University. He recently received the Young Talents and IACS Awards at the 18th International Congress on Catalysis. His current research focuses on the precise synthesis of monometal, alloy, and multi-element clusters and nanoparticles, as well as the application of these materials to challenging hydrocarbon upgrading reactions.

Research Keyword (3-5 keywords use commas to separate each word):

Heterogeneous catalysis, Clusters, Nanoparticles, Alloys