Nano-Scale Metal Clusters and Metal Cluster Complexes: Theoretical Insight into Electronic Structure, Geometry, and Reactivity

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Nano-scale metal clusters and particles play important roles as catalyst in many reactions such as oxygen reduction reaction (ORR) in fuel cell, NOx reduction in three-way catalyst for cleaning automobile exhaust gas, and so on. To make new development in catalytic chemistry of metal clusters and cluster complexes, we need to elucidate reactivity and catalysis based on electronic structure.

Our group has started theoretical approach to nano-scale metal cluster/particle and metal cluster complexes. We elucidated stability and its determination factors of core-shell particle consisting of low-cost metal core and platinum shell[1] and reactivity of metal particle for NO.[2] In this talk, we wish to report our theoretical approach to enhanced activity of core-shell particle $M_{13}@Pt_{42}$ (M = Ni and Co) for ORR compared to Pt particle[3] and stability and electronic structure of Pd_{13} cluster complex $[Pd_{13}(C_7H_7)_6]^{2+}$ bearing highly symmetrical cuboctahedral structure. In the study of ORR, we elucidated the reason why core-shell particle $M_{13}@Pt_{42}$ is more active than Pt_{55} based on d valence band energy. In the study of Pd_{13} cluster complex, we succeeded in explaining why a highly symmetrical cuboctahedral structure is obtained but similar anti-cuboctahedral and icosahedral structures are not.

[1] L. Jing, et al., *J. Phys. Chem. C*, **2018**, *122*, 9081.
[2] N. Takagi, et al., *J. Phys. Chem. A* **2019**, *123*, 7021.
[3] B. Zhu, et al., *J. Cat.* **2021**, *397*, 13.