

DFT study on the hetero-junction effect of precious metal clusters

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Lately, precious metal nanoparticles have received much attention as electronic devices, spintronics materials, catalysts, etc. In the case of catalysis, the catalytic activities of Pd/Pt bimetallic clusters for hydrogenation were changed depending on its constituent parts and the structures of the nanoparticles. Especially, the core/shell type Pd/Pt bimetallic cluster exhibit extremely high catalytic activity for cyclooctadiene partial hydrogenation¹. This result suggests that the characteristics of the core/shell type bimetallic clusters are dramatically changed from the catalytic point of view.

It is also well known that precious metal nanoparticles immobilized on the several types of the supports showed different catalytic activities from the unsupported precious metal nanoparticles itself. As it is an interesting issue to modify the electronic state of the nanoclusters in order to increase its catalytic activity for several catalytic reactions, Pd clusters supported on the model single wall carbon nanotubes (Pd/SWCNT) are also examined.

It would be presumed that the variation of the catalytic activities of the catalysts mentioned above is related to the hetero-junction in those systems. In order to discuss the hetero-junction effect of the bimetallic core/shell clusters and Pd/SWCNT, UB3LYP calculations for N₁₃, N-M₁₂, (N,M=Pd, Au or Pt), Pd₃₈, Pt₆-Pd₃₂ and Pd_n/CNT(4,4) and Pd_n/CNT(5,5) model systems were examined as a first step for understanding the hetero-junction effect on the cluster model catalysts.

[1] N. Toshima, et al., *J. Phys. Chem.* **95**,7448-7453 (1991).

[2] M. Okumura, S. Tsubota, and M. Haruta, *Cat. Lett.* **51**, pp. 53-58(1998).

[3] M. Okumura, S. Tsubota, and M. Haruta, *J. Mol. Catal. A-Chem.* **199**, pp. 73-84(2003).