The collaboration research for the Dual Graduate School between VNU and JAIST

[Title of collaboration research]:

Computational design of catalyst using nano-metal-cluster on nanotube and its application to fuel cell

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[Reference home-page address]:

[Other references]:

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1. Purpose

The catalysis plays an innovative role in the development of new technologies, and electrocatalyst design is a key factor for enhancing their performances, which are becoming big issues accompanying the industrialization. Nanotechnology is believed to be important in heterogeneous catalysis for its peculiar properties and potential applications. The carbon nanotube with beautiful tubular structure and a large effective surface which could facilitate the adsorption of catalyst small particles is expected as supports for catalyst. In this study, we use theoretical calculation techniques to design new nanocatalyst system using carbon nanotube and metal nano-clusters.

2. Method

In this research, physical properties of several metals nano clusters and carbon nanotubes will be investigated together with catalyst in several reactions, such as oxygen reduction reaction in cathode of fuel cell. Effect of dispersity and cluster size of nanocatalyst particles on electrocatalytic activities, and method for size control of clusters on carbon nanotube supports will be investigated carefully in order to establish new concept for catalyst design.

Ab initio calculation based on the Density Functional Theory (DFT) will be main technique in this research. First principle molecular dynamics simulation also will be carried out for investigation of reaction process. Plane wave and localized pseudo numerical atomic orbitals methods are applied as basis functions for computation of clusters and periodic systems.

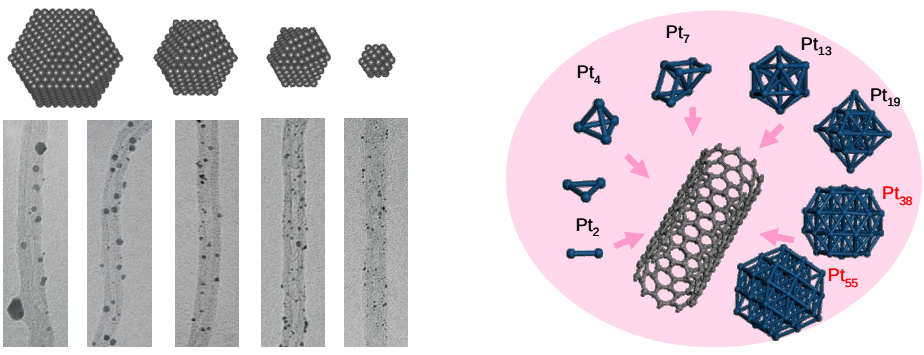

Fig. 1: Experimental observation (HRTEM) and calculation model for Pt clusters adsorbed carbon nanotube.