DFT calculations of electronic structure of Pd nanoparticles

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Palladium (Pd) are attractive material for many scientific and industrial fields such as catalysis and hydrogen energy. In many cases, Pd is used as nanoparticles (NPs) because of the high specific surface area and high active surface sites (edge, corner and terrace). In other words, the catalytic activity is determined by the diameter and shape of NPs. I have studied the hydrogen storage property of Pd NPs [1]. Pd bulk can absorb the hydrogen uo to 0.6 per Pd atom. On the other hand, Pd NPs absorb hydrogen less than 0.4. The reason why the hydrogen absorption amount decrease with the reduction of the size is not clear. In order to clarify the hydrogen absorption property and mechanism of Pd NPs, one idea is investigation of the stability of the hydrogen in the Pd NPs by means of abinitio calculation. It is expected that the prediction of the hydrogen storage amount by the calculation of the electronic structure.

As the first step, in this study, the electronic structure of Pd NP has been investigated by means of the abinitio calculation based on the density functional theory (DFT). The DFT calculations were performed using the Quantum Espresso [2] and WIEN2k [3] packages. The structure optimization of Pd NP was carried out with Quantum Espresso. After the structure optimization, the all electron calculation of the Pd NP was done by using of WIEN2k to obtain the density of state (DOS) of the valence band. Three models were assumed for the Pd NP, octahedron (Oh), cube and cuboctahedron (CuboOh). Pd Oh has (111) face and Pd cube has (100). Pd CuboOh has both faces. The DOS of the Pd NPs were compared with the valence band spectrum of the Pd NPs obtained by X-ray photoelectron spectroscopy using synchrotron radiation.

References:

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