Energetical effects of the edges and vertices of face-centered-cubic Pd and Au nanoparticles: A density functional theory study

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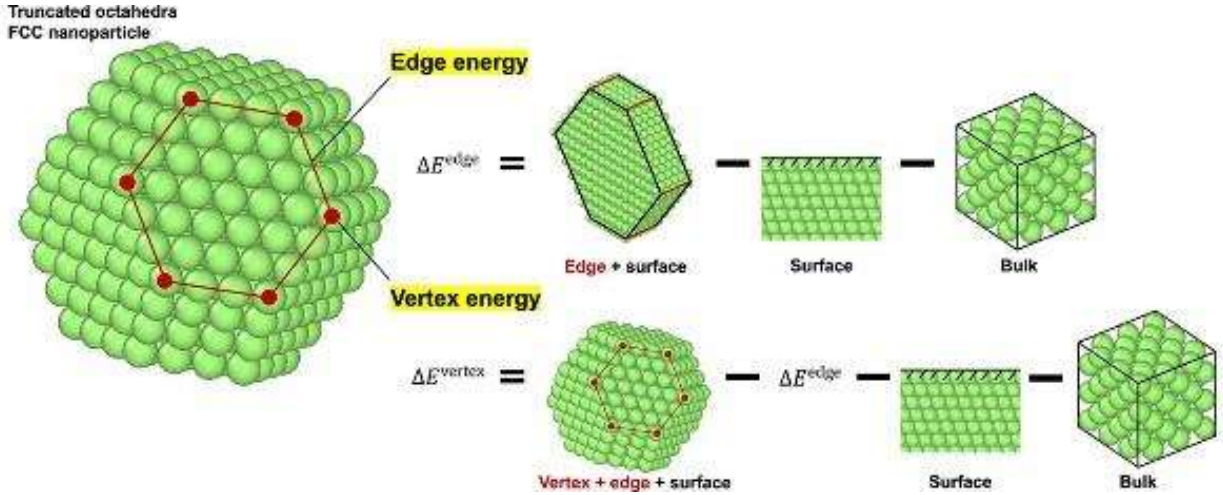

Purpose

Quantitative analysis of effect of edges and vertices of nanoparticles to the energy

Computer: SQUID

Abstract

The properties of nanoparticles depend on their sizes, and these size effects in face-centered-cubic (FCC) nanoparticles are attributed to the edge and vertex effects. However, the effects of edges and vertices on the properties of nanoparticles have not yet been explicitly investigated. In this study, we propose a method to evaluate the edge and vertex effects in FCC nanoparticles using density functional theory atomistic simulations. Pd and Au FCC nanoparticles are modeled as conventional truncated octahedra with and faces. The changes in the excess energy due to the edges and vertices are separately described and are calculated with respect to the size of the nanoparticles. Through explicit calculations, we confirmed that for Pd and Au nanoparticles with several hundred atoms, the vertex effects are negligible, whereas the edge effects are still significant.