

Title:

Ideal vs Real: Simulated Annealing of Experimentally Derived and Cuboctahedral Platinum Nanoparticles

Abstract:

Platinum nanoparticles continue to be of great interest due to their catalytic properties. Computational approaches have been extensively used in order to determine the effects of size and shape of nanoparticles on their chemical properties. Ideal structures, such as truncated octahedra, are often used in these studies, and while they can be very reasonable models, they are not realised experimentally. Performing calculations on the structures of real nanoparticles allows us to study the effects of deformations (such as stacking faults), adatoms and other phenomena that are observed experimentally. It also provides a means to verify the models used for our calculations.

The coordinates of a number of platinum nanoparticles have been obtained by high resolution annular dark-field scanning transmission electron microscopy by the group of Professor Peter Nellist (Department of Materials, University of Oxford). They range in size from 2.0 to 5.5 nm. These structures are compared with idealised cuboctahedra within this size range using annealing simulations. We have adopted a classical molecular dynamics approach using the Gupta many-body potential. These simulations are used to determine structural stability and to predict the effects of heating and electron beam damage, as well as to search a thermally restricted configuration space. We find that the annealing process results in very similar structures for both the real and ideal nanoparticles, and these final structures are much more similar to the former than the latter. Finally, we have used accurate large-scale first principles density functional theory calculations on a number of these structures to verify the classical potential.