Combined aberration-corrected in-situ TEM characterization and ab initio calculations on the morphological changes of platinum nanoparticles

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Among metal catalysts, platinum is by far the most efficient for most industrially relevant catalytic reactions. It is the most popular electrocatalyst for PEM fuel cells and is also used in catalytic converters for automobiles. Due to the extreme high price of platinum, much of the recent research effort has been driven by reducing the amount of platinum used in catalysts. This effort has mostly concentrated on reducing particle sizes, better dispersion of particles, adding second metallic components to make bimetallic catalysts and particle shape control to maximize the catalytically active surfaces. However, metal nanoparticle catalysts are often used at elevated temperature and in gaseous environments for heterogeneous catalytic reactions. Under these environments, metal particles can experience morphology changes and such changes can alter their catalytic properties. Understanding the dynamic behavior of metal nanoparticles in their operating conditions is therefore important in designing a better catalyst.

Here we use aberration corrected transmission electron microscopy (TEM) to study the morphological changes of 5-10 nm platinum colloidal nanoparticles at elevated temperature and in an O_2 environment. Aberration-corrected TEM has the advantage over conventional TEM of reduced delocalization due to the reduction of objective lens spherical aberration, allowing direct interpretation of the shape, particularly for small nanoparticles. In addition, we have also conducted ab-initio calculations to determine the equilibrium shape of the platinum nanoparticles for the experimental conditions. The combination of experimental observations using aberration-corrected in-situ TEM with theoretical calculations of the morphological changes of the nanoparticles gives us insight into the behavior of metal nanocatalysts in their operating conditions.