

Supplementary Information

“The preparation and characterization of novel Pt/C electrocatalysts with controlled porosity and cluster size”

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Calculation of theoretical electroactive surface areas of Pt/C catalysts

Using the modeling data of de Graaf, et al.,¹ the number of Pt atoms per cluster was plotted as a function of cluster size, as shown in Figure S1. One additional datum point is included for a single Pt atom, using the atomic radius of 0.278 nm as the cluster diameter.

A third-order polynomial was fit to the data and constrained to pass through the origin, as indicated in Figure S1. This polynomial equation was used to calculate the number of atoms per cluster in the templated Pt/C catalysts based upon the calculated mean cluster sizes from EXAFS data. The mass of the cluster was determined from the number of Pt atoms it contained. The theoretical electroactive surface area (ESA) was then calculated from the geometric surface area of the cluster and its mass.

The calculation of theoretical ESA is shown in eq. S1 (C, B and A are coefficients from the polynomial fit to the data in Figure S1).

$$ESA = \frac{4\pi\left(\frac{d}{2}\right)^2 * N_A}{AM_{Pt}(Cd^3 + Bd^2 + Ad)} \quad \text{eq. S1}$$

d = cluster diameter / m

N_A = Avogadro's number / atoms mole⁻¹

AM_{Pt} = atomic mass of Pt / g mole⁻¹

C = 34.906

B = -29.431

A = 12.742

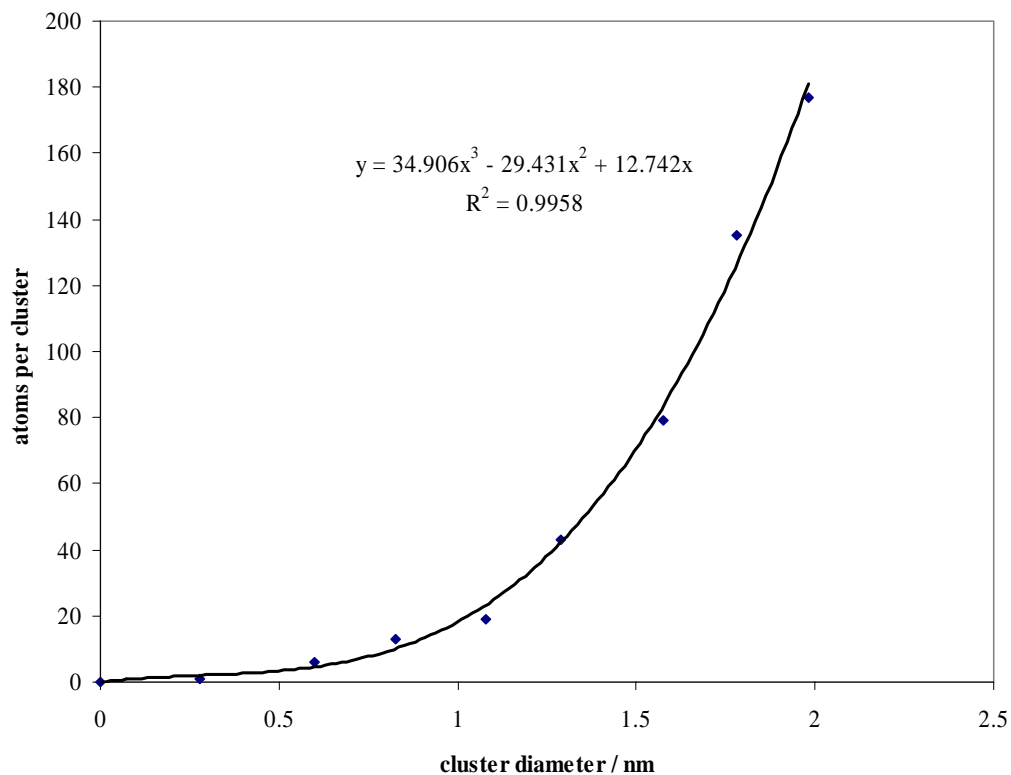


Figure S1. Third-order polynomial fit of modeled number of Pt atoms per cluster as a function of cluster size.

The principal assumptions, which limit the accuracy of the calculations, were:

- 1) the clusters were all equal in size to the mean size determined through EXAFS analysis;
- 2) the clusters were all spherical.

Reference

- 1 J. de Graaf, A. J. van Dillen, K. P. de Jong and D. C. Koningsberger, *J. Catal.* 2001, **203**, 307-21.