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# How does the percentage of atoms on the surface of fcc metals nanoparticles change with their shape and the size?

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**Abstract**

Metal nanoparticles are used for different applications both in the industry and universities mainly for fundamental researchs in several fields of science. In (electro)catalysis, metal nanoparticles are used to speed up (electro)chemical reactions. As these reactions occurs on the electrode surface, the high ratio area/volume of nanomaterials have turned them very attractive for application in catalysis. Another important aspect of these materials is the atom arrangement at the surface, because it affects their (electro)chemical properties. In this work, a structure simulation software was used to create nanoparticle models of different shapes (cubic, octahedral and spherical) to find correlations between the the nanoparticles' size and the amount of atoms at their surface. For Pt nanoparticles, we find that the size is a critical parameter for diameters <8 nm where the atoms at the surface change from about 20% to 80-100% (1 nm). On the other hand, the percentage of atoms at the surface do not change appreciably with the shape, except for nanoparticles <2nm.

***Key words:***

*Nanoparticles, Platinum, Catalysis.*

## Introduction

Most of the chemical reactions performed in industries and laboratories use catalysts to accelerate and or /driven the reaction to an efficient production of the target molecule[1]. Nano-catalysts, those that have size in the order of $10^{-9}$ m, show a great advantage due to the wide superficial area (where the reactions occur) in a small amount of material, enhancing the price-performance ratio[2].

Apart from the high area/mass ratio, nanoparticles (NPs) with different shapes (Image 1) have different atoms arrangements at their surfaces. Modifications in the atoms arrangements generate different electronic structure altering the interaction between the NPs and the reactant and impacting in the catalytic properties of the material. Last but not least, the size is also important. As the properties of atoms at the surface are different to that of those "inside" the material, the properties of NPs are also affected by the percentage of the atoms at the surface.

In this work, a structure simulation software was used to create Platinum NPs of different shapes (cubic, octahedral and spherical) and find correlations between the NPs' size and shape with the number of atoms at their surface.

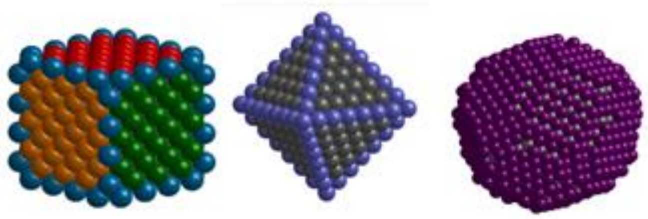

**Image 1.** Cubic, Octahedral and Spherical models of NPs. It is important to note the difference in the atoms arrangement between NPs and also in each NP.

## Results and Discussion

Image 2 shows an exponential decreasing of the percentage of the atoms at the surface for the three shapes analyzed in this work. The result agree with the fact that the area of these geometric forms is proportional to $a^2$ and the volume to $a^3$, being "a" the edge of the cubes and octahedrons or the radii for a sphere.

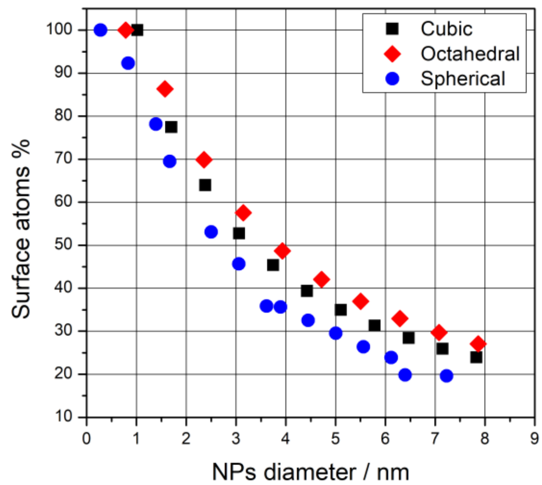


**Image 2.** Dependence of the percentage of atoms at the surface of NPs with their size and shape.

## Conclusions

The amount of surface atoms is a lot more sensitive to the size than to the shape of the NPs.

The model constructed in this work can be used to perform similar analysis for any *fcc* metal.

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