# Synthesis of Hollow Nanoparticles by Laser Irradiation: A Computational Analysis

Alejandro Prada[1*], Felipe Valencia[1,2†], Lukas Cornejo[1], Max Ramirez[2,3], Alejandro Varas[2,3], José Rogan[2,3]

[1]Departamento de Computación e Industrias, Facultad de Ciencias de la Ingeniería, Universidad Católica del Maule, Talca.

[2]Centro para el desarrollo de la Nanociencia y Nanotecnología (CEDENNA), Santiago.

[3]Departamento de Física, Facultad de Ciencias, Universidad de Chile, Santiago

*aprada@ucm.cl, †fvalencia@ucm.cl

## Abstract

Nowadays, hollow nanoparticles are one of the most technologically interesting shapes. They have allowed a more precise distribution of drugs in the human body, the development of larger volume gas storages, more efficient catalysts, structures with better mechanical properties than solid materials, and many other advances.[1] They are synthesized by physical, chemical and biological processes, that have achieved a large volume of nanoparticles; but with a low degree of perfection, sometimes with undesired porosities or incipient fractures. In recent decades, the study of localized surface plasmon resonance (LSPR) for metallic nanoparticles has allowed the development of a new synthesis technique based on the use of laser irradiation[2,3].

By means of molecular dynamics simulations, we analyzed in more detail the formation of these holes, both in monometallic and bimetallic nanoparticles. Atomistic simulations shows to be useful tool to in-situ observe and analyze the formation thresholds in nanoparticles with different sizes, allowing us to know the energies and environmental conditions that promote the formation of hollow nanospheres. The same simulations are extrapolated for the laser irradiation of Ag and Au nanoparticles which leads the formation of an AgAu alloy nanostructure. Our results shows, how the energy deposition can be used as a fundamental parameter to control the synthesis of alloyed nanoparticles.

Acknowledgement: This work was supported by the Fondo Nacional de Investigaciones Científicas y Tecnológicas (FONDECYT, Chile) under grants #1190662 (JR, MR, AV, FV), #11190484 (FV) y #3190123 (AP). The authors thanks to Financiamiento Basal para Centros Científicos y Tecnológicos de Excelencia AFB180001. Powered@NLHPC: this research was partially supported by the supercomputing infrastructure of the NLHPC (ECM-02).

## References

[1] Valencia F.et al.The Journal of Physical Chemistry C122, (2018) pp25035-25042.
[2] Castro-Palacio JC. The Journal of Physical Chemistry Letters11, (2020) pp5108-5114
[3] González-Rubio G.The Journal of Physical Chemistry Letters11, (2020) pp670-677