# Molecular dynamics simulations of cavity formation in gold nanoparticles upon ultrashort laser irradiation

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The irradiation of gold nanoparticles (AuNPs) in a colloid with nanosecond laser pulses can give rise to the formation of cavities [1]. The concentration of the surfactant used to stabilize the particles, the laser fluency, and the size of the nanoparticles, determine the efficiency and features of the process. The resulting hollow particles are obtained when the right balance between the heating and cooling processes is given. The first process induces an expansion and the melting of the particle, while the second, leads to the recrystallization, keeping the extraneous matter trapped in the inside. These experimental observations have been satisfactorily explained by the molecular dynamics (MD) simulations carried out in reference [2]. Specifically, the simulations have confirmed that it is necessary the existence of trapped molecules in the inside of the cavities to stabilize the cavities. MD simulations and calculation of optical properties when gold nanoparticles (in a colloid) are irradiated with femtosecond laser pulses have been developed in reference [2]. The simulations allowed the prediction of shape changes under different conditions for the laser fluency and duration, the size of the nanoparticles and the cooling rate, which is driven by the properties of the solvent and the surfactant. These simulations provide a guidance for the synthesis of nanoparticles with specific morphological features. The results show that the nanospheres should be heated up to 2500 y 3500 K, followed by a fast cooling (time constant of 120 ps). Therefore, the experimental conditions for the efficient production of hollow nanoparticles are described what opens a broad range of possibilities for applications in areas such as energy storage and catalysis. Finally, MD simulations are carried out to gain insights into the pump-probe experiments using AuNPs in reference [3]. Upon femtosecond laser irradiation and deposition of energy, the nanospheres vibrate which can be measured by means of the scattering cross section. Hyper spherical coordinates are used to follow the breathing modes of the particles and to determine the vibrational frequencies for each particle size.

## References:

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