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## **Map of Structural and Optical Properties of Plasmonic Nanoparticles at Thermal Equilibrium**

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### Abstract:

It is well known that the optical Properties of Nanoparticles (NPs) depend on its composition, size and morphology [1]. For example, a colloidal system of silver NPs can show a greenish or yellowish hue whether the NP is cubic of about  $d \approx 80$  nm or cuboctahedral of about  $d \approx 150$ -200 nm [2]. However there is not an obvious relationship between color, size and morphology at different temperatures.

Recently, a phase map relating NPs morphology as a function of temperature and size ( $T, d$ ) was generated, where ab initio methods were employed to calculate the energetically most stable shapes at a given ( $T, d$ ) [3].

Most of the times experts in the synthesis of nanoparticles use a trial and error method, which sometimes entails time, money and effort wasted. Motivated by this, we present a color phase map of gold and silver NPs in vacuum, which can be a useful tool to experimentalists to determine the appropriate size and shape depending of temperature conditions. To build up this color map, we employ the morphologies from the ( $T, d$ ) phase map, and calculate the optical extinction using the discrete dipole approximation [4]. Then, we calculate the NP's real color that would be observed by a human eye in a dilute colloid containing such NPs. Finally, we construct a color phase map showing the relationship between temperature, size, shape and color associated to gold or silver NPs [5,6,7].

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