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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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