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# Synthesis of gold nanoparticles with different atomistic structural characteristics

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**Abstract**

A chemical reduction method was used to produce nanometric gold particles. Depending on the concentration of the main reactant compound different nanometric sizes and consequently different atomic structural configurations of the particles are obtained. Insights on the structural nature of the gold nanoparticles are obtained through a comparison between digitally-processed experimental high-resolution electron microscopy images and theoretically-simulated images obtained with a multislice approach of the dynamical theory of electron diffraction. Quantum molecular mechanical calculations, based on density functional theory, are carried out to explain the relationships between the stability of the gold nanoparticles, the atomic structural configurations and the size of nanoparticles.


*Keywords:* Nanoparticles; Gold; Structural determination; High-resolution electron microscopy; Density functional theory; Molecular simulation

## 1. Introduction

Nanoparticles are defined as atomic arrangements with nanometric dimensions and usually with a small number of constituent atoms. The structural configurations of these small particles induce new types of physical properties. Therefore, the selection of a synthesis method which can give rise to a particular structural particle configuration is very important for new technological applications [1,2]. Depending on the nanometric particle size, the nanostructures can have different applications. These applications include fields such as: catalysts, photography, medicine, information storage in magnetic devices etc. In recent years, the high-resolution electron microscope (HREM) has been one of the main tools used to study the physical properties of nanometric particles. Metallic nanoparticles usually display simple geometric atomic arrangements, mainly with tetrahedral, octahedral and decahedral forms [3,4]. They even present atomic configurations which display five-fold symmetry [5]. In the reduction synthesis method used in this investigation, particles of different average sizes and different geometrical arrangements have been obtained.

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The morphological nature of the nanometric particles depends on the concentration of the main reagent compound used in the reduction process. In this study, the structural characterizations of gold nanoparticles with different structural morphologies have been carried out through a comparison between experimental and theoretical HREM images. The stability of the nanoparticles is also evaluated using density functional theory based on quantum mechanical calculations.

## 2. Experimental procedures

Ultra fine gold particles have been obtained using the chemical reduction method reported earlier [6,7]. Methanol solutions of gold ions were prepared by dissolving crystalline hydrogen tetrachloroaurate ($HAuCl_4 \cdot xH_2O$) in methanol (0.033, 0.044, 0.099, 0.11 and 0.12 mmol in 25 ml of methanol). A methanol solution of PVP [poly (*N*-vinyl-2-pyrrolidone) (150 mg of PVP in 25 ml of methanol), was added to the metal ion mixture. To reduce the metal ions, 6 ml of an aqueous solution of $NaBH_4$ (0.066 M) was added to the mixture solution dropwise at room temperature. A homogeneous colloidal dispersion was formed after the addition of the $NaBH_4$ reductant in the solution containing the metal ions.

The structural and morphological characteristics of the dispersed metallic nanoparticles have been studied using a transmission electron microscope, Philips Tecnai F20, which has a field emission gun attachment, an operating voltage of 200 keV, a spherical aberration of 1 mm, and a direct maximum resolution dot to dot of 0.23 nm. TEM specimens were obtained from the homogeneous colloidal solution. Drops of this solution were deposited on a copper grid (3 mm in diameter) with an amorphous carbon film. The HREM images have been digitally processed. Theoretical simulations based on the multislice approach of the dynamical theory of electron diffraction [8] have been carried out to generate HREM images of gold nanoparticles.

Studies on the stability of the nanoparticles were carried out using quantum molecular calculations. These simulations were carried out using the Dmol$^3$ software by Accelrys [9], which is based on the density functional

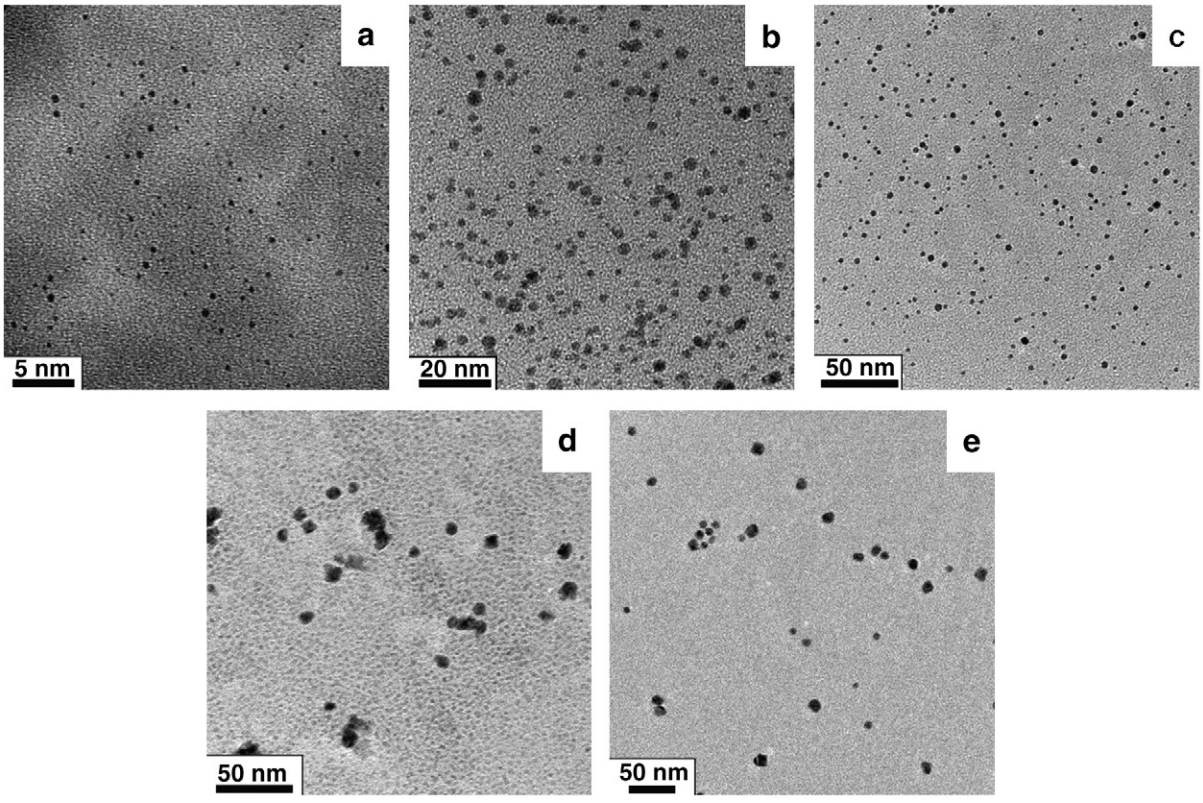


Fig. 1. Low magnification TEM images of the gold nanoparticles synthesized with different concentrations of gold ions; a) 0.033 mmol, b) 0.044 mmol, c) 0.099 mmol, d) 0.11 mmol and e) 0.12 mmol in 50 ml of reaction mixture.