The University of Texas at San Antonio

UTSA Physics and Astronomy

Qualifying Exam

Mohammad Hoque

Date: **: Monday, July 2nd 2018**

Time: **11:00 am to 1:00 pm**

Location: **AET 3.328**

Campus: **Main Campus**

Advisor: **Dr. Kathryn Mayer**

Abstract

Microanalysis of larger metallurgical molecule

For the most applications, control of the core size, shape, and dispersity and the nature of the ligand shell is desirable, along with a simple and widely applicable preparation method. Highly stable and functionalizable larger aqueous ~4.5 nm gold nanoparticles have been synthesized and functionalized by replacing the flexible carboxylic terminated group of citrate/tannic acid using monothiols (11-mercaptoundecanoic acid, MUA), dithiols (□- lipoic acid, LA), and aromatic thiols (para mercaptobenzoic acid, p-MBA). The particles are then characterized by UV-Vis spectroscopy for optical properties, X-ray Diffraction (XRD) for structural analysis, high resolution transmission electron microscopy (HR-TEM) for structure and size determination, hydrodynamic diameter profiles extracted from dynamic light scattering (DLS) as a complementary method for size distribution study, and zeta potential to study the colloidal stability. Electronic charging of the Au nanoparticle core, shift in the surface plasmon responses possibly due to quantized charge effect is being investigated. These highly stable aqueous ~4.5 nm Au NPs could be used for a potential biomedical application like photothermal cancer therapy exploiting their localized surface plasmon resonance (LSPR) characteristic.

The study of the crystalline structure of nanoparticles for local atomic arrangement (interatomic distance) is challenging due to the fact that some are stable in nontranslational symmetry configurations. Crystal symmetries and geometrical reconstruction of the nanoparticles can be determined by electron diffraction but nearest neighbors from an atomic reference are not directly provided using electron diffraction. In this way, atomic pair distribution function (PDF) has evolved as an essential experimental tool to ease this challenge. The reduction of the dynamic scattering produced as a result of the strong interaction of the electron with atoms is obtained using precession electron diffraction (PED) at room and low temperatures and later used for e-PDF postprocessing data in synthesized ~4.5 nm gold nanoparticles. The e-PDF measurements under PED are comparable with x-PDF offset differences between experimental data and PDF calculated from theoretical models. The factor used to quantify the agreement between the calculated PDF and the experimental e-PDF obtained with the method herein reaches 25% using two different structure models, face-centered cubic (fcc) and truncated octahedron (TO) after a fine subtraction of the carbon film that supports the nanoparticles.

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