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MS-1-P-3507 STEM Electron Diffraction and High Resolution Used in the Determination of Thiolated Gold Clusters

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Gold nanoparticles protected by thiolate ligands have attracted extensive research activity because of their enhanced optical, electrochemical, and other application-related properties. The desired physicochemical properties are strongly dependent upon size, composition, and structure. It is therefore critical for improved materials design to correlate the cluster structure and bonding with the properties sought for applications. However, the determination of atomic structures of nanomaterials is a challenging task even for composition elucidated gold−thiolate nanoclusters where gold cores span various symmetries. Determination of the total structure of molecular nanocrystals is an outstanding experimental challenge that has been met, in only a few cases, by single-crystal X-ray diffraction. Described here is an alternative approach that is of most general applicability and does not require the fabrication of a single crystal. The method is based on rapid, time-resolved nanobeam electron diffraction (NBD) combined with high-angle annular dark field scanning/transmission electron microscopy (HAADF-STEM) images in a probe corrected STEM microscope, operated at reduced voltages. In the current presentation, we will show the new structures of Au130 and Au144 thiolated clusters explored in a combined experiment-theory approach [1-2]. A full map in reciprocal space has been simulated and compared with the experimental patterns using STEM diffraction as well as atomically resolved images obtained through aberration-corrected STEM-HAADF images. The nanobeam diffraction (NBD) through the STEM imaging mode is controlled by the condenser lens system. The combination of probe-corrected STEM imaging and quasi-parallel beam diffraction (D-STEM) is obtained by positioning the beam in the STEM image at a single nanoparticle using the Digiscan control. The scan is stopped and positioned arbitrarily at a xy position on the screen. Subsequently, the electron diffraction pattern is recorded using a digital charge couple device (CCD) camera. D-STEM mode works in the diffraction plane, the overlapping of the convergent disks is optimized by a compensation of the last condenser lens (C3) and the use of the adaptor lens (ADL) at the hexapole coils of the CEOS corrector.

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