

Supporting Information

CuS₂-passivated Au-core, Au₃Cu-shell nanoparticles analyzed by atomistic-resolution C_s-Corrected STEM

Subarna Khanal,[†] Gilberto Casillas,[†] Nabraj Bhattarai,[†] J. Jesús Velázquez-Salazar,[†] Ulises Santiago,[†] Arturo Ponce,[†] Sergio Mejía-Rosales[‡] and Miguel José-Yacamán^{†*}

[†]Department of Physics and Astronomy, University of Texas at San Antonio, One UTSA Circle, San Antonio, TX, 78249

[‡]Center for Innovation, Research and Development in Engineering and Technology, and CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450, Mexico until

E-mail: miguel.yacaman@utsa.edu

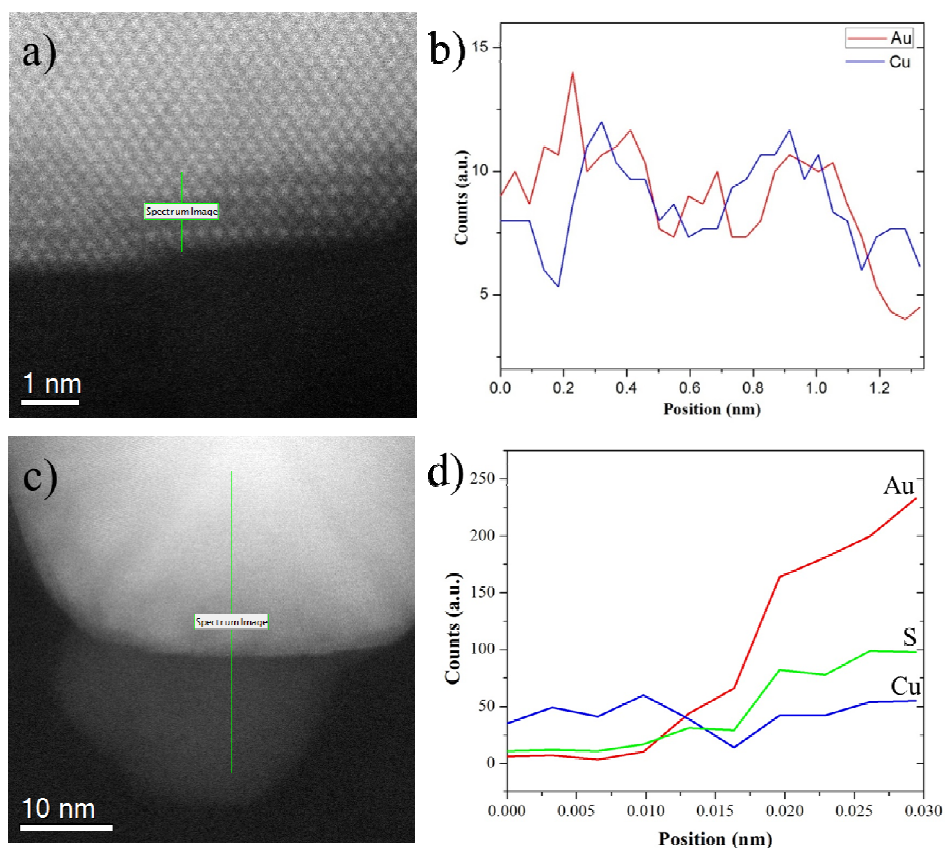


Figure S1. STEM-EDS line scanning (a) along interface, (b) showing the presence of Au and Cu, (c) along core-shell region with surface layer, (d) showing the presence of Au, S and Cu. It can be seen clearly that Au signal is very strong while Cu and S signals are flat, indicating that CuS₂ surface layer is present.

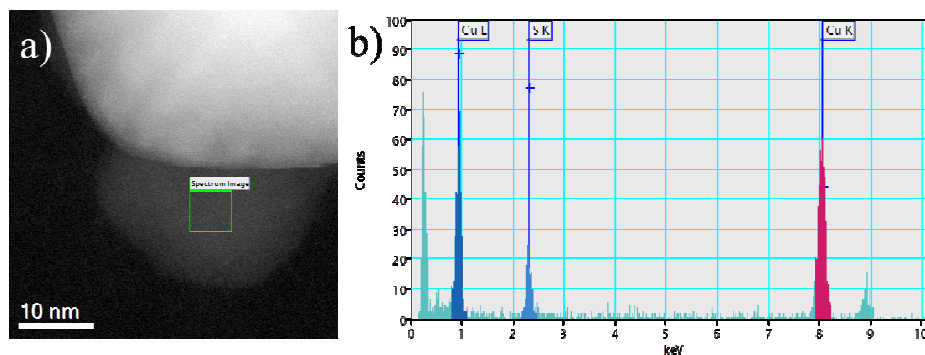


Figure S2. EDS spectrum of CuS_2 surface layer, which shows the presence of Cu and S in the elemental composition of the surface layers.

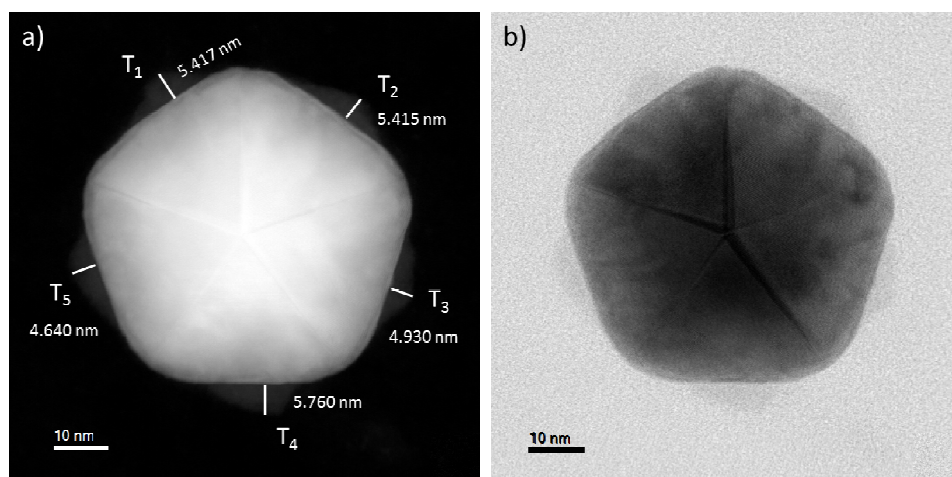


Figure S3. (a) High angle annular dark field (HAADF) and (b) Bright Field (BF) STEM micrographs of Decahedral Au- CuS_2 Core-shell nanoparticles, shows the average thickness of the shell is 5.23 nm.

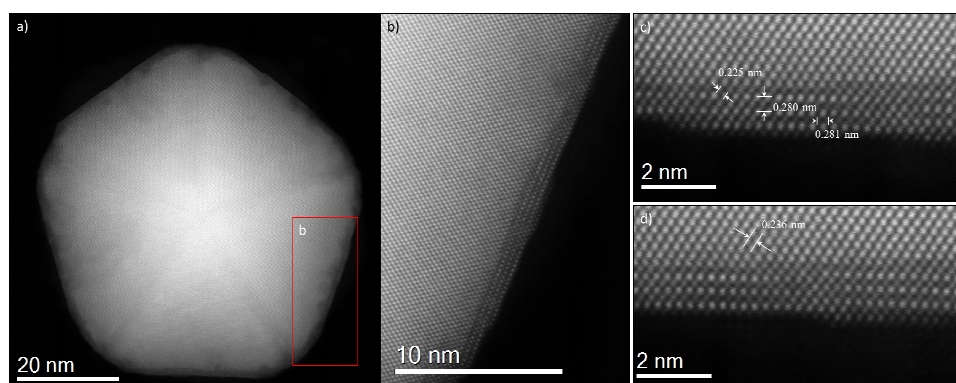


Figure S4. HAADF STEM image of decahedral nanoparticles different magnification and lattice spacing between Au and Cu interface boundary region.

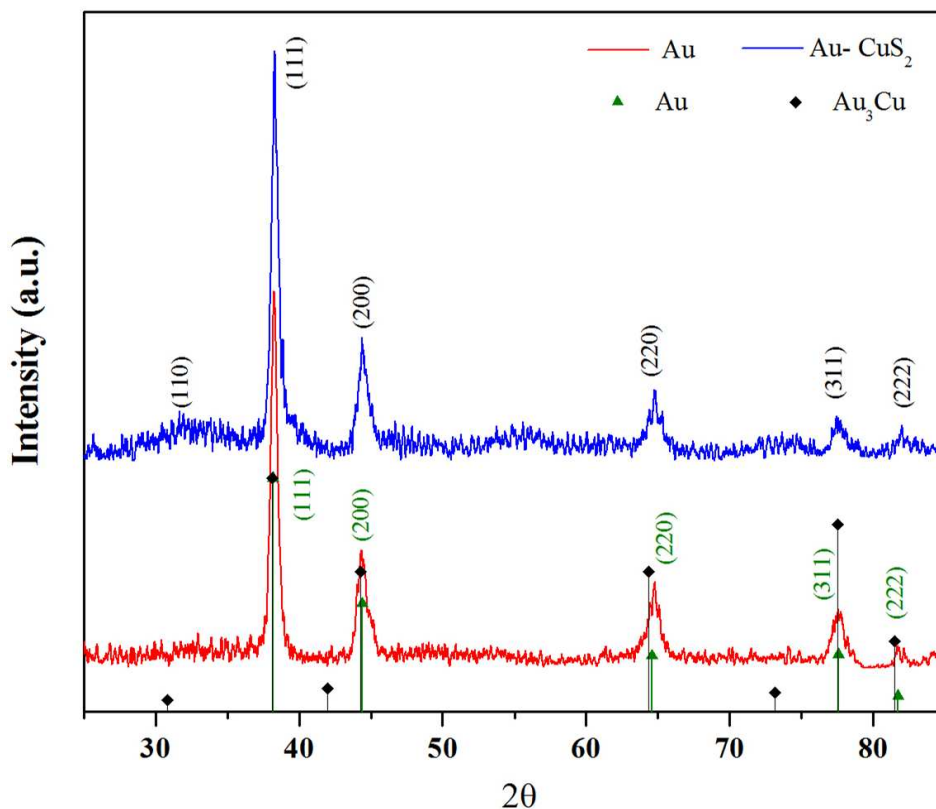


Figure S5. X-Ray diffraction patterns of Au core and Au-CuS₂ nanoparticles. Standard patterns for Au and Au₃Cu are also inserted in the figure. Full width half maxima (FWHM) value is measured for Au and Au₃Cu. The obtained values for Au is 0.93°, 0.97° and 1.17° while for Au₃Cu is 0.97°, 1.25° and 1.67° corresponding to (200), (220) and (311) planes, suggesting broader diffraction peak for Au₃Cu than for Au core.

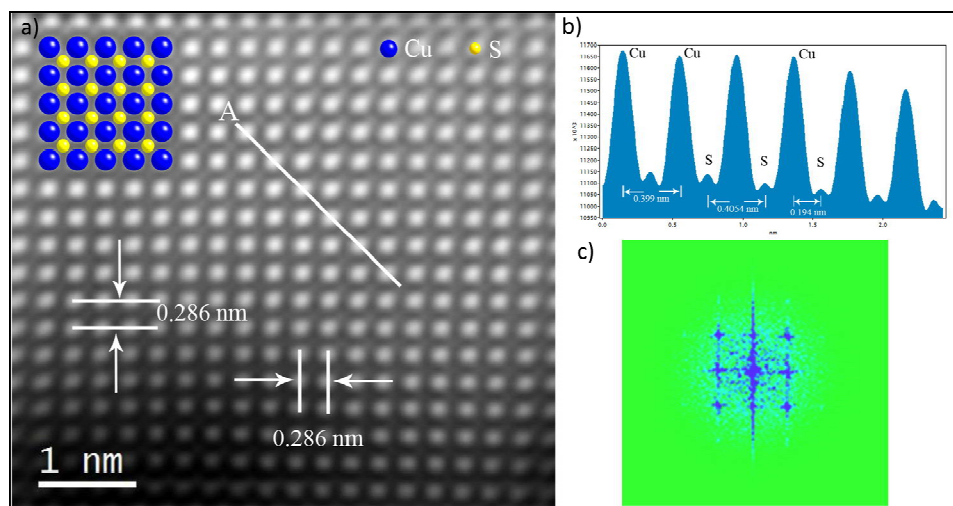


Figure S6. (a) Atomic resolution HAADF image of CuS₂ surface layer, the inset model structure of CuS₂ is exactly match with this image, (b) Intensity profile of surface layer shows the disparity of the Cu rich and S rich atomic columns, (c) The fast Fourier transform (FFT) pattern of the shell region.