replacing MAR17-2016-008021

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic structure and optical properties of $Ag_{44}(MNBA)_2$ nanoclusters: An ab initio study [1] ZAHRA HOOSHMAND, DUY LE, VOLODYMYR TURKOWSKI, TALAT S RAHMAN, University of Central Florida — In a recent study,Abdulhalim et al. have presented a new strategy for tailoring the optical properties of thiol-protected small Ag nanoclusters by protonation-deprotonation of the ligand shell[1].Specifically,the absorption spectrum of the 44-atom Ag nanoparticles with 30 MNBA (5 mercapto-2-nitrobenzoic acid) ligands, showed dependence on the pH environment.Here we present results of our density functional theory (DFT) and TDDFT based calculations of the effects of the MNBA ligand on the electronic and optical properties of Ag_{44}.In particular,we find when 2 MNBA molecules are adsorbed on Ag_{44} there is a strong tendency of dimerization between adjacent molecules via H...O-H groups.This dimerization is proposed to be the origin of the experimentally observed nanocluster's optical behavior at lower pH values. In the case of high pH environment, the deprotonation significantly modifies the binding of sulfur atoms to the silver cluster,and as a result the optical properties of the system.TDDFT results for the excitation energies of the system demonstrate that the optical absorption spectrum is defined by transitions that involve hybridized ligand-nanoparticle states.Obtained results may lead to a better understanding of the connection between the electronic structure and the optical response of noble-metal nanoparticle-ligand systems.[1] Abdulhalim,L.,et al., *Inorg.Chem.*,2016,55 (21), p 11522.

[1]Work support in part by DOE Grant DE-FG02-07ER46354

Zahra Hooshmand Gharehbagh
University of Central Florida

Date submitted: 13 Nov 2016 Electronic form version 1.4