Electronic structure effects of a palladium impurity in a thiolate protected gold cluster.

Katarzyna A. Kacprzak, Olga Lopez-Acevedo, Hannu Häkkinen

Department of Physics, Nanoscience Center, University of Jyväskylä
Department of Chemistry, Nanoscience Center, University of Jyväskylä

katarzyna.kacprzak@jyu.fi

The stability of the thiolate protected cluster anion Au_{25}(SR)_{18}^{-1} can be explained by the “superatom” model where the gold core supports delocalized electrons in a 1S^2 1P^6 closed shell configuration. Here, we investigate the effects of a palladium atom impurity on electronic structure of Au_{25}(SR)_{18}^{-1} and derive simple rules to apply the super-atom model to bimetallic systems containing both gold and d-metals. In particular for this system we have found that the most preferable position of the palladium atom is at the center of the gold core. In that position it does not contribute to the delocalized cluster orbitals inducing a hole in the cluster P shell. Other positions considered that break the icosahedral symmetry also decrease the degeneracy of the cluster P shell. Charging properties of the palladium-doped nanoparticle will also be discussed.

Figure: The relaxed configuration of the PdAu_{24}(SR)_{18}^{-1}

