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Chirality and Electronic Structure of the Thiolate-Protected Au_{38} Nanocluster OLGA LOPEZ-ACEVEDO, Department of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, Finland, HIRONORI TSUNOYAMA, TATSUYA TSUKUDA, Catalysis Research Center, Hokkaido University, Japan, HANNU HÄKKINEN, Department of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, Finland, CHRISTINE M. AIKENS, Department of Chemistry, Kansas State University, US — Our joint computational and experimental investigation of the structural properties of the $Au_{38}(SR)_{24}$ gold protected nanocluster will be presented [1]. We have identified a new low-energy, chiral, D_3 symmetric structure that yields an excellent match between computed and measured powder XRD function. We have characterized the electronic shell structure of this nanocluster in terms of a particle-in-a-cylinder model. The CD response in the low-energy region (below 2.2 eV) of the new structure is very similar to the one reported several years ago from experiments for $Au_{38}(SG)_{24}$. The mechanism of the chiral response for low excitation energies is related to the chiral arrangement of the gold-thiolate ligand shell around the bi-icosahedral Au_{23} core. The determination of the total structure of $Au_{38}(SC_2H_4Ph)_{24}$ nanoparticles by single crystal X-ray crystallography confirmed our results [2].

[1] O. Lopez-Acevedo et al J. Am. Chem. Soc., 2010, 132 (23)
[2] Qian et al J. Am. Chem. Soc., 2010, 132 (24)

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