INTERPRETING THE ELECTRONIC STRUCTURE OF SUPERATOMIC $AU_8(PPH_3)_7^{2+}$

JONATHAN WOOD FAGAN, CHRISTOPHER J. JOHNSON, *Chemistry, Stony Brook University, Stony Brook, NY, USA*.

Atomically-precise gold nanoclusters (AuNCs) in the tens to hundreds of Au atoms size range can exhibit superatomic characteristics where the geometric and electronic stability of the cluster is driven by "shell-closing" electronic configurations. The superatomic model predicts that Jahn-Teller-like distortions stabilize clusters near the closing of a shell by rearranging the molecular orbitals. We have collected a highly-resolved electronic absorption spectrum of an ellipsoidal phosphine-protected AuNC that supports the qualitative model for non-spherical superatomic clusters. The lower energy transitions reasonably match the metal-metal transitions predicted by density functional theory (DFT) calculations. In addition, we confirm these results by a qualitative "particle-in-a-box" numerical calculation that treats the core electrons as particles in an ellipsoidal potential. The results of this qualitative model are consistent with both the results of the DFT calculation as well as the electronic structure predicted for superatomic clusters with non-spherical cores.