Optical Properties of Cage Versus Space-Filling Gold Clusters: A TDLDA Study WERONIKA WALKOSZ, JUAN C. IDROBO, SERDAR OGUT[1], University of Illinois at Chicago, JINLAN WANG, JULIUS JELLINEK[2], Chemistry Division, Argonne National Laboratory — Recent DFT computations[3] have revealed that medium size Au_n clusters form hollow cage and space-filling structures that are energetically competitive. In fact, for $n = 32$ and 50 the cage structures are more stable than their space-filling counterparts. Here we report results of large-scale computations on the optical absorption spectra of the most stable cage and space-filling forms of Au_n, $n = 32, 38, 44, 50$. The computations are performed using the time-dependant linear-response density functional formalism within the local-density approximation (TDLDA). We examine the trends in the low-energy (< 6 eV) parts of the spectra as a function of the cluster size and structure and compare them with the predictions of the classical Mie theory.

[3]J. Wang *et al.*, J. Chem. Phys. A **109**, 9265 (2005).

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