Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First Principles Absorption Spectra of Intermediate Size Ag_n ($n = 10 - 20$) Clusters KOPINJOL BAISHYA, JUAN CARLOS IDROBO, SERDAR OGUT[1], University of Illinois at Chicago, MINGLI YANG, KOBLAR A. JACKSON[2], Central Michigan University, JULIUS JELLINEK[3], Chemical Sciences and Engineering Division, Argonne National Laboratory — First principles optical absorption spectra, obtained within time-dependent density functional theory (TDDFT), for the ground state and low-energy isomers of Ag_n ($n = 10 - 20$) are presented. Overall, our theoretical results exhibit quite good agreement with spectra obtained for Ag clusters trapped in rare- gas matrices. We show that the classical predictions from Mie- Gans theory using the bulk dielectric function of Ag are in rather good agreement with experimental results and TDDFT spectra for isomers of various shapes. We analyze the orbital character of the optical excitations, and unexpectedly find that the d electrons of Ag_n clusters in this size range have a significant contribution to low-energy optical excitations, unlike the case for smaller Ag_n ($n < 9$) clusters.

[1]Supported by DOE Grant No. DE-FG02-03ER15488
[2]Supported by DOE Grant No. DE-FG02-03ER15489
[3]Supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, under Contract No. DE-AC-02-06CH11357

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Date submitted: 27 Nov 2007 Electronic form version 1.4