Abstract Submitted
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Isomeric Forms, Polarizabilities, and Optical Absorption Spectra of Ag_{11} SERDAR OGUT, JUAN C. IDROBO[1], University of Illinois at Chicago, KAROLY NEMETH, JULIUS JELLINEK[2], Chemistry Division, Argonne National Laboratory — First principles based computational results on the atomic structures, static polarizabilities, and optical absorption spectra of eight low-energy isomers of Ag_{11} are presented and discussed. The computations were performed using the static and time-dependent formalisms of the density functional theory. Comparison of the computed spectra with those measured for Ag_{11} embedded in Ar and Ne matrices[3] shows that it is the spectrum of the lowest energy isomer that exhibits the best overall agreement with the experiment. The theoretical analysis indicates that the d electrons play a more important role in optical transitions in Ag_{11} than in smaller Ag_n,$n \leq 8$, clusters.[4]

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