

Abstract Submitted  
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**Size Dependence of the Static Polarizabilities and Absorption Spectra of Gold Clusters** SERDAR OGUT, JUAN CARLOS IDROBO<sup>1</sup>, University of Illinois at Chicago, JINLAN WANG, JULIUS JELLINEK<sup>2</sup>, Chemistry Division, Argonne National Laboratory — We present results for static polarizabilities and absorption spectra for ground state structures of  $\text{Au}_n$ ,  $n = 2 - 14, 20$ , clusters calculated within static and time-dependent density functional theory. The static polarizabilities of the clusters with less than 14 atoms exhibit even-odd oscillations. The polarizabilities of  $\text{Au}_{14}$  and  $\text{Au}_{20}$  are noticeably lower. This change in the behavior of static polarizability is correlated with the transition from two-dimensional to three-dimensional structures at  $n = 14$ . The  $d$  electrons have a large effect on the optical spectra as they quench the oscillator strengths significantly and are heavily involved in low-energy excitations. The calculated spectra are compared with available experimental data and spectra obtained for  $\text{Ag}_n$  clusters.<sup>3</sup>

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<sup>3</sup>J. C. Idrobo, S. Ogut, and J. Jellinek, Phys. Rev. B **72**, 085445 (2005)

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