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Comparison of TDLDA and GW-Bethe-Salpeter Methods for Optical Excitations in Noble Metal Clusters SHING F. YIP, JUAN C. IDROBO, SERDAR OGUT[1], University of Illinois at Chicago, MURILO TIAGO, JAMES R. CHELIKOWSKY[2], University of Texas at Austin, JINLAN WANG, JULIUS JELLINEK[3], Argonne National Laboratory — We perform a comparative analysis of first principles results for optical spectra of Ag_n and Au_n ($n \leq 8$) clusters calculated within the time-dependent local density approximation (TDLDA) and the GW-Bethe-Salpeter (GW-BSE) technique. Both the TDLDA and GW-BSE calculations are performed entirely in real space based on the higher-order finite difference *ab initio* pseudopotential method. In the GW-BSE method, the screened Coulomb potential is calculated from the TDLDA polarizability. The convergence of the results with respect to various computational parameters is carefully examined. In general, the TDLDA and GW-BSE methods are in reasonable agreement with respect to peak positions at low energies, while high-energy excitations and oscillator strengths can be different. The GW-BSE results are found to be in a somewhat better agreement with the available experimental data.

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Serdar Ogut
University of Illinois at Chicago

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