Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Novel magnetism in gold and silver nanoclusters WEIDONG LUO, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Ferromagnetic (FM) ordering in transition-metal systems (solids, surface layers, nanoparticles) arises from partially filled d shells. Thus, recent observations of FM Au nanoclusters were unexpected, and an explanation has remained elusive. We report first-principles density-functional spin-polarized calculations for Au and Ag nanoclusters. We find that in highly symmetric Au nanoclusters, the highest-occupied molecular orbital (HOMO) is highly degenerate and partially filled by Au $6s$ electrons with spins aligned according to Hund's rule. The nanoclusters behave like "superatoms," with the spin-aligned electrons being itinerant on the outer shell of atoms. Similar results obtain for Ag nanoclusters. In contrast, the same kind of calculations for Pt nanoclusters find that FM ordering is controlled by the partially filled d states in the usual way, and spin polarization generally occurs in many eigenstates of the Pt clusters. This research was sponsored in part by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and by the McMinn Endowment at Vanderbilt University. Computations were performed at the National Energy Research Scientific Computing Center.

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Date submitted: 29 Nov 2007 Electronic form version 1.4