Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Magnetism of small Co clusters as a probe of *ab initio* theory
CLAUDIA TROPAREVSKY(*), The University of Tennessee and Oak Ridge National Laboratory, FERNANDO REBOREDO(+), Oak Ridge National Laboratory, ADOLFO EGUILUZ(*), The University of Tennessee and Oak Ridge National Laboratory — We report *ab initio* calculations of the electronic and magnetic properties of small Co clusters. We performed pseudopotential-based and all-electron calculations. In view of the "unwritten theorem" that electron localization enhances the electronic correlations, we have also considered the LDA+U functional, which is tailored for the strong-correlation problem associated with, e.g., partially-filled d shells. As a result of the weak dependence of the total energy on the calculated magnetic moment, the latter is very sensitive to the method employed. Thus, the magnetic moments obtained in the all-electron and pseudopotential calculations are quite different. Furthermore, the on-site Hubbard U enhances the magnetic moment significantly. The available experimental data for the magnetic moment of small clusters [Billas et al., Science **265**, 1682 (1994)] are consistent with this enhancement. Additional Stern-Gerlach measurements for smaller clusters would, in combination with our *ab initio* results, constitute a direct determination of the U for these prototypes of correlated-electron behavior. (*) Supported by NSF Grant ITR DMR-0219332 (+) Managed by UT-Battelle for the U.S. DOE under contract DE- AC05-00OR22725

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Date submitted: 20 Nov 2006 Electronic form version 1.4