

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Magnetization of iron clusters from first-principles calculations¹

JAMES R. CHELIKOWSKY, University of Texas, MURILO L. TIAGO, University of Minnesota, SHEN LI, Rutgers University, MANUEL M.G. ALEMANY, Universidade de Santiago de Compostela, Spain, YUNKAI ZHOU, YOUSEF SAAD, University of Minnesota — The magnetic moment of Fe clusters as function of number of atoms has been observed to show a slow decrease from the isolated atom value (4 Bohr magnetons) to its bulk value of 2.2 Bohr magnetons per atom. In addition, a series of peaks has been observed, for which the causes are not yet fully understood (see Billas, Chatelain, and de Heer, *Science*, 1994). We analyze the dependence of total magnetic moment, local magnetic moment, cohesive energy and other physical quantities in iron clusters Fe_n ($1 < n < 250$), and compare these results with available experimental data. We use a real-space method, pseudopotentials and first-principles DFT to obtain the properties of the cluster in its ground state. Calculations are done using the PARSEC code (www.ices.utexas.edu/parsec). We also discuss some of the recently developed capabilities of PARSEC.

¹Supported by DOE under Grants DE-FG02-03ER25585/15491, NSF grant DMR-0551195 and NERSC

Murilo L. Tiago
University of Minnesota

Date submitted: 16 Jan 2006

Electronic form version 1.4