Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electron- and Spin-Density Distributions around Zn Impurities in Cuprates CHRISTOPHE BERSIER, SAMUEL RENOLD, ERICH P. STOLL, PETER F. MEIER, Physics Institute, University of Zurich, TOM A. CLAXTON, Department of Chemistry, University of York — First-principles density-functional calculations have been performed with clusters comprising up to thirteen copper atoms in the CuO_2-plane for La_2CuO_4, $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$. The differences in the electron- and spin-density distributions that occur upon replacing one planar Cu by a Zn atom are worked out. In general, the charge densities at the oxygens adjacent or in the next shell to Zn are smaller than those calculated without Zn. Simulating in addition the influence of hole doping, it is found that Zn repels holes and favors the formation of antiferromagnetic bubbles in its neighborhood. Furthermore, a comparison of the calculated electric field gradients (EFGs) with NMR and NQR data on Zn substituted cuprates suggests that the copper satellite peaks with an EFG value somewhat smaller than that of the main line are due to Cu which are second nearest neighbors to Zn. For Cu atoms adjacent to Zn, the calculated EFG values are marginally larger and will contribute to broaden the main line.

Samuel Renold

Date submitted: 01 Dec 2004 Electronic form version 1.4