Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Test of Variational Ab Initio Methods for Studying Magnetic Hyperfine Interactions in the Phosphorus Atom. R.H. PINK, S.R. BADU, SUNY Albany, H. PAUDEL, ARCHANA DUBEY, LEE CHOW, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, T.P. DAS, SUNY Albany — The half-filled 3p valence shell of the phosphorus atom provides an interesting test of the accuracy of calculated instantaneous correlation effects. When no correlation effects are included, one obtains a sizable negative magnetic electron-nuclear hyperfine constant [1] while experiment [1] predicts a sizable positive hyperfine interaction. This is because static spin polarization effects are dominated by the 2s shell which is exchange polarized by the 3p electrons. When dynamic correlation effects are included [1], providing instantaneous admixture of s-states with the p-states, one obtains a positive contribution which overcomes the static spin-polarization effects with good agreement with experiment. We have compared the magnetic hyperfine constants calculated by currently used variational methods involving HFMBPT and DFT procedures with the earlier results [1] to examine the extent to which these two procedures successfully include instantaneous correlation effects. [1] N.C. Dutta, C. Matsubara, R.T. Pu and T.P. Das, Phys. Rev. Lett. 20, 1139(1968).

R.H. Pink
SUNY Albany

Date submitted: 19 Nov 2009 Electronic form version 1.4