Abstract Submitted
for the SES05 Meeting of
The American Physical Society

Performance of Small and Medium Split Valence Basis Sets in the Calculation of Hydrogen Bonding Properties with DFT Methods KEVIN RILEY, KENNETH MERZ, University of Florida — As the speed of modern computers increases while their cost decreases it becomes possible to consider the use of ab initio methods to calculate properties of very large molecules. These types of calculations promise to greatly enhance our understanding of the structure and function of large molecular systems. It seems that the first step to take in making calculations on very large systems would be to use a relatively inexpensive method along with small and medium basis sets such as 3-21G*, 6-31G*, etc. The least computationally expensive ab initio methods are the density functional theory (DFT) methods. One concern that one might have regarding this approach is that the accuracy of DFT methods along with smaller basis sets in describing intermolecular interactions is not very well characterized. In this study we calculate the binding energies and hydrogen bond distances for a set of three hydrogen bonded systems, $(H_2O)_2$, $(NH_3)_2$, and H_2O-NH_3 along with several density functionals and basis sets. The functionals used in this study represent each of the five categories (LSDA, GGA, meta-GGA, hybrid, and meta-hybrid) of functionals. The basis sets used here are 3-21G*, 3-21+G*, 6-31G*, 6-31+G*, and 6-31++G*.

Kevin Riley
University of Florida

Date submitted: 04 Aug 2005 Electronic form version 1.4