

**SYSTEMATIC COMPARISON OF DENSITY FUNCTIONALS.** *Xuelin Wang, Alan Lowe, Qi Wang, Justin Briggie, and Angela K. Wilson, Department of Chemistry, University of North Texas, Box 305070, Denton, TX 76203-5070, Fax: 940-565-4318, [akwilson@unt.edu](mailto:akwilson@unt.edu)*

The performance of several density functionals including B3LYP, BLYP, B3PW91, BPW91, B3P86, BP86, and MPW1K has been investigated for a series of first- and second-row molecules. The basis sets used in the calculations include the correlation consistent basis sets (cc-pVxZ, where x=D(2), T(3), Q(4), 5), augmented correlation consistent basis sets (aug-cc-pVxZ), and the new pc sets [Jensen, Journal of Chemical Physics, 201, 9113, (2001)]. Atomization energies and molecular structure are reported. A statistical error analysis including mean error, standard deviation, mean absolute deviation, and maximum error has been performed.