

ADF Calculation of Core-Electron Binding Energies

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Abstract

A total of 54 core-electron binding energies were studied with the ADF program and compared with the observed values. The results indicate that a polarized triple-zeta basis set of Slater-type orbitals is adequate for routine assessment of the performance of each method of computation. With such a basis set, seven density functionals were tested. In addition, the performance of twenty-one energy density functionals were computed from the density calculated with the statistical average of orbital potentials. Among all the choices tested, the best density functional for core-electron binding energies of C to F turns out to be the combination of Perdew-Wang 1986 functional for exchange and the Perdew-Wang 1991 functional for correlation, confirming earlier studies based on contracted Gaussian-type orbitals. For this best functional, five Slater-type orbital basis sets were examined, ranging from polarized double-zeta quality to the largest set available in the ADF package. For the best functional with the best basis set, the average absolute deviation of the calculated value from experiment is only 0.13 electron volts.