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Comparative study of Density Functionals for Calculation of Core Electron Binding Energies in First-row Hydrides and Glycine IOGANN TOLBATOV, DANIEL CHIPMAN, Notre Dame Radiation Laboratory, Notre Dame, IN 46556 — In our study we use the ΔSCF approach and a wide variety of pure and hybrid density functional approaches to study CEBEs in glycine, methane, ammonia, and water. We focus on establishing methods having potential to improve analysis of experimental X-ray photoelectron spectra of amino acids, DNA nucleosides, and large polypeptides in various environments. Several well performing density functionals are found that can reproduce experimental results within 0.2 eV on average for the absolute binding energies and also for the intramolecular and intermolecular shifts in the studied molecules. Accuracy in each approach is evaluated in reproducing experimental values for the absolute CEBEs in all four molecules and for the intramolecular and intermolecular chemical shifts between like nuclei in the same or different molecules. Promising candidates that we have found are recommended for future analysis due to their accuracy and efficiency in computation of CEBEs and chemical shifts.

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