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Electron binding energies using perturbative delta-SCF method SHUSIL BHUSAL, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — The knowledge of fundamental and optical gaps is of significant importance for organic photovoltaics. The electron binding energies estimated from the Kohn-Sham eigenvalues are significantly underestimated. Here, we use our recently outlined perturbative delta-SCF approach to compute the electron binding energies of a number of aromatic organic molecules commonly used in organic photovoltaics. Further, the electron affinities are also computed for the C60, C70 and PCBM. The results show that the perturbative delta-SCF provide adequate description of valence electron binding energies. We also applied the method to compute the core binding energies and the core-valence excited states. While the method can successfully predict the core-valence excited states the results on the core-binding energies are mixed. The strategies for improvement of the core binding energies will be discussed.

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