Computational Apparatus to Accurately Acquiring Experimental Observables: Study of Cyclopenta-Fused Polycyclic Aromatic Hydrocarbons

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Great progress has been made in electronic structure calculations through a lot of efforts towards developing accurate methods to solving the Schrödinger equation using wave functions or the Kohn-Sham equations using densities. The accuracy of computational results was mostly measured by comparison with experimental measurements. As in any experimental measurements, the system of interest is perturbed with an external component that is often not incorporated in the methods of electronic structure calculations. One of the examples is to obtain the HOMO and LUMO energy levels of a molecule that can be calculated and measured experimentally using CV or UV-Vis measurements. The HOMO and LUMO energies are important parameters in the study of electron excitation, most extensively through photoexcitation studies, and are critical in the field of catalysis, photovoltaics, photoelectronics, and luminescence. The disagreement between the electronic structure calculations and the experimental measurements comes from two sources. One is the accuracy of the method and the second is the lack of inclusion of the external component to reflect the experimental perturbation to the system being measured in the method.

In this poster, we present our efforts to include the external component in the electronic structure calculations and show the results from the studies of Cyclopenta-Fused Polycyclic Aromatic Hydrocarbons shown below that are important molecules as potential electron acceptors on photovoltaics.