ANY PARTICLE BINDING ENERGY CALCULATIONS USING PROPAGATOR THEORY

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Although accurate correlated calculations have reached an advanced state in terms of theory and computational implementation, interpretation of these results in terms of the orbital concepts based on an one particle picture is still a difficult issue. In the case of electronic structure calculations, propagator theory (PT) has been successfully used to overcome this problem, since this theory offers a systematic treatment of correlation allowing for the calculation of one particle properties, such as binding energies, while keeping a good comprimising between accuracy and computational cost [1].

We have recently extended the electron propagator theory to the treatment of any type of particle using an Any Particle Molecular Orbital (APMO) wavefunction as reference state. In the APMO approach, all particles are treated at the same level of electrons, applying the idea of a mean field of particles. The new method, called APMO/PT, have been implemented in the LOWDIN code to calculate correlated binding energies not only for electrons but also for any type of particle species in molecular systems.

Our method is a promising prediction tool for a large number of ionization experimental techniques that study processes involving nuclear and electronic dettachment, such as Electron Impact Ionization (EII) and Threshold Ion Pair Production Spectroscopy (TIPPS). In the same way, the APMO/PT approach allow us to study binding of exotic particles, such as muons and positrons, to molecules. Comparison of our predictions with the availabel experimental data and highest level calculations shows that our method can properly predict binding energies for a large range of particle species with the advantage of a low computational cost. Details of the formulation and ilustrative results will be discussed.

References

[1] Yngve Öhrn and J.V Ortiz, *Mol. Phys.* **108**, 2871, (2010).