A GENERALIZED ANY PARTICLE PROPAGATOR THEORY: PREDICTION OF PROTON AFFINITIES AND ACIDITY PROPERTIES WITH THE PROTON PROPAGATOR

J. Romero[1], M. Diaz-Tinoco[2], J. V. Ortiz[3], R. Flores-Moreno[2], A. Reyes[1]

[1]Departmento de Química, Universidad Nacional de Colombia,
Av. Cra. 30 # 45-03, Bogotá, Colombia.
[2]Departmento de Química, Universidad de Guadalajara
Blvd. Marcelino García Barragán 1451, Guadalajara, 44430, México.
[3]Department of Chemistry and Biochemistry, Auburn University,
Auburn, Alabama, 36849-5312, USA.

Electronic structure methods based on the electron propagator theory (EPT) are nowadays well established for the accurate computation of electron binding energies (EBEs) in molecular systems. One of the most appealing features of the EPT is that only a single calculation is required to obtain a detailed description of the ionization phenomena, offering a systematic treatment of correlation while keeping a good compromise 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 [2]. In the APMO approach, all particles are treated under the same footing of electrons in electronic structure methods. This new method, called APMO/PT, has been implemented in the LOWDIN code to calculate correlated binding energies, not only for electrons but also for any type of particle in molecular systems.

In this work we present the application of the APMO/PT approach to study the proton detachment process, called proton propagator (APMO/PPT). We employed this method to calculate Proton Binding Energies (PBEs), Proton Affinities (PAs) and proton hydration properties. Comparison of our predictions with the available experimental data reveals that the second order proton propagator reproduces quantitatively the experimental trends.

Results presented in this work suggest that the APMO/PPT approach is a promising tool for studying proton transfer processes and acid/base properties.

References

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

[2] J. Romero, E. Posada, R. Flores-Moreno and A. Reyes, *J. Chem. Phys.* **137**, 074105 (2012).