Analyzing Proton Acidity with the Proton Propagator Approach

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We have extended the electron propagator theory [1] using an Any Particle Molecular Orbital (APMO) reference wavefunction [2,3]. This approach, called APMO/PT is capable of describing the binding energies of any type of quantum species. In this work we present an overview of the applications of APMO/PT to study proton binding energies in molecular systems. Results obtained so far demonstrate the potential of APMO/PT to provide a common framework to study and understand one particle properties in composite systems (system containing several types of particles)

References:

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