Investigation of Isotope Effects from First Principles

Sergio A. González, Néstor Aguirre and **Andrés Reyes**
Department of Chemistry, National Universidad of Colombia, Bogotá.
areyesv@unal.edu.co

Recently, a number of theoretical methods have been proposed to include nuclear quantum effects in regular electronic structure calculations. Different applications of these methods to molecular systems containing hydrogen atoms such as hydrogen bonds have been considered and the results are very encouraging. However, the current computational implementations of the methods reported in the literature (MCMO, NEO, DEMO) present some limitations related to the number quantum nuclei types supported or the availability of the implementation. For these reasons, we have created the program Any Particle Molecular Orbital APMO/HF, where we implement the nuclear-electronic orbital method at a Hartree-Fock level of theory for electrons and nuclei.

We present some applications of the method on the study of isotope effects on molecular acidity and basicity, as well as the primary and secondary isotope effect on inter and intra-molecular hydrogen bonding and dihydrogen bonding.

The trends for electron densities, geometries and bond strength follow experimental and other theoretical results.

The current implementation of the code and theory can easily be extended to include different levels interparticle correlation.