Electronic structure theory of exotic atoms and molecules

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Theory can provide important support at all the stages of spectroscopic experiments, from planning the measurements, through extracting the properties of interest from the data, and to the interpretation of the results and their comparison to theoretically predicted values. To this end, highly accurate calculations of atomic and molecular properties are needed. In order to be reliable, such calculations must include both relativistic effects and electron correlation on the highest possible level. This is especially important for heavy and radioactive systems, where the relativistic effects have a crucial effect on the electronic structure and properties and the large number of electrons requires state-of-the-art treatment of correlation.

Relativistic coupled cluster is considered one of the most powerful methods for accurate calculations of properties of heavy many-electron systems. This approach can be used to obtain ionization potentials, electron affinities, excitation energies, hyperfine structure constants, and other properties, including the various coupling parameters needed for the interpretation of experiments that search for signatures on physics beyond the Standard Model with atoms and molecules. This method has been shown to be extremely reliable and to have very strong predictive power. Recently, we have developed a scheme that allows us to use extensive computational investigations to assign uncertainties on the theoretical predictions, facilitating the use of these predictions in experimental context.

A brief introduction to the relativistic coupled cluster method will be provided and the new development for estimation of uncertainties will be presented. The talk will focus on recent successful applications of the coupled cluster approach to properties of heavy atoms and molecules, in particular in connection to recent and planned experiments.