CIM – Ph.D. project: simulations of muonic X-ray and other new spectroscopic experiments using the novel features of muons.

Research Area and Environment

The suggested Ph.D. project focus on new emerging experimental techniques using muons (a heavy short-lived cousin of the electron) to explore the electronic and nuclear wavefunction. This new technique is still in the crib – four muon sources are available in the world at the moment - the first atomic muonic X-ray measurements has just been reported in the literature. The aim of this project is to simulate and understand the benefits and advantages of this new experimental tool. The project will develop tools for and apply simulations on atomic and molecular muonic X-ray spectroscopy, muonochromic shift spectroscopy, and ultra-fast chemical reactions with muonic molecular systems.

Your Ph.D. advisor will be Prof. Roland Lindh (principle Ph.D. advisor) and Dr. Ignacio Fdez. Galván at the Department of Chemistry – Ångström, Division of Theoretical Chemistry, and Prof. Sverker Holmgren at the Department of Information Technology, Division of Scientific Computing. The Theoretical Chemistry group has a long experience in the development of multi-configurational electron-structure methods and models, and state-of-the-art simulations of molecular reactions, electronic and X-ray spectroscopy, and photochemically induced reactions. The development of a general fermionic wavefunction model will require the development of new computational tools and procedures, these will be developed in close collaboration with our IT partners at Uppsala University.

This Project

This Ph.D. project contains three components:

(1) The development of wavefunction simulation tools that can contain fermions of different types (electrons and muons). This will be achieved by generalizing existing simulation tools in the MOLCAS quantum chemistry program suite. In particular, modules for multi-configurational electron-structure simulations including both dynamic and static electron-electron correlation will be updated. Non-relativistic and relativistic approximation will be considered. Additionally, resources specific for muons has to be developed (for example, one-particle basis sets).

(2) Simulations of atomic muonic X-ray experiments already performed. This to verify the developed methods and to provide insights into the experimental results, for example, how the nuclear charge distribution is different in isotopes with the same atomic number (see the difference of the $^{86}$Sr and $^{88}$Sr spectra above).

(3) Simulations of new spectroscopic methods based on the novel features of muons. Molecular muonic X-ray spectroscopy with chemical fingerprint (compare to ESCA and Mössbauer spectroscopy) is obvious. Muonochromic shift spectroscopy – a comparison of spectra of a molecule with a muonic molecule with the same electronic structure and total charge – will reveal imperfections in the muonic screening of the heavy atom due to the chemical bonding. Finally, muonic molecules will effectively allow us to produce transmuted species with novel isotopic composition, in that mass effects on chemical reactions can be observed and measured for non-existent isotopic atoms (for example, hydrogen exists as the isotops $^1$H, $^2$H and $^3$H, however, muonic helium will effectively be a $^4$H atom).

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