Ground and excited state properties of heavy element systems from relativistic (embedded) coupled cluster calculations

HALBERT Loïc[A], YUAN Xiang[A,B], RÉAL Florent[A], VALLET Valérie[A], <u>SEVERO PEREIRA GOMES André</u>[A]

A) Univ. Lille, CNRS, UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, F-59000 Lille, France; B) Department of Chemistry and Pharmaceutical Sciences, Faculty of Science, Vrije Universiteit Amsterdam, de Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

andre.gomes@univ-lille.fr

Accurate electronic structure calculations have become an indispensable tool to understand the molecular properties of heavy and superheavy elements. Such approaches help make sense of the underlying complex physical processes probed by experiments, or in the case such experiments are unfeasible due to the heavy elements' radiotoxicity. In this presentation I will outline our contributions to developments of coupled cluster approaches based on four-component Hamiltonians for ground[1] and excited/ionized states[2], as well as response properties[3], and discuss their application to investigating species such as actinides[4]. Furthermore, I will show how these can be combined with more approximate approaches through embedding theories, to enable the investigation of species in complex environments such as in solution[5] or at interfaces[6].

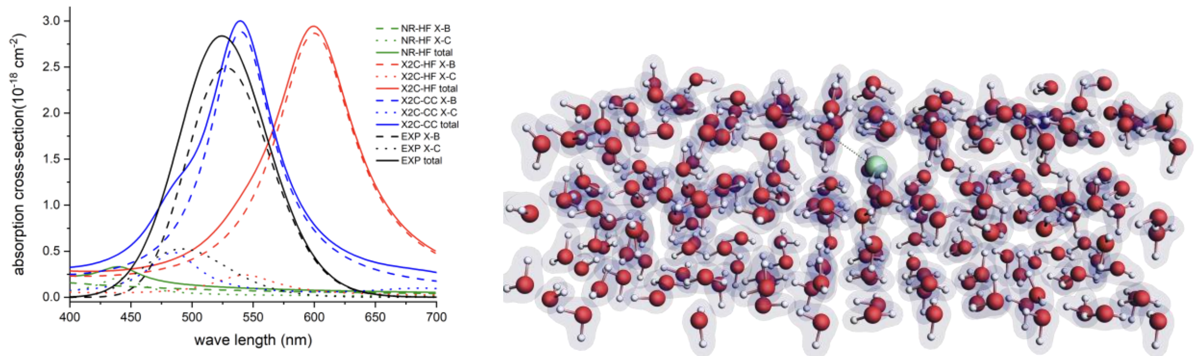

Figure 1. Left: one-photon absorption spectrum of the I_2 molecule obtained from with non-relativistic (NR) and relativistic (X2C) Hartree-Fock and coupled cluster damped response theory calculations[3]. Right: Structural model employed in CVS-EOMIP-in-DFT calculations to determine the 2p core electron binding energies of chloride and HCl on amorphous ice[6.]

<u>Keywords</u>: relativistic coupled cluster, response theory, core spectra, embedding

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