Université de Lille

FACULTÉ DES SCIENCES ET TECHNOLOGIES

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Laboratory:PhLAM

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Eventually CaPPA Work Package: WP-6 Hazard: dispersion, reactivity, deposition of radionuclides

Implementation of an efficient approach for equation of motion coupled cluster calculations of electronic excitations and ionizations of core electrons

Spectroscopic techniques involving the excitation or ionization of core electrons provide a wealth of information on the interactions of atoms within a molecule, of of a molecule with their surroudings. The outcome of experiments is, however, rather difficult to interpret without support from accurate theoretical models describing the electronic structure of the target systems.

Among the available electronic structure approaches that can be used to treat electronic states arising from the excitation or ionization of core electrons, the equation of motion coupled cluster approach, in combination with the core-valence separation (CVS) approximation (CVS-EOM-CC), has been shown to provide very accurate results [1]. While the implementation of CVS-EOM-CC can be done in a straightforward manner using projection techniques, the latter can be particularly costly in terms of memory usage and number of operations, a fact that motivation the introduction of more efficient schemes, combining CVS-EOM-CC and the frozen-core approximation (fc-CVS-EOM-CC) [2].

The goal of this project is to devise a prototype implementation of fc-CVS-EOM-CC, employing the Psi4Numpy framework [3], and employ it in the calculation of core spectra for species of environmental interest. Such an implementation can then serve as a basis for an implementation of CVS-EOM-CC in a newly developed relativistic coupled cluster code for massively parallel architectures [4].

[1] L. Halbert, ML Vidal, A Shee, S Coriani, ASP Gomes, *Chem. Theory Comput.* 2021, 17, 6, 3583
[2] ML Vidal, X Feng, E Epifanovsky, AI Krylov, S Coriani, . *Chem. Theory Comput.* 2019, 15, 5, 3117
[3] DGA Smith *et al.*, *J. Chem. Theory Comput.* 2018, 14, 7, 3504
[4] JV Pototschnig *et al.* https://arxiv.org/abs/2103.08473

Key words: core-valence separation, python implementation, equation of motion coupled cluster, core excitation, core ionization