Master 2 “Photonics, Complex and Quantum Systems (PhoCQS)”: Research Training 2023-2024

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Topic: Molecular physics

Simulating excitations and ionizations with efficient electronic structure methods

Spectroscopic techniques involving the excitation or ionization of core or valence 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. Simulation methods based on a quantum mechanical treatment of the electrons in the molecules have become invaluable tools to simulate the electronic states arising from ionization and excitation of core electrons. Among these methods, the equation of motion coupled cluster method (EOM-CC) has been shown to be very accurate and reliable [1], and treat elements acroos the whole periodic table [2] but it can be computationally very expensive and therefore less expensive, approximate methods can replace it in practice [3], including for processes involving core electrons [4].The goal of this project is to devise a pilot implementation of approximate methods for core spectra [3,4], with the help of the Psi4Numpy framework [5], and employ it in the calculation of excited and ionized states for species of environmental interest such as halide anions and halogenated molecules, and subsequently integrating it to the relativistic electronic structure code DIRAC [6].

[1] A. I. Krylov, DOI: 10.1146/annurev.physchem.59.032607.093602 (2008)
[2] A. Shee et al. DOI: 10.1063/1.5053846 (2018); L. Halbert, et al.DOI: 10.1021/acs.jctc.0c01203

(2021)
[3] L. Halbert, ASP Gomes, arXiv:2307.01342 (2023)
[4] ML Vidal et al. DOI: 10.1021/acs.jctc.9b00039 (
[5] DGA Smith *et al.* DOI: 10.1021/acs.jctc.8b00286 (2018)
[6] T Saue et al. DOI: 10.1063/5.0004844 (2020) ; Pototschnig et al. DOI: 10.1021/acs.jctc.1c00260 (2021)

Key words: python, scientific computing, equation of motion, theoretical spectroscopy