Research Project

Spectroscopic lines of ions are currently used as diagnosis tools of astrophysical and laboratory plasmas. To extract an accurate information on the plasma conditions, it is necessary to have a precise knowledge of the electronic structure of the ions chosen for the spectroscopic study. In this context, my research project regards the computational study of molecular ions such as SiHn+, CHn+ and OHn+ (n=1, 2, 3). I also simulate the x-ray absorption spectra of these molecular ions, and compare them with the results of experiments performed on the synchrotron facility SOLEIL (Bizau, J.M., et al., 2014). My simulations are performed with standard quantum chemistry packages and home-made codes. The description of the electronic structure is based on a post Hartree-Fock method - Configuration Interaction and spin-orbit coupling. The nuclear dynamics of core excited systems is treated using a wavepacket propagation method. The effects of the plasma temperature are taken into account through the population of valence excited states (triplet/singlet states).

I already performed the simulation of the x-ray absorption spectra of some mono-protonated species (SiH+, CH+, OH+). The next step is to consider the di- and tri-protonated species.

Scientific Results and Impact

I already performed the simulation of the x-ray absorption spectra of some mono-protonated species (SiH+, CH+, OH+). My calculations agree quantitatively with the experiments, which validate our computational approach. The next step is to consider the di- and tri-protonated species. In particular, we will investigate the changes in the spectrum profiles when adding hydrogen atoms to the central element (for instance in the case of SiH2+ and SiH3+).

Principal Key Facts, Communications Related to the Project and Distinctions
