Spécialité de Master « Optique, Matière, Plasmas »

Stage de recherche (4 mois minimum, à partir de début mars)

Proposition de stage (ne pas dépasser 1 page)

Date de la proposition : 24/10/2014

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Lieu du stage / *internship place*: LCP-MR, 11 rue Pierre et Marie Curie 75005 Paris

Titre du stage / *internship title*: Double Core-Hole Spectroscopy

Résumé / *summary*

The photoionisation of isolated molecules leading to formation of double core-hole (DCH) states has recently become a hot topic. Two inner shell holes can be located either at the same atomic site (single site DCH: ss-DCH) or at two different sites (two sites DCH: ts DCH). It was predicted (*J. Chem. Phys. 85, 6513 (1986)*) that for DCH states the corresponding chemical shift is much higher than for single core-hole (SCH) states and that the energy of ts-DCH states is very sensitive to the chemical environment of the atoms and to the molecular bond lengths due to the interplay between Coulomb repulsion and relaxation energies.

Due to the relatively low cross sections of DCH states and a difficulty to identify them, the first experimental observations have been performed only recently. These experiments were performed using either synchrotron radiation in combination with multi-electron coincidence spectroscopy [*Phys. Rev. Lett.* ***105****, 213005 (2010), Phys. Rev. Lett.* ***106****, 063003 (2011), Phys.Rev. Lett.* ***107****, 193004 (2011)*] or intense XFEL radiation [*Phys. Rev. Lett.* ***105****, 083005 (2010), Proc. Natl. Acad. Sci. U.S.A.* ***108****, 16912 (2011)*]. In 2013, multi-electron coincidence technique enabled detection of the so-called pre-edge states with two core holes and one electron in an excited orbital [*Phys. Rev. Lett.* ***110****, 163001 (2013)*] corresponding to simultaneous ionization and excitation of two core electrons ($K^{-2}V$).

We propose to study these novel DCH pre-edge states in molecules using a new technique, which does not require challenging multi-coincidence measurements, and provides high-resolution data with high collection efficiency. This technique takes advantage of a high-resolution high-energy electron spectrometer HAXPES (HArd X-ray PhotoElectron Spectroscopy), which was installed in 2012 as a permanent end-station at the GALAXIES beamline of the French synchrotron radiation facility SOLEIL and has since demonstrated an excellent performance [*J. Electron Spectrosc. Relat. Phenom.* ***190****, 188 (2013), J. Phys. B* ***47****, 124031 (2014), Nature Communication* ***5****, 4069 (2014)*]. The outstanding instrumental performance of HAXPES spectrometer in combination with the extremely narrow bandwidth of the GALAXIES beamline so far has no analogue in the world and provides an unprecedented opportunity to perform high-resolution high-energy electron spectroscopy in the hard x-ray regime for dilute systems. The recently performed preliminary measurements of the DCH pre-edge states in CS_2 molecule demonstrate good agreement with the theoretical simulations.

We expect to record complete pre-edge spectra related to DCHs in each of different representative samples, Ar, SO2, OCS, H2S, CF3Cl, CH3Cl, CH3SH, CH3SeH, CH3I, CF3I and Xe. This is possible due to the photon energy range available at the GALAXIES beamline, which covers the DCH states of the $K^{-2}V$ shells of the molecules containing the second row elements such as S, Cl, Ar and the DCHs in the $L^{-2}V$ shells of the third row elements (Se, I, Xe). We will take advantage of a close collaboration with Stéphane Carniato, professor at LCPMR, for theoretical simulations of the experimental spectra.

Toutes les rubriques ci-dessous doivent obligatoirement être remplies

Ce stage pourra-t-il se prolonger en thèse ? *Possibility of a PhD* **? : YES**

Si oui, financement de thèse envisagé/ *financial support for the PhD***:** LabEx MiChem and Gothenburg University (Sweden)

Lasers, Optique, Matière		Lumière, Matière, Interactions	**X**
Plasmas : de l'espace au laboratoire			

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