Probing quantum phenomena in atoms and molecules with soft X-ray RIXS at Sirius

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The quantum mechanical properties of small molecules provide the basis for our quantitative understanding of chemistry and a testing ground for new theories of molecular structure and reactivity. The chemical properties of small molecules continue to present rich challenges at the chemistry/physics interface since these molecules exhibit properties in isolation, and interact with their environments, in ways that are not yet fully understood. From a theoretical point of view, these features can only be explained if the quantum nature of the atomic nuclei is considered together with the possible couplings between nuclear and electronic degrees of freedom. With modern methods, small molecular systems can be investigated in extraordinary detail by high-resolution spectroscopic techniques, and by complementary theoretical and computational advances. This combination of cutting-edge approaches provides rigorous tests of our understanding of quantum phenomena in molecules and atoms. Among the new developments, the Resonant Inelastic X-ray Scattering (RIXS) stand out as a versatile technique to probe the electronic structure of molecular systems in gas, liquid and solid state [1]. For instance, the coupled electronic and nuclear motions may lead to complex structural or dynamical features that can now be observed experimentally [2]. This valuable tool will be soon available to the Brazilian community at the IPE beamline of Sirius, the 4th generation synchrotron source under construction in Campinas. In this seminar, we will present an introduction to IXS methods with particular attention to the resonant inelastic X-ray scattering technique (RIXS). We will discuss the basic aspects of the techniques using selected examples from the literature and present the current status of the development of the beamline, spectrometer and associated instrumentation.
