Resonant Inelastic Soft X-ray Scattering with Vibrational Resolution

Jan-Erik Rubensson

Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

E-mail: jan-erik.rubensson@fysik.uu.se

Resonant inelastic X-ray scattering (RIXS) reflects fine details in electronic structure and dynamics. The process is site specific on the atomic length scale (sub-nanometer) and time specific on the timescale for nuclear and electronic rearrangements (femto- to attoseconds). Consequently, RIXS spectroscopy has a tremendous potential in atomic and molecular, chemical and condensed matter physics. RIXS techniques have, however, suffered from the lack of adequate radiation sources. In practice this has limited the spectral quality and only a fraction of the inherent advantages have been exploited.

The performance of the SAXES set-up at the ADRESS beamline has changed the picture completely, and now many of the inherent features of the RIXS method can be exploited. The energy resolution ($E/\Delta E \sim 10000$) allows for a clear separation of vibrational excitations in molecular systems. This directly provides detailed information about ultrafast dynamics, and facilitates accurate mapping of ground and excited state potential surfaces. In addition, the phenomenology in simple systems gives new information about the scattering process itself.

Measurements on free molecules (O_2, NO, N_2, NO_2, CO_2) and liquids (acetone, water) will be presented, and discussed in terms of *ab-initio* multimode scattering calculations. Implications for RIXS studies for molecular materials and processes will be discussed.