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Charge order as seen by resonant X-ray scattering: crystallography in the twilight zone

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The recent years have witnessed an extraordinary development in the study of electronic orderings in strongly correlated systems, a subject that was initiated back in the mid fifties. This development is, to a large extent, due to the advent of high flux, high brilliance 3rd generation synchrotron light sources (ESRF, APS, Spring-8 and many others actually being built) and the possibility of directly measuring the electronic orderings themselves and not the lattice distortions induced by them. Charge orderings, orbital orderings and particularly odd magnetic orderings have been thus revealed for the first time and studied in resonant X-ray scattering (RXS) experiments. By virtue of its wavelength tunability these X-ray sources can easily operate at the absorption edges of a given atom and probe unoccupied final states of the atom. As we are dealing with electronic orderings, both crystallography and resonant atom spectroscopy are concerned and the goal is to optimize both simultaneously: to be able to collect data with the resolution of the spectroscopy techniques and in wide variety of Bragg reflections to finally be capable to render all data consistent within a model. Thereby the experimental protocol is of tantamount importance and has to be worked out prior to any such undertaking. Note that the accuracy needed here is orders of magnitude greater than that required by, for instance, MAD techniques. The underlying crystallography that one may end up doing in these electronic orderings is thus the twilight zone of both well known disciplines. In this presentation we will discuss several examples where charge ordering is at the core of relevant features of the compounds: (a) NaV_2O_5 [1,2] and the onset of a spin-singlet quantum ground state, (b) NdNiO₃ [3] where charge disproportionation at the metal sites or a ligand hole ordering bond center ordering, triggers the magnetic ordering and further stabilizes the magnetic structure and finally (c) Fe_3O_4 [4] where the observation of charge ordering by RXS requires a very special care of the experimental conditions. Recipes and insights on the way RXS experiments should be carried out and further analyzed will be given as well.

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Elucidating the structure of liquid crystal phases using resonant x-ray scattering

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The use of resonant x-ray scattering to determine structures in liquid crystal systems is a powerful experimental technique that utilises 'forbidden reflections' to determine the subtle differences in interlayer orientation that can differentiate several smectic systems. The technique relies on the materials containing an atom to which the x-ray energy can be tuned, usually Sulfur or Selenium. Experiments are often carried out on freestanding films that provide a highly monodomain structure that allows high resolution measurements to be made, and hence structural details to be determined. This talk reviews the successful use of resonant x-ray scattering in the study of the ferroelectric, antiferroelectric and ferrielectric phases of liquid crystals. It reports recent high-resolution, resonant, polarized x-ray scattering experiments performed on free-standing films of several materials that exhibit remarkably wide ferrielectric phases. Polarized resonant x-ray scattering is shown to be an unrivalled method in determining the detailed structure of these complex phases.

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