

Séminaire SOLEIL

Nonresonant inelastic x-ray scattering spectroscopy : recent applications at the University of Helsinki

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Invité par Jean-Pascal RUEFF

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Séminaires

Inelastic x-ray scattering spectroscopy is a photon-in/photon-out method that has developed into mature but novel tool for studies of energetics of electron states in matter. Some of the latest results and ideas on using it for three-dimensional imaging [1], and studying various complex and less complex materials, will be presented.

One of the powerful inelastic x-ray scattering methods is so-called x-ray Raman scattering, where a core electron is excited by an inelastic scattering process. This method yields similar spectra to those of soft x-ray absorption spectroscopy (sXAS) but the results can be obtained using hard x-rays in the 10 keV photon-energy regime. For example, the structure of water in elevated temperatures and pressures up to the supercritical regime has been studied using this method [2], and comparisons to density-functional-theory calculations based on ab-initio molecular dynamics simulations yield insight to the microscopic structure of this elusive system in extreme conditions.

X-ray Raman scattering spectroscopy has also been used to reveal fine structures of the 4d-4f excitations in various rare earth compounds; recent high-energy-resolution results on La, Ce, Pr, Nd, Sm, and Tm will be presented.

Inelastic x-ray scattering can also be used to create excitations within the 3d manifold in transition metal oxides, i.e. so-called crystal field excitations that typically span energy ranges of 1-3 eV.

Results for the metal-to-insulator transition in V₂O₃ and for the temperature dependence of the crystal-field excitations in CuO [3] will be presented.

[1] "Direct tomography with chemical-bond contrast"; S. Huotari, T. Pylkkänen, R. Verbeni, G. Monaco, and K. Hämäläinen, *Nature Mater.* 10,489 (2011)

[2] "Microscopic structure of water at elevated pressures and temperatures"; Ch. J. Sahle et al., *PNAS* 110, 6301 (2013)

[3] "Temperature dependence of crystal field excitations in CuO"; S. Huotari, L. Simonelli, Ch. J. Sahle, M. Moretti Sala, R. Verbeni, and G. Monaco, arXiv:1310.6730 [cond-mat.str-el] (2013)

**Ce séminaire sera suivi d'une pause-café**

Formalités d'entrée : accès libre dans l'amphi du Pavillon d'Accueil. Si la manifestation a lieu dans le Grand Amphi SOLEIL du Bâtiment Central, merci de vous munir d'une pièce d'identité (à échanger à l'accueil contre un badge d'accès).

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