

Séminaire SOLEIL

# Tools for a Next Generation Theoretical X-ray Beamline : XAS, XES, and RIXS

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Invité par Fausto SIROTTI

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Grand Amphi SOLEIL

Prospects for the development of a next generation theoretical x-ray beamline are discussed. Such tools are important for a quantitative analysis of experiments carried out at next generation x-ray sources. In particular we discuss the theoretical tools needed for improved simulations of x-ray spectra, e.g., XAS, XES, and RIXS, including real-time probes from XFEL sources. First we review current techniques and extensions for core-spectra based on the GW/BSE method, i.e., 1) a real-space Green's function approach now implemented in the FEF9 code [1]; and 2) a k-space approach implemented in the code OCEAN (Obtaining Core Excitation using ABINIT and NBSE)[2]. Both of these methods include ab initio treatments of inelastic losses and vibrational effects. In addition improvements are discussed for treating correlation effects including Hubbard corrections, multiplets, satellites, and multi-electron excitations, which are observed in many systems. Third we discuss an alternative real-time approach based on real-time methods for obtaining core-level x-ray response in time-dependent sources. These approaches are illustrated with applications to several core-level spectra including XAS and RIXS in complex systems.

To complete these developments, we discuss how such a theoretical beamline can be implemented within a scientific cloud computing environment, e.g., on the Amazon EC2 [3]. All the relevant codes for this beamline can be precompiled and optimised on such cloud-computing resources and thus readily available to the scientific community.

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[1] J. J. Rehr et al., Comptes Rendus Physique 10,548 (2009).

[2] J. Vinson et al., Phys. Rev. B 83, 115106 (2011) [3] J. J. Rehr, et al. Scientific Computing in the Cloud, CISE, 12, 34 (2010).



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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