Réunions scientifiques

Séminaires

Séminaire SOLEIL

Unraveling the mysteries of complex systems with x-ray spectroscopies : ab initio theory and computation vs experiment*

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Invité par A.M. FLANK et N. JAOUEN

Lundi 10 mai à 14h00
Grand Amphi SOLEIL

There has been dramatic progress in recent years both in ab initio calculations and in the interpretation of various x-ray spectroscopies, e.g., x-ray absorption spectra (XAS) and inelastic x-ray scattering (IXS). Together with advances in analysis methods, these developments now permit an interpretation of experimental data in terms of structural and electronic properties of a material. We first summarize these advances, focusing on a heuristic explanation of the real-space Green's function (RSGF) approach used in the FEFF code [1]. The RSGF approach builds in some key many-body corrections to the independent particle approximation, and thus differs from conventional electronic structure and quantum chemistry calculations based on wave-functions and density functional theory. The method is illustrated with applications to complex materials ranging from catalysts and minerals to bio-structures and aqueous systems. Finally we discuss some recent theoretical developments leading to a new generation of codes including FEFF9 [2] and the Bethe-Salpeter Equation code OCEAN [3].

[1] J. J. Rehr and R. C. Albers, Rev. Mod. Phys. 72, 621 (2000).
[2] J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, Y. Takimoto, F. Vila, Comptes Rendus Physique, 10, 548 (2009).
[3] J. Vinson, E. L. Shirley, J. J. Rehr and J. J. Kas, UW Preprint (2010).

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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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