THEORETICAL SPECTROSCOPY
The ETSF Users' Newsletter

ETSF Users' Meeting and Training Day for Experimentalists

Friday 22 October 2010 at the Ecole Polytechnique (Paris) will take place a one day training specifically dedicated to experimentalists. The emphasis is on excited states theory and calculations, in particular valence electron excitations. The aim is not to learn technical details of theoretical methods, but to get insight about the fundamental ideas, in-principle possibilities and limitations, and in-practice performance and shortcomings.

The 2010 ETSF users' meeting will be integrated in the programme. It aims to exchange ideas between ETSF scientists and users, collect suggestions to improve the services offered by the ETSF to the scientific community and foster future collaborative projects.

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Programme: http://www.etsf.eu/system/files/2010ETSFSchool.pdf

ETSF
European Theoretical Spectroscopy Facility

Welcome to the sixth edition of the ETSF Users' Newsletter. In this issue, the beamline presentation and the User Corner are both dedicated to X-ray Spectroscopy. Besides, you are invited to a one day introductory training on theoretical spectroscopy (see page one). Don't miss the upcoming events listed on page two.

Submission deadline for the Autumn evaluation of the ETSF call for proposals: 26 October 2010, 17:00 (CET).

X-ray Spectroscopy Beamline

The x-ray spectroscopy (XRS) aims to develop theoretical techniques for quantitative calculations of the various core-level spectroscopies measured at modern x-ray synchrotron facilities. These include x-ray absorption spectra (XAS), i.e., x-ray absorption fine structure (XAFS) and x-ray absorption near edge structure (XANES), and related spectra such as x-ray magnetic circular dichroism (XMCD), which are widely used to understand structural, vibrational and magnetic properties of materials.

The primary engine for these calculations is the FEFF code [1]. This approach uses a Real-space Green's function (RSGF) approach that builds in many-body effects such as inelastic losses, core-hole screening, and Debye-Waller factors [2,3]. Additional many body effects are treated with TDDFT, BSE, and spectral functions [3]. The RSGF approach in FEFF can also calculate core-level x-ray scattering factors (including diffraction anomalous spectra), x-ray emission spectra (XES), non-resonant X-ray Raman scattering (XRS) and core-level electron energy loss spectra (EELS) and various optical constants from the UV-x-ray energies. The approach is generally applicable to aperiodic systems throughout the periodic table, including bulk, surfaces, nano-structures, liquids, biostructures and other disordered materials as illustrated, e.g., in [4,5].

Beamline Coordinator: Prof. John Rehr
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[1] See http://leonardo.phys.washington.edu/feff/
[2] J. J. Rehr and R. C. Albers, Rev. Mod. Phys. 72, 621, (2000).
[3] John J. Rehr et al., Comptes Rendus de Physique 10, 548 (2009).
[4] John J. Rehr et al., Phys. Chem. Chem. Phys. 12, 5503 (2010).
[5] Veronesi et al., Phys. Rev. B 82, 020101 (2010).

User Corner: X-ray Spectroscopy

1) Prof. Boscherini, you work on X-ray spectroscopy at the Department of Physics, University of Bologna (Italy). Which scientific problem are you currently working on?

We are investigating novel ways to analyze and interpret X-ray Absorption Fine Structure (XAFS) spectra of metalloproteins. One of the problems in this field is the difficulty of taking into account thermal vibrations avoiding *ad hoc* or "blind fitting" approaches, also in consideration of the high number of multiple scattering contributions. Our method is to use *ab initio* DFT calculations to determine the equilibrium structure and the dynamical matrix as a starting point to interpret the XAFS spectrum. This leads to a very robust analysis ap-proach which avoids the pitfalls of fitting with many free parameters.

2) How (and when) did you get in touch with the ETSF?

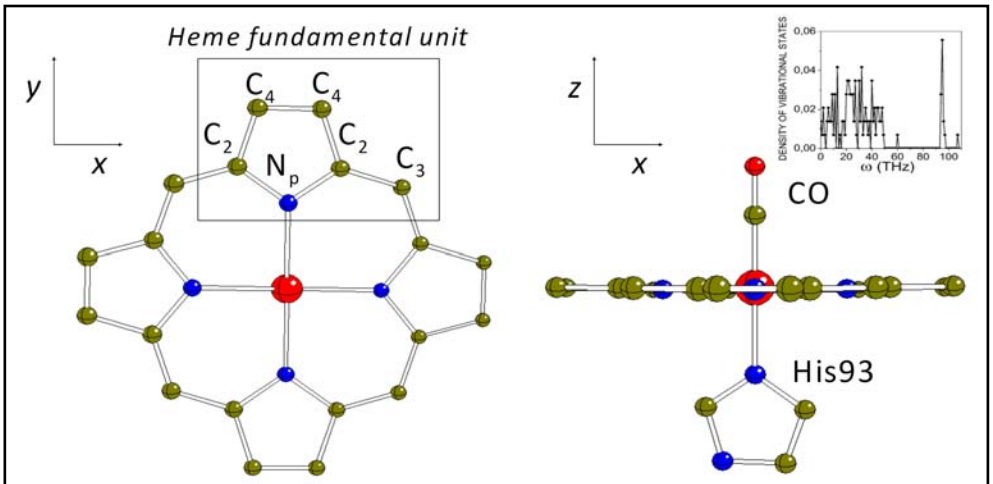
We received the announcement of the call for proposals by email in 2008. We submitted a proposal and were successful. The project started in April 2009.

3) What did you expect from your ETSF user project?

We expected support on the simulation method and especially on the way to handle thermal vibrations.

4) What was the result?

In the case of carbonmonoxy myoglobin we obtained an excellent comparison between the experimental spectrum and its simulation for the main part of the molecular structure (the heme plane), without any structural fitting parameters. Also, we were able to determine the geometry of the CO ligand by fitting, using as free parameters only those related to this residue. This result, recently published in Physical Review B as a Rapid Communication [Veronesi et al., PRB 82, 020101 (R) (2010)] illustrates the power of this kind of joint experimental – theoretical approach.



Graphical representation of the Fe site in MbCO. The inset reports the vibrational density of states calculated using density-functional perturbation theory.

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ETSF Agenda

11-15 October 2010 ETSF Workshop on Electronic Excitations (Berlin)

22 October 2010 Introductory Training on Theoretical Spectroscopy and ETSF Users' Meeting (Paris)

26 October 2010 Submission deadline for the Autumn evaluation of the ETSF call for proposals

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