THEORETICAL SPECTROSCOPY
The ETSF Users' Newsletter

ETSF training modules and tutorials

A major concern of the ETSF is to spread its knowledge and experience in theoretical spectroscopy both from the view point of theoretical physics and the implementation in software packages. Training events and online modules are available for **users, both theoreticians and experimentalists, and students** with different background in theoretical physics.

The ETSF regularly organizes **training events** such as the hands-on TDDFT schools and workshops or in the Spectroscopy Lectures. Training material of past schools and events are available on the ETSF website. The next tutorial addresses experienced users. It focuses on the development and maintenance of atomic-scale software (CECAM, Spain, 21-25 June 2010, www.cecam.org/workshop-467.html).

Besides these events, an **on-line training portal** on theoretical spectroscopy methods is being developed. The training modules are organized in two levels, an introductory level that outlines all the essential topics and a tutorial level that complements more complex subjects and derivation.

www.etsf.eu/services/training

ETSF
European Theoretical Spectroscopy Facility

Welcome to the fifth edition of the ETSF Users' Newsletter dedicated to training. On page 2, you will find the agenda and the User Corner: Lorenzo Sponza presents his training project. Don't miss it! More training opportunitites are presented on the first page. The beamline presented in this issue is Photoemission Spectroscopy.

Submission deadline for the Spring evaluation of the ETSF call for proposals: 21st April 2010, 17:00 (CET).

Photoemission Spectroscopy Beamline

The Photoemission Beamline is dedicated to studying, describing and predicting the outcomes of electron spectroscopies such as Photoemission (PES) and Auger Spectroscopy (AES). PES probes the energy levels of electrons or, more in general, the nature of chemical bonding and electron motion in a substance. The electronic transitions are selected by tuning the energy of the incident radiation and the electrons bring information via the Kinetic Energy, the direction of their momentum and the electron spin.

In a photoemission experiment, the main structures are due to photoelectrons. There are however also other peaks, of similar width but different energy, unrelated to incident photons, due to Auger recombination. In a proper theoretical formulation, PES and AES should be treated on equal footing as a single coherent process.

Typical topics of interest of the Photoemission Beamline are quasiparticle energies and band-gaps, core and valence photoemission, angle resolved photoemission, thermal effects and electron-phonon coupling, lifetimes of electrons and holes, spectral functions, Auger spectra. The main theoretical methods used are Density Functional Theory and Many-Body Techniques. Such investigations are performed for systems such as metals, semiconductors, molecules, surfaces, nanosystems, including e.g. transition metals and their alloys, transition-metal oxides, graphite and graphene, to mention some representative examples.

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User Corner: Dedicated Training at the ETSF

1) Mr Sponza, you work on magnetized materials at IOM-CNR with the group BEAR of S. Nannarone (Trieste, Italy). Which scientific problem are you currently working on?

We are presently studying the propagation of electromagnetic fields inside magnetized materials. My role was to write a code to simulate the reflectivity from anisotropic media, arranged, if necessary, in a layered structure. As a basic input of this code, we need the dielectric tensor for each layer. For a correct description of the field inside the sample, the reflected and the transmitted ones, it is essential to have an accurate description of the dielectric tensor, and ab-initio techniques are a good way to reach it.

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

The code written in Trieste was running properly on model systems. But to run the code on real systems, we needed complementary competences in ab initio techniques. In April 2009, with the help of S.Nannarone, I asked for a training of 4 months in order to learn techniques to compute the dielectric tensor of the material we want to simulate.

3) Why did your group chose to submit a training project rather than a collaborative research project?

Stefano Nannarone and the group preferred me to learn the methods rather than to apply them blindly. On one hand, it is a gain of competences for our group in Trieste, and on the other hand, it was didactic for me, and I am happy for this.

4) What did you learn during your stay at the ETSF Paris node?

I worked essentially on DFT and TDDFT using both ABINIT and DP codes. Of course, in university, I had courses about DFT, but I had to learn a lot to finally understand TDDFT... If I have. Also learning how to use the two codes has been a long procedure.

Moreover there are many things linked to these main topics. For instance, I had to learn how to use DOS and band-structure calculations. I also started some simulation in the GW approximation. And, last but not least, I learned more about computers, compilers and libraries.

And French, too!

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ETSF Agenda

21 April 2010 Submission deadline for the Spring evaluation of the ETSF call for proposals

21-25 June 2010 CECAM Tutorial - development and maintenance of atomic-scale software (Spain)

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

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