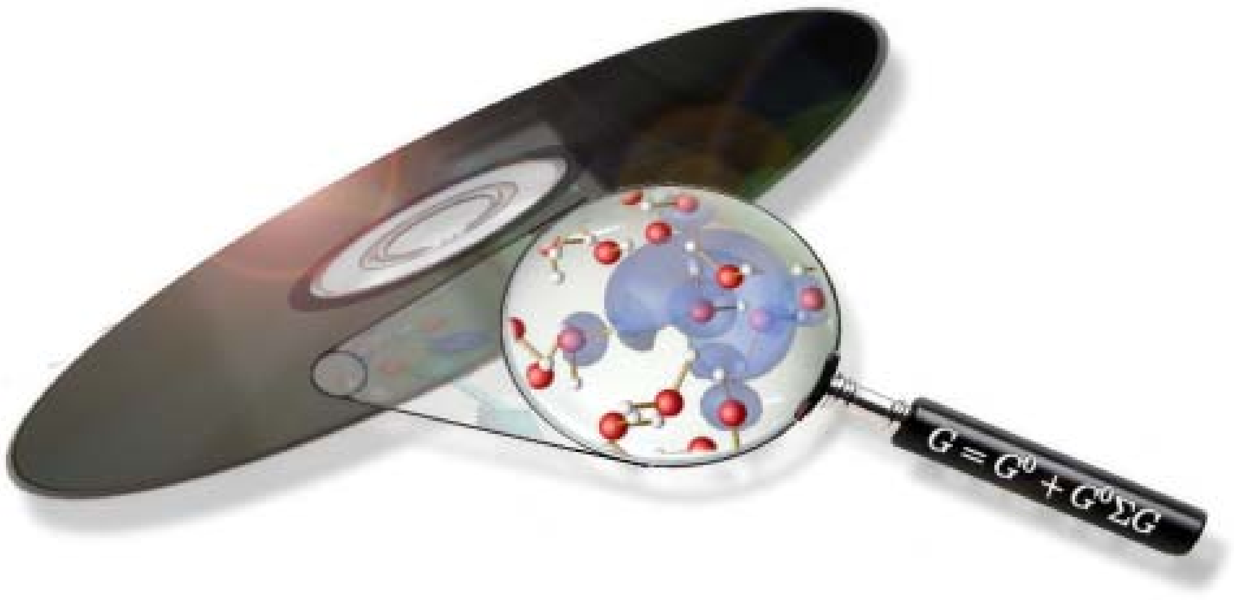
# INTRODUCTION PACKAGE FOR NEW USERS

## (version 1.2)



# Opening new eyes to the Nanoworld

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CAPACITIES

e-infrastructure

# THE ETSF IN A NUTSHELL

## WHAT IS THEORETICAL SPECTROSCOPY?

Theoretical Spectroscopy is the study, using a powerful combination of quantum-based theories and sophisticated computer simulations, of the interaction between matter and radiation (electrons, light, X-rays, lasers, and other modern photon sources). Such an interaction leads to the appearance of electronic excitations whose characterization allows the researchers to be able to:

- analyse and explain experimental data (ellipsometry, EELS, Raman, IR, NMR, X-Ray, ARPES, STS, I/V transport, etc.)
- predict properties of new materials, beyond experiments
- achieve remarkable technological and fundamental breakthroughs, such as new functionality (optoelectronics) or biological applications

## THE ETSF CONCEPT: OUR MISSION STATEMENT

The **European Theoretical Spectroscopy Facility (ETSF)** is a research and knowledge centre dealing with problems of spectroscopy and the properties of electronic excited states in matter, particularly nanostructures, nanoelectronics and the energetics of atomic motion on the nanometre scale. Within the ESTF, expertise, theory and the associated software are used in different ways according to the interest and background of the users.

The ETSF concept is summarized in our **mission statement**:

> The **European Theoretical Spectroscopy Facility** (ETSF) is a User Facility charged with providing support and service to research under way in academic, government and industrial laboratories. All domains that need knowledge about electronic excitations, transport and spectroscopy will benefit from the ETSF, such as condensed matter physics and chemistry, biology, materials and nano science. The ETSF provides users with *computer codes*, *background knowledge*, *training* and *collaborators* to enhance their studies of the electronic and transport properties of complex or nanoscale materials. Its focus is on the rapid transfer of groundbreaking fundamental knowledge of matter on the quantum-mechanical level to detailed understanding and future-oriented design of prototypical or technologically relevant systems.

The ETSF can be seen as the *theoretical equivalent of a synchrotron* structured around "theory beamlines" delocalised over the available infrastructure of the different nodes that constitute the core of the ETSF.

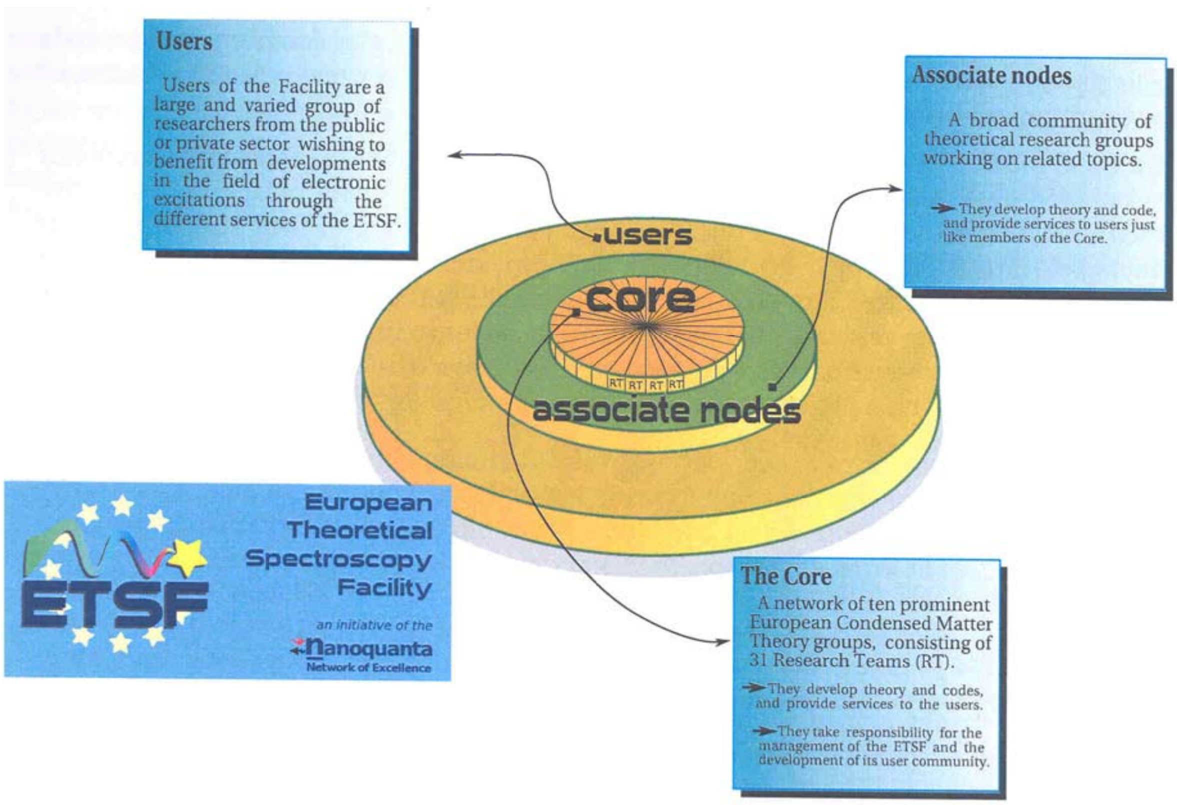
# THE STRUCTURE OF THE ETSF

The ETSF is built around a **core of ten scientific nodes**, whose primary research interest is focused on theoretical spectroscopy and/or electron transport. The core nodes are committed to the scientific, structural and service development of the ETSF. The core nodes take responsibility for management and out-reach in the ETSF. One of the core nodes (Louvain la Neuve) is the central node that hosts the President of the ETSF and the ETSF executive director, thus coordinating the ETSF overall strategy.

The ETSF also incorporates a community of expert research groups, the **associate nodes,** also working in the field of theoretical spectroscopy and electron transport. Their competences are complementary to those of core or other associate nodes, and are included in the scientific dynamics of the ETSF, developing new theories and/or scientific codes. However, they do not contribute to the ETSF management and administration.

**Users** are a much larger and more varied group of researchers from the public or private sector wishing to benefit from developments in the field of electronic excitations, through the use of the ETSF theoretical and numerical tools and services.

In addition, the ETSF has an **administrative structure** formed by a Steering Committee, a Governing Board, and an Advisory Board.



## OBJECTIVES

**We aim to broaden the access to the knowledge and the expertise we have built in the field of theoretical spectroscopy across the public and private sector.**

We are able to achieve this by:

- Developing **theory**
- Developing **scientific software**
- Providing **training** in theoretical and computational techniques
- **Undertaking scientific projects on demand**

## BEAMLINES

Reflecting the structure of a synchrotron facility, the ETSF is divided into seven beamlines, each of which is concerned with a specific scientific topic. The following short descriptions will help you to decide in which part of the ETSF your project fits. Please contact the beamline scientist for further details.

**A beamline scientist is responsible for the contact with the users of each line. In particular, he/she serves as the contact person for users who want to submit a proposal to the ETSF.**

### Optics Beamline

**Coordinator:** Dr. Olivia Pulci (Olivia.Pulci@roma2.infn.it)
University of Rome Tor Vergata, Rome, Italy

**Phenomena**: Linear optics (absorption spectra, cross sections, reflectance anisotropy, surface differential reflectivity, birefringence, chirality). Second Harmonic Generation.

**Systems**: Surfaces, dots, wires, nanotubes, molecules. Bulk materials. Amorphous materials. Liquids.

**Theoretical methods:** Density Functional Theory (DFT), Time-Dependent DFT (TDDFT). Many-body methods: *GW* approximation, Bethe-Salpeter equation (BSE). Tight binding, etc.

**Codes:** Abinit, EXC, Yambo, Quantum Espresso, CPMD, FHI96, Octopus, DP

### Energy Loss Beamline

**Coordinator:** Dr. Francesco Sottile (francesco.sottile@polytechnique.edu)
Ecole Polytechnique, Palaiseau, France

**Phenomena**: Electron Energy Loss Spectroscopy. Reflection Electron Energy Loss

Spectroscopy. Inelastic and Coherent X-ray Scattering.
**Systems:** Bulk, surfaces, and nanostructures.
**Theoretical methods**: DFT, TDDFT, BSE.
**Codes:** DP, EXC, Yambo

## Quantum Transport Beamline

**Coordinator**: Dr. Peter Bokes (peter.bokes@stuba.sk)
Slovak University of Technology, Bratislava, Slovakia

**Phenomena**: Transients, memory effects, bound states, electromigration. Conductance and/or I-V curves of molecular and atomic junctions. STM, STS.
**Systems:** Metals, organic chains, atomic chains, carbon nanotubes
**Theoretical methods:** Tight-binding, classical nuclear dynamics. DFT, TDDFT. *GW*, non-equillbrium Green's Functions.
**Codes:** ABINIT, SfhingX, GWST

## Time-resolved Spectroscopy Beamline

**Coordinator**: Dr. Miguel Marques (marques@teor.fis.uc.pt)
CNRS, University of Lyon, France

**Phenomena**: Time-resolved excitations, photoinduced chemical reactions, time-resolved fluorescence spectroscopy. Strongly non-linear optics, attosecond dynamics, ionization yields, high-harmonic generation. Quantum-control of electronic/ionic processes.
**Systems**: Molecules and clusters.
**Theoretical methods**: TDDFT
**Code:** Octopus

## Photo-emission Spectroscopy Beamline

**Coordinator**: Dr. Claudio Verdozzi (Claudio.Verdozzi@teorfys.lu.se)
Lund University, Lund, Sweden

**Phenomena**: Core and valence photoemission, angle resolved photoemission, thermal effects and electron-phonon coupling. Auger spectra
**Systems**: transition metals and their alloys, transition-metal oxides, surfaces, molecules, simple metals, semiconductors, graphite.
**Theoretical methods**: DFT, *GW*, T-matrix approximation.
**Code:** ABINIT

## X-ray Spectroscopy Beamline

**Coordinator**: Prof. John Rehr (jjr@phys.washington.edu)
University of Washington, Seattle, USA

**Phenomena**: Core level X-ray absorption spectra (XAS): X-ray absorption fine structure (XAFS), X-ray absorption near edge structure (XANES), and X-ray magnetic circular dichroism (XMCD). X-ray scattering factors, X-ray emission

spectra, non-resonant X-ray Raman scattering and electron energy loss spectra.
**Systems**: Bulk, Surfaces and Nanostructures. Liquids.
**Theoretical methods**: Real-space Green's function (RSGF) approaches including *GW*, core-hole screening, and Debye-Waller factors. TDDFT, BSE.
**Code:** ABINIT

## Vibrational Spectroscopy Beamline

**Coordinator**: Prof. Gian-Marco Rignanese (gian-marco.rignanese@uclouvain.be)
Université Catholique de Louvain, Louvain-la-Neuve, Belgium
**Phenomena**: Infrared absorption: IR frequencies and intensities; Raman scattering: Raman frequencies and intensities.
**Systems**: Bulk, Surfaces and Nanostructures.
**Theoretical methods**: Density Functional Perturbation Theory (DFPT).
**Codes:** Abinit, Octopus, and Yambo

# SERVICES PROVIDED BY THE ETSF

## BECOMING A USER OF THE ETSF

**A potential user of the Facility would be any researcher from the public or private sector wishing to benefit from developments in the field of electronic excitations.**

The services and benefits that you will obtain from being an ETSF user are:

- **Direct use of ETSF software** with the help of publications, manuals and tutorials published by the ETSF. You can download the programs and documentation from our web page **http://www.etsf.eu**. Read more on page 10.
- **Participation in training events** on the use of ETSF software. Read more on page 12.
- **Proposition of an ETSF project.** If there is a simulation of spectroscopy that would be of interest to you but that you cannot fully develop by yourself, you may propose a project that requires partial- or full-work of ETSF personnel. The typology of the projects comprise:
  - **research projects** address specific scientific problems. ETSF scientists will work in close collaboration with the proposer, employing computational resources and scientific software provided by the ETSF;
  - **training projects** provide dedicated trainings on topics in theoretical spectroscopy (theory, methodology, software, *etc.*), delivered to individuals or groups, at the user's site, an ETSF node, or at another suitable place.

  The full procedure to submit a project is explained in the subsection "user-projects", on page 13.
- **Receipt of the electronic Users' Newsletter** twice a year. It informs you of the latest news of the ETSF, its services and the next submission deadline.
- **Discuss on the ETSF Users' Forum**: ask a question about the call, about ETSF capabilities, discuss needs for theoretical spectroscopy, etc.
  http://www.etsf.eu/forum/7

To become a user of the ETSF is very simple. Just use one of the following ETSF services and you will be added to the ETSF User Community:

- submit a proposal, no need to be successful
- subscribe to a training session

or ask for it directly to the ETSF Centre for Users and Technology (see page 13).

To unsubscribe, you should also contact the ETSF Centre for Users and Technology

# ETSF SOFTWARE AND TOOLS

The ETSF highly efficient computational software plays a crucial role in bridging the gap between theoretical methods and real applications. ETSF scientists have developed a great variety of efficient computational programs, libraries and tools aiming at first principle modelling of real materials. Another important component of ETSF is the integration of code developments. Steps have been taken in the direction of standardization of files, easing the transferability and widespread use of ETSF software.

## ETSF *ab-initio* scientific codes

*Ab initio* codes developed within the ETSF cover different application regimes ranging from molecules and nano-scale clusters to 1D, 2D and 3D extended systems. Basic physical quantities provided by these programs include

- ground state electron density and total energy from density functional theory
- quasi-particle energy within GW approximation and its extensions
- linear (and beyond) electric response

Through these physical quantities, a large variety of physical properties can be addressed:

- structural properties
- electronic properties
- optical and dielectric properties
- magnetic properties

Currently, the ETSF offers the following codes. Further information, downloading procedures, documentation, etc. can be found in the ETSF web site (www.etsf.eu).

- **Abinit:** a computational package based on pseudopotentials and using the plane waves basis set. It is mainly an implementation of density-functional theory (DFT) and density-functional perturbation theory (DFPT), but also of time-dependent density functional theory (TDDFT) in the Casida's approach, as well as many-body perturbation theory in the GW approximation.
- **DP:** a Linear Response TDDFT code working in reciprocal space, frequency domain and using a plane waves basis set. Its purpose is to calculate dielectric and optical properties, like optical absorption, reflectivity and refraction indexes.
- **EXC:** a Bethe-Salpeter Equation code working in reciprocal space, frequency domain, and using a plane waves basis set. Its purpose is to calculate dielectric and optical properties, like optical absorption, reflectivity and refraction indexes.
- **Yambo:** a multipurpose Ab-Initio Many-Body code, which uses the Green's function theory to calculate response functions and quasiparticle energies and lifetimes.

- **TOSCA:** a package for computing optical spectra of solids in the so-called RPA approximation. The full power of TOSCA is revealed when studying complex systems like surfaces or clusters.
- **OCTOPUS:** a code to solve the time-dependent Kohn-Sham (TDKS) equations in a non-perturbative way by propagating the TDKS orbitals in real time and real space. It is therefore particularly geared to the calculation of non-linear (and of course also linear) optical properties. It also allows for the classical motion of ions and it includes (low-order) relativistic effects.

## ETSF libraries and tools

To handle files produced by ETSF software, following the ETSF recommendations of standardization, we propose a set of libraries and tools:

- **ETSF_IO:** a library of F90 routines to read/write the ETSF file format. It is available under LGPL. The tar file, that can be downloaded from the ETSF web page, contains a full documentation, several tutorials, compilable and highly documented programs, and a complete self test suite.
- **pspconvert.py:** a command-line pseudopotential conversion program. The development of such a code aimed to address several needs felt by the scientific community, like allowing the use of older datasets with newer codes and facilitate dataset exchange between researchers. Furthermore **pspconvert** will be a very useful tool to help in the process of unification of pseudopotential file formats, helping everyone to migrate to the newer format.
- **V_Sim** (http://www-drfmc.cea.fr/sp2m/L_Sim/V_Sim/index.en.html): a visualization tool also able to read the crystallographic data from the ETSF file format since its 3.3 release. It proposes the capability to render atomic structures and to load density files to draw iso-surfaces.

## ETSF TRAINING EVENTS

The ETSF regularly organizes training events targeted at young researchers pursuing, or wishing to pursue, a career in the area of theoretical spectroscopy. This service can be extended upon request to other users, e.g. experimentalists, scientists working in industry, or researchers working in a similar field.

Examples of regular training events are the Theoretical Spectroscopy Tutorials organised every year and the Benasque TDDFT Workshop and School organised every year and a half.

ETSF users are informed about coming events through the ETSF Users' Newsletter sent every six months by email. Updated information are posted in the ETSF web page, where the user can access to the full description of the activity, relevant dates, and application forms.

**The ETSF web page (www.etsf.eu/services/training) is the main source of information about training activities, which is regularly updated.**

# USER PROJECTS

In analogy to large experimental research infrastructures, such as synchrotron facilities, the ETSF users can propose projects for which scientific and technical support is provided by ETSF researchers. As mentioned above, such projects range from specific training to full scientific projects.

**An ETSF user project is a work provided by ETSF scientists for the user on his/her demand. The ETSF provides competences, not funding.**

More specifically, user projects can fall in with one of the following categories:

- Collaborative Research projects on demand:
  - Specific development of the theory and codes
  - Specific development of a code
  - Specific calculations
- Training projects on demand:
  - Visit of the user and/or one of his colleagues at an ETSF node to learn theory, methodology, software, *etc (weeks or months)*
  - Lectures about theory, methodology, software, *etc.* at the users' place or elsewhere given by ETSF scientists (few days)
  - Participation to a school

**Any user from the public or private sector can submit proposals all along the year using the form provided in our web page.**

Before submitting a proposal, we encourage you to contact an ETSF scientist or the coordinator of the beamline that you believe is the most appropriate for your project. You can also ask for general advise by contacting one of the ETSF administrators (see page 15).

The information that you have to include in your proposal is rather simple:

- Project title
- Names and e-mails of the proposer and his/her team
- For research proposals, a two-pages project description (scientific background, objectives, description, impact)
- For training proposals, a one page presentation of your needs and background
- Information priory discussed with an ETSF scientist or Beamline coordinator (see page 16).
- A statement about the possibility of co-funding. Note that depending on the nature of the project, the ETSF will need to charge for some of the services provided.

**The evaluation of research proposals takes place twice a year, in spring and autumn. Training proposals are evaluated within three weeks after submission.**

Once your **research proposal** has been submitted, it will follow a three-step evaluation:

- A feasibility report by the Beamline coordinators. In addition to feasibility, they assess effort and CPU time needed. Their report is sent to the External evaluators to help them understand the work asked, but it is indicative only.
- An evaluation by an external panel of experts. They assess the scientific excellence of the project and, for industrial projects, the impact in the final research/product.
- A "Beamline time" allocation by an internal panel of ETSF scientists representing the ETSF Steering Committee. "Beamline time" is allocated to as many proposals as possible, within the available resources and following the ranking of the External Scientific panel.

**Training proposals** are evaluated in a quick one-step process. They are sent to an internal training evaluation panel constituted of the Beamline coordinators. They evaluate the scientific excellence of the proposals and, for industrial users, the impact in the final research/product.

As a final step, and before the actual development of your project, the ETSF will contact you to close all the pertinent administrative, technical and (if needed) economical issues related to your project. Proposers are informed of the outcome of the call within three months after the call deadline for research projects, and within three weeks after submission for training proposals. An ETSF scientist will be assigned to your project, acting as the primary contact person as well as coordinating your project.

**Note that strict confidentiality rules are applied to your project before, during, and after its evaluation.** Submitted proposals are accessible only to ETSF Steering Committee members. They are required to maintain confidential and secure all proprietary information belonging to the applicant. Experts of the external and internal panels sign a declaration of confidentiality before beginning their work. Confidentiality holds also on the working phase, involving now the implied ETSF scientists too. If necessary, a contract will be signed with the user, dealing with confidentiality and intellectual property rights.

# CONTACTS

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# ETSF on-line

## At www.etsf.eu you can find further information about theory, code development, potential applications, training events and other ETSF activities

**ETSF scientists are looking forward to rewarding discussions and collaborations!**
**Subscribe to the ETSF website and chat on the ETSF users' forum:**
**http://www.etsf.eu/forum/7**