



The Event is hosted at the École Polytechnique, Amphithéâtre Sauvy. How to reach:

- ◆ RER B + walk
Get off in Lozère and take the indicated walking path. Around 15 minutes (and 300 steps).
- ◆ RER B + Bus
Get off in Massy-Palaiseau and get the TransEssonne bus 91-06. See <http://www.albatrans.net/> for the timetable. Stop in Polytechnique-Lozère (5th stop).
- ◆ by Car
Coming from Paris, follow the exit Palaiseau both on the A6 or on the N118. Main entrance GPS coordinates are 2° 12mn 9s Est, 48° 42mn 51s Nord. Follow the map below to the closest parking area.



ETSF France
Bât. 411, LSI, Ecole Polytechnique
91128 Palaiseau cedex, France

22 October 2010 | Amphithéâtre Sauvy
École Polytechnique, Palaiseau, France
<http://etsf.polytechnique.fr>



2nd Introductory Training Day on

Theoretical Spectroscopy

INVITATION
1-Day Event



European Theoretical
Spectroscopy Facility



**Moving Theory
to Applications**

2nd Introductory Training Day on
Theoretical Spectroscopy

INVITATION
1-Day Event



22 October 2010 | Amphithéâtre Sauvy
École Polytechnique, Palaiseau, France
<http://etsf.polytechnique.fr/>



e-infrastructure





Summary and Scopes

Electronic excitations, caused for example by irradiation with electrons, light or modern photon sources (synchrotron, ultra-fast lasers), are key quantities for the study of materials, ranging from solids to atoms, from surface to nanoscale systems.

Experimental techniques measuring electronic excitations have seen rapid progress (high spatial resolution, short measurement time, low temperature), which continuously requires and stimulates a more precise theoretical description and analysis. The joint use of theory and computer simulation has in fact, over the last decades, permitted to achieve big improvements in the description of optical and electronic properties of finite and infinite systems.

The main scope of this introductory training day is to provide attendees with both the theoretical foundations and the knowledge about ab initio calculations.

After a brief introduction about the programmes and training solutions proposed by the European Theoretical Spectroscopy Facility (ETSF, <http://www.etsf.eu>), theoretical approaches along two different lines will be presented: on one side, methods based on density functionals and on the other side, methods based on Green's functions in many-body perturbation theory. 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.

Lecturers and Contributors:

- G. Bruant, F. Sottile,
M. Gatti, J. Rehr, L. Reining
- M. Bertocchi, A. Berger, A. Cucca

Information and registration:

- France.Pochard@polytechnique.edu
+33 (0)1 6933 4470

Scientific contact:

- Francesco.Sottile@polytechnique.fr

Program

- 09h30 Introduction to ETSF: training solutions
- 09h55 An ETSF training project: experience of an undergraduate student
- 10h00 Introduction to ab initio approaches for electronic structure calculations
- 10h10 Density Functional Theory: description through electron density
- 10h40 Caffeine Break
- 11h10 Green's Functions theory: description through (quasi)particles
- 11h40 Industry meets Theory: experience of a post-doc

Lunch

The afternoon is dedicated to the presentation of ETSF "beamlines", i.e. to theory and applications centred around particular experimental approaches.

- 13h30 Photo-emission beamline
- 14h00 Presentation of the ETSF liveCD
- 14h30 Optics beamline
- 15h00 Caffeine break
- 15h30 Loss Spectroscopy beamline
- 16h00 X-ray beamline
- 16h30 Discussions



http://etsf.polytechnique.fr/Training_Theoretical_Spectroscopy