European Theoretical Spectroscopy Facility

Introduction to ETSF: Training Solutions

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Outline

1. Introduction to ETSF
   - 1.1 Why the ETSF?
   - 1.2 What kind of infrastructure is it?
   - 1.3 How does it work?
2. Training opportunities
   - 2.1 Hands-on schools
   - 2.2 Online training modules
   - 2.3 On demand training
   - 2.4 Collaborative projects

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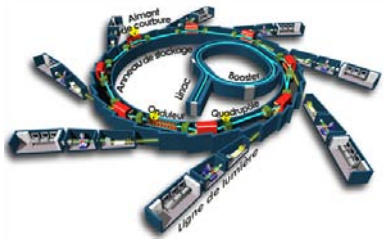
Why the ETSF?

Experimentalists



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Theoreticians

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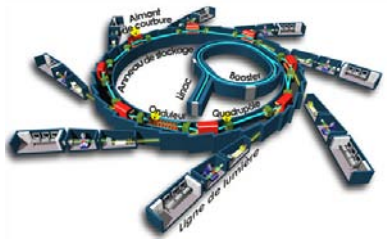
Why the ETSF?

Experimentalists



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Theoreticians

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What kind of structure is the ETSF?

✓ It is not a funding agency

✓ It does not provide computer time

✓ It is not a machine somewhere

✓ It is not a company

So, what is the ETSF?

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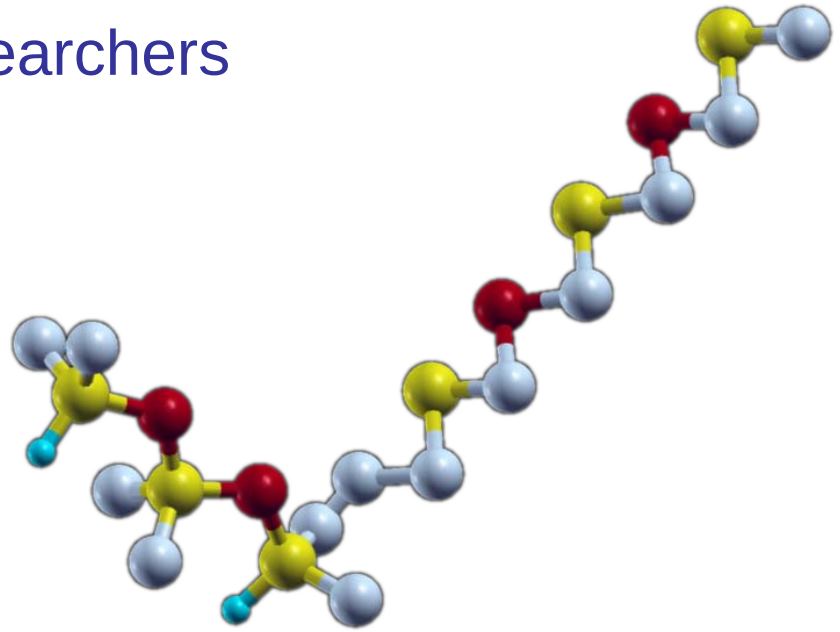
A new type of facility!

A knowledge center for theoretical spectroscopy:

- ► carrying out state-of-the-art research
- ► gathering the experience and know-how
- ► offering its expertise to researchers

To Design and Optimize

√ opto-electronic devices
√ photovoltaic materials
√ biological devices
√ nanostructures



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How does it work?

Core nodes

They created the ETSF and ensure its management.

Central Node

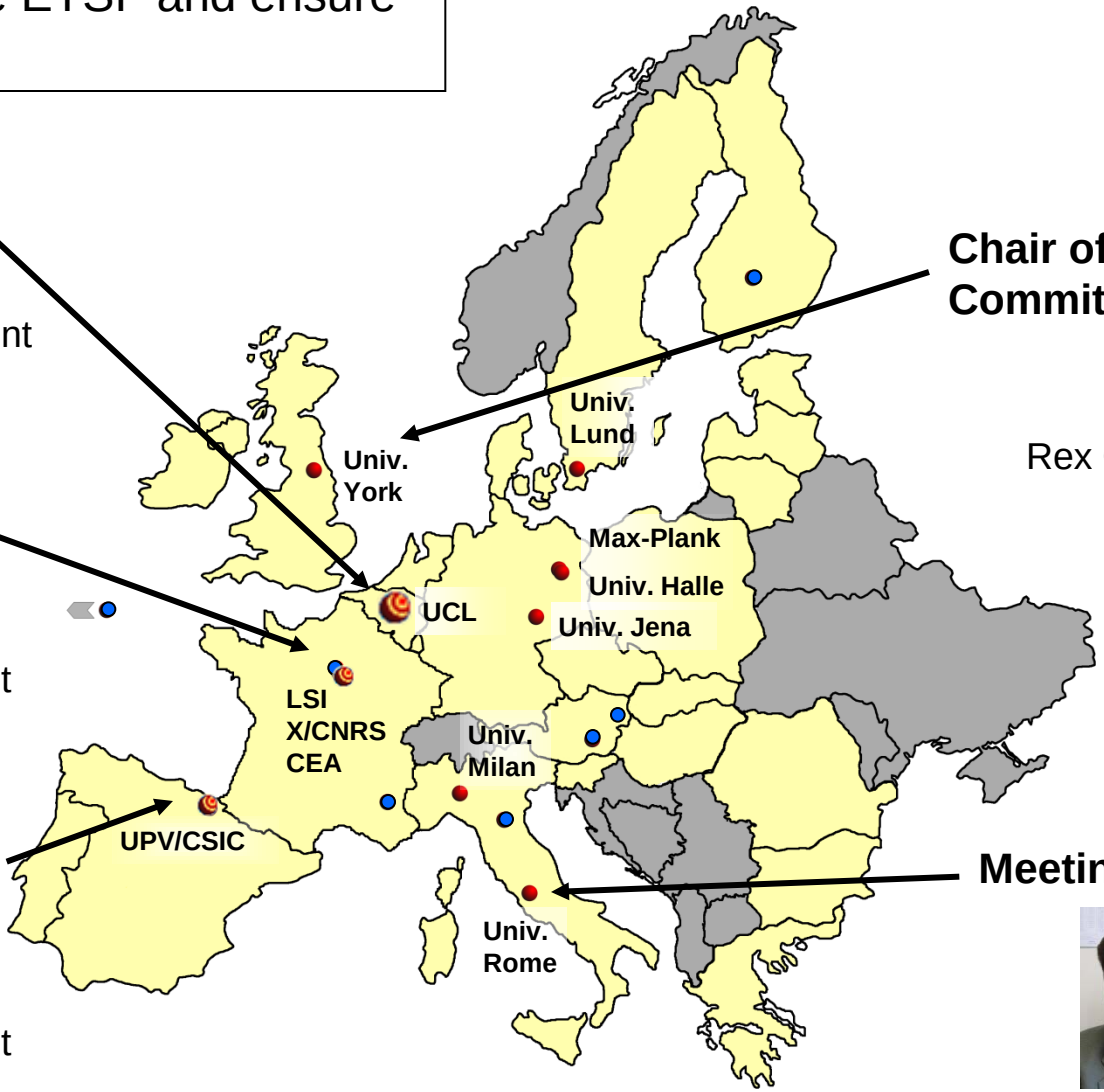
Xavier Gonze
ETSF President

Centre for Users and Technology

Lucia Reining
Vice-President

Centre for Scientific Development

Angel Rubio
Vice-President



Chair of the Steering Committee

Rex Godby

Meeting Centre

Rodolfo
Del Sole

Associate nodes

They bring in complementary competences.

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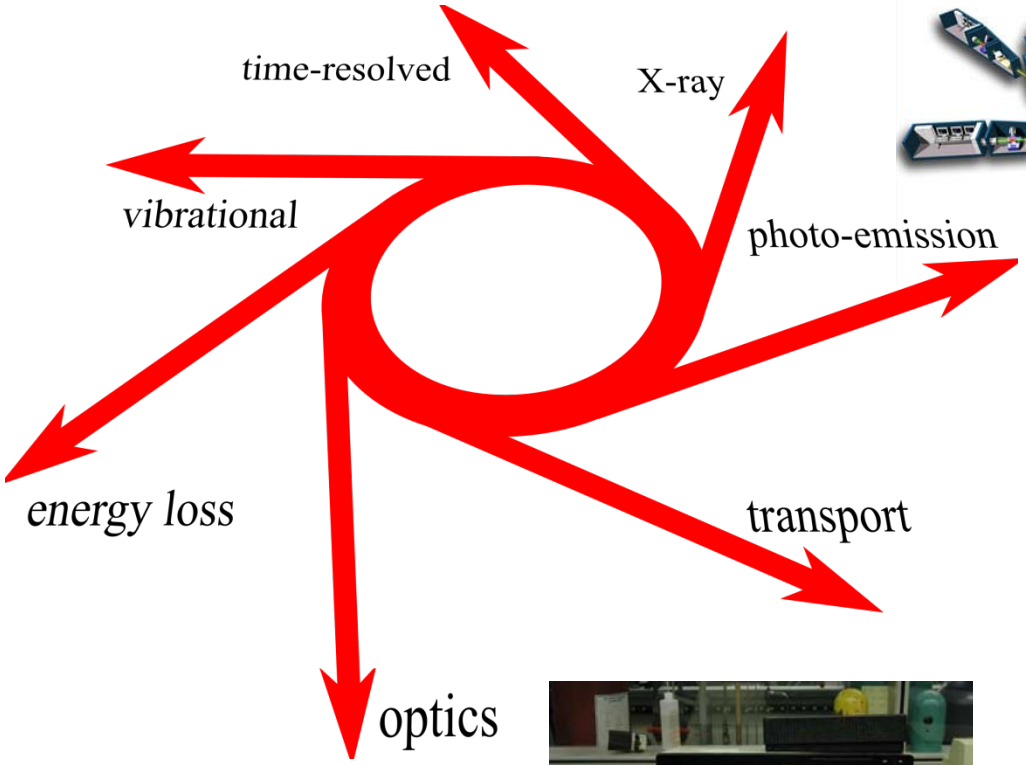
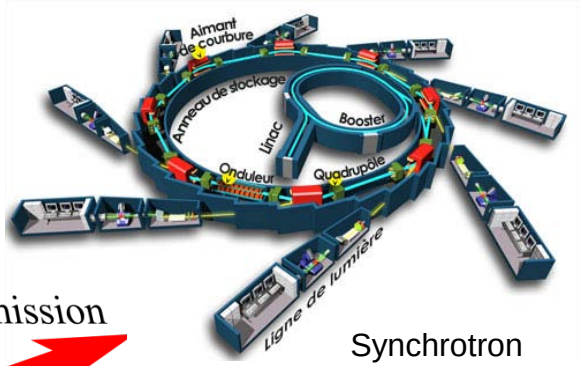
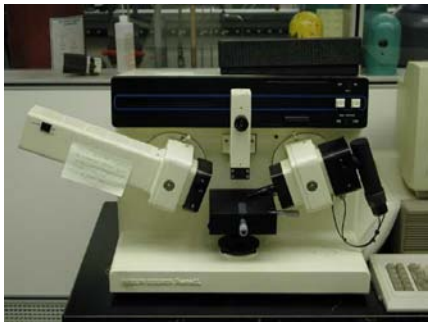
ETSF Beamlines





Synchrotron
SOLEIL

Microscope LPS
Orsay University



Elipsometer
Yale University

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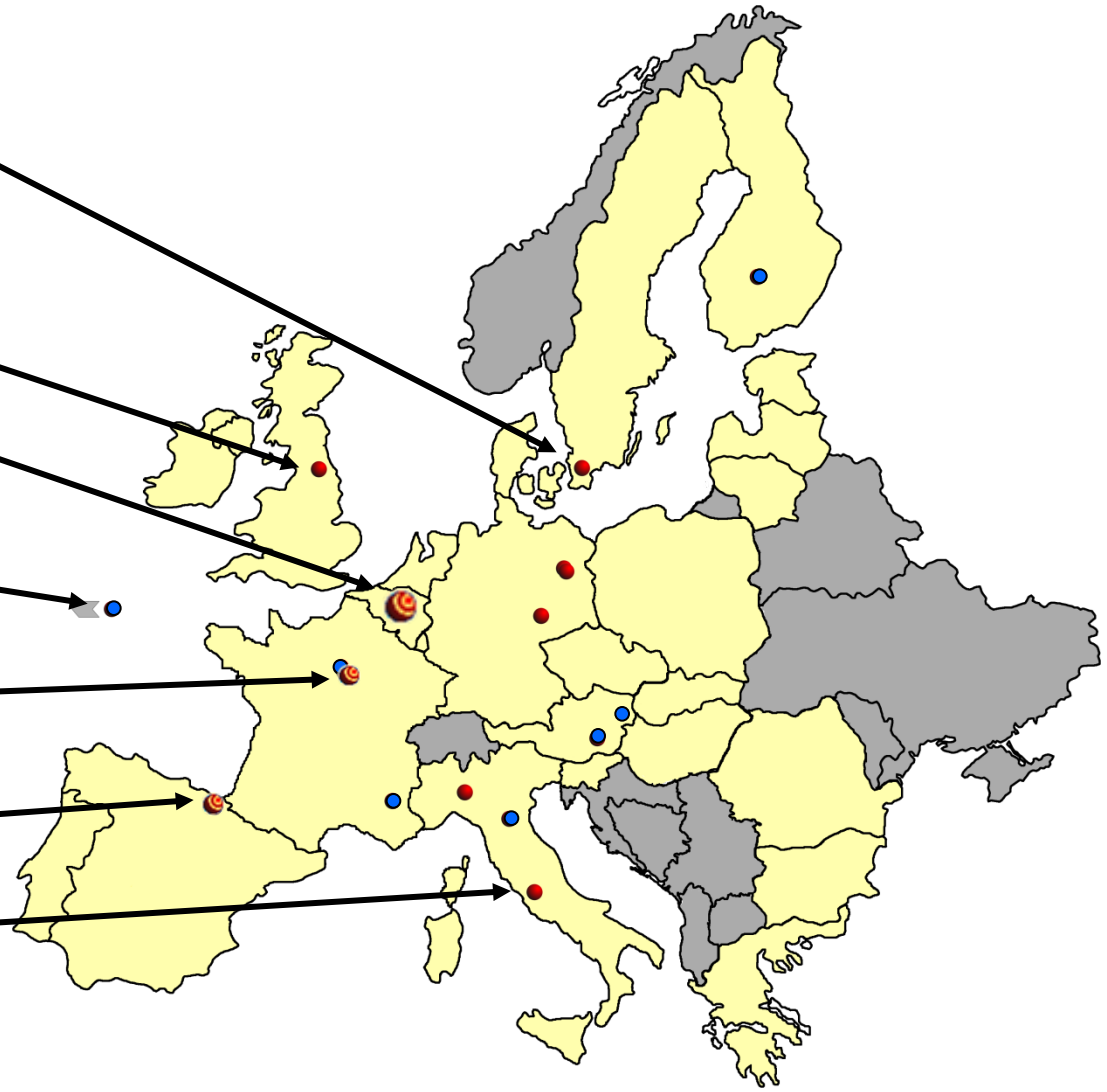
ETSF Beamlines

- Photoemission spectroscopy
  (Claudio Verdozzi)
- Quantum transport
  (Peter Bokes)
- Vibrational spectroscopy
  (Gian-Marco Rignanese)
- X-ray spectroscopy
  (John Rehr)
- Energy loss spectroscopy
  (Francesco Sottile)
- Time resolved spectroscopy
  (Miguel Marques)
- Optics
  (Olivia Pulci)



ETSF Beamlines

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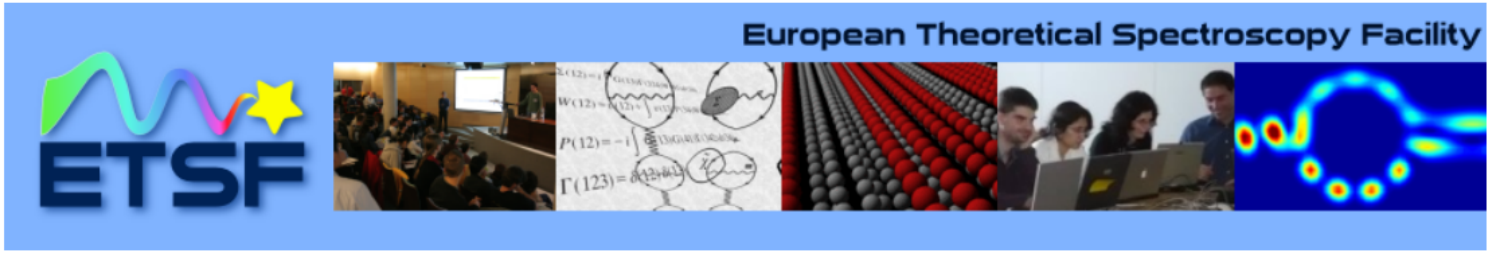

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- About the ETSF
- *Beamlines*
  - Optics
  - Energy Loss Spectroscopy
  - Quantum Transport
  - Time Resolved Spectroscopy
  - Photoemission Spectroscopy
  - X-Ray Spectroscopy
  - Vibrational Spectroscopy
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Intranet

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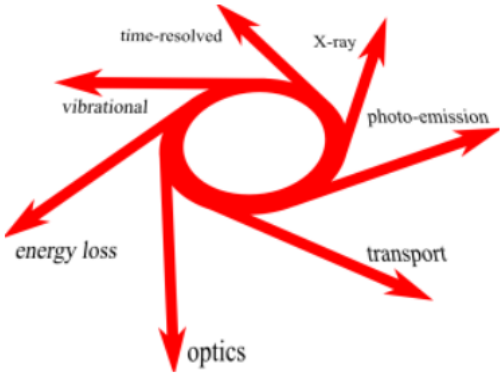
Beamlines

The ETSF is divided into 7 beamlines, each of which is concerned with a specific scientific topic. A beamline coordinator is responsible for the contact with the users of each line. He/She also serves as the contact person for users who want to submit a proposal to the ETSF.

Further details are available on the beamlines' description.

Beamlines and Coordinators



Optics

Dr. Olivia Pulci
University of Rome Tor Vergata, Rome, Italy
Olivia.Pulci@roma2.infn.it

Energy Loss Spectroscopy

Dr. Francesco Sottile
Ecole Polytechnique, Palaiseau, France
francesco.sottile@polytechnique.edu

Quantum Transport

Dr. Peter Bokes
Slovak University of Technology, Bratislava, Slovakia
peter.bokes@stuba.sk

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ETSF services

- Availability of ETSF codes

abinit.org EXC SIESTA dp™ Octopus Yambo etc.

- Training

- Hands on schools
- Online Training Modules
- On demand training

- Biannual call for proposals

submit a proposal

- Scientific collaboration
- Commissioning of theory and software developments

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Training: hands-on schools

- Spectroscopy Lectures at CECAM (Zürich)
- Hands-on TDDFT schools and workshops in Benasque (Spain)

  - Full time intensive programs
  - Limited enrolment
  - Highly available computer facilities
  - Exercices
  - Informal environment → easy to ask deeper questions to the lecturers
  - ECTS credits delivered
  - Starting point for more substantial web-based distance learning

Online Training Modules

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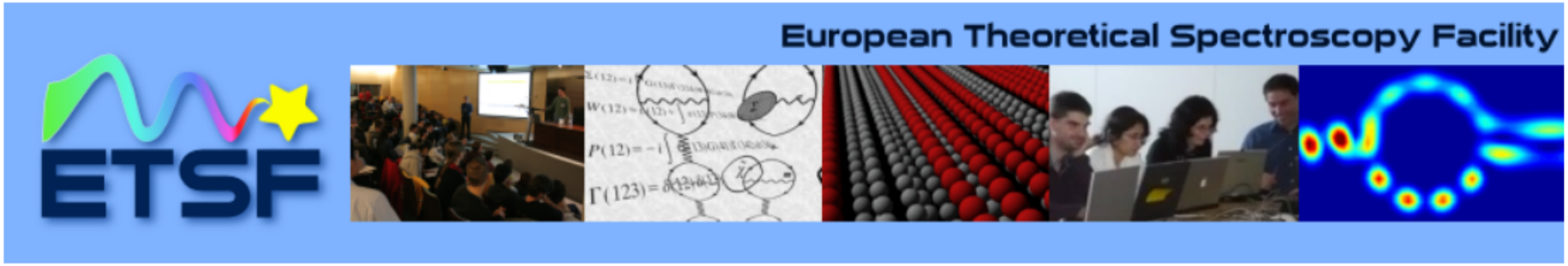
- Introduces the methods of theoretical spectroscopy
- Addresses ETSF users, both theoreticians and experimentalists
- First modules online, other under construction



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- Beamlines
- Services
  - Collaborative Research
  - Training
    - Online Training Modules
      - Electrons and Nuclei
    - Tutorials and

Home

The Hartree-Fock approximation and beyond

With the Born-Oppenheimer approximation the general problem of the electron and nuclei is separated. The first problem awaiting solution now is the Schrödinger equation of the interacting electrons moving in the potential of the momentary configuration of the nuclei

$$\left(\hat{T}_e + \hat{V}_{ee} + \hat{V}_{ek}(\{\mathbf{R}_I\}_{N_k})\right) \Phi_n(\{\mathbf{r}_i\}_{N_e}; \{\mathbf{R}_I\}_{N_k}) = E_n(\{\mathbf{R}_I\}_{N_k}) \Phi_n(\{\mathbf{r}_i\}_{N_e}; \{\mathbf{R}_I\}_{N_k})$$

The potential of the electron-nuclei interaction $\hat{V}_{ek}$ can be cast into the form $\hat{V}_{ek}(\{\mathbf{r}_i\}_{N_e}, \{\mathbf{R}_I\}_{N_k}) = \sum_i V_{ext}(\mathbf{r}_i)$, where the single particle potential $V_{ext}(\mathbf{r})$ in our context is the Coulomb

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On Demand Training

- Delivered to individuals or groups,
- At the user's site, an ETSF node, or at another suitable place.
- Training projects may be submitted all year round
- Evaluation every two weeks by an internal panel constituted by the ETSF beamline coordinators

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Call for Proposals

- Specific scientific problem (calculation, development of theory and code, consultancy, *etc.*)
- Work done by ETSF scientists in collaboration with the users
- Proposals may be submitted all year round
- Evaluations twice a year by an independent panel of experts

Questions?

I will be happy to answer any question you may have about the ETSF and its services.

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