



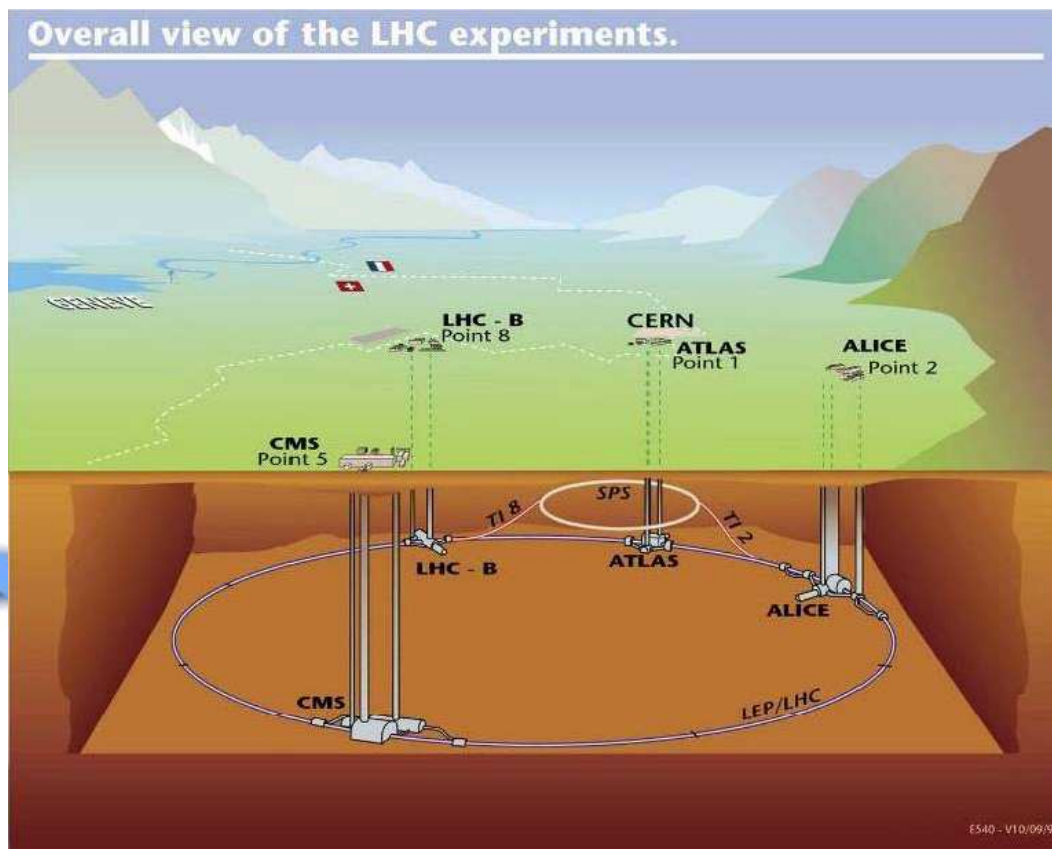
**European Theoretical  
Spectroscopy Facility**

A Theoretical Facility:  
Interfacing with Industrialists &  
Experimentalists

*Anne Matsuura, Ph.D.- UCL, chief executive of the ETSF*

# Research infrastructures

Genève : the CERN



# ETSF: An E-Infrastructure

Vol 450|6 December 2007

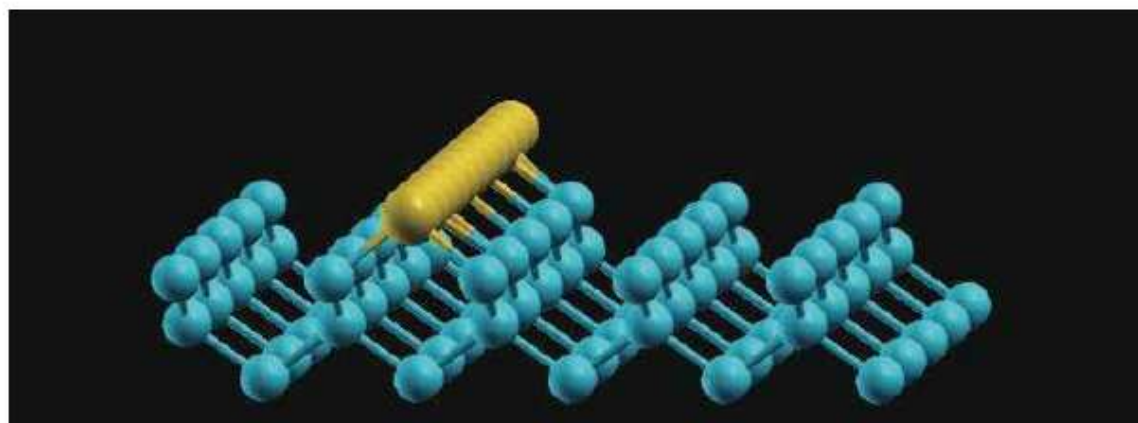
nature

BUSINESS

## Smart networking

Theoreticians have combined their expertise to form a network to help other scientists design materials or understand biological pathways. **Katharine Sanderson** reports.

For the past three months Joerg Schaefer, a physicist at the University of Würzburg in Germany, has been waiting for a group of theoretical spectroscopists to calculate the exact position of gold and platinum atoms in nanowires made from single atoms of the metals. When laid out on a semiconductor surface, the wires could potentially be used to transfer data at high speeds in microprocessors by acting as switches. Once the theoreticians have worked out what combination of metal and semiconductor should produce a



M. VERSTRAETE

# ETSF - Much in Common with Physical Research Infrastructures

- International Collaboration
- Long-Term Projects
- Cutting-Edge Science for a Large Community
- Complex Organization



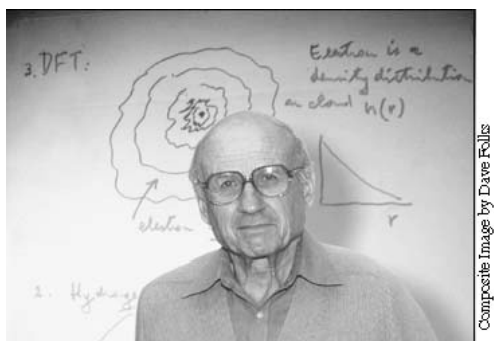
European Theoretical Spectroscopy Facility:  
*the emergence of a new infrastructure*

Louvain-la-Neuve  
28 november 2008



# Theoretical tools

Equations and formalism  
from quantum mechanics  
and electromagnetism ...

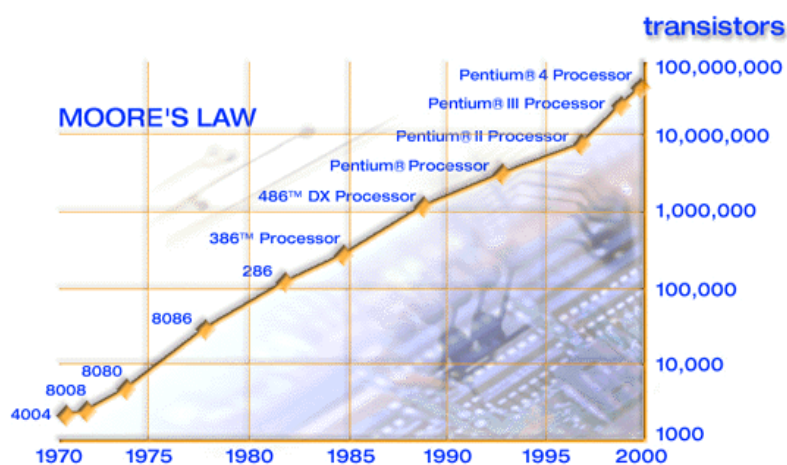


*W. Kohn, chemistry Nobel prize 1998*



*H. Bethe, physics Nobel prize 1967*

... computers ...



# Theoretical tools

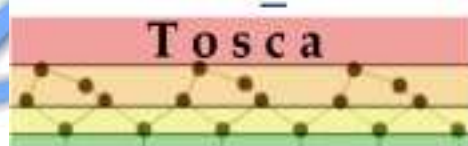
... and software programs for simulation ...



phi98PP



abinit



PP2PP



structure

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September 2008

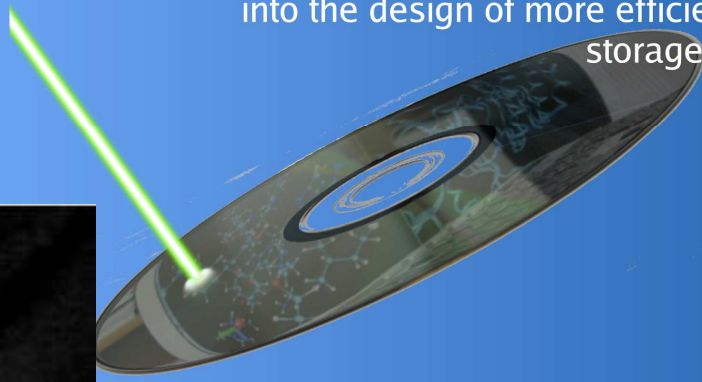
Formalism + computers + programs  
=> *new investigation tools*



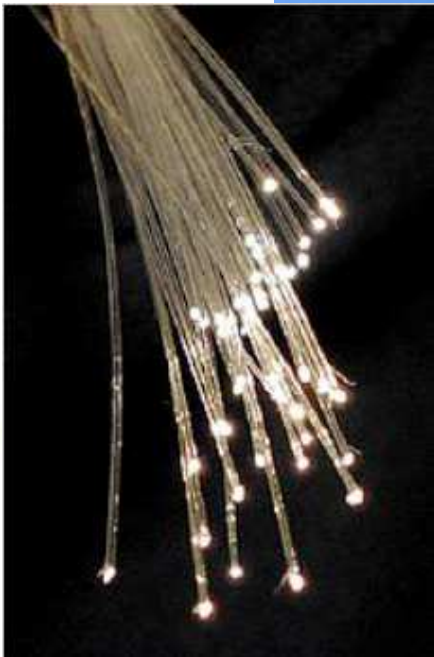
# Domains of application : materials for ...

## Optical data storage and rewritable DVDs

Computer simulation gives new insight  
into the design of more efficient data  
storage media.



Light-emitting devices (LED)

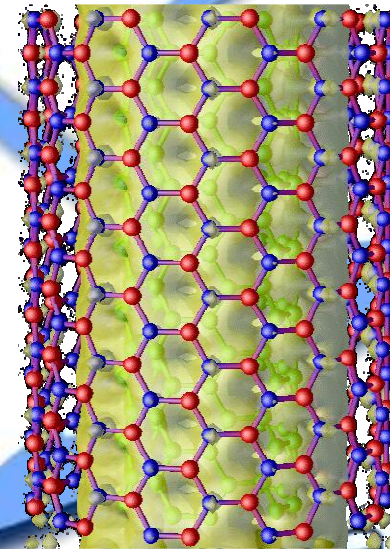
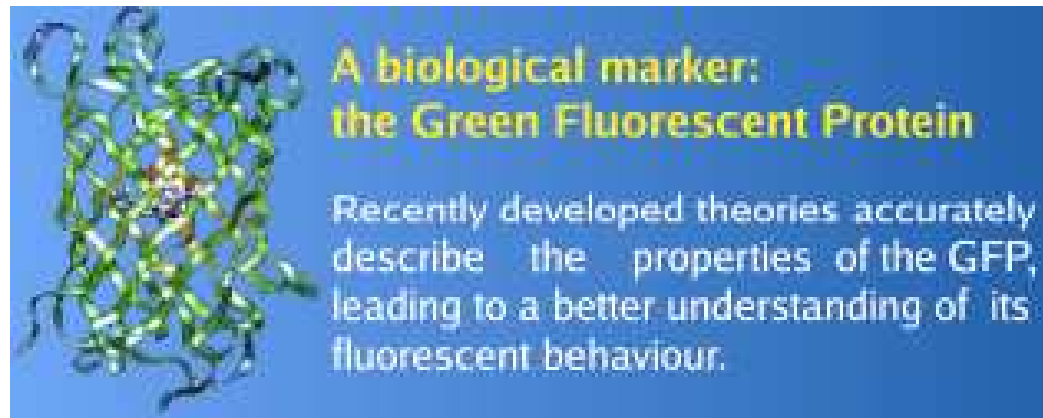


Optical fibers



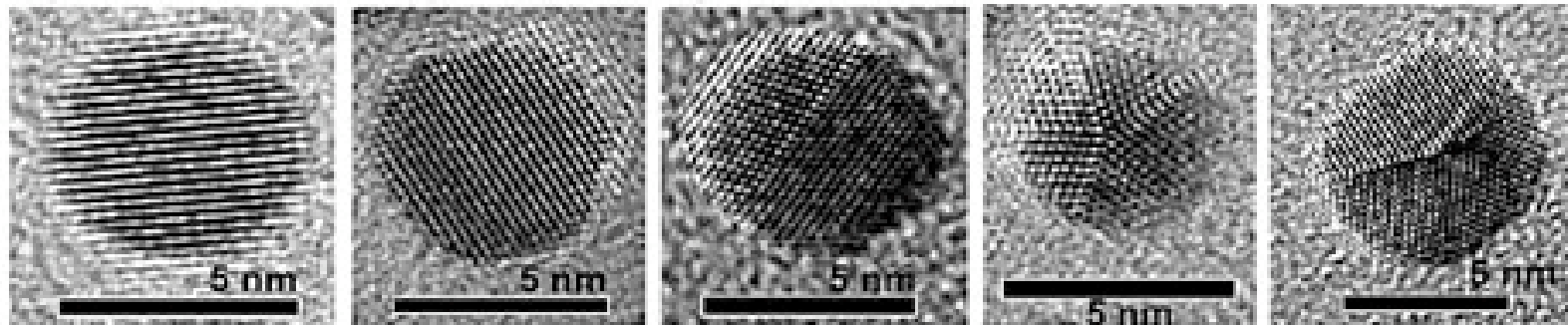
Photovoltaics

# Domains of application : biology, nanoscience, ...



European Th  
the

High resolution TEM images of Au and Ag nanoparticles:



Aqueous  
colloidal gold.



# From tools to an infrastructure

How to achieve an effective match between such capabilities and the needs of users ?

... A new infrastructure ...

- networking
- integration of tools (formalism, software)
- maintenance of tools
- support, service, formation

Then, calls for proposals + peer review by international experts in field to select top quality proposals

# User profiles

- Call for proposal : ETSF satisfies a variety of needs

Category	Type of projects
Theo, expert	automatic
Theo, non-exp.	rapid training
Experimentalist: .....hands-on	teach in collaboration
.....hands-off	provide collaboration
Industry	results at date
Training need	customized training

# History

2000-4

Nanophase RTN: close scientific collaboration and training

2004-8

**Nanoquanta Network of Excellence:**

research integration, established of the ETSF, added ETSF Associate Nodes, created Young Researcher Network

2007-8

First call for **user projects**

2009-11

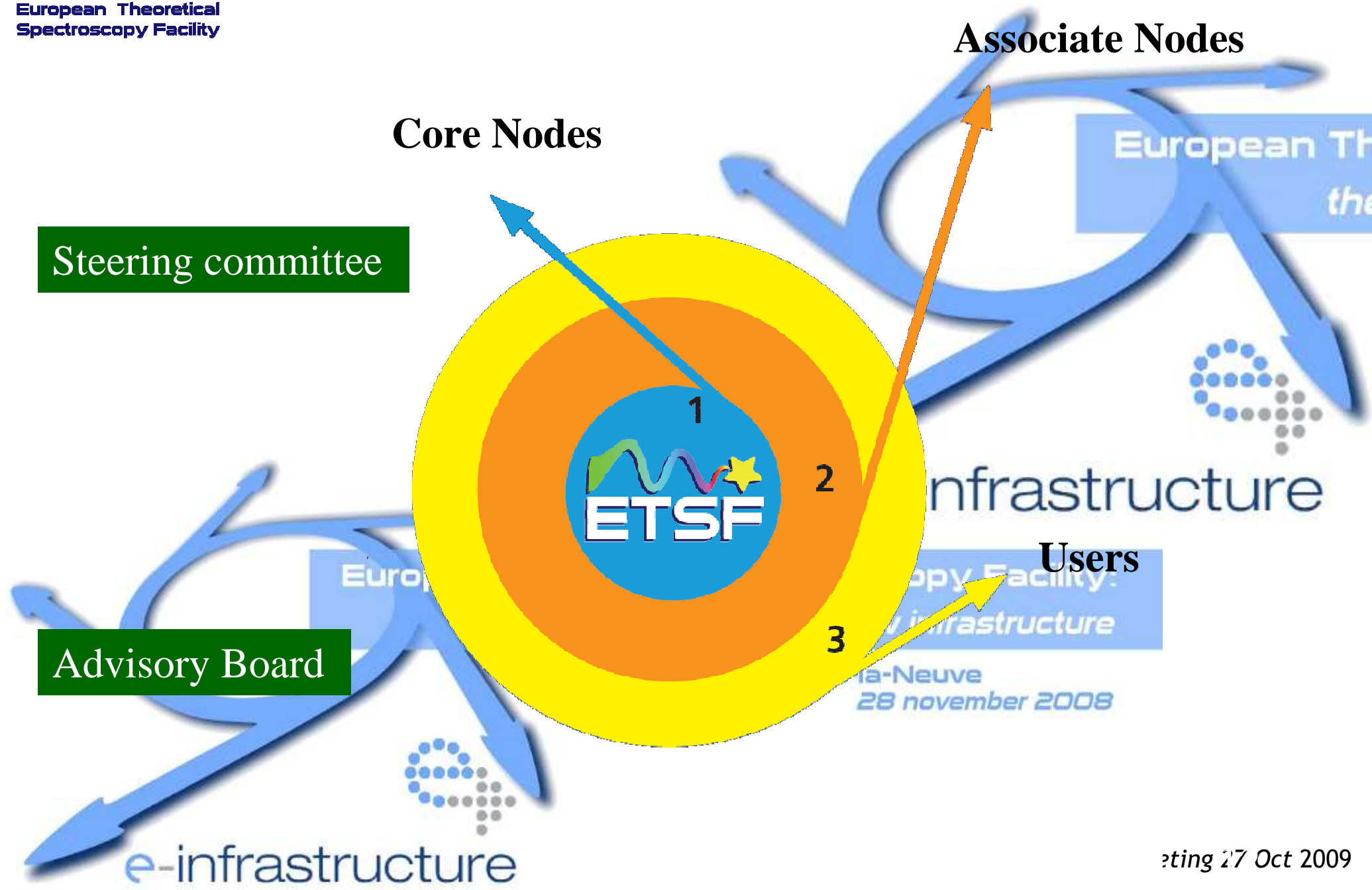
**EU e-I3 grant** : up to now 3 calls,  
next one Oct 2009

Aug 2009

Dr. A. Matsuura -chief executive



# ETSF Structure



# *A distributed infrastructure ...*

... integrates complementary skilled experts :  
developers, maintainers, practitioners, teachers ...



A frontier-of-science research : in 2006-2008, from the 10  
ETSF « core nodes », 397 publications, including 45 Phys. Rev. Lett.,  
5 Appl. Phys. Lett., 1 Science, and 386 invited talks.

# *A distributed infrastructure ...*

... helps users find the best experts, and get these experts to provide the theoretical help they need

## *ETSF Beamlines:*

*The ETSF is structured in beamlines to ease access to its theoretical tools. The ETSF beamlines are:*

- + Optics
- + Quantum Transport
- + Time-Resolved Spectroscopy
- + X-Ray Spectroscopy
- + Energy Loss Spectroscopy
- + Photoemission Spectroscopy

Until now :  
three calls,  
>140 proposals received,  
+ schools, on-line tutorials,  
+ 9 open-source programs,  
+ continuing improvements to  
maintain world-class quality



# *A distributed infrastructure ...*

... maintains the Web site (<http://www.etsf.eu>)



Home

**European Theoretical Spectroscopy Facility**

**ETSF**

Welcome to the European Theoretical Spectroscopy Facility

The ETSF is a knowledge center for theoretical spectroscopy carrying out state-of-the-art research on theoretical and computational methods for studying electronic and optical properties of materials. The ETSF gathers the experience and know-how of more than 200 researchers in Europe and the United States, facilitating collaborations and rapid knowledge transfer.

The ETSF offers its expertise to researchers, industry, and students in the form of collaborative projects, free scientific software and training. Proposals to benefit from these services can be submitted at any moment, and are evaluated twice a year by an external scientific panel.

The ETSF is co-funded by the EU under the FP7 Capacity programme.

**Intranet**

- Login

# *A distributed infrastructure ...*

... maintains and integrates open source software

Creation of a “LiveCD”, by a software engineer

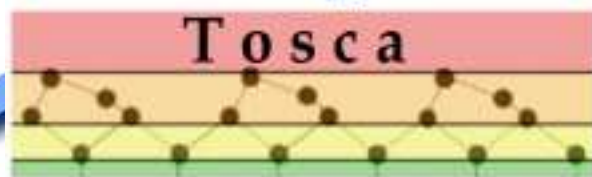
Dissemination of our softwares (Web availability, creation of RPM and Debian packages)



fh98PP



abinit



PP2PP



e-infrastructure

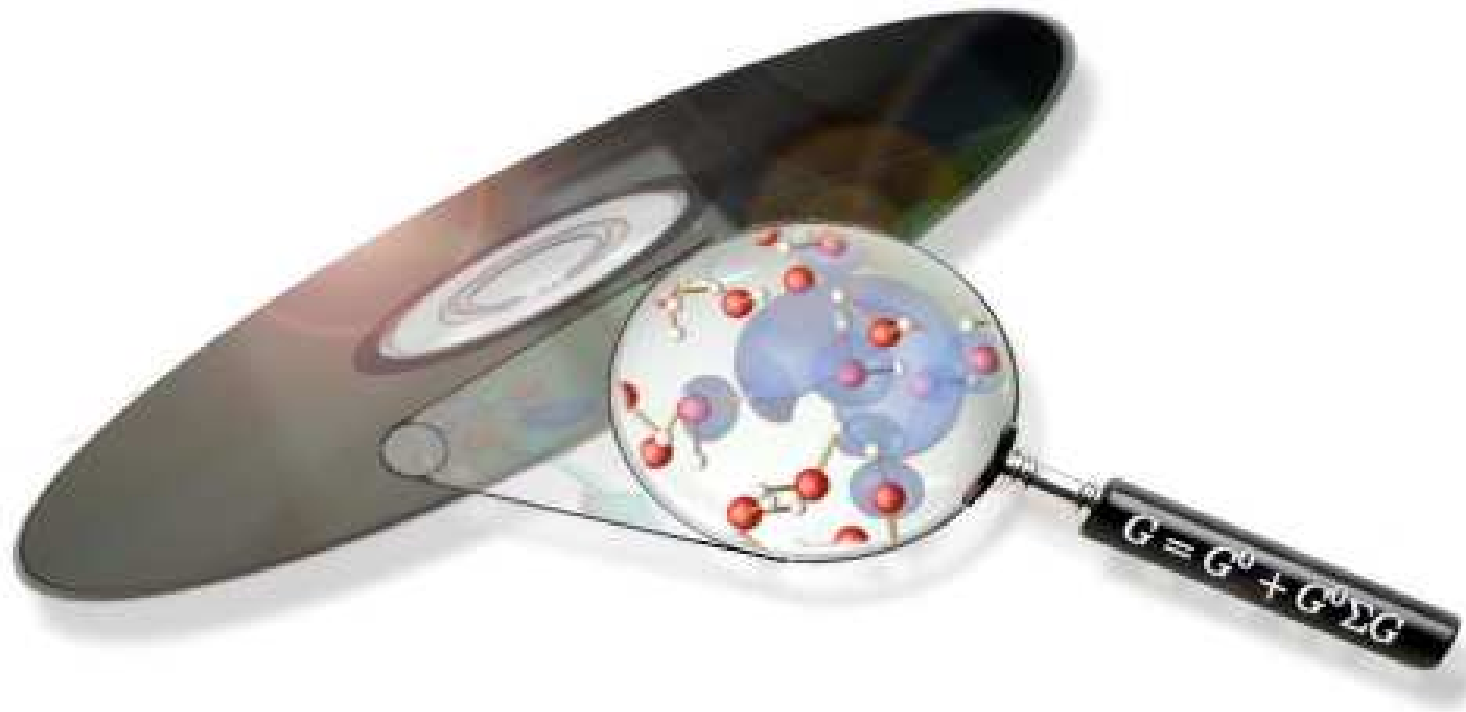
# Bridging theory to experiment

$$\Sigma(1, 2) = -i \int d^3x d^3y v(5, 1^+) G(1, 4) \frac{\delta G^{-1}(4, 2)}{\delta V(3)} \frac{\delta V(3)}{\delta U(5)}. \quad (4)$$

The 3-point irreducible vertex function is defined with respect to the effective potential

With Eq. (2) and equation for  $\bar{\Gamma}$

$$\bar{\Gamma}(1, 2; 3) =$$



<animation : plasmons>



# Outreach to Experimental Users

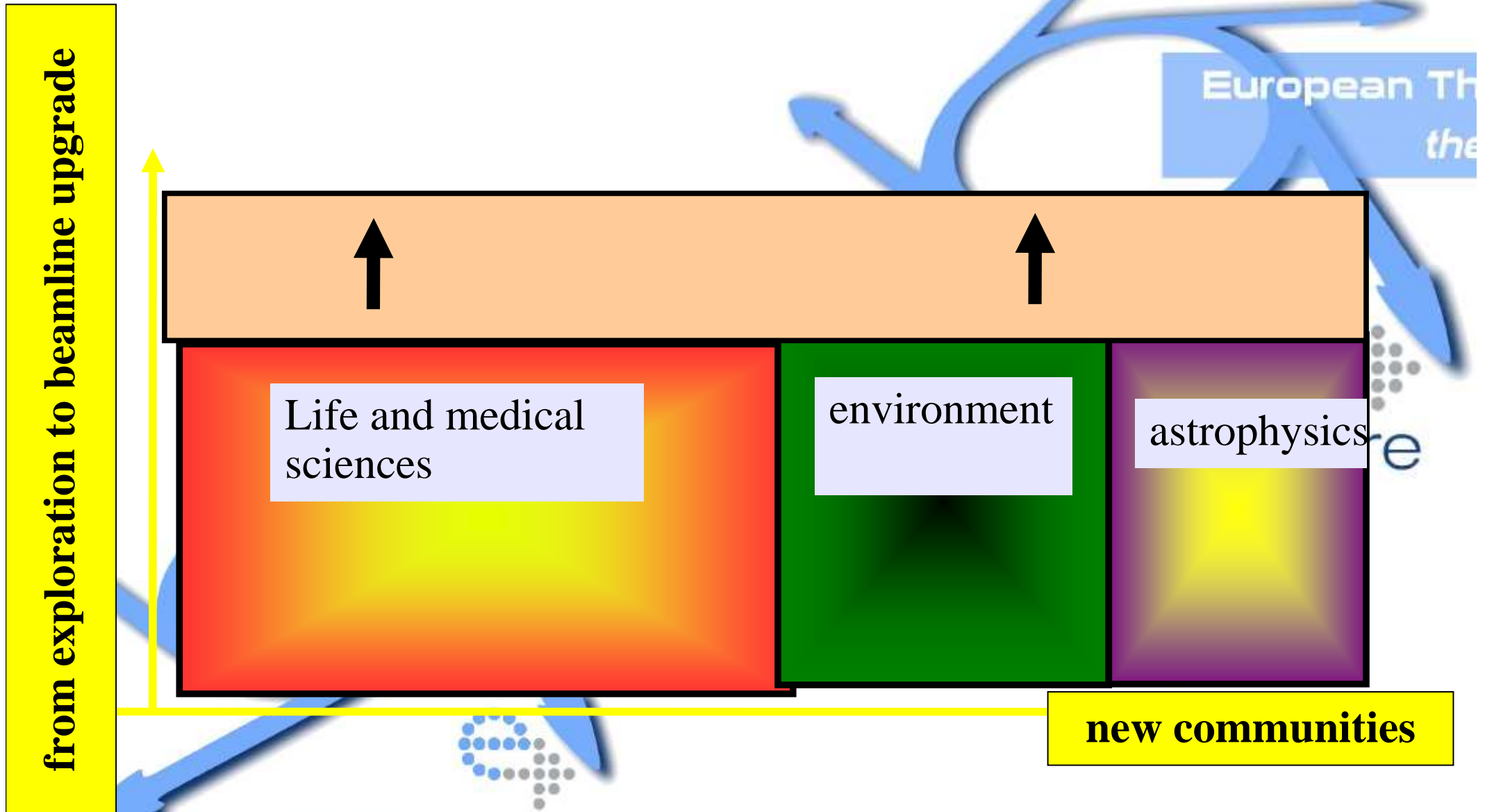
- Strengthen ties between ETSF Nodes and experimental community
  - Look for new user communities
- Software E-library/Online public
- Customized Training
- Workshops & Schools
  - Annual Users' Meeting



Louvain-la-Neuve  
28 november 2008

# “Large” ETSF:

Users’ communities & beamline development



# Ideas for Outreach to Industrialists

- Expand corporate connections that already exist with ETSF Nodes
  - Include corporate connections that ETSF Node Universities have (low-hanging fruit)
- Publicity for non-scientists
- Events such as Company Days
  - Consultancy sessions
- Partner with experimental facilities/resources to offer theory & experiment to industrial user





# Links

*Diamond*

*XFEL*

*MAX-Lab*

*SOLEIL*

*Swiss Light Source*

*ESRF*

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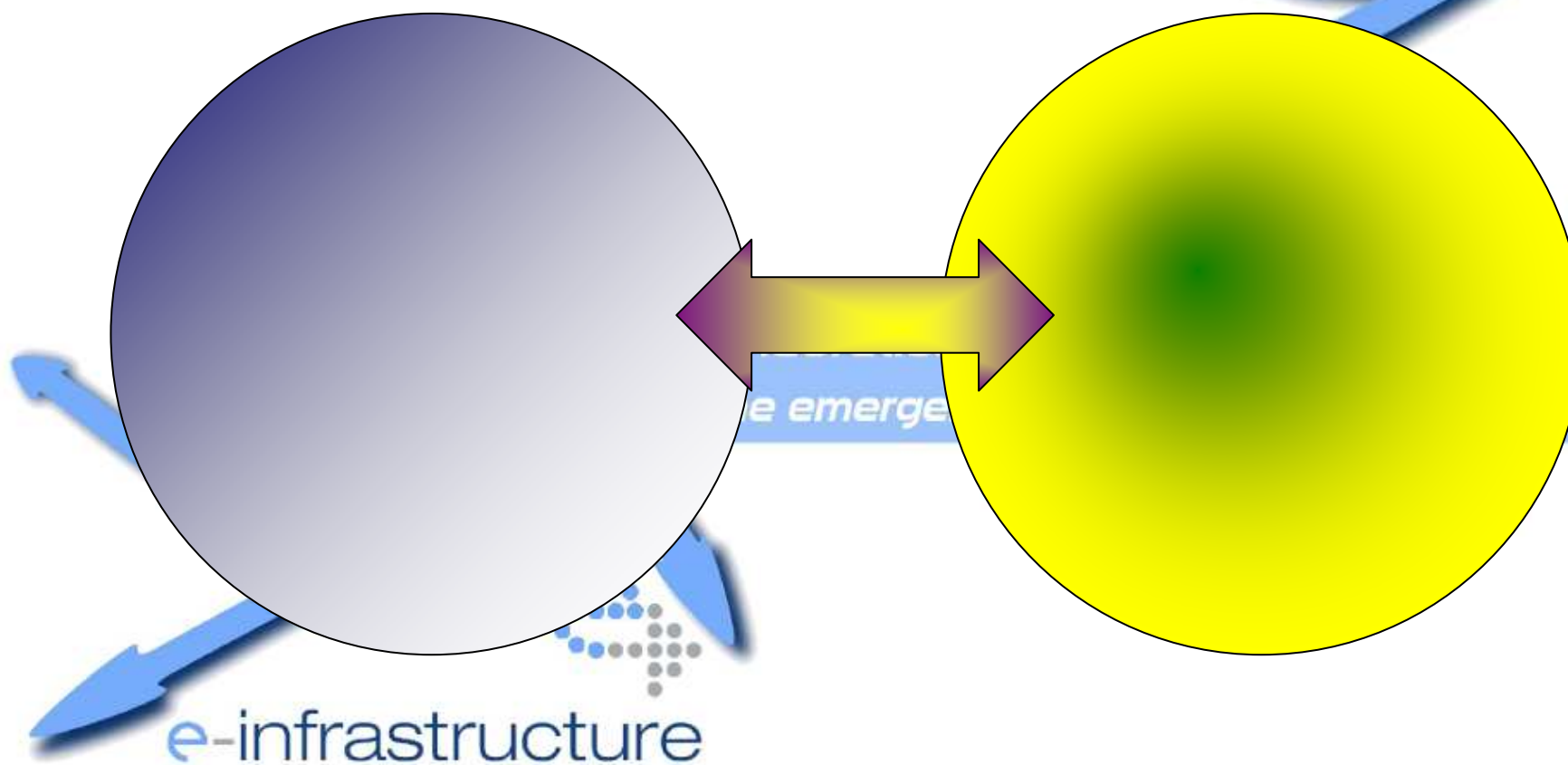
Paris La Neuve  
28 november 2008

# Together Can Offer Companies...

Theoretical + Experimental Resources = Complete Package

**Experimental**

**Theoretical**





European Theoretical  
Spectroscopy Facility

# Company Day



Le Laboratoire des Solides Irradiés,  
Unité Mixte de Recherches  
Ecole Polytechnique /  
CNRS / CEA (UMR 7642).



en liaison avec le réseau d'excellence européen Nanoquanta et la nouvelle infrastructure ETSF (I3), vous invite à assister à un séminaire d'information :

## « Les nouveaux outils de calculs des structures électroniques »

organisé le **lundi 4 février 2008**

à l'École Polytechnique, en Amphithéâtre Becquerel, de 9h30 à 16h.

Ces outils logiciels sont développés dans le cadre de Nanoquanta et du European Theoretical Spectroscopy Facility, et s'appliquent en particulier aux nano-matériaux, aux polymères ou aux bio-molécules (<http://www.etsf.eu/>).

Le programme du séminaire, en français, laissera une place importante aux applications de ces méthodes dans le secteur industriel, avec présentation d'exemples dans différents domaines.

### Programme prévisionnel de la journée :

à partir de 9 h 30 : Accueil  
10 h 00 - 11 h 00 : l'ETSF  
- présentation générale (Lucia Reining, LSI)  
- présentation institutionnelle  
(Gaëlle Bruant, LSI)  
Pause café  
11 h 15 - 12 h 15 : Utilisateurs industriels :  
trois exemples  
pause déjeuner - buffet  
(avec session posters et démos.)

13 h 30 - 14 h 15 : l'appel à projets ETSF  
- l'appel pilote (Giovanni Onida,  
Université de Milan)  
- la soumission (Francesco Sottile, LSI)  
14 h 15 - 14 h 30 : Modes de collaboration,  
(François Plais, DRIP)  
Pause café  
14 h 45 - 16 h 00 : Table ronde,  
questions / réponses,  
conclusions du séminaire

A l'issue de cette journée, vous pourrez évaluer l'intérêt de ces outils de modélisation dans le cadre de vos activités de R&D et vous disposerez des contacts pour concrétiser un projet de collaboration.

Participation aux frais 100€,  
incluant CD rom avec présentations, pauses et déjeuner – buffet  
préinscription par mail, ([gaelle.bruant@polytechnique.edu](mailto:gaelle.bruant@polytechnique.edu))

Avec le support du Conseil Régional d'Ile-de-France.





## Future : develop, open and link

- Open the ETSF to many users
- Open new user communities to the ETSF
- Attract more corporate interest in the ETSF
- Partner with experimental facilities/resources
- Keep and develop ETSF virtual beamlines at the forefront of science

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# ETSF

The EU, national, regional, local sponsors,  
and the support of our institutions ...

