

6 may 2014 – Grand Amphi Soleil

Soleil Theory Day

Journée de rencontre avec la
spectroscopie théorique



Scope of the day

- Present the ab initio **theoretical approaches** and **computational codes** that are developed by the ETSF
- Stimulate new **discussions** and **collaborations** between experimentalists and theoreticians
- Collect the demands of **training on theory and codes** in order to plan specific tutorials at Soleil

Scope of the day

- Present the ab initio **theoretical approaches** and **computational codes** that are developed by the ETSF
- Stimulate new **discussions** and **collaborations** between experimentalists and theoreticians
- Collect the demands of **training on theory and codes** in order to plan specific tutorials at Soleil



Program

- 9h30-10h00 Matteo Gatti - Theory activities at Soleil
- 10h00-10h30 Lucia Reining - Key concepts of theoretical spectroscopy
- 10h30-11h00 Coffee break
- 11h00-11h40 Giorgia Fugallo - Basics of density-functional theory
- 11h40-12h30 Matteo Gatti & Claudia Roedl - Photoelectron spectroscopy
- 12h30-13h30 Lunch break
- 13h30-14h20 Francesco Sottile - Absorption and energy-loss spectroscopy
- 14h20-15h10 John Rehr & Keith Gilmore - Core-level spectroscopies
- 15h10-16h00 Poster session: ongoing theory developments and collaborations with experimentalists

Matteo Gatti

Theory activities @ SOLEIL

Laboratoire des Solides Irradiés – CNRS - Ecole Polytechnique
European Theoretical Spectroscopy Facility (ETSF)
Synchrotron SOLEIL

matteo.gatti@polytechnique.fr
<http://etsf.polytechnique.fr> - <http://www.etsf.eu>

Room: O1.1.17 @ SOLEIL

Matteo Gatti

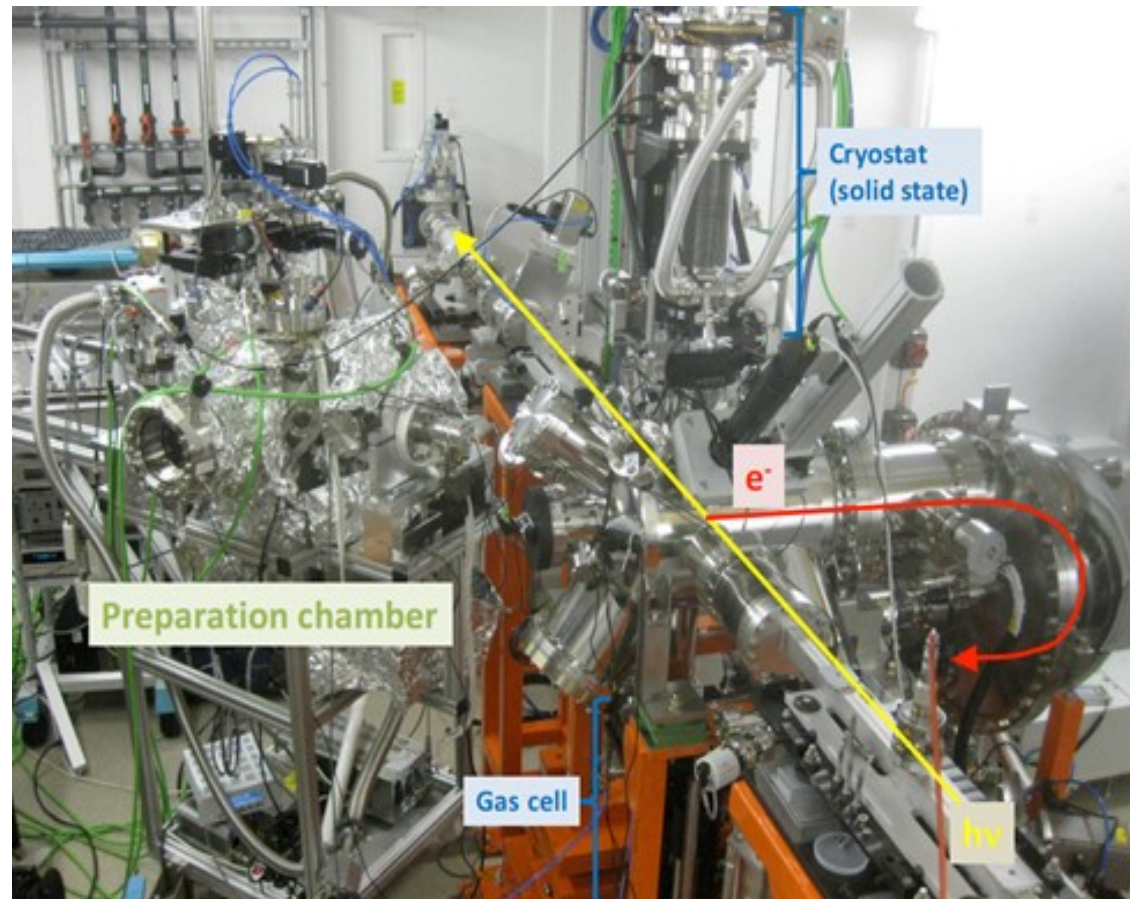
How can a theoretician @ SOLEIL be really useful?

Laboratoire des Solides Irradiés – CNRS - Ecole Polytechnique
European Theoretical Spectroscopy Facility (ETSF)
Synchrotron SOLEIL

matteo.gatti@polytechnique.fr
<http://etsf.polytechnique.fr> - <http://www.etsf.eu>

Room: O1.1.17 @ SOLEIL

Performing experiments ???



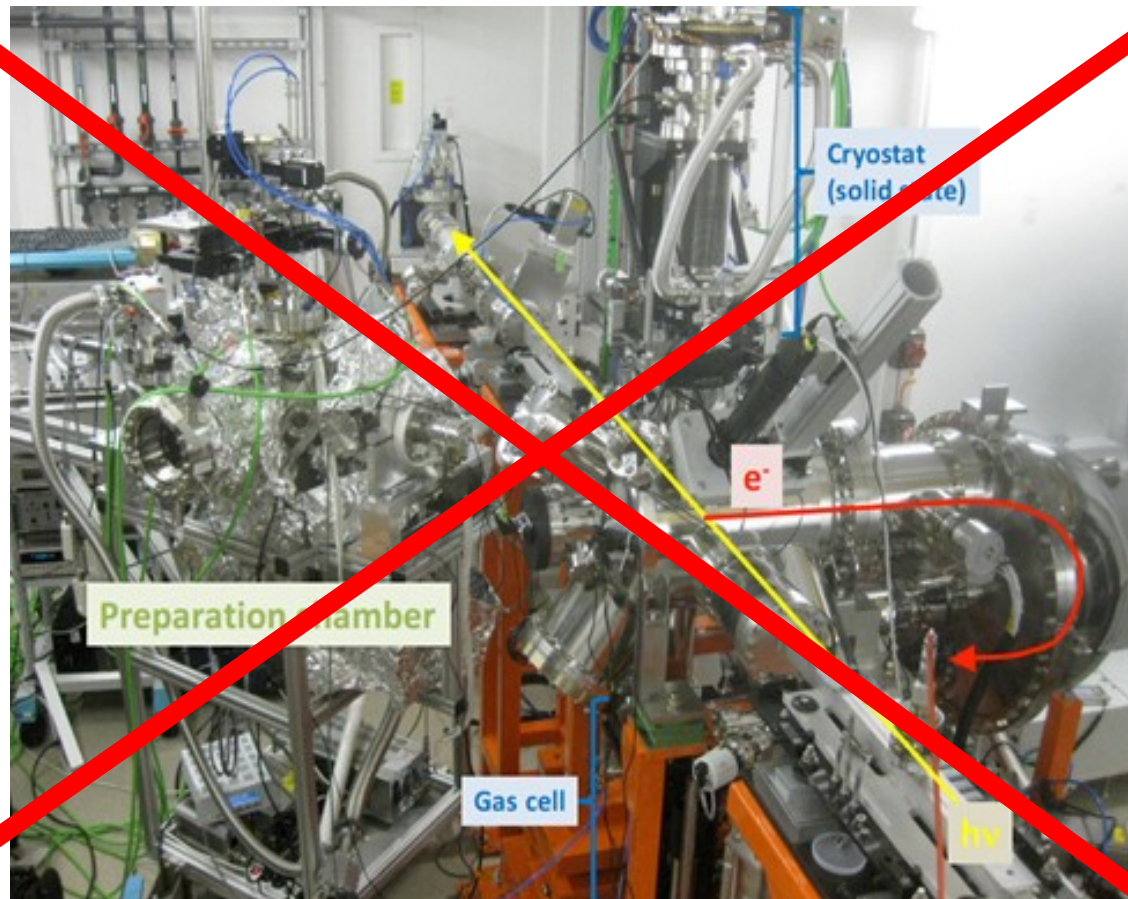
HAXPES station @ GALAXIES



WARNING

THEORETICIAN

Performing experiments ???



HAXPES station @ GALAXIES

Developing theory

- **Bridging theory and experiment**
→ what we calculate = what we measure?
- **Complementing theory and experiment**
→ different expertise, different language

Bridging theory and experiment

- Supporting experimental results and their interpretation
- Benchmarking theoretical development and predictions
- Developing theory upon request
- Theory antenna: Consulting and training
- ...

Learning a lot

Both directions

Bridging theory and experiment

- Supporting experimental results and their interpretation
- Benchmarking theoretical development and predictions
- Developing theory upon request
- Theory antenna: Consulting and training
- ...

Your ideas?
Your suggestions?

One theoretician alone?

Theoretical spectroscopy group LSI Ecole Polytechnique



See: <http://etsf.polytechnique.fr>



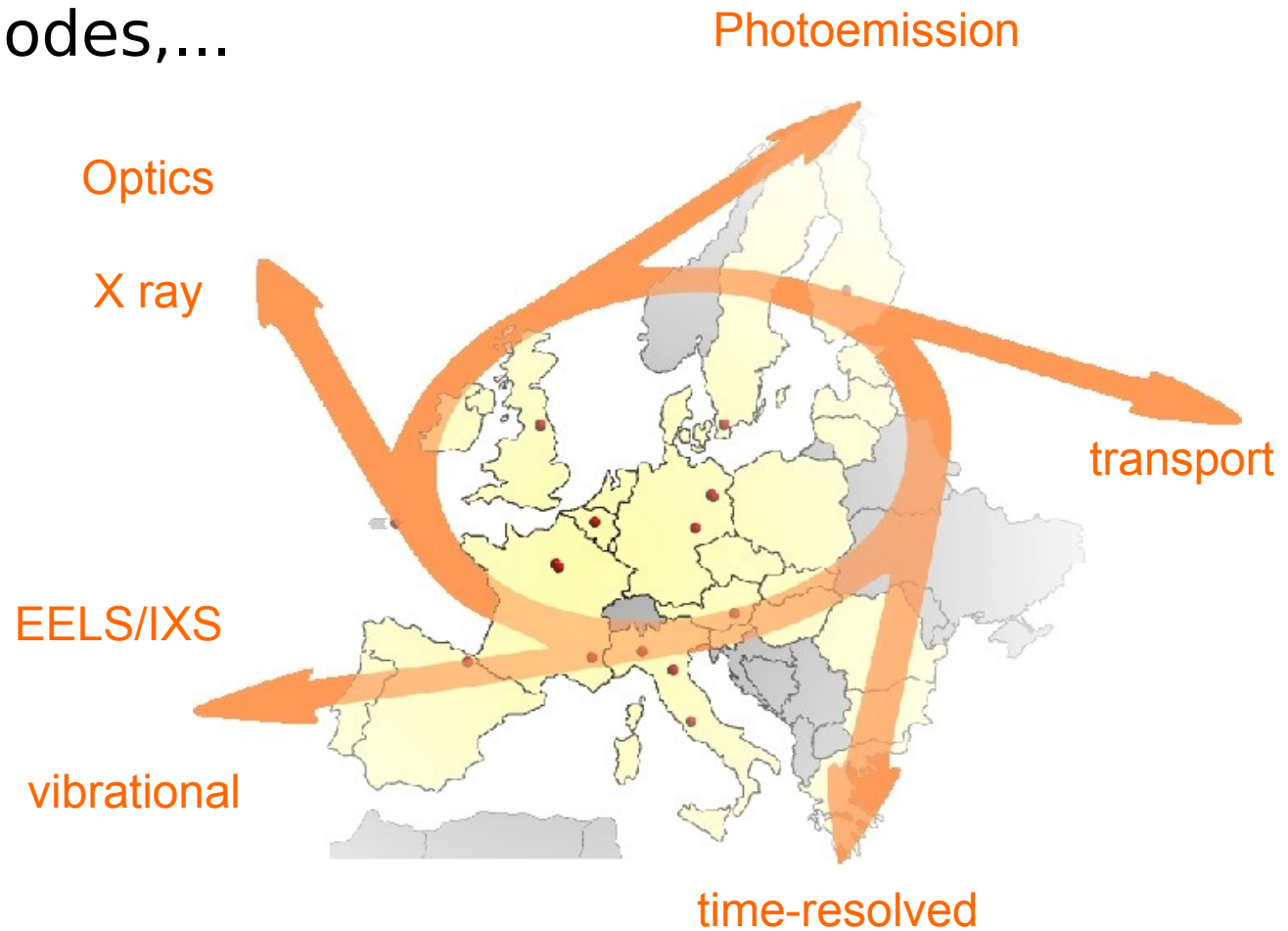
European Theoretical Spectroscopy Facility



68 research teams – more than 200 researchers in EU+US

See: <http://www.etsf.eu>

Collaborative projects Training, Codes,...



Next call: autumn 2014
See: <http://www.etsf.eu>

Experiments help improving theory

Theory helps improving experiments

$$1 + 1 > 2$$

Theory + Experiment
Working together

Experiments help improving theory

Theory helps improving experiments

$$1 + 1 > 2$$

The whole is greater than
the sum of its parts