GATHERING THE EFFORT TO MODEL SPECTROSCOPIES AT EUROPEAN LEVEL: THE COST ACTION MP1306 *EUSpec*

D. SÉBILLEAU[1], H. EBERT[2] and H. HERPER[3]

[1]Groupe Théorie, Département Matériaux-Nanosciences, Institut de Physique de Rennes, UMR CNRS-UR1 6251, Université de Rennes-1, 35042 Rennes cedex, France
[2]Department Chemie, Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81377 München, Germany
[3]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

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Roscoff : 23-27 May 2016

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Introduction

With the increasing complexity of physical, chemical, biological systems studied and the technological need for new materials with pre-defined tunable properties, there is a growing necessity to structure and federate research effort around common objectives. This has many advantages:

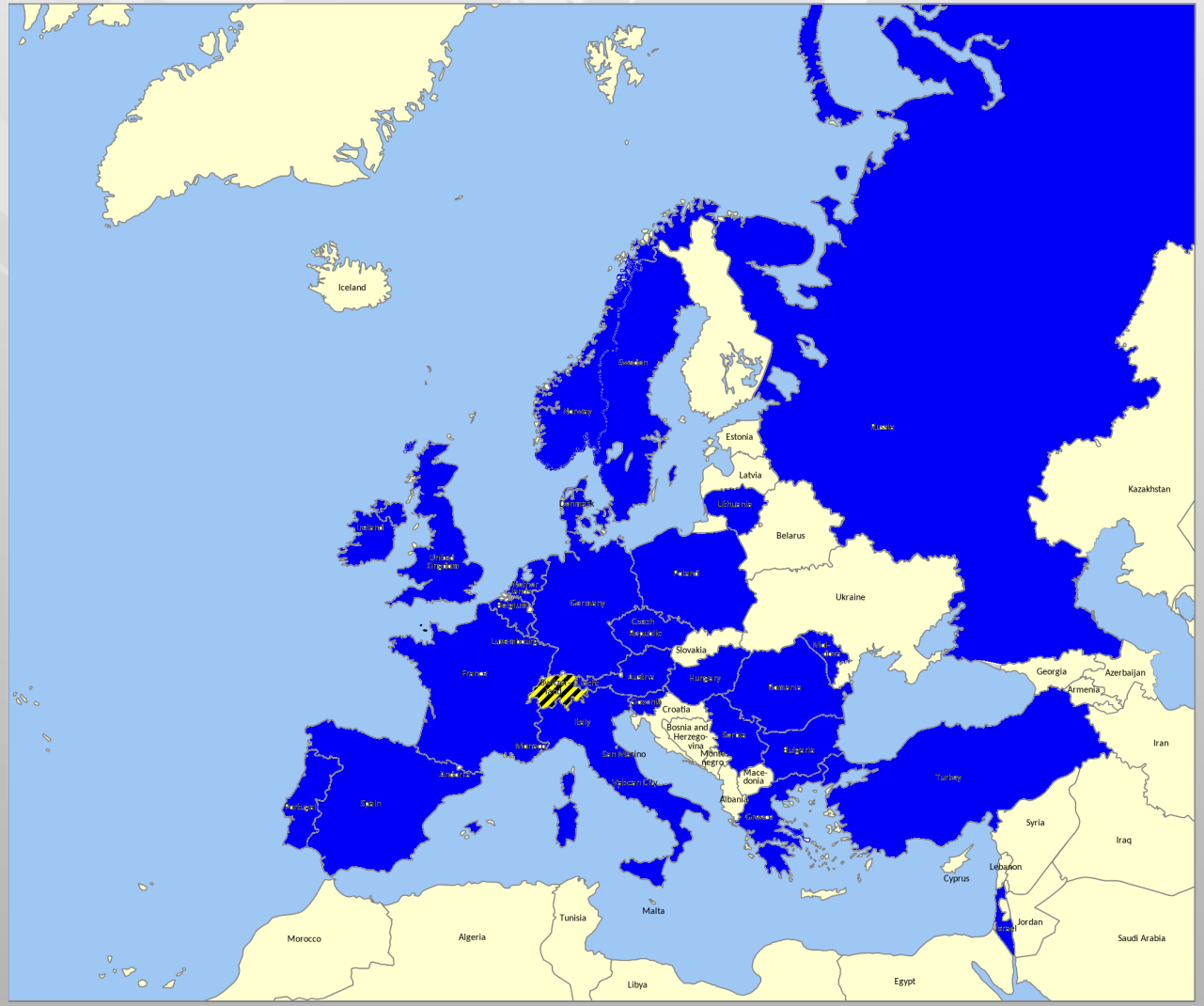
1. share the effort
2. do not reinvent the wheel in several places more or less at the same time
3. reach a critical size to be more visible at international level

EUSpec is such a structuration effort in the field of theoretical spectroscopy for the characterisation of materials

Introduction

- *EUSpec*: *"Modern Tools for Spectroscopy on Advanced Materials: a European Modelling Platform"*
- duration: 18th March 2014 – 17th March 2018
- objective: modelling of spectroscopies from different and complementary points of views (real space, reciprocal space and quantum chemistry methods, ...)
- means: gather scientists developing codes in all these areas in close contact with experimentalists
- so far: 26 COST countries, 2 NNC (Russia and Moldova) and 1 IPC (Japan), have joined
- so far: $>$ 200 physicists/chemists involved after 2 years
- tools: scientific missions (5 days-3 months), workshops, training schools, summer/winter schools (2 weeks)

Introduction



The *EUSpec* consortium so far:

Blue: COST countries who have joined

Switzerland is in the process of joining

+ IPC: Japan

Objectives

The main objectives of the *EUSpec* COST Action, as described in the MoU, are:

- gather theory activities in spectroscopy to supply high level support for demanding experiments using large-scale facilities or laboratory radiation sources performed within academic as well as industrial fundamental and applied research groups
- devise new methods to improve the description of the spectroscopies used to study the properties of nano-materials, strongly correlated systems, proteins, and to model promising new spectroscopies
- develop fundamental methods to better describe the intrinsic properties of ground and excited states in a wide range of materials

Objectives (cont.)

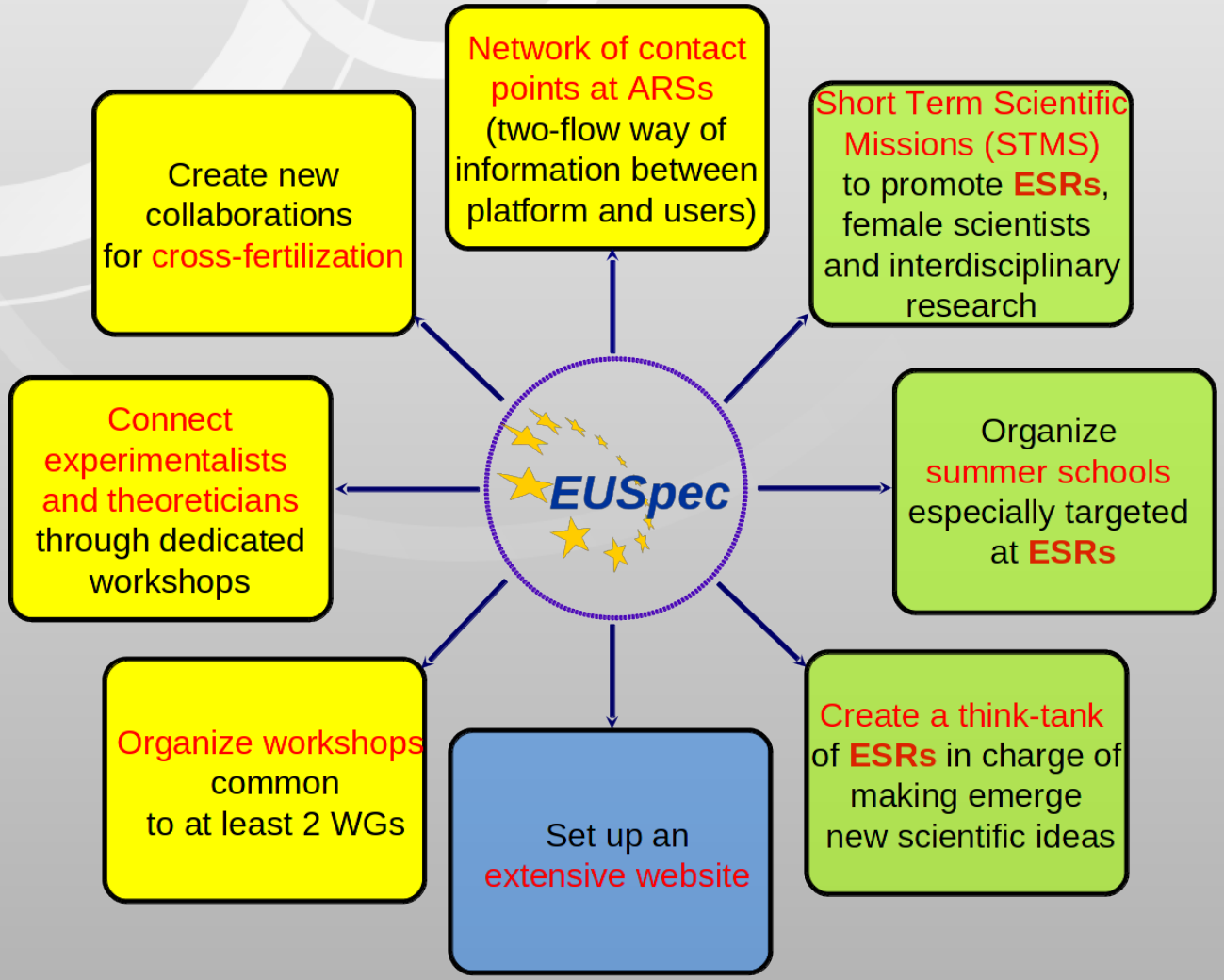
- implement these new methods in the codes of the consortium and test them against experiments specifically prepared by the experimental Working Group (WG) of the consortium
- transfer of recent achievements in the field of electronic structure calculations to spectroscopy codes. This applies, in particular, to full potential mode calculations, the advanced treatment of correlations effects and the description of all type of dichroic as well as time-dependent phenomena
- extend the applicability of the available spectroscopy codes to a very wide range of materials and spectroscopies. For this purpose a coherent platform with a common data format and interface to current electronic structure codes will be introduced

Objectives (cont.)

- Enhance the interaction between theory and experiment:
  1. by attracting and introducing new users to the theoretical tools provided by *EUSpec*
  2. by encouraging companies working on materials and computing to join
  3. by extending the community from SR/XFEL users to users of standard laboratory sources and of neutron sources

This last point is achieved through the a network of contact points at Advanced Radiation Sources (ARS) whose role is to ensure that the achievements of *EUSpec* are disseminated at ARSes and that information coming from ARSes is taken into account by *EUSpec*

Objectives: activities



Means: working groups

Work in *EUSpec* is organised into 5 Working Groups (WG):

1. WG1 Correlation: in charge of the description of electron correlation
2. WG2 Spectroscopy: in charge of the description of a wide range of spectroscopies and their implementation into the codes of the Action
3. WG3 Time-resolution: in charge of the description of femtosecond SR and XFEL spectroscopies
4. WG4 Platform: in charge of the integration of the codes into the platform website
5. WG5 Experiment: in charge of setting-up and establishing experiments to test and push theoretical models to their limits

Means: workshops, ...

EUSpec organises regularly meetings, training schools and summer/winter schools which are open to everyone. However, only Action participants are eligible for financial support. More precisely:

- 2 whole Action meetings (☞ 1st WAM : Louvain-La-Neuve, Belgium, 15-17 Sep. 2014)
- 4 scientific workshops (☞ 1st one : Aveiro, Portugal, 25-26 Jun. 2015)
- 4 hands-on training workshops (☞ 1st one: Plžen, Czech Republic, 23-26 Feb. 2015) (☞ 3rd one: Rennes, France, 27-30 Jun. 2016)
- 2 summer/winter schools (☞ 1st one: Ajdovščina, Slovenia, 1-11 Feb. 2016)

EUSpec funds short-term scientific missions (STSM: from 5 days to 3 months). Their number is defined annually by the Management Committee (☞ this year: ∼ 12-15 STSMs)

Annual budget: 134000 € ... reduced now to 125000 €

Means: the *EUSpec* website

The *EUSpec* website is the core of the Action. At the end, it will offer:

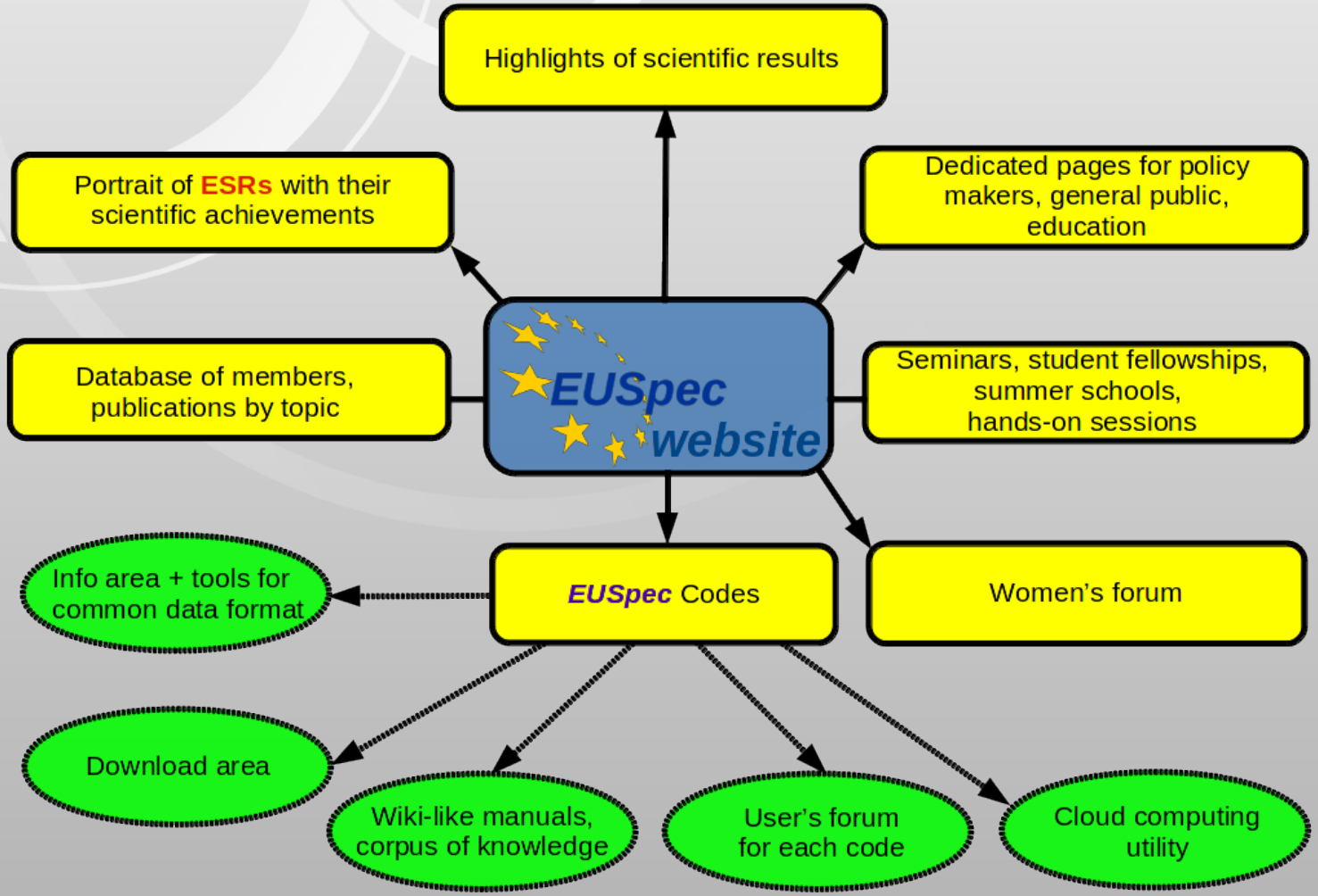
- a download platform
- extensive user's guides
- wiki-organised manuals
- information about the theoretical methods underlying the codes
- users' forum for certain codes and for certain topics
- information about training courses
- etc

Means: the *EUSpec* website

In addition, it will also contain:

- highlights of scientific results
- portraits of young researchers with their scientific achievements
- database of the members of the Action
- a topical selection of publications

Means: the *EUSpec* website



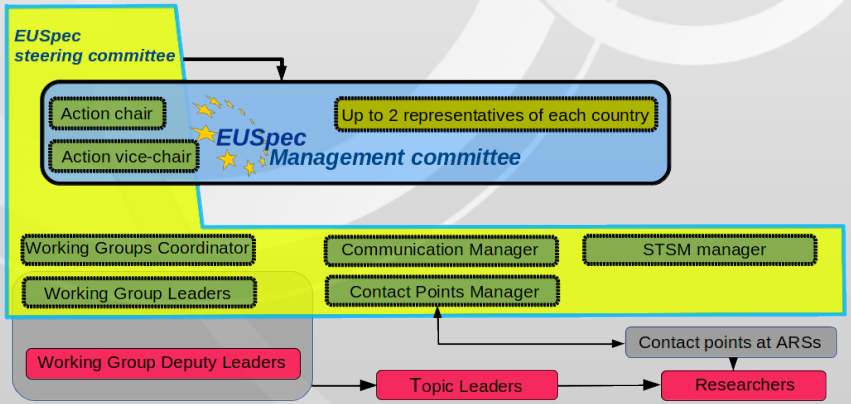
Means: the *EUSpec* website

At present, 18 codes are involved in *EUSpec*. Among them

1. electronic structure codes: SPR-KKR, WIEN2k, CRYSTAL, ABINIT, QUANTUM ESPRESSO, OCTOPUS, ORCA, QUANTY, GPAW, ...
2. spectroscopy codes: MsSpec, MXAN, GNXAS, FDMNES, CTM4XAS, CTM4RIXS, ...
3. visualisation: XcrySDen

The full list with details on the codes is available from our website
A newsletter is also be available both by direct mail and through the website. 2 issues have been published so far. The third one is due anytime now.

Means: the management structure



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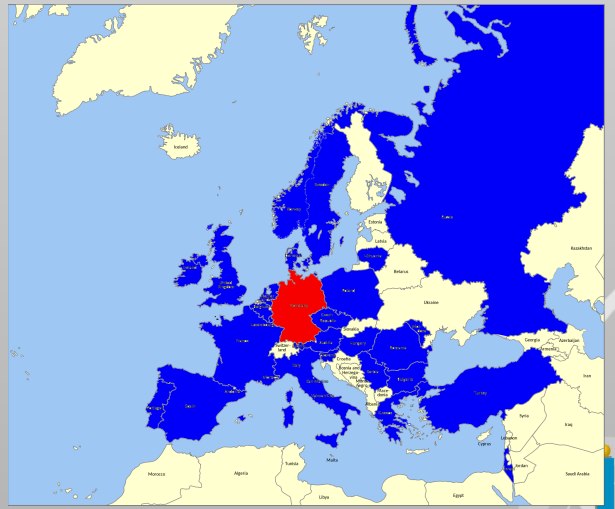

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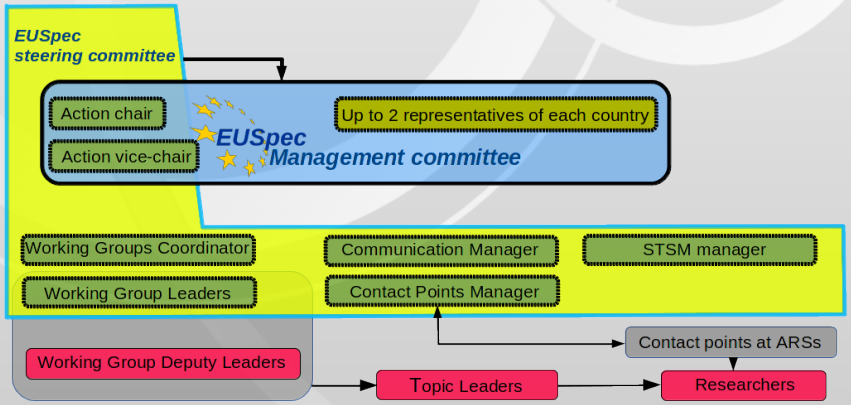

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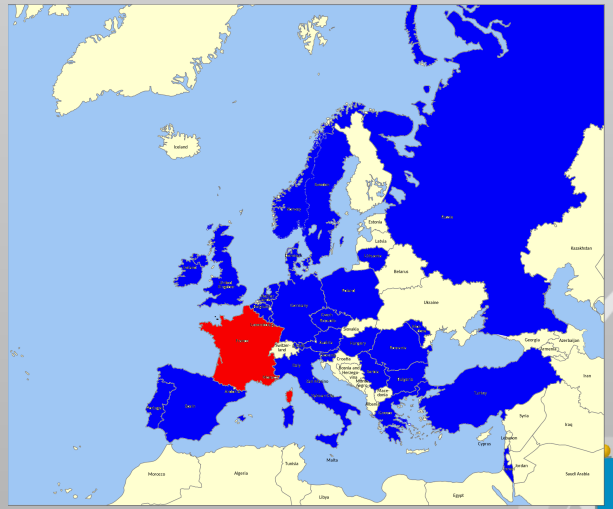

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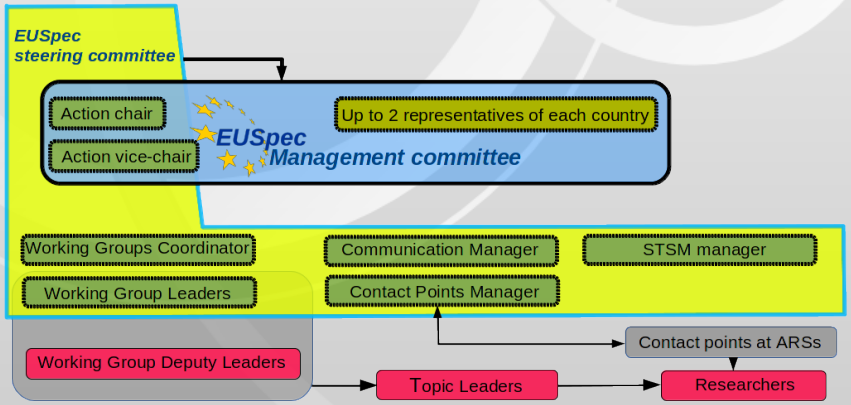

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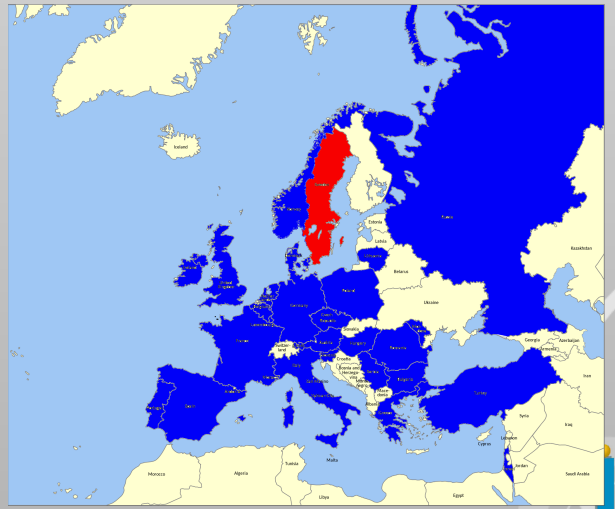

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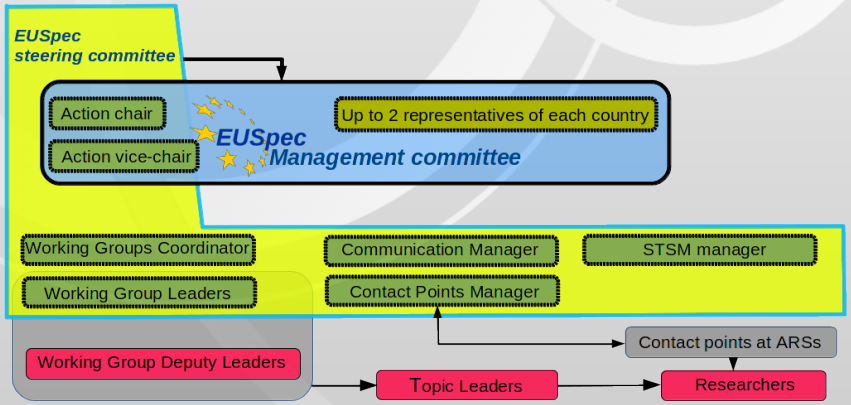

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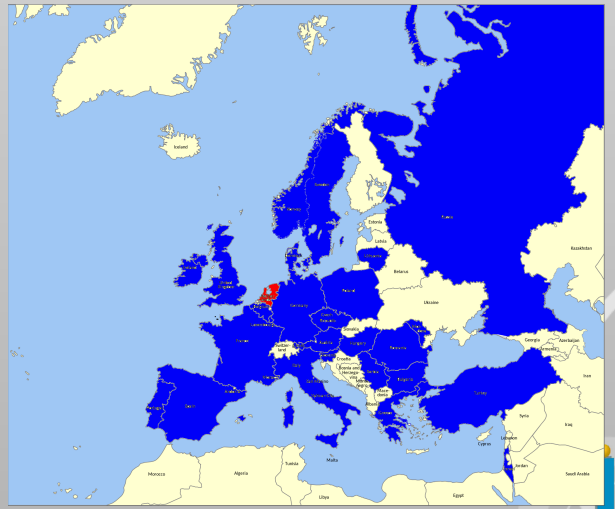

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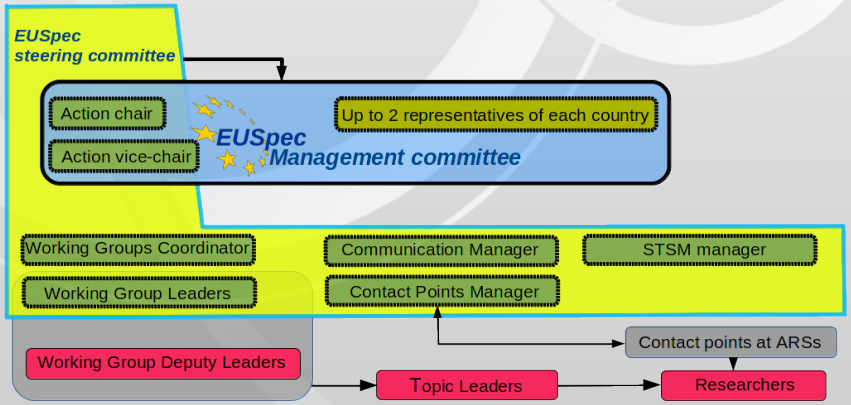

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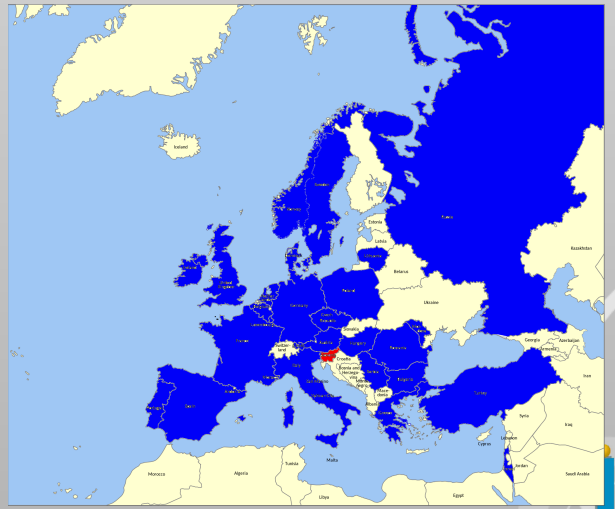

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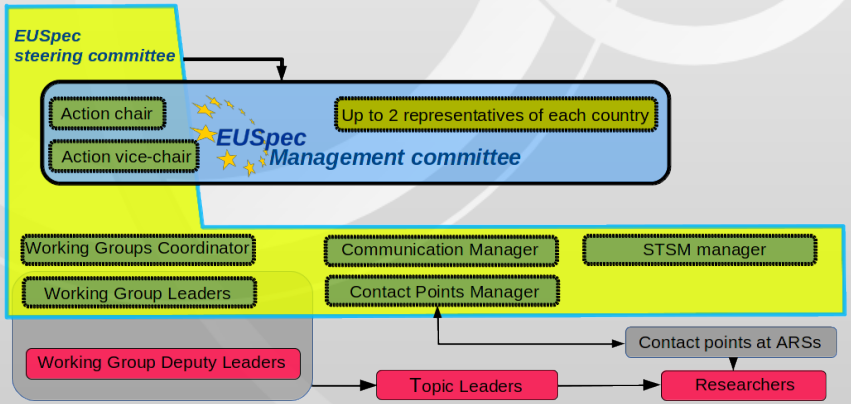

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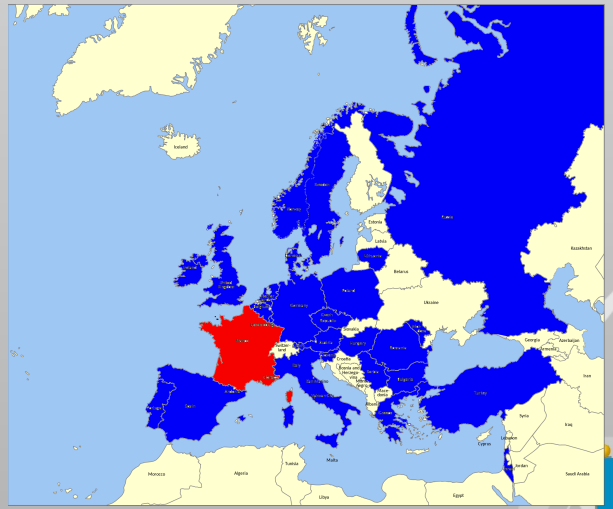

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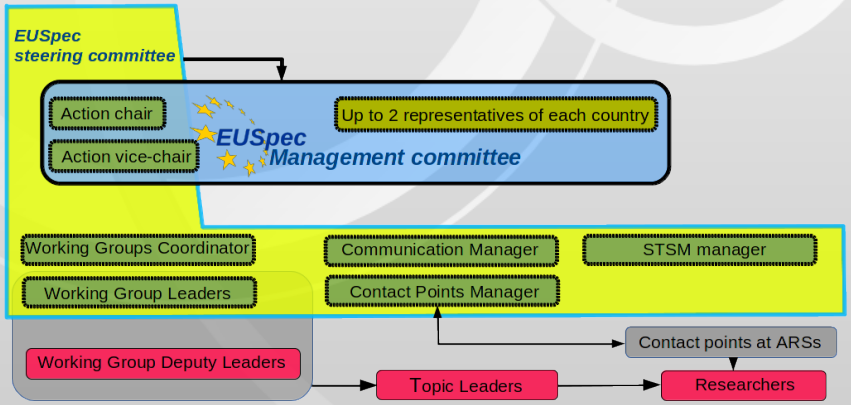

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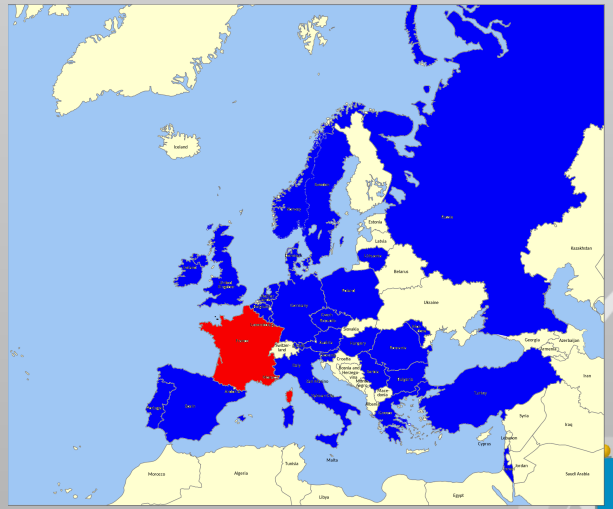

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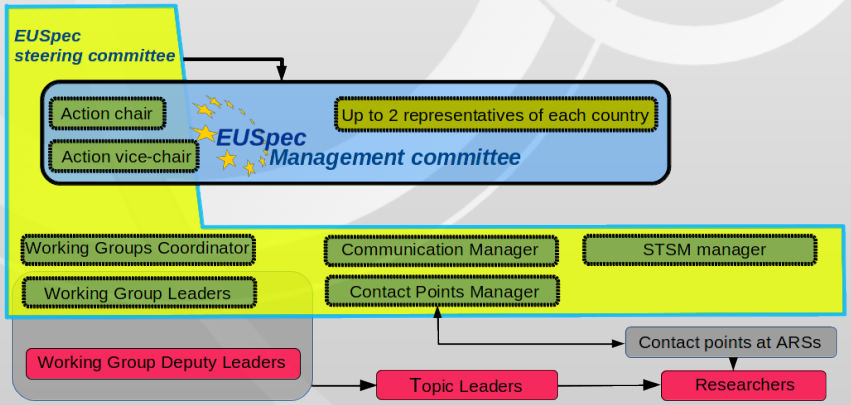

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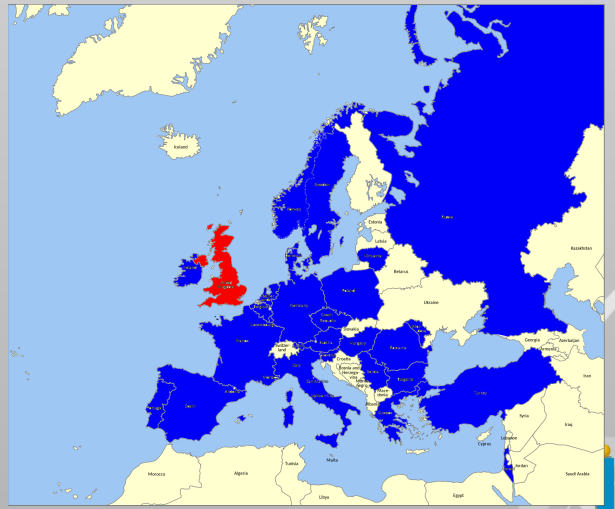

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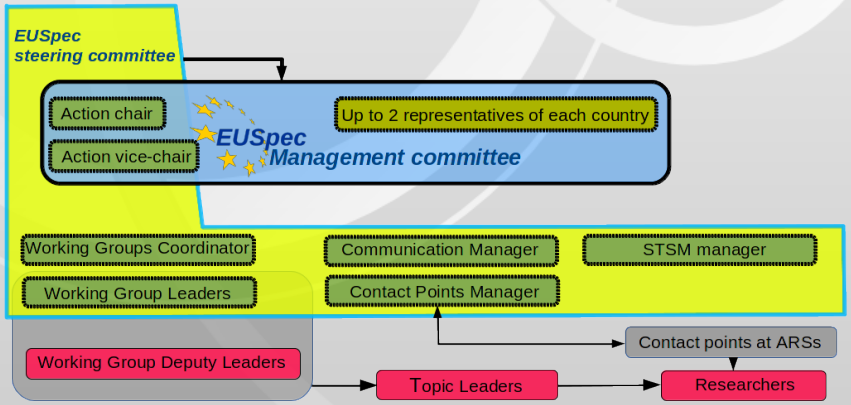

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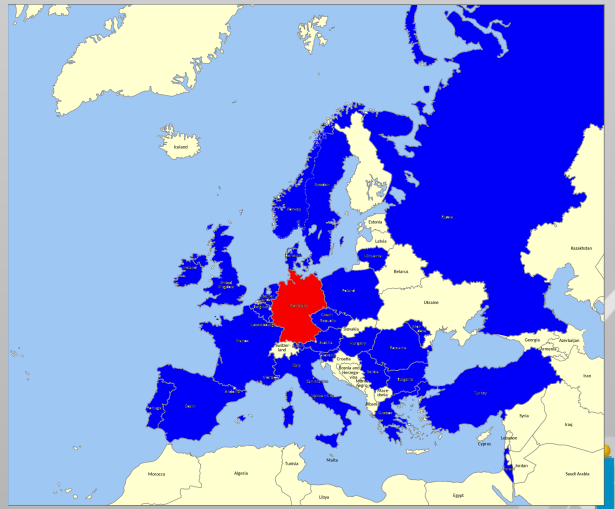

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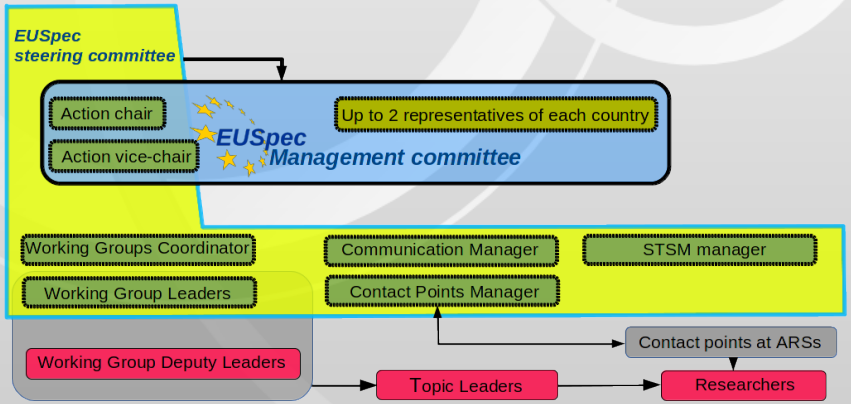

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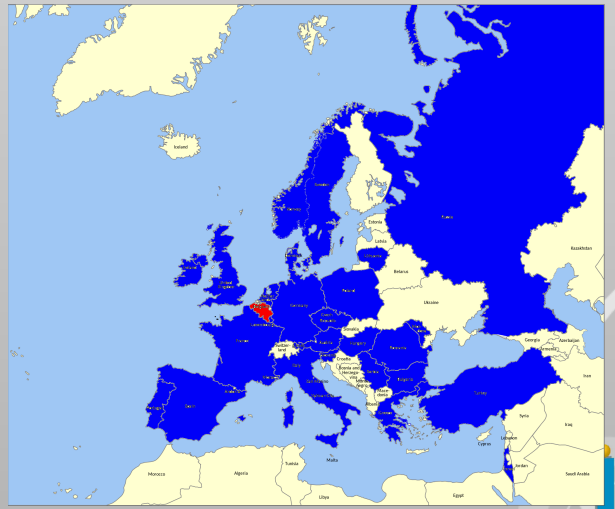

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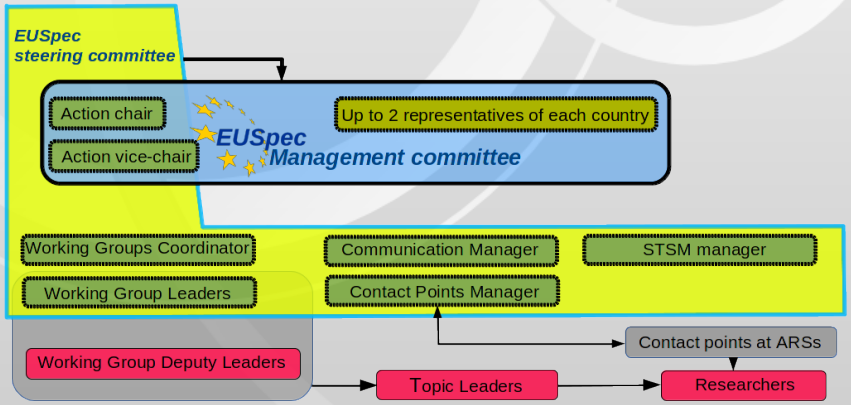

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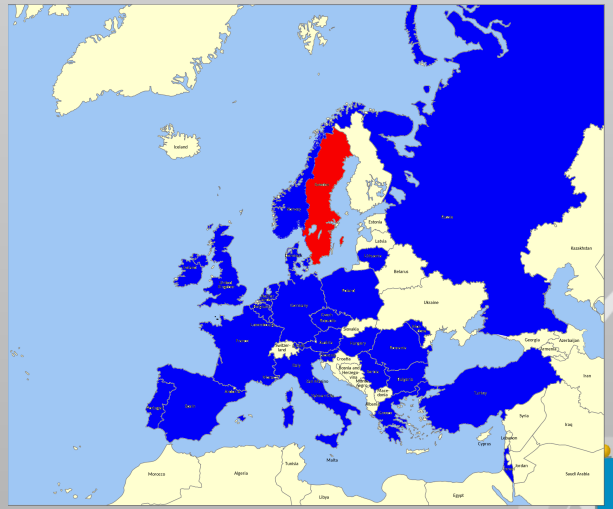

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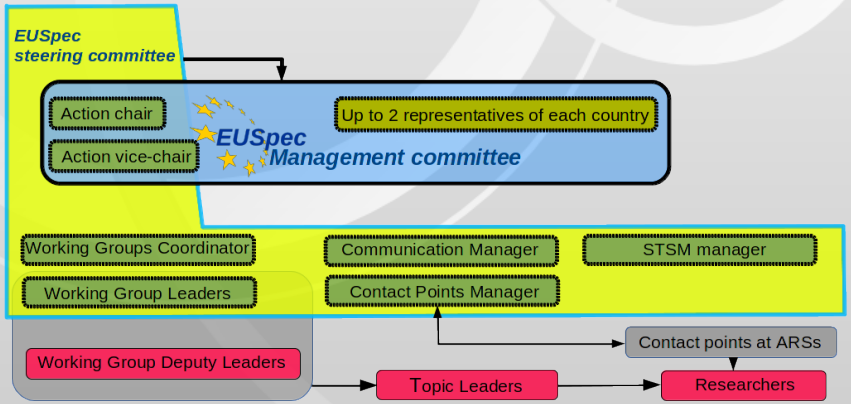

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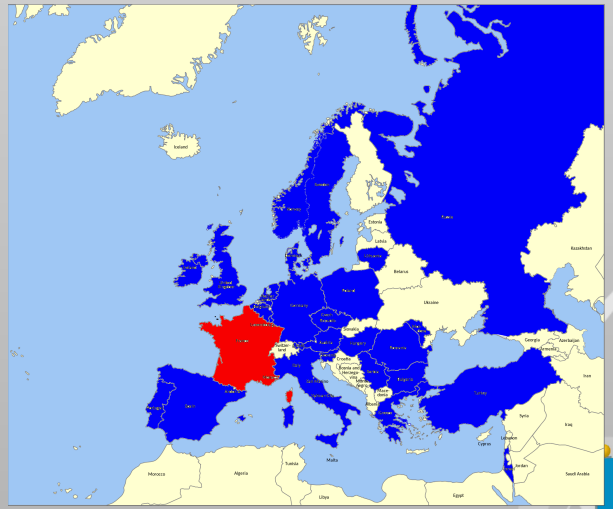

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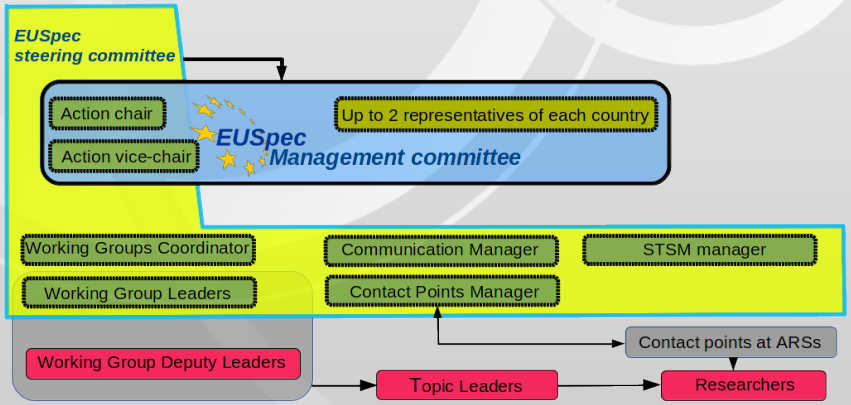

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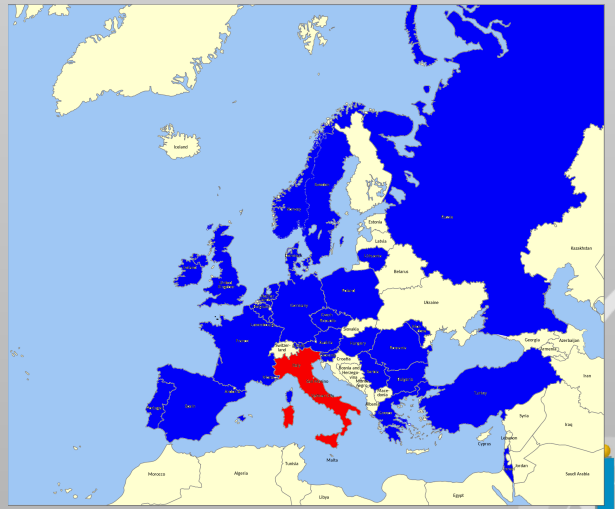

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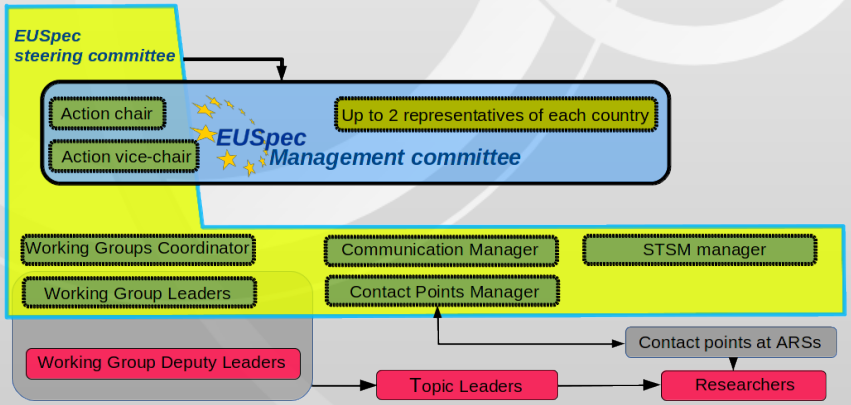

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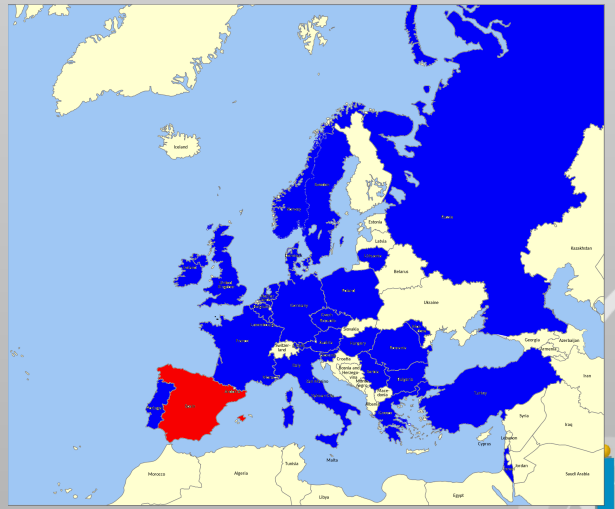

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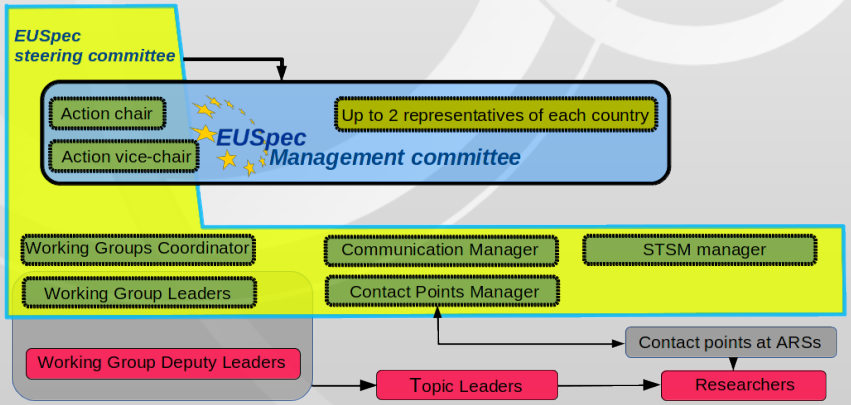

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- WG2 spectroscopy: Barbara Brena (SE)
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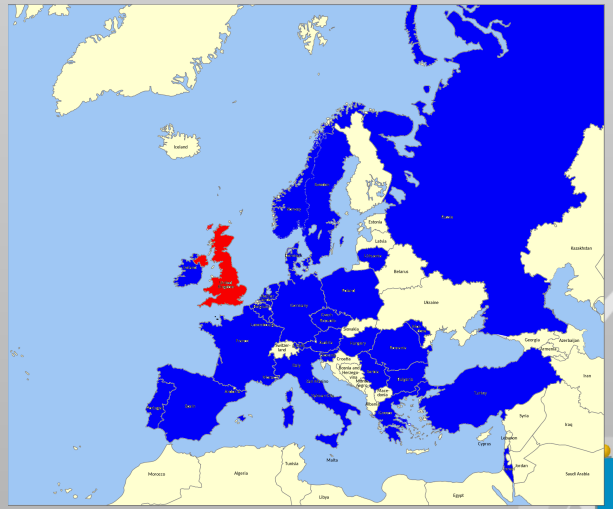

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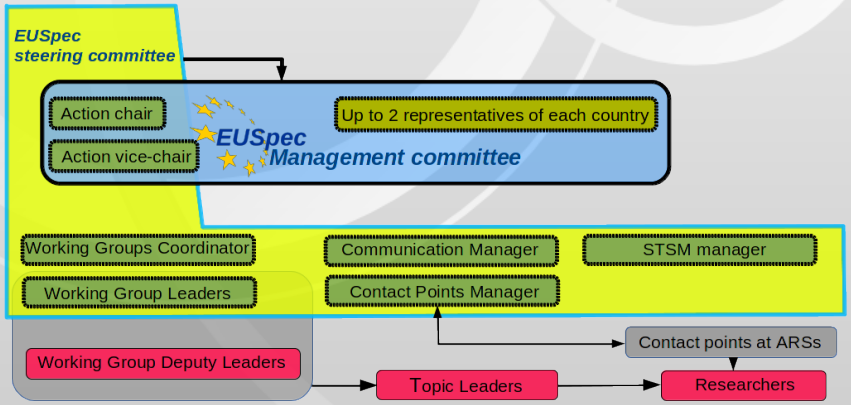

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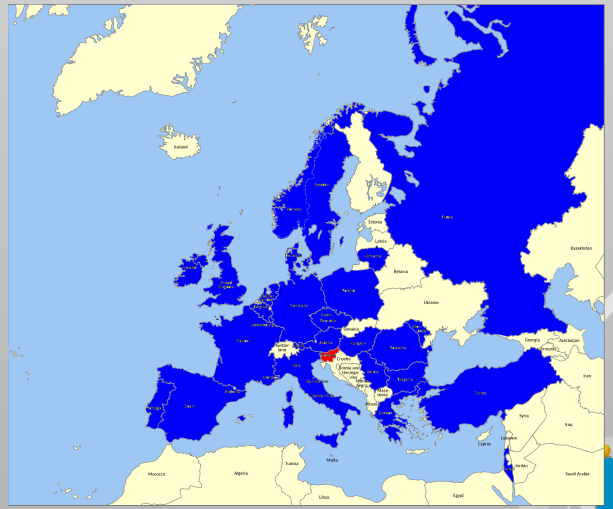

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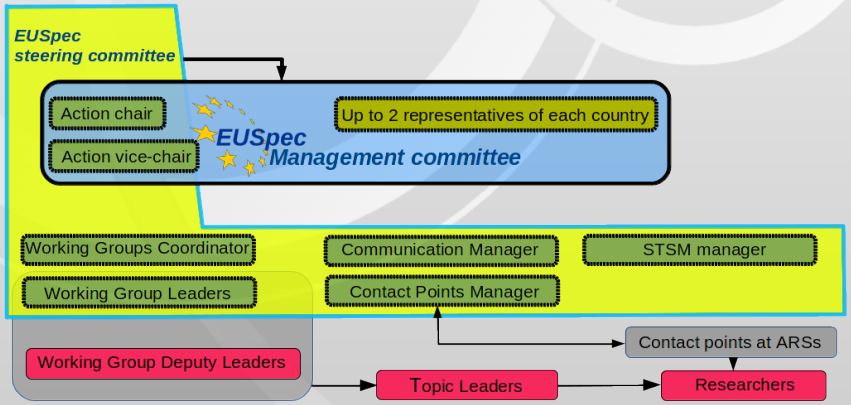

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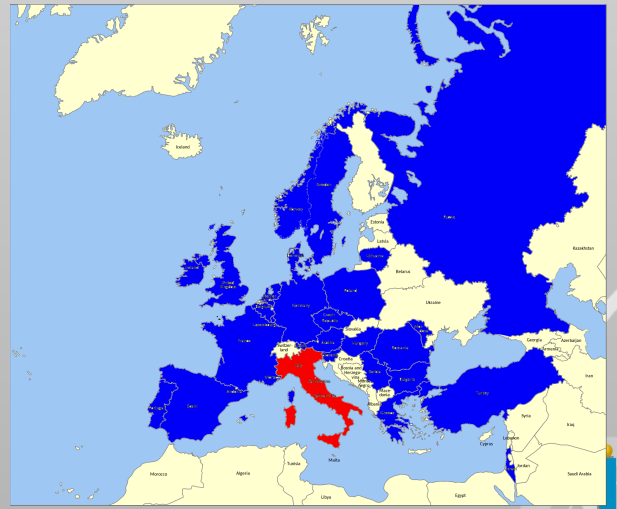

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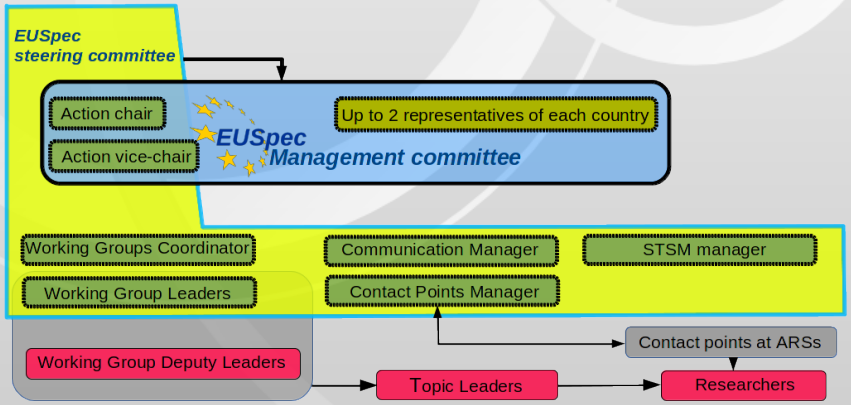

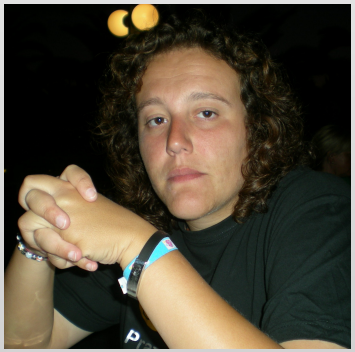

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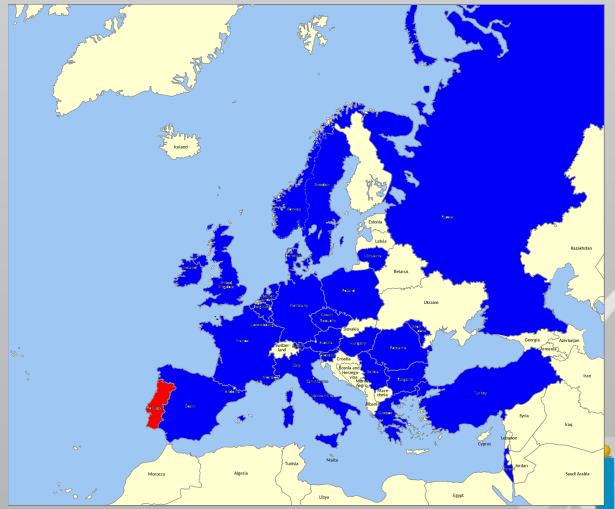


Means: events planned this year

- Training school on multiple scattering codes : Rennes (France) 27-30 June 2016
- WG2-WG5 meeting : Rennes (France) 30 June 2016
- Support for MSNano conference : Rennes (France) 1-2 July 2016
- Support for Benasque TDDFT school (Spain) 12-19 September 2016
- WG4 meeting : coding workshop Budapest (Hungary) 18 October 2016
- Hands-on DFT/MS codes : Daresbury (UK) 12 December 2016. Co-funded by CCP

Means: events planned this year (cont.)

- WG1 meeting : Prague (Czech Republic) 6-8 February 2017. Co-organized by Claudia Draxl
- WG/MC meeting : Athens (Greece) 16 February 2017
- WG2-WG5 meeting : Krakow (Poland) 14-15 March 2017
- $\sim$ 12 STSMs (24600 €) including one coding mission

The following table shows the scenarios available to eligible STSM applicants:

Home Institution	Host Institution
From a Participating COST Country	To another Participating COST Country
	To an approved NNC institution
	To an approved IPC institution
	To an approved Specific Organisations (EC and EU Agencies, European RTD Organisations, International Organisations)
From an approved NNC institution	To a Participating COST Country
From an approved European RTD Organisation	To a Participating COST Country

Example of work done: data format in WG4

Idea: define a common data format to exchange data between our codes (based on NetCDF/HDF5), building on the experience of work already done by other networks (ETSF, MSNano, ...). Idem for a format to exchange data between experiments and codes

- we have organized several one-day WG meetings to discuss the subject (Munich, Frascati, ...) where people from ETSF were invited (Micael Oliveira, Yann Pouillon, Matteo Giantomassi) or from synchrotron (Keith Gilmore)

Example of work done: data format in WG4 (cont.)

- participation to a common ETSF/EUSpec/NOMAD CECAM coding workshop that was held in Lausanne. Jan Minár was involved in the one-week coding session during which the foundations for the new ESCDF were laid (Electronic Structure Common Data Format). He worked in particular on the ESL (Electronic Structure Library)
- Ongoing discussions with the E-CAM project to use one of the E-CAM postdocs to complete the implementation of the ETSF library
- we are discussing with IXAS (H. Oyanagi, Photon Factory, Japan) as IXAS has also a working group on the subject

Means: interaction with existing networks

COST Action *EUSpec* interacts with the following networks:

- European FP7 network *ETSF*
  - based on pseudopotential description
  - optical spectroscopies for semiconductors
  - chair: X. Gonze (Louvain), vice-chair: L. Reining (Paris)
- European FP7 IRSES network *MSNano*
  - restricted to multiple scattering method
  - coordinator: D. Sébilleau (Rennes)
- COST Action MP1302 *Nanospectroscopy*
  - aims at nanospectroscopic methods
  - emphasis on optical experiments
  - chair: M. Fleischer (Tübingen), vice-chair: P.-M. Adam (Troyes)

Means: interaction with existing networks (cont.)

- CECAM : organisation of a common CECAM/ETSF/*EUSpec* workshop on data format on 25-27 January 2016

  + following coding sessions

⇛ Proposal: have common meetings EUSpec-REST

Conclusion

The *EUSpec* COST Action

- provides a common platform for theory
- coordinates theory activities
- enhances theory-experiment interactions
- provides experimentalists with program packages for interpreting results
- collects feedback from experiment

Websites: http://www.cost.eu/COST_Actions/mpns/MP1306
http://www.euspec.eu/

The COST action EUSpec cordially invites to...

EUSpec TRAINING SCHOOL

cost Action

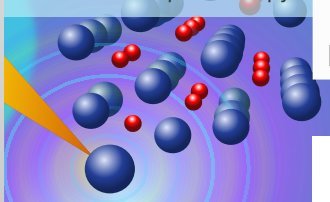
European Cooperation in Science and Technology

MULTIPLE SCATTERING CODES

June 27-30, 2016 - Université de Rennes 1, France

MXAN | GNXAS | MsSpec | FPMS | MCMS

This training school will focus on codes using the multiple scattering framework to model core-level spectroscopies such as X-ray Absorption, Photoelectron Diffraction, Auger Electron Diffraction, or Auger Photoelectron Coincidence Spectroscopy.



Registration and more information at :

EUSpec.sciencesconf.org

REGISTRATION : before the 8th May 2016 & limited to 40 participants

Invited Plenary Speakers

M. Benfatto *(LNF-INFN, Frascati)*
C. R. Natoli *(LNF-INFN, Frascati)*
A. Di Cicco *(Università di Camerino)*
D. Sébilleau *(IPR, Rennes)*
K. Hatada *(IPR, Rennes)*
H. Ebert *(LMU-Munich)*
J. Minár *(LMU-Munich)*
O. Šipr *(Inst. Phys. ASCR, Prague)*
P. Krüger *(Chiba University)*
A. Taranukhina *(SFedU, Rostov on Don)*

Codes descriptions :

MXAN : *to fit XAS data in terms of selected structural parameters from the edge to 250 eV*
GNXAS : *advanced software for EXAFS data analysis with a rigorous fitting procedure of the raw experimental data*
MsSpec : *to model 5 different spectroscopies including photoelectron and Auger electron diffraction*
FPMS : *full-potential XAS calculations that can treat very large clusters*
MCMS : *R-matrix multi-channel calculations of XAS spectra*

Satellite conference on multiple scattering: 1st-2nd July 2016 (same place)
More information at : MSNano.sciencesconf.org

cnrs | UNIVERSITÉ DE RENNES 1 | ipr Rennes

D. SÉBILLEAU, H. EBERT and H. HERPER

MSNano | EUSpec | cost European Cooperation in Science and Technology

July 1-2 2016

4th MSNano conference on recent advances in the multiple scattering approach to spectroscopies

University of Rennes 1, France

A tribute to C.R NATOLI for his 75th birthday

The first day will focus on recent developments in the description of spectroscopies within the multiple scattering framework proposed in the FP7 MSNano network and on experiments performed to test these models. On the second day detailed overviews of work involving multiple scattering will be given by many leading researchers in the field. These talks are dedicated to Rino Natoli on the occasion of his 75th birthday, in honour of his outstanding lifetime achievements in the multiple scattering modeling of spectroscopies and his tutoring work in the training of two generations of multiple scattering physicists.

International invited speakers

R. Choubisa (Pilani, India)
W. Chu (Hefei, China)
H. Daimon (Nara, Japan)
A. Di Cicco (Camerino, Italy)
H. Ebert (Munich, Germany)
C. S. Fadley (Berkeley, USA)
T. Fujikawa (Chiba, Japan)
J. García (Zaragoza, Spain)
R. Gunnella (Camerino, Italy)
T. Jaouen (Fribourg, Suisse)
P. Krüger (Chiba, Japan)
A. Marcelli (Frascati, Italy)
J. Minár (Munich, Germany)
T. Miyanaga (Hirosaki, Japan)

International invited speakers

C. R. Natoli (Frascati, Italy)
F. Palumbo (Frascati, Italy)
M. Pedio (Trieste, Italy)
N. Perkins (Minneapolis, USA)
J. J. Rehr (Seattle, USA)
O. Šipr (Prague, Czech Republic)
G. Stefani (Roma, Italy)
A. Taranukhina (Rostov/Don Russia)
M. A. Van Hove (Hong Kong, China)
R. Zeller (Jülich, Germany)
C. Zou (Hefei, China)

Local invited speakers

C. Brouder (IMPMC, Paris)
M. Cammarata (IPR, Rennes)
S. Di Matteo (IPR, Rennes)
C. Godet (IPR, Rennes)
K. Hatada (IPR, Rennes)
Y. Joly (Néel, Grenoble)
P. Sainctavit (IMPMC, Paris)
D. Sébilleau (IPR, Rennes)
P. Turban (IPR, Rennes)

MSNano.sciencesconf.org

METROPOLE Rennes | cnrs | UNIVERSITÉ DE RENNES 1 | ipr | Région BRETAGNE