European Cooperation in the field of Scientific and Technical Research
- COST -

Brussels, 22 November 2013

COST 075/13

MEMORANDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action MP1306: Modern tools for spectroscopy on advanced materials: a European modelling platform

Delegations will find attached the Memorandum of Understanding for COST Action MP1306 as approved by the COST Committee of Senior Officials (CSO) at its 188th meeting on 14 November 2013.

MEMORANDUM OF UNDERSTANDING
For the implementation of a European Concerted Research Action designated as

COST Action MP1306
MODERN TOOLS FOR SPECTROSCOPY ON ADVANCED MATERIALS: A EUROPEAN MODELLING PLATFORM

The Parties to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the "Technical Annex to the Memorandum", have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of document COST 4114/13 "COST Action Management" and document COST 4112/13 "Rules for Participation in and Implementation of COST Activities" , or in any new document amending or replacing them, the contents of which the Parties are fully aware of.

2. The main objective of the Action is to gather theory activities in spectroscopy to supply high level support for demanding experiments using large facility or laboratory radiation sources performed within academic as well as industrial fundamental and applied research.

3. The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at EUR 56 million in 2013 prices.

4. The Memorandum of Understanding will take effect on being accepted by at least five Parties.

5. The Memorandum of Understanding will remain in force for a period of 4 years, calculated from the date of the first meeting of the Management Committee, unless the duration of the Action is modified according to the provisions of section *2. Changes to a COST Action* in the document COST 4114/13.

A. ABSTRACT AND KEYWORDS

This Action called EUSpec brings together the expertise of experts working in the science of advanced materials in order to build a coherent theory and computing platform with a new common data format to model sophisticated spectroscopy experiments performed at advanced radiation sources (ARS) as well as at academic and industrial research laboratories. Complementary theoretical approaches will allow to deal with a wide variety of materials. Ultimately, the accurate interpretation of spectroscopies will provide the means to access the intimate origin of the macroscopic behaviour of materials, for which a detailed knowledge of the electronic, magnetic and geometrical structure at the atomic level is a prerequisite. The platform established through this Action will be widely available to academic as well as industrial users. Close contact with them will be kept through an extensive webpage, a series of workshops and a network of contact points at European synchrotron radiation (SR), X-ray free electron laser (XFEL) centres and neutron sources (NS). As the Action primarily aims at coordinating and synchronizing on-going developments and research activities as well as enhancing the interaction between theory and experiment in the wider field of spectroscopy, COST is the most suitable framework to reach these goals.

Keywords: Computational Materials Science, Theory of Spectroscopy, Advanced Radiation Sources research, Time-Resolved Spectroscopies

B. BACKGROUND

B.1 General background

The study of materials is of central importance for progress in science and technology, and it is relevant in domains as different as physics, chemistry, biology, geology or archaeology. Other disciplines (space sciences, domotics) deeply rely on the mastering and integration of advanced devices and multifunctional materials including their complex interaction with fields and matter. A deep knowledge of the properties of the materials on the atomic scale is necessary in order to understand the origin of their macroscopic behaviour. New discoveries in this area quickly find their way into applications. For example, in condensed matter, nano-systems and transition-metal oxides are expected to lead to a whole new range of electronic devices based on spin transport. In biology, the study of the interaction of molecules with hybrid systems promises essential improvement in drug delivery and manipulation. Nano-structures exhibit new properties that can be tuneable. Their control

requires a precise knowledge of the structure, which may differ radically from that of standard materials. Indeed, the reduced dimensionality would enhance the importance of valence electron correlations. To make significant progress in the field, however, a proper understanding of the mechanisms and in particular their entanglement is a prerequisite that has to be met. To achieve these goals, non-destructive spectroscopies are a fundamental tool of analysis at the nanoscopic level, allowing to probe matter and its constituents with an atomic resolution, and to monitor their time evolution down to the femtosecond range, transforming them into unique methods to trace chemical reactions.

Corresponding spectroscopic experiments are done in academic and industrial labs, but also to a rapidly increasing extent at sophisticated radiation sources such as synchrotrons, free electron laser facilities or neutron sources. The continuously increasing resolution concerning space, energy, momentum, spin and time, gives much more detailed information as obtained in the past. To make full use of this, complementary theoretical support is indispensable. This has to go in general far beyond simple simulation of experimental data as it is well established in the field of X-ray diffraction. In fact many theoreticians are working more or less independently at an advanced level on this subject within the EU member states, using different theoretical frameworks and languages and targeting different materials, which results in a fragmentation of the research into separate communities. The lack of communication between them hinders rapid progress as new developments are not communicated as fast as possible and often work on the same subject is done in parallel. Also the communication between theory and experiment has to be improved. On the one hand side, new types of experiments are important benchmarks for the status of theory and often require and trigger new formal theoretical and corresponding code developments. On the other hand, experimental groups are not always aware of the available tools and program packages provided to them by the colleagues from theory.

To deal with the situation described it is first of all necessary to enhance the communication and interaction between the various theory groups as well as their link to experiment. The efforts and developments necessary to reach this goal and to allow, in particular, an easy exchange of data will be more than compensated by the exchange of know-how as well as common program modules. In fact, the primary aim of the Action EUSpec is to start synergy effects between existing activities scattered over many theory groups and to enhance the communication of theory with experiment. Accordingly, the COST scheme, providing the basis for an efficient networking and exchange is the ideal platform for this Action. Performing the Action EUSpec within the COST framework, it will

benefit obviously from the provided support perfectly fitting to its needs. In particular, the flexibility of the COST scheme will be of great advantage compared with other schemes as it is expected that more expert groups involving also additional countries will join the Action.

This Action will lead to a large-scale network in order to give a strong impetus to the spectroscopy research and to give Europe a decisive lead. It will establish a platform that goes far beyond the applicability of the actual individual codes in order to address the relevant questions and problems for many more materials and spectroscopies. This will be achieved by gathering the expertise of European researchers (theoreticians and experimentalists) working with various solid state and quantum chemistry methods that do not usually interact.

B.2 Current state of knowledge

Accompanying experimental data by theoretical simulations is well established for many techniques that probe materials at the atomistic level, with the most prominent example given by X-ray diffraction. Important examples for electron spectroscopies aiming to probe structural properties are LEED (low energy electron diffraction), EXAFS (extended X-ray absorption fine structure) and XPD (X-ray photo electron diffraction). In fact several programs are available that allow non-expert users to perform detailed simulations and in this way reliable data analysis. Also, for spectroscopies that provide primarily information on electronic and magnetic properties corresponding computer codes are available that provide valuable support to experimentalists. In this case, however, the supply of an adequate description of experimental observations is much more demanding. This applies on the one hand side for the description of the underlying electronic structure of the systems that may be strongly influenced by electronic correlations. This is a field of modern quantum mechanics that has seen many important developments during the last one or two decades allowing for a more and more improved treatment e.g. for nano-systems, oxides or organic solids. An equally important issue is to account for experiment-specific issues and aspects as for example the geometrical set-up, selection rules imposed by the relevant matrix elements or the spin-polarization in photo emission or Auger experiments. Another important example is the demanding description of time-resolved spectroscopy experiments. These continuously increasing demands from the experimental side have triggered many theoretical developments during the last years that to some extent are incorporated in corresponding computer codes accessible to interested users.

In spite of the ongoing need for theoretical support and developments, only very few networks have

been initiated in the past devoted to the promotion of the theory of spectroscopy. At present, the European FP7 network ETSF is based on a pseudopotential description of optical spectroscopies for semiconductors. Some members of the present Action EUSpec are part of the FP7-IRSES network MSNano restricted to the multiple scattering (MS) method. A similar DOE-funded network (Computational Materials Science Network) is running at the moment in the US. It has to be emphasized that all of these networks are focused on a certain class of materials, type of spectroscopies or theoretical framework and do not always provide computer codes to interested users.

In contrast to previous and present networks, the involvement of experts from physics and quantum chemistry, experimentalists and theoreticians in the present Action, will act as a cross-fertilizer to make new ideas rapidly emerge. In particular, the new approach of the Action EUSpec will allow to deal with a wide range of materials. Likewise, building a common platform that supplies a sophisticated interface between complementary codes also allows to deal with many more materials. The platform will not only provide codes for downloading but also critical assessment of the different methods through the sieve of sophisticated experiments on complex materials, on-line courses and by a close interaction of developers and users. It will act as a reference that will provide a wide body of knowledge.

B.3 Reasons for the Action

Within academic and industrial research, full use of spectroscopic data can be achieved only by an adequate support from theory. The rapidly growing and challenging tasks for theory require an improved interaction of European theoreticians to keep pace with developments on the experimental side, but also theoretical activities outside Europe, and especially in the US. Theoretical investigations on spectroscopic properties consist in general of two steps: a detailed and reliable calculation of the electronic structure of the investigated material and the subsequent determination of its spectroscopic properties. At present, most of the electronic structure codes are European-based, while for spectroscopies, the most widely used code is from the US. Obviously, there is a clear need for a stronger interaction of theory groups in Europe to link steps one and two much better than so far. This means that new developments in the field of electronic structure calculations - in particular concerning correlation effects and time-dependent phenomena - have to be communicated and spread much more effectively to be incorporated within step two. This step, in turn, provides the direct link to experiment that has to work properly in a mutual way: providing theoretical support for the

interpretation of experimental data and also giving feedback for further theoretical developments.
The Action EUSpec will establish Europe as the leader in theoretical spectroscopy research by providing the same level of excellence as achieved by European electronic structure codes. This in turn will boost European science to devise new materials and trigger the research on faster, more powerful and intelligent devices. It will reinforce European assets in the highly competitive and volatile market of consumer electronics. Being at the core of a wide range of applications in science and technology, the sophisticated analysis tools provided will benefit many communities, starting from the advanced radiation sources (ARS) academic and industrial users to material research (and development) laboratories who will be offered a coherent platform and support to analyse materials and therefore unravel the various properties of nano-structures, proteins, etc. Spectroscopies combined with efficient tools for analysis play a key role in these domains. Furthermore, these tools will also be useful for neutron scattering experiments as they deliver detailed information not only on the electronic and magnetic ground state but also on spectroscopic properties.

B.4 Complementarity with other research programmes

As mentioned, the present FP7 theory networks ETSF and MSNano are rather focused concerning the materials investigated and the applied theoretical tools. In contrast to these, the Action EUSpec is based on a much wider range of methods and will therefore serve a much larger number of target groups and end users. Nevertheless, strong interaction and exchange with these networks is planned allowing the Action EUSpec to benefit from recent developments and achievements of these networks. In fact, both networks strongly support the extended concept of the Action EUSpec and are interested at joining it in the future.

C. OBJECTIVES AND BENEFITS

C.1 Aim

The main objective of this Action is to gather theory activities in the field of spectroscopy to supply outstanding high level and up-to-date support for demanding and sophisticated spectroscopy experiments using advanced large facility or laboratory radiation sources performed within academic as well as industrial fundamental and applied research.

C.2 Objectives

To reach its main goal the Action EUSpec will devise new methods to radically improve the description of the spectroscopies used to study the properties of nano-materials, strongly correlated systems, proteins, and to model promising new spectroscopies appearing during the time of the Action. Fundamental methods will be further developed to better describe the intrinsic properties of ground and excited states in a wide range of materials covering not only metals and semiconductors, but also transition-metal oxides and more generally compounds exhibiting strong correlation effects. They will be implemented in the codes of the consortium and will be tested against specifically prepared experiments by the experimental Working Group (WG) of the consortium. Although most proposers of the Action EUSpec are from the SR/XFEL community, NS and standard laboratory sources users as well as companies working on materials will be encouraged to join the Action. The consortium, built to cover most of the available methods, as different kind of materials are best tackled by different theoretical methods, will also establish a strong link with theory groups geographically far from ARS.

Various secondary objectives imply the following deliverables.

- 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.
- Extending 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.
- Enhancing the interaction between theory and experiment. This will be achieved among other things by installing communication points (mediators) at the European synchrotrons, contributions to newsletters and providing a user-friendly and extensive website, with a download platform, wiki-like organized manuals, various communication tools and specific search machines.
- To promote collaborations, the transfer of know-how and the introduction of new users to the programs-specific workshops and hands-on courses will be organized.

C.3 How networking within the Action will yield the objectives?

The objectives of the Action EUSpec will be achieved by

- closely connecting experimentalists and theoreticians through dedicated workshops
- enabling a two-flow way of information between the platform and the ARS through a network of contact points who will act as mediators between the Action and end users
- setting up an extensive website proposing theoretical courses of spectroscopies and frameworks to describe them, wiki-like organized manuals for each code, download area, discussion forum and a dedicated user forum for each code, cloud computing facility, list of contact points at ARS, forthcoming events (workshops, hands-on courses, etc.)
- creating of a think tank of early-stage researchers (ESR) in charge of making emerge new scientific ideas
- enabling cross-collaboration between the different WGs by organizing workshops common to at least 2 WGs
- organizing summer schools specially targeted at ESR
- creating new collaborations for cross-fertilization
- using Short Term Scientific Missions (STSMs) as a tool to encourage interdisciplinary research (theory and experiment, physics and chemistry, etc.)

C.4 Potential impact of the Action

The outcome of the Action EUSpec will impact research on materials in the following ways:

- by the creation of a vast community of physicists and chemists centred around its web platform. This platform will continue after the completion of the Action therefore gathering this community on the long term
- by tutoring a new generation of theoreticians and experimentalists (the ESR of the Action) in the field of spectroscopies for the characterisation of materials
- by gathering on the platform a vast corpus of knowledge thought as a reference on the state of the art, a large amount of expertise and the most advanced computer codes for modelling

As a result, the Action will lead to important advances in the knowledge on materials and on the

possibility to design new materials that will shape tomorrow's technology (such as materials for spintronics that will lead to greener - less power consuming - electronics or quantum computing devices). Likewise, the control of the time variable in experiments that the Action will enable will lead to the mastering of the time-behaviour of physical and chemical processes in materials. In turn, this will push Europe to the leading position in the competition for the modelling and designing of new materials.

C.5 Target groups/end users

In the short term, the target groups will be academic and industrial scientists who are using spectroscopies to study materials. This will include theoreticians working in the field of spectroscopy and experimentalists who need an advanced interpretation of experimental data so as to extract accurate information from this data. These end-users will be reached through the dedicated platform (which will be made widely public) but also through the mediation of the contact points in ARS whose action will be to orientate experimentalists to the tools provided by the platform or to Action participants that could help them solve their problem.

Another short-term target group will be both decision makers and the general public who will have dedicated pages on the Action website where they can find specific information explaining in general words the outcome of the Action EUSpec and its impact on the future.
In the longer term, as the tools devised during the course of the Action will pave the way to the emergence of completely new functionalized materials, not only European academic and industrial research and development but also industrial production and competitiveness will benefit from the Action EUSpec.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

The Action EUSpec proposes to establish a computing platform dedicated to the modelling of spectroscopies used to characterize materials on the atomic scale and on the nanoscale, as well as a corpus of knowledge on the subject. To cover the largest possible range of spectroscopies and materials, the platform will propose very different and complementary frameworks, depending on the probe energy and state of the matter/material involved. From the material point of view, the Action will cover a wide range of applications such as photonics, charge and spin storage/transport, energy

generation, ultra-high sensors including nano-bio probes and complex biological structures determination like proteins. Therefore, it will consider theoretical models developed within mono-electronic as well as multi-electronic approaches. The latter are more suited to systems with strongly correlated electrons such as transition metal oxides, or reduced dimensionality structures. In this view, the Action will gather scientists working on computer codes using a real space approach (multiple scattering, Korringa-Kohn-Rostoker method, etc.) particularly suited to nano-materials, a reciprocal space approach (Full Potential Linearized Augmented Planewave method, pseudo-potentials, etc.) ideal for periodic materials, or a quantum chemistry approach (Complete Active Space Perturbation Theory, Configuration Interaction, etc.), fundamental for strongly localised electrons. This work on the description of the intimate behaviour of the matter and its interaction with advanced probing radiation particles on the (sub)nanoscale will be coupled to cutting-edge experiments whose purpose will be to test the theories and to trigger new developments by posing new challenges.

The scientific work will be organized in 5 WGs:

1. **Working Group 1 Correlation:** Most electronic structure calculations supplying the basis for spectroscopic investigations are performed in the framework of density functional theory (DFT). However, in its local density approximation (LDA) electronic correlations are often insufficiently accounted for. The many recent developments in this field that improve upon the treatment of electronic correlations have to be transferred and exploited for spectroscopy calculations. New functionals in DFT, that are self-interaction free, promise certain improvements. For example, the LDA+U method incorporates correlation effects into LDA by an additional Coulomb term in a way that allows a straightforward link to subsequent spectroscopy calculations. Such calculations can now be based on a specific calculation of the Coulomb parameter U. There are also several implementations of the GW-method for moderately correlated materials that express correlation effects in terms of a wave vector dependent self-energy. Nevertheless, a direct link to spectroscopic properties, however, is so far rarely made. For moderately and strongly correlated systems dynamical mean field theory (DMFT) has become a new and powerful tool. First applications in X-ray absorption and valence band photo emission were very successful and therefore supply a very promising starting point for further work in this direction. Recently, a unifying method has been proposed to account for electronic correlations both in the ground state and excited states of correlated systems in the framework of a configuration interaction (multi-channel), real-space multiple scattering scheme. It will offer a further, alternative possibility to tackle the correlation problem.

2. Working Group 2 Spectroscopy: The ongoing refinement of established spectroscopic experiments as well as the introduction of new ones continuously increases the demands to the accompanying theory. An example for the first one is the description of spin-resolved photo emission for circularly polarized radiation. This is a central issue when dealing with the spin-polarized surface of topological insulators that are a new promising material class in spintronics. The ongoing development of new and more efficient spin detectors will clearly enhance the importance of the related issues. Standard angle-resolved photo emission has recently been extended to its resonant version combining element-specific and wave vector resolved information. While first steps for an adequate description of this experiment have been made, further work is urgently needed. Apart from refining and extending the theoretical description of spectroscopic experiments there is a strong need to incorporate dynamical correlations in an experiment-specific way to lead to a complete and quantitative theory. This important issue is strongly linked to those of WG 2, but includes schemes that go much beyond the treatment of ground state properties. For example, one can make use of the Bethe-Salpeter equation and time-dependent DFT as a formal platform. Obviously, this provides a natural link to WG 3.

3. Working Group 3 Time-resolution: The appearance of femtosecond and attosecond physics has opened a whole new area of physics and chemistry. For example, the reactivity of molecules, whether they are biochemical in nature and located in the human body, or catalytic in the exhaust system of an automobile, is determined by the interplay between their electronic and geometric structures. Thanks to their spatial and temporal resolution, free electron laser (FEL) and last generation SR have disclosed the possibility to study the reactions of molecules spatially and in real-time. This WG will consider the following actions: (1) the study of the dynamics of chemical reaction and the probing of matter under extreme and/or metastable conditions by X-ray absorption spectroscopy (XAS) supported by specific theoretical approaches mimicking time-dependent Hamiltonian for excitation processes in molecules and quasi-equilibrium relaxation time approximation of the Boltzmann equation in solids/liquid systems; (2) in the case of FEL, the assessment of calculation frameworks commonly in use, when extremely high intensity ultrafast pulses with high coherence degree will be accessible by such facilities in the X-ray energy range; (3) for pump-probe X-ray, the simulation of relevant spectroscopic quantities of interest describing the systems dynamics for a few picoseconds like time resolved luminescence, pump and probe absorption reflectivity, four wave mixing and spin-echo; (4) use of time resolved X-ray emission spectroscopy to complement XAS by enhancing sensitivity to low Z atoms and to electronic details; (5) the dissemination of state-of-

the-art techniques and know-how among European researchers to allow to bridge separate fields of disciplines (physics, chemistry, biology, engineering, and other natural sciences).

4. Working Group 4 Platform: The platform will be part of the Action webpage, i.e., accessible through a dedicated webpage. The main components of this platform will be: (1) a reference corpus containing theoretical courses on the spectroscopies and on the provided frameworks to describe them, (2) a download area where each code will be accessible according to its licensing status, (3) for each code, a wiki-like organized manual and a user's forum, (4) for some codes, a cloud computing utility allowing to run the code in a restricted configuration mode for testing before downloading the most appropriate one, (5) a data exchange interface so that the different codes can interact easily whenever necessary (6) a critical assessment of the various methods and codes, with their limits of validity to help the user to decide which one is the most appropriate for the problem at hand, (7) a Who's Who database on spectroscopy that will provide information on the expertise (theoretical as well as experimental) of the people working in the field.

5. Working Group 5 Experiment: The main objective of the WG is the design and realization of new experiments to test the theoretical models and their limitations. The ultimate goal will be to achieve a quantitative agreement between theory and experiment with the aim to provide a complete description of the geometric and electronic states at the atomic level either of the excited state or the ground state. This knowledge allows experimentalists to correlate this microscopic characterization with the macroscopic properties of different systems. In particular, the WG is interested in the understanding of exotic properties, including the HTC superconductors, the colossal magnetoresistive manganites and recently, the occurrence of multiferroicity, which strong correlated electron systems such as mixed-valence transition-metal compounds present. In these systems, charge, spin and orbital degrees of freedom are highly mixed and offer therefore a challenge to theory. In order to provide a unified description of the electronic ground state is then mandatory to carry out experiments using different electronic spectroscopies such as X-ray absorption spectroscopy, X-ray emission spectroscopy, resonant X-ray scattering in the soft and hard X-ray regimes and X-ray magnetic circular dichroism. One key point is to reach a common interpretation of K- and L2,3-edges absorption spectra for the transition-metal atoms that nowadays is made on the basis of different theoretical approaches, multiple scattering versus charge transfer multiplet approach, respectively.

D.2 Scientific work plan - methods and means

The following tentative work plan for the various WGs will offer the possibility to be amended to account for new participants joining the Action or to new spectroscopies or materials that would require the Action to adjust in real time. It will be put into practice by a close coordination of the WGs that are linked as described above (see D.1). The organisation of the Action EUSpec and its periodical meetings and workshops as outlined in section E will ensure a strong and efficient interaction and exchange among the WGs.

1. **Working Group 1 Correlation:** All activities of WG 1 will be based on the common data format introduced by WG 4 together with the corresponding input and output routines. Interfaces for these will be incorporated into the various program packages to allow first of all the transfer of the self-consistent potential created by any electronic structure code to any spectroscopy code. Additional interface routines will be developed to also transfer of a complex and energy-dependent and possibly wave vector dependent self-energy. These are of interest in the cases of GW- and DMFT-based calculations. To implement DMFT in electronic structure codes as a new scheme to deal with electronic correlations a standard interface of DMFT-solvers will be provided to available packages. The various corresponding code developments will be mutually supported by providing data sets for testing and benchmarking. For example, using exact diagonalisation scheme as a DMFT-solver gives access to atomic multiplet effects in solids. This approach will be checked against schemes using an atomic multiplet description within the crystal field approximation and against accurate first principles quantum chemical embedded cluster methods. This way it will ultimately offer an alternative for the computation of $L_{2,3}$-edge spectra of transition metals. In addition it will be exploited to provide the necessary input for the recently developed multi-channel multiple-scattering scheme.

2. **Working Group 2 Spectroscopy:** As a first step the WG will define and install a common set of test cases for a wide range of spectroscopic calculations. Corresponding cross checks of the programs will certainly reveal in particular improvements when adopting the so-called full-potential techniques. Another central issue will be the impact of spin-orbit coupling that gives rise to many important dichroic effects. Here comparative studies will monitor the differences resulting from a treatment via perturbation theory and via the Dirac equation. In a similar way the various levels to incorporate correlation effects will be compared with respect to their

impact on spectroscopic properties. Another main activity of the WG is to promote schemes that account for dynamical correlations in spectroscopy that go well beyond the simple final state or Z+1 models. Again the exchange of experience and program modules together with the supply of benchmark data sets will accelerate corresponding program developments. This will be used for example when implementing the solution of the Bethe-Salpeter equation for disordered systems using multiple scattering theory. Finally, the rapid exchange of new ideas will be used to develop in the future the adequate theoretical description of new experiments on demand. An example for this will be the extension of a recent theory for resonant photo emission to the angle-resolved case.

3. Working Group 3 Time-resolution: Large scale apparatus and infrastructures providing access to external users will experience large benefits from the support of the present COST networking. Such benefits could be quantified in cooperation between different expertises and more efficient preparations of experiments and exploitation of the resources involved in the running such facilities. Furthermore the analysis of data will be faster, leading in a more systematic way by dedicated resources to the establishment of portals to access computing tools and to the huge amount of novel experimental data that have been being collected in the last few years. The open structure of the COST network will represent a support structure for scientists interested in starting new experimental/theoretical investigations in the field by using such large facilities for an efficient dealing with data depending largely on preparation and operation of the advanced experiments. To this aim the application of good practices of data handling already in use in large research infrastructures for high energy physics experiments will be promoted.

4. Working Group 4 Platform: The main points in the work organised under this WG are: (1) establishment of a common data format for the main files of the codes involved in the Action to facilitate passing data from one to another (potential files, crystal or molecular files, etc.), (2) building of a common web interface for the cloud computing facility. This interface will allow users to run each code of the facility in a restricted mode directly from his/her own computer without having to download it, (3) writing by each code development team of a wiki-based web user's manual based on a common wiki template allowing cross-hyperlinking between them, (4) assessment of the pros and cons, limits of each framework. This will be the case not only for the general frameworks (real space, reciprocal space, quantum chemistry

approach, etc.), but also for more specific points such as for example the description of correlation (see WG 1 for more details) or vibrational effects.

5. **Working Group 5 Experiment:** The experimental plan consists mainly in the realization of new experiments using different electronic spectroscopies. The data will be sent to the different theory working groups (WG 1 and WG 2) to check their models with the aim to get a complete geometrical and electronic characterization. Two strategies will be followed in the experimental design. On the one hand, the WG carries out experiments on test systems using different spectroscopies, as for example, hard X-ray coupled to soft X-ray absorption, photo emission and X-ray emission spectroscopy (XES). The simultaneous modelization gives a unified description and it serves as a check of the used approaches. On the other hand, and as a second strategy, the WG carries out experiments on systems whose macroscopic properties change abruptly as a function of external parameters as temperature (phase transitions), composition, magnetic field, pressure, etc. The theoretical description of these systems in the different phases will provide the geometrical and electronic changes responsible for their singular behaviour. Finally, a series of spectroscopic investigations will be conducted in systems with an almost full 3d-electron shell (CuO, NiO, etc.) to study the effect of the Pauli exclusion principle. This is a challenging field for theoretical interpretations, since the treatment of exchange effects, as implemented up to now, is not adequate to treat these extreme cases.

E. ORGANISATION

E.1 Coordination and organisation

The COST Action EUSpec is managed by a **Management Committee (MC)** headed by an Action Chair (AC) and an Action Vice-Chair (AVC). It is composed of up to two representatives of each participating countries and acts according to the Rules and Procedures for Implementing COST Actions. It issues the reports and interacts with the COST office. To help it in the management and to be able to react efficiently, the MC appoints:

Working Group Leaders (WGL) and **Deputy Leaders**. They will coordinate the WGs both scientifically and administratively. Each WGL appoints **Topic Leaders (TL)** who are in charge of a specific topic within the WG.

Working Groups Coordinator (WGC). The WGC looks at the synergies between the WGs and makes proposals to the WGLs to increase these synergies. He/she is also in charge of the organisation of workshops common to two or more WGs.

Communication Manager (CM). The CM is responsible for the dissemination and outreach activities in the Action. He/she presides in particular over the building, updating and maintenance of the Action's website and ensures that the Action website provides all the necessary information. In addition, he/she is the editor of the quarterly newsletter.

Short Term Scientific Missions Manager (STSMM). The STSMM receives the proposals for STSMs. He/she controls their adequacy of the aims of the Action and if necessary ranks them in view of their quality and the budget available. He/she works in close contact with the Steering Committee which he/she is a member of.

Contact Points Manager (CPM). The CPM manages the network of contact points in the different ARS. He/she works with the CM to ensure that the achievements of the Action are disseminated towards the ARS and with the WGL so that information coming from the ARS can be taken into account by the WGs.

Steering Committee (SC). The SC prepares the agenda of the MC meetings and makes proposals and recommendations to be discussed at these meetings. It is composed of the following members: the AC, the AVC, the WGLs, the WGC, the CM, the STSMM and the CPM. The SC will also be in charge of the elaboration of a white paper presented at the last Action meeting and discussing prospective ideas for the continuation of the work initiated by the Action, in particular to make the platform perennial.

The Action EUSpec will promote and coordinate the networking and dissemination of the research in the following way. The core of the Action is its website which, in addition to the usual information, will contain a download area, a forum for each code of the platform and a cloud computing utility to run the codes directly from the platform. In addition to this central tool, the Action will organize:

Whole Action Meetings (WAM) will take place in the first and fourth year, preferentially as a satellite meeting to a prominent international conference on spectroscopy as the VUVX or XAFS conferences. They will also be open to external scientists. **MC meetings** and **WG meetings** will take

place every year and - if applicable - the day before the WAM. The last WAM will synthetise the achievements of the Action and make proposals for the future. One **Scientific Workshop (SW)** every year will be focusing on at most two WGs. Each SW will be followed by a **Hands-On Training Workshop (HOTW)** centred on at least two codes of the platform and more specifically targeted at ESR. In addition, a **Summer School** will take place every two years. They will be organized by ESR. **Short Term Scientific Missions (STSMs)** will be organized all along the Action with a priority to ESR to promote exchanges between the participants.

E.2 Working Groups

The Action is organized into 5 WGs:

- the WG1 Correlation in charge of the description of electron correlation (ground state and excited state)
- the WG2 Spectroscopy in charge of the description of a wide range of spectroscopies and their implementation into the codes of the Action
- the WG3 Time-Resolution in charge of the description of femtosecond SR and XFEL spectroscopies
- the WG4 Platform in charge of the integration of the codes into the platform website and of the cloud computing facility
- the WG5 Experiment in charge of setting-up and establishing experiments to test and push theoretical models to their limits

Each participant will be asked to join at least one of the WGs. Each WG will be the dedicated environment for scientific communication outside the workshop thanks to WG mailing lists and forums, and under the supervision of the WGL and the deputy WGL. Each WGL will be in charge of the organisation of the WG meetings.

E.3 Liaison and interaction with other research programmes

There are complementary research projects in Europe with which the Action EUSpec will establish discussion and seek cooperation. The COST Action MP1302 Nanospectroscopy aims at consolidating European expertise on all aspects of nanospectroscopic techniques. There may be common interest in the modelling. Likewise, the FP7-IRSES network MSNano is interested in the modelling of

spectroscopies within the multiple scattering framework, while the FP7 network ETSF aims at optical spectroscopies for semiconductors using essentially a pseudopotential approach. The Action EUSpec will interact with them through its Correlation and Spectroscopy WGs. Speakers from the various mentioned networks will also be invited at the EUSpec workshops and meetings. Both the MSNano and the ETSF networks have already shown their strong interest in collaborating with the Action EUSpec.

E.4 Gender balance and involvement of early-stage researchers

This COST Action will respect an appropriate gender balance in all its activities and the Management Committee will place this as a standard item on all its MC agendas. The Action will also be committed to considerably involve early-stage researchers. This will also be placed as a standard item on all MC agendas.

For this, the MC will explore and adopt the best practice across Europe. It will promote the active participation of female scientists at responsibility positions and monitor the evolution of the gender balance during the Action. The STSMM will continuously encourage female ESR to apply for STSMs and take into account specific issues as far as possible.

The involvement of ESR in the managing of the Action will also be a top priority of the MC. Specific measures for ESR will include:

- setting-up of a think-tank of ESR. It will make new proposals and will have a dedicated section in the website of the Action
- in each WG, when the WGL is not an ESR, its deputy should be.
- ESR will be encouraged to act as session chairs during Action meetings and to organise Action events. In particular, they will be in charge of the organisation of the two summer schools. This will enable them to learn administrative and organisational skills
- ESR will get the priority for STSMs to promote their mobility. Moreover, STSMs will be decided through proposals so that ESR learn to write proposals.

F. TIMETABLE

Activity	Year 1	Year 2	Year 3	Year 4

Kick-off meeting	x															
Set-up website		x														
SC, MC meeting		x				x				x				x		
WG meeting		x				x				x				x		
WAM		x												x		
Scientific workshop				x				x				x				x
Hands-On Training Workshop				x				x				x				x
Summer school							x								x	
Report							x								x	

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: AT, CH, CZ, DE, ES, FR, HU, IT, NL, PL, RO, SE, SI, UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 56 Million € for the total duration of the Action. This estimate is valid under the assumption that all the countries mentioned above but no other countries will participate in the Action. Any departure from this will change the total cost accordingly.

H. DISSEMINATION PLAN

H.1 Who?

The Action identifies two separate groups for its dissemination plan, an internal group and an external group. The internal group comprises:

- the staff scientists and ESR registered as participants
- graduate and undergraduate students at the institutions part of the Action, and in particular those of the Mamaself Erasmus Mundus 2 European programme

The external group contains:

- other scientists interested, including industrial scientists
- national and European funding agencies

- research policy decision makers, including those at the local level
- media and the general public
- high school students and their science teachers

H.2 What?

The promotion of the Action and the dissemination of its achievements will be done under the authority of the Management Committee (MC) by the Communication Manager (CM). The channels considered are the following:

- collaborative publications in peer-reviewed high-impact factor journals
- communications at Action meetings (internal) and international conferences (external). Communications and advertising of the Action at ARS users meetings
- promotion of the Action (through posters) at conferences, workshops as well as users meetings to encourage female scientists and ESR to join, and make the Action more widely known
- creation of a network of contact points at ARS
- mailing list among each WG for dissemination among participants
- round table discussions with industry
- administrative and technical help for Action members organizing specific topical sessions at large meetings
- participation to outreach activities like the ”Fête de la Science” in France
- press release to advertise outstanding results or events

Moreover, the Action website will gather all the information to and from the Action and will be a central tool in the dissemination plan. A password-protected area for MC and SC members will give access to the minutes of the meetings, budget tables, mail lists and other confidential information.

The open-access area will contain:

- information about activities, seminars, job opportunities, students fellowships, students summer schools (Mamaself for instance)

- databases of members, of publications by topic
- highlights of scientific results
- portraits of ESR with their scientific achievements
- dedicated pages for the general public and for decision makers
- download area for the codes
- an users forum for each code
- a cloud computing facility for some codes

H.3 How?

The dissemination of the results of the Action will be regularly monitored by the MC. To facilitate this dissemination, the Action will take the following measures:

- Action acknowledged in all related publications
- Action involved in outreach activities targeted to the general public
- all workshops, summer schools open to invited speakers from outside as well as participants financed by own sources
- Action meetings organised just before or just after international conferences to facilitate the attendance of external experts
- conference grants established for ESR, summer schools planned by ESR for ESR
- slides of workshops/schools made available on the Action website. Likewise for talks aimed at the general public
- seminars at Action participating institutes shared by videoconferencing whenever possible (through the Action website)
- quarterly newsletter edited by the CM on behalf of MC to inform participants and subscribers about new publications, upcoming events, open positions, etc.
- creation of a “Who’s Who” database in the field of spectroscopy
- participants asked for suggestions for new participants

- STSMs: particularly targeted at ESR for exchanges of PhD students and post-docs (following a proposal submission to the STSM manager and approval by the MC)
- exchange between participating expert groups and existing European student schemes such as the Mamaself Erasmus Mundus master located at the same institution