EUSpec
COST Action MP1306:
Modern Tools for
Spectroscopy on Advanced Materials
newsletter

Recent activities:
The third EUSpec training school

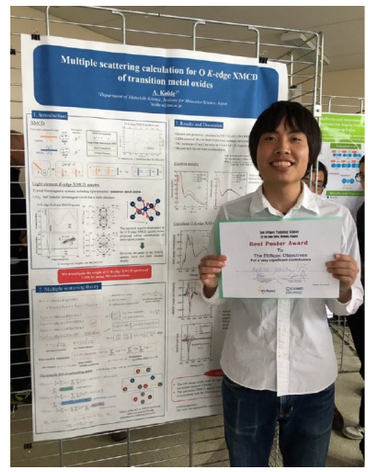
Decmber 2016, 4th issue
visit also: www.euspec.eu

Inside

The third EUSpec training school was organized in Rennes (France) from the 27th of June until the 30th of June 2016. Its focus was on multiple scattering codes. More precisely, the codes involved in this school were: MXAN, GNXAS, MsSpec, FPMS and MCMS. These codes allow to model spectroscopies such as X-ray absorption, photoelectron or Auger diffraction. Over 30 students attended the course. Unfortunately, several others could not arrive on time due to visa problems. The first day was devoted to 9 lectures on multiple scattering theory given both by the code developers and by other theorists involved in related codes. Subjects encompassed the basics on scattering theory, how to use multiple scattering to describe the electronic properties or to take into account correlation effects and the full-potential approach to multiple scattering.

Hands-on during the EUSpec training school

The next three days were devoted to hands-on courses on the use of the codes, with half a day dedicated to each code and two to three trainers for each code. Each student was provided a desktop computer with a virtual machine with the codes installed on it, and a bootable USB key containing the same virtual machine to take away home. During the last afternoon, trainers from each code took care of the students who wanted to specialize more on a given code. In parallel to the last day of training, a WG2-WG5 meeting was organized by Barbara Brena (Sweden) and Maddalena Pedio (Italy), followed by a management committee meeting.



Best poster award to Akihiro Koide (Inst. Molecular Science Okazaki Japan)

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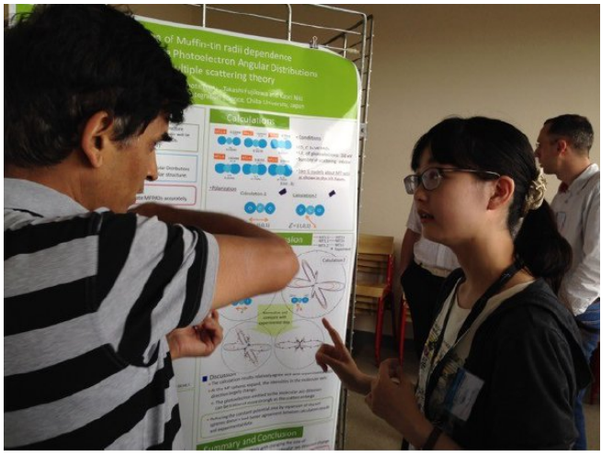
Report of third EUSPEC training school -- continued

A poster session was also organized and a jury of four scientists had a look at all the posters to award a best poster prize. This EUSpec poster prize was awarded to Akihiro Koide from the Institute of Molecular Science in Okazaki (Japan). Hands-on during the EUSpec training school.

The welcome talk of the deputy mayor of Rennes



During the poster session

On the social side, the first day finished with a beer tasting session organized by a local micro-brewery, with one of the brewers answering the questions from the audience. Students and trainers alike enjoyed it. The following day, a guided 90-minute tour of the Parlement of Brittany was organized. It was followed by the training school dinner which was taken at a renown restaurant. Finally, in order to conclude the school, a reception was staged at the town hall, with a welcome talk given by a deputy-mayor.

During the reception at the town hall

The group photograph of the EUSpec Training School and Management Committee Meeting

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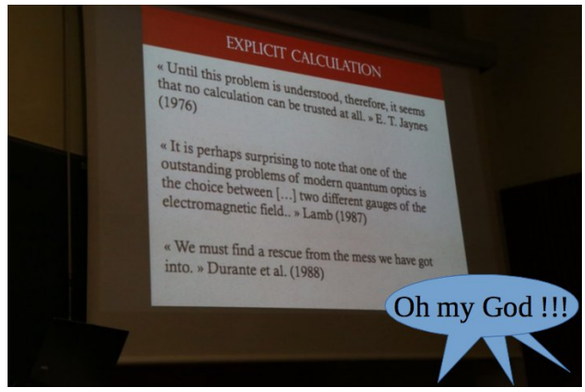
The EUSpec Training School was followed by a two-day MSNano conference co-funded by EUSpec. The first day of the conference was devoted to the presentations of the latest developements in the multiple scattering modeling of spectroscopies that have been done within the MSNano network. MSNano, which has ended now, was a precursor of EUSpec but focused on the multiple scattering approach.

C. R. Natoli (Italy) concluding the conference



C. Brouder (France) "shocking" the audience during his talk on gauge invariance in X-ray spectroscopy and scattering

The second day of the conference involved a series of 24 short talks to honour Calogero Natoli on the occasion of his 75th birthday. Both scientific talks and talks sketching Calogero Natoli's influence on the multiple scattering modeling of spectroscopies were delivered. It was followed by a garden party attended by over 70 persons.

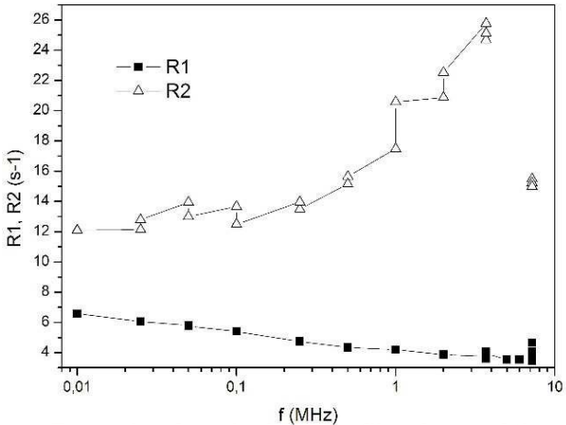
(Didier Sébilleau)

Short Term Scientific Missions

The Short Term Scientific Missions (STSM) in the COST action have been successfully carried out since its 1st call. Here we report three STSM activities happened in the first half of 2016.

Dr. Nuno Silva (Dep. FÍsica Universidade de Aveiro) visiting Prof. Alessandro Lascialfari (Dipartimento di Fisica Universita' degli studi di Milano).

The STSM took place between 2016-04-03 and 2016-04-09. This mission aimed at the development and study of a nanomaterial combining Hyperthermia, Thermometry and Imaging.
During the mission Dr. Nuno Silva and Prof. Alessandro Lascialfari have evaluated the H-NMR relaxivity of water-based ferrofluids containing iron selenide magnetic nanoparticles and nanothermometers as a function of frequency (i.e. applied magnetic field) and temperature around room temperature. Transverse and longitudinal Nuclear relaxivities were measured (see example in graph below). The magnetic nanoparticles affect mainly the transverse relaxation, as found for iron oxide nanoparticles. Values of the order of r2~2.5 s-1mM-1L were obtained at 7.2 MHz, still quite below than the commercial iron oxide-based contrast agent Endorem (~ 100 s-1mM-1L). Some of the samples were not stable with time. In total, 5 samples were studied in a total of about 35 h of machine time. During the visit Dr. Nuno Silva had also the opportunity to learn concepts associate to Magnetic Resonance Imaging and to learn how to operate the relaxometer at an end-user level.
In the view of the present experiments, it is clear that stability of the nanoparticles in water solution must be



Example of a relaxivity profile of one of the studied samples

improved. Nanoparticles are obtained in organic media and subsequently transferred to water solution and this step must be improved, while keeping or improving their thermometric ability. The nuclear relaxivity of the ferrofluids must also be improved, possibly by tuning the size of the nanoparticles and their surface capping. The possibility of performing measurements at higher fields, particularly at those used in clinical practice,

STSM -- continued

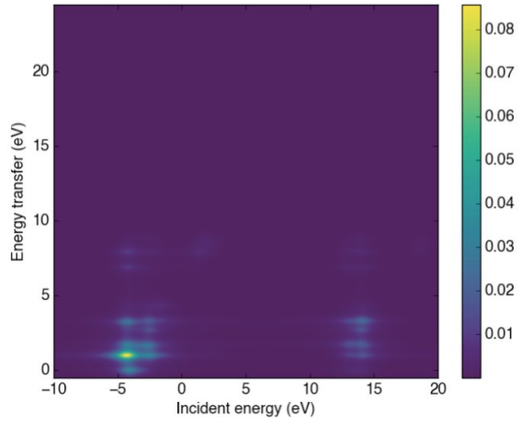
with temperature control will be tested in future experiments. Finally, the team agreed that interesting results were obtained and that new studies should be performed after stability issues are solved.

Dr. Ondřej Šipr (Fyzikální ústav AVČR, Praha, Czech Republic) visiting Prof. Hubert Ebert (Ludwig-Maxmilians-Universität München, Germany).

The STSM took place between 2016-04-04 and 2016-04-09. The purpose of the STMS was to discuss and analyze numerical results concerning the T_z term for Co monolayers and Co adatoms of 3d elements on (111) surfaces of Cu, Ag, Au, Pd, and Pt. Dr. Ondřej Šipr and Prof. Hubert Ebert wanted to assess and critically evaluate to what degree the values of T_z as well as the dependence of T_z on the direction of the magnetization can be described via the approximate expression. This was supposed to give them information on whether the magic-angle-based elimination of T_z from XMCD data can be used for adatoms, clusters and monolayers or not.
During the stay they focused on understanding and explaining why the effect of spin-orbit coupling (SOC) on the T_z term does not show any systematic dependence on the SOC in the host. Dr. Ondřej Šipr and Prof. Hubert Ebert analyzed the data obtained so far and tried to identify systematic patterns depending on the dimensionality and the SOC. They also analyzed the DOS to understand the chemical effects on the T_z term. For this purpose they evaluated the phase-shifts of Co atoms and of Cu, Ag, Au, Pd, Pt atoms forming the substrate and analyzed common patterns in terms of resonance, split bands and hybridization.
They found that the crucial factor for the importance of SOC on the Tz term is not the nominal value of the substrate SOC but rather the dimensionality. They argue that the importance of the SOC should be weighted against the width of the band: smaller width of the band means that the relative importance of the SOC is larger. Further, they found links between coincidence of resonances in energy between Co atoms and host atoms on the one side and importance of hybridization on the other side. This seems to explain the somewhat peculiar dependence of the importance of SOC on the chemistry.
Further collaboration between the groups on studying the effects of SOC on various spectroscopic properties is probable. Dr. Ondřej Šipr and Prof. Hubert Ebert expect that the STSM concerned will result in a joint publication on the importance of SOC for the Tz term in XMCD spectra.

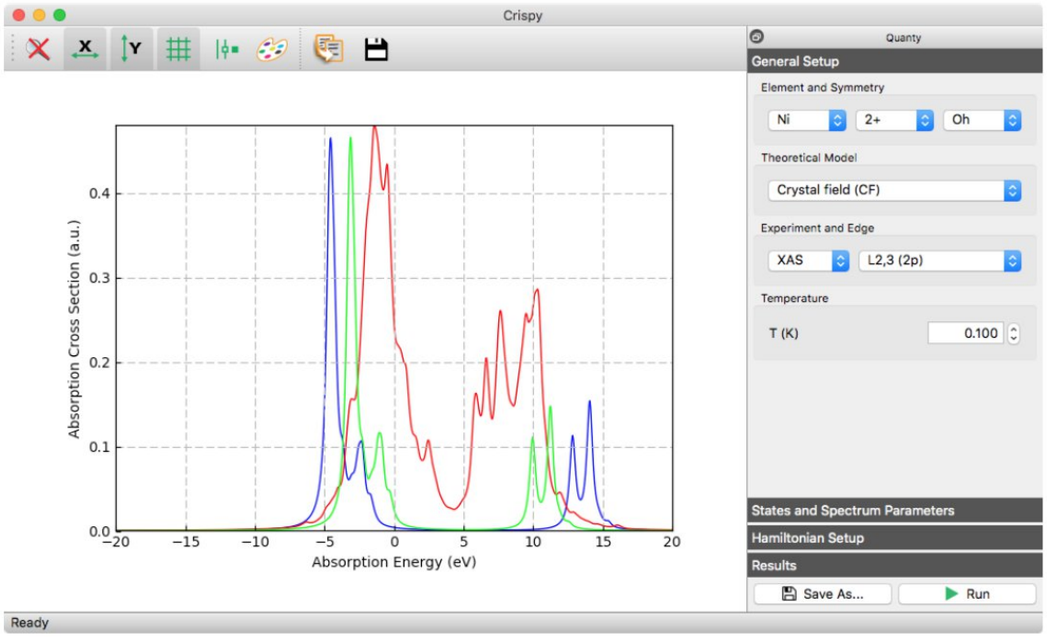
Dr. Marius Retegan (ESRF - The European Synchrotron, Grenoble, France) visiting Dr. Maurits Haverkort (Max Planck Institute for Chemical Physics of Solids in Dresden, Germany).

The STSM took place between 2016-04-11 and 2016-04-15. The main goal of the mission was to extend Crispy—a core-level spectroscopy oriented graphical user interface developed at the ESRF—to include more of the capabilities present in the Quanty software. Problematic to this task was the fact that the two programs are developed using different programming languages. To better integrate with the current development strategies of the ESRF, Dr. Marius Retegan developed the interface using the Python programing language, which provides a large number of support libraries and allows for extended flexibility in the development. Quanty, on the other hand, is developed using the C programming language, a choice motivated by the heavy computational tasks that are required during the calculation of core-level spectra. Having a scripting language, Lua, on top of the compiled C code, facilitates its usage. This last aspect allows a pragmatic approach to integrate Quanty's features into the GUI by writing template files for the different simulations, and then fill them with parameters introduced via the GUI. Alternative integration schemes were left for future developments.
In the first part of the mission, with the help from Dr. Maurits Haverkort, Dr. Marius Retegan wrote template files for the simulation of advanced spectroscopic techniques such as resonant inelastic X-ray scattering using a ligand field approach. The plot below shows the initial results obtained for a model system (NiO). These templates should be easily transferable to other systems, covering a larger part of the periodic table.
During the second half of the mission, Dr. Marius Retegan worked on integrating part of the templates into Crispy. An example of the type of core-level spectra simulation performed directly from the interface is shown below.



Simulation of X-ray scattering from ligand field theory for NiO. For details see text.

STSM -- continued



Screenshot of Crispy's main window showing three L-edge spectra simulations of Ni(II) using a crystal field approximation, for details see text.

The figure shows a screenshot of Crispy's main window, with three L-edge spectra simulations using a crystal field approximation: two for a Ni(II) system using different parameters for the 2p–3d spin-orbit interaction and a third for a Mn(IV) system.
Dr. Marius Retegan and Dr. Maurits Haverkort have also discussed about having an easier way to extract the parameters required for the simulations of core-level spectra directly from ORCA, an ab initio and density functional theory code. This however requires additional development on the Quanty side, to be done in the next months.
The STSM to Dresden has helped Dr. Marius Retegan to extend his knowledge of Quanty.
The user interface has since been significantly extended. The current version can be found at https://github.com/mretegan/crispy. The software is released under the MIT license, which allows contributions from other members of the EUSpec community to be done transparently and with appropriate attributions.

Dr. Dominik Legut (IT4Innovations Center, Czech national supercomputer center Tech. Univ. Ostrava, Czech Republic) visiting Prof. P. M. Oppeneer (Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden).

The STSM took place Feb. 1st – 9th 2016. The short scientific mission was planned to establish and prolong discussions with researchers at host institutions about topics related to the magneto-optical effects, core-level spectroscopy employing density functional calculations. Based on the symmetry analysis concerning the space and point groups, available basis functions in the collinear code, the initial structure of the highly oriented pyrolytic graphene (HOPG) was set up for first-principles calculation modeling consisting of only 4 carbon atoms. The electronic structure of the HOPG was calculated using the local density approximation (LDA) [1] approach using the full potential augmented plane wave code (FLAPW), WIEN2k [2] employing the spin-orbit interaction as an addition to the scalar-relativistic calculations. To acquire the dielectric tensors for the dipole transitions across the carbon K-edge the code using linear response (Kubo formula) had to be modified for the non-magnetic system. Similarly to the graphene (DPG 2015), the discrepancy of the XAS between theoretical and measured spectra indicates the necessity to employ the core-hole calculations within certain supercell. The core-hole calculations were tested first for the XAS and XMCD of the simpler Gd at the M4/M5 edges (d—f transition). Firstly, the electronic structure within the single-electron framework (without the core-hole taken into account) and magnetic moments were calculated using LDA for the exchange and correlation effects for the hcp lattice with a=3.629 Å and c/a = 1.597 in accord of Ref. [3]. The magnetic

STSM continued

moment per Gd atom of 7.44μ_B is practically the same, with value of 7.41μ_B per atom as reported in [3]. Similar values of magnetic moments of Ref. [3] were also obtained for the calculations employing the so-called Hubbard U technique for the f-shell of Gd with U=6.7eV and J=0.7eV. Then Dr. Dominik Legut and Prof. P. M. Oppeneer calculated the XAS of M_4/M_5 edges that shows not to be satisfactory in comparison w.r.t. experiment. The electronic structure of the core-hole calculations with 1 and half core-hole using LDA and LDA+U technique and the optical calculations are underway at present. Within this STSM the initial research collaboration between partners countries of EUSPec project MP 1306 started and this project therefore is acknowledged in the future publications resulting from the applicant stay within this STSM.

[1] J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992).
[2] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, *An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties*, Techn. Univ. Wien, Austria (2001).
[3] Ph. Kurz, G. Bihlmayer, and S. Blügel, J. Phys. Cond. Matter. **14**, 6353 (2002).

News from EUSpec

CNRS Bronze medal 2016 to Amélie Juhin

(IMPMC équipe Minéralogie magnétiquede basse dimensionnalité (MIMABADI), France)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Amélie Juhin was honoured with the "Médaille de bronze 2016 du CNRS" for her outstanding research in the field of magnetic spectroscopy (XMCD, RIXS-MCD). Her main research interest is the magnetism of molecules and nanoparticles. Aged 36 she is already known as an expert in her field and her theoretical and experimental contributions to magnetic spectrocopy are well recognized.
After her Phd in 2008 which she got from the University of Pierre-and-Marie-Curie (France) Amélie Juhin headed for a Postdoc to the Debye Institure of Materials Science (Netherlands). In 2010 she was offered her current position at the IMPMC. In the EUSpec network she is as deputy manager responsible for the Short Term Scientific Missions within this COST action.
More information (in French only) can be found at
http://www.cnrs.fr/fr/recherche/prix/medaillesbronze.htm

Gender Balance and Early Career Investigators: EUSpec initiatives

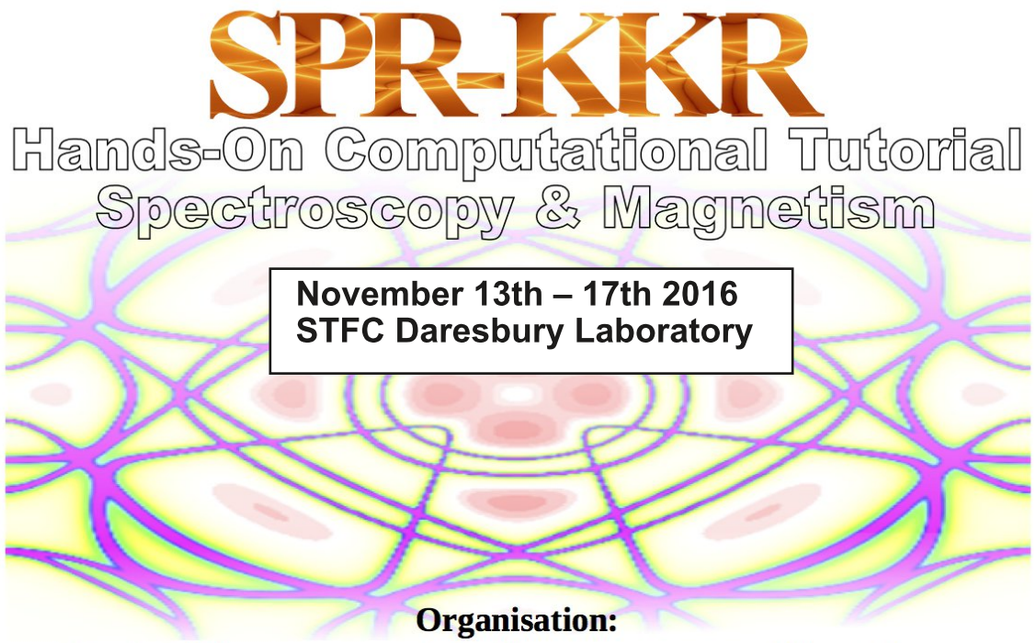
During the last EUSpec MC meeting that was held in Rennes on June the 30th, it was proposed to set up the EUSpec Prize, as an award to be given to young scientists in the early career stage. The precise details, like the criteria for the selection of the recipients, will be further discussed during the coming MC meeting in Athens which will take place in winter 2017. However, several important issues were already pointed out in Rennes. The nominees will be early career investigators (ECI), members of the EUSpec. At present EUSpec includes 66 ECI's in a total of 214 registered members. The prize will be given to a male and to a female researcher each time. A suggestion is to proceed with the nominations during the year, and then in Athens to appoint a committee to take care of the selections.

This was not the only initiative directed toward gender balance in EUSpec. In fact, a webpage called *women in EUSpec* has been recently created, which will host scientific portraits of women in EUSpec, and will provide for example statistics about women participants in EUSpec as well as it will provide useful links.

Also the activity of ECI's has been supported by EUSpec. ECI's have been given preference in STSM's, and they have been in charge of several events like the 2016 Winter school. In addition, the creation of a webpage with ECI scientific portraits has been discussed. The latter, has been argued, could also be an important platform for ECI for networking within EUSpec.

(Barabara Brena)

Recent events



Organisation:

Martin Lüders
STFC Daresbury Laboratory
Daresbury, England

Julie Staunton
University of Warwick
Coventry, England

Hubert Ebert
Ludwig-Maximilians-Universität
München, Germany

The aim of the course is to introduce theoreticians as well as experimentalists into the KKR bandstructure method and its use to calculate various electronic and magnetic properties of solids.

Emphasis will be put on the fully relativistic formulation, on the implementation of clusters, surfaces and ordered as well as disordered solids, on linear response phenomena and on the calculation of spectroscopic processes and magnetic properties. In addition to the general features of the code, particular focus of the course will be on the calculation of magnetic properties, such as exchange couplings and magnetic anisotropies, as well as applications to angle resolved photoemission spectroscopy (ARPES) experiments based on the one step model.

To comprehend the formal background and technical details of the KKR method several lectures on corresponding topics will be given by our speakers. For direct applications the first sessions will be devoted to introduce the *Munich SPR-KKR program package*, including its graphical user interface called *xband*. The participants will individually work with the various calculation possibilities of SPR-KKR while being guided by tutors. These sessions are meant in particular to introduce the field to inexperienced users, but also more adepted users will have the opportunity to discuss individal problems with the tutors and authors of SPR-KKR.

For further information & registration:

https://eventbooking.stfc.ac.uk/news-events/spr-kkr-hands-on-course-2016

(there are limited resources available to cover accomodation costs)

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in collaboration with CCP MAGNETISM and CCP Computational Electronic Structure of Condensed Matter

For the recent STSM call please visit our webpage

www.euspec.eu

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