newsletter

COST Action MP1306: Modern Tools for Spectroscopy on Advanced Materials

News from the Platform

-- Report on recent activities in WG 4--

by Martin Lüders

One of the deliverables of the "platforms" working group is the creation of a standardized data format, which can be used to connect various codes and calculations together. For instance, the electronic structure of a material has been calculated from first principles (ab initio) using one of the electronic structure codes. This electronic structure shall then be used to simulate the corresponding photo-emission spectrum. Very often, this task would be complicated by the fact, that the codes for calculating the electronic structure, and the code performing the spectroscopy use different file formats and, even worse, different physical representations of the fundamental quantities, such as potentials, densities or wave functions.

In order to facilitate such exchange of data, first conversions between different representations (in particular pseudo-potential versus all electron) have to be developed, and secondly, a standard for storing certain data elements has to be established. Both tasks have been started and are well on the way.

Keisuke Hatada and co-workers have just published a paper [1] in which they describe how muffin-tin densities and potential, for KKR based spectroscopy codes, can be obtained from self-consistent densities and potentials, generated with VASP.

The second task started by a review of existing file formats. A potential candidate was the ETSF file format, which was developed with the same goals in mind, but was not sufficient for the needs of our community. The main shortcomings were the lack of support for all-electron methods, and the lack of support for parallel I/O, which is getting more and more important for large calculations.

Together with the main developers of the ETSF library, which is now embedded in the CECAM electronic structure library (ESL) activity, it was decided to apply for a CECAM coding workshop to address the shortcomings. CECAM suggested to merge the proposal with a similar one by the NOMAD activity, which is interested in storing the results of ab initio calculations into a database for future data mining. The common workshop took place in February in the CECAM headquarter at Lausanne. The first three days have been devoted to discussions and decision-making about how to structure the data. In the following two weeks, a smaller group of developers remained to start the actual implementation.

The major outcome of the workshop was that the two communities, which followed quite similar aims, exchanged their experiences, and more importantly, what has already been developed in each, so that repeating the work can be avoided. Technical details about the emerging library are published on the web pages of the ESL activity [2], in particular on the pages on the new ESCDF I/O format [3].

[1] J. Xu, C. R. Natoli, P. Kruger, K. Hayakawa, D. Sebilleau, L. Song and K. Hatada, Comp. Phys. Comm. **203**, 331 (2016)
[2] http://esl.cecam.org
[3] http://esl.cecam.org/mediawiki/index.php/ESCDF_-_Electronic_Structure_Common_Data_Format

More activities in EUSpec:

EWinS 2016
EUSpec Winter School on core level spectroscopies
February 1–11, 2016 | Ajdovščina, Slovenia
http://ewins2016.ijs.si/

Report of first EUSPEC Winter School on core-level Spectroscopies

February 1st-11th, 2016
University of Nova Gorica, Ajdovščina, Slovenia
(by Layla Martin-Samos)

The idea that a two-week school should be in Slovenia first emerged during the first Whole Action Meeting (WAM 2014) in Louvain-la-Neuve, Belgium. In compliance with the naming of other action meetings, the school was nicknamed as "EWinS", standing for "EUSPec Winter School". The preparations for the school started in spring 2015 and in autumn they become rather intense with many skype calls between the local organizers and Hubert Ebert, Didier Sebilleau, Amelies Juhin as well as other members of school international committee. The ideas on the table were many and the uncertainties on practical aspects were even more. Let us introduce the context. "EWinS" is the first two-week school organized within the context of EUSpec. "Being the first" is already a source of concerns. "Being the first" in a small town of 6600 inhabitants in the middle of west Slovenia becomes an epic quest. Fortunately, with the help of volunteers, long and difficult budget plans, creative accommodation and transportation plans, on Monday the 1st of February all trainees were attending the first lecture given by Prof. Maria N. Piancastelli. After the coffee break Prof. Lucia Reining explained the basis of electronic excitations under a theoretical point of view.

In the afternoon, the network infrastructures of the University of Nova Gorica and the computer facilities provided by the Chemical Department of the University of Munich, have been intensively tested by 46 trainees running remote computer simulations. Prof. Peter Blaha explained in a very clear and easy way, how to calculate core-level shifts from first-principles all-electron approaches, using the Wien2k code. The first

Visiting ELETTRA

training day ended late in the afternoon. On Tuesday, the program smoothly continued and the local organizers got some time to breath. On Wednesday Prof. Frank de Groot introduced core level spectroscopies and Prof. Cécile Hébert presented recent developments and new perspectives of EELS. After the "Wine testing at poster session" on Wednesday evening, we noticed a marked difference in the overall school atmosphere: maybe the wine, maybe the whether helped in promoting friendship and scientific discussions. Thursday and Friday were dedicated to pseudo-potential approaches with hands-on sessions on Quantum-Espresso/XSpectra package. After a hard week, finally the weekend arrived. A group of trainees went to visit one of the national parks: the Skocjan caves (a karst cave system that is on UNESCO list of the natural heritage sites) guided by one of the local students Matija Stupar. On Monday the 8th, the participants went to visit the Elettra Synchrotron in Trieste (Italy). On Tuesday the lectures continued, this time with more emphasis on the Quantum Chemical perspective, whereas Prof. Claudio Masciovecchio presented frontier research at FERMI. The ORCA trainers provided a very nice two-

day introduction to Quantum Chemical modeling approaches followed by the hands-on courses.

Thursday was dedicated to the young researchers (ECIs) and Yaroslav Kvashnin animated the round table on STSM. Despite the intensity of the school, the last day was very exciting with many original contributions from the trainees.

Thank you to all participants, to the international committee, to Sasa Badalic, to Rita Römling, to Gerald Derondeau and to all volunteers that made possible the school! We had a wonderful time! Thank you again!

The detailed school program, abstracts and presentations can be found at the school webpage: http://ewins2016.ijs.si/.

Plenary Invited lecturers:
Maria N. Piancastelli (Uppsala University)
Lucia Reining (Ecole Polytechnique)
Frank de Groot (Utrecht University)
Stefano Baroni (SISSA)
Claudio Masciovecchio (Elettra Sincrotrone)
Cécile Hébert (EPFL)
Dimitrios Manganas (MPI für Chem. Energiekonversion)

Invited speakers and trainers:
Peter Blaha (TU Wien)
Stefano de Gironcoli (SISSA)
Guillaume Radtke (University P. et M. Curie-CNRS)
Iztok Arčon (University of Nova Gorica)
Matteo Amati (Elettra Sincrotrone)
Keisuke Hatada (University of Rennes 1)
Dean Cvetko (University of Ljubljana)
Yaroslav Kvashnin (Uppsala University)

Local Organizers:
Layla Martin-Samos (University of Nova Gorica)
Anton Kokalj (Jožef Stefan Institute)
Barbara Ressel (University of Nova Gorica)

International Committee:
Hubert Ebert (University of Munich)
Didier Sébilleau (University of Rennes 1)
Amélie Juhin (University P. et M. Curie-CNRS)
Frank de Groot (Utrecht University)
Maddalena Pedio (CNR-IOM)
Jarmila Savkova (University of West Bohemia)
Sara Lafuerza (ESRF)
Nicholas Hine (University of Warwick)
Yaroslav Kvashnin (Uppsala University)

Short Term Scientific Missions

The 3rd call for Short Term Scientific Missions (STSM) in the COST action has been announced. Here we report four STSM activities happened in the second half of 2015.

Claudio Attaccalite (CNRS/Université Grenoble Alpes, Institut Néel, F-38042 Grenoble, France) visiting Myrta Grüning (School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom)
The STSM took place from 20/07/2015 to 28/07/2015. The goal of the mission was to develop an ab-initio code for the electro-optical response.

The electro-optic effect corresponds to a change of the propagation of an electromagnetic wave in a material by a static external electric field. This term covers a number of different phenomena consisting of the change of refractive index or absorption in a medium. The variation of the refractive index has both a fundamental and applicative interest. In particular the variation of the absorption spectrum induced by a static electric field is a common experimental tool to identify the excitons character in molecular and atomic solids. In fact the different kinds of excitons respond in different ways to the external electric field.

Electro-absorption is not only important from a fundamental point of view but it is currently used to build very efficient photo-receptors and laser modulators. Designing this kind of devices requires a deep knowledge of the response of bulk materials in the presence of an external electric field. Claudio

Attaccalite and Myrta Grüning have recently developed a new methodology to study optical properties of materials where the coupling between electrons and the external field is described by means of Modern Theory of Polarization while correlation effects are derived from Green's functions.[1]

During the STSM they extended this approach to the electro-optical response in bulk materials. A publication is expected in the

Figure 1: Schematic representation of the electro-absorption

next months. These advances will benefit all community gathered by the COST action and facilitate new collaborations between theoreticians and experimentalists.

[1] C. Attaccalite and M. Grüning, Phys. Rev. B **88**, 235113 (2013).

Fabio Iesari (University of Camerino, Italy) visiting Didier Sébilleau (University of Rennes 1, France)
The STSM took place from 28/08/2015 to 30/09/2015. The main goal of the mission was the development of different codes for data analysis of EXAFS data and the construction of a collaboration between Rennes and Camerino.
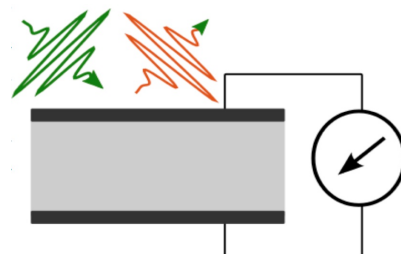
During his stay Iesari worked in strict contact with Dr. Keisuke Hatada to finish the development of the graphical interface for the suite of programs GNXAS [1], which will help the use of the program by a wider audience with a more user-friendly window. Iesari also kept working on his thesis project, the Reverse Monte Carlo program [2] for EXAFS data of highly-disordered systems. In particular he worked on the implementation of multi-atomic, multi-edge cases. Since this upgrade requires heavy computation and memory usage, the computational expertise of the Rennes group has been very helpful. They also discussed how to parallelize the program using GPUs instead of classical CPUs to decrease the computation time.

Iesari believed this was an amazing opportunity for his training as a Ph.D thanks to the profitable exchange of ideas and experiences.

[1] A. Filipponi, A. Di Cicco, and C. R. Natoli, Phys. Rev. B **52**, 15122 (1995).
[2] A. Di Cicco, F. Iesari, S. De Panfilis, M. Celino, S. Giusepponi and A. Filipponi, Phys. Rev. B **89**, 060102 (2014).

Alla Zak (Faculty of Sciences, HIT - Holon Institute of Technology, Israel) visiting Sabrina Sartori (Department of physics, University of Oslo, Norway)

The STSM took place between 02/09/2015 and 11/09/2015, for investigation of Na-ion batteries as renewable energy storage system based on WS2 nanotubes.

The development of sustainable energy systems is among the greatest challenges of nowadays. Nanotechnology potentially can provide new solutions because energy conversion processes occur at interfaces and surfaces, which are abundant in nanostructured materials. In this project Dr. Zak and Prof. Sartori propose to investigate the use of inorganic nanotubes (INT) of WS_2 and MoS_2 as materials for Na-ion batteries (NIB). This application is intended for stationary storage systems, where the size and weight of the storage system is of lesser concern.

Meeting this target Dr. Zak team synthesized the inorganic nanotubes of WS_2, and together with Prof. Sartori, head of the Norwegian group, they managed to obtain uniform thick composite films of polymer with INT-WS_2 – the active material for electrodes. During this STSM they have developed the method for dispersion of this material to prepare composite with chosen polymer polyvinylidene fluoride (PVDF) for preparation of the proper samples.

INT-WS_2 of up to 50 micron long and ~100 nm in diameter were synthesized in the quartz-made reactor specially designed for this process.

Three electrodes were made using aluminum and copper foils, and prepared by mixing the active material (WS_2), the conductive material (glassy CarbonSuperP (CSP)) and the polymer binder PVDF in N-Methyl-2-pyrrolidone (NMP).

The first samples were tested, however these attempts were not satisfactory from the electrochemical performance point of view. The analysis of the samples to clarify the reason for the devices failure showed that the method used for dispersion of the INT might not have been suitable. Moreover, the synthesis of nanotubes will be further study in order to prepare nanotubes with less size distribution. Newly prepared nanotubes will be mixed with PVDF and their performance as NIB will be tested according to the above described procedure. Moreover, Prof. Sartori will test these samples with the aim of performing innovative measurements in real-time, for instance, charging/discharging the battery while simultaneously collecting structural information and absorption spectroscopy measurements.

Finally, Dr. Alla Zak and Prof. Sabrina Sartori can conclude, that the purpose of the proposed STSM – to develop method for the sample preparation, was fully achieved. The STSM was very fruitful and important, as both groups got an opportunity to share their experience in properties and handling of nanotubes, and in the preparation of anodes for Na-ion batteries in "real life".

Davide Sangalli (Istituto di Struttura della Materia, CNR, Italy) visiting Pina Romaniello (Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, France)

The STSM took place between 01/11/2015 and 14/11/2015. Dr. Sangalli and Dr. Romaniello are two scientists working on optical properties of extended systems from first principles. One of them uses a current-based approach, via the calculation of the current-current response function χ_{jj}, whereas the other one uses a density-based approach, via the calculation of the density-density response function $\chi_{\rho\rho}$. The two formalisms are very similar but with some subtle aspects which they often discuss about. The STMS scientific mission was the perfect occasion to finally tackle some of these questions.

During his stay at the "Laboratoire de Physique Théorique" in Toulouse (1st-14th November 2015), Dr. Sangalli worked with Dr. Romaniello on a systematic and detailed theoretical and numerical comparison of the two approaches. First, along the line of Ref.[1], they established an exact relation between dielectric function constructed from χ_{jj}, $\varepsilon[\chi_{jj}]$, and the one constructed from $\chi_{\rho\rho}$, $\varepsilon[\chi_{\rho\rho}]$. Then they showed that, in practical calculations, this relation might not hold anymore if the equations are not properly treated. To do this they worked both at the level of independent as

STSM -- continued

well as interacting particles, using the Bethe-Salpeter equation (BSE). In particular they showed that solving the BSE using the so-called excitonic hamiltonian requires a redefinition of the current operator in order to get the same results from the density-based approach and the current-based approach.

A draft on these results is in preparation. To the collaboration took part also the researcher Arjan Berger from the Laboratoire de Chimie et Physique Quantiques.

[1] J. E. Sipe, and E. Ghahramani, Phys. Rev. B **48**, 11705 (1993).

**NEW call open from
1st of June 2016**
(Mission period: 10/06/2016 to 15/11/2016
Max funding per mission: 1200 EUR)

For details see:
www.eusepc.eu/STSM

Upcoming event

**3rd EUSpec Training School:
multiple scattering codes
Université de Rennes-1, Rennes, France
June 27-30 2016**

The aim of this Training School is to introduce experimentalists and theoreticians to the multiple scattering framework for the descriptions of spectroscopies, so that they are able to run any multiple scattering code. The first day will be entirely devoted to the basic knowledge about multiple scattering theory. The next three days will involve hands-on on five different codes that model core-level spectroscopies:

* **MXAN:** to fit XAS data in terms of selected structural parameters from the edge to 250 eV, recovering in this way the complete geometry around the absorbing atom

* **GNXAS:** advanced software for EXAFS data analysis with a rigorous fitting procedure of the raw experimental data

* **MsSpec:** to model five different spectro-scopies including photoelectron and Auger electron diffraction. REXS and EELS are under implementation and will be released soon

* **FPMS:** full-potential XAS calculations that can treat very large clusters. It is an ideal tool to study open systems (molecules, graphene, etc.) when the muffin-tin approximation fails

* **MCMS:** R-matrix multi-channel calculations of XAS spectra featuring in particular particle-hole multiplet effects

One specialized training session will be devoted to each code, with a sixth one free in order to allow trainees to go deeper into one of the codes. Poster sessions will also take place and trainees are encouraged to bring one (or more) poster. This training school is limited to 40 participants. There is no registration fee. Trainees from COST countries belonging to the EUSpec Action and the two institutes from the Near Neighbour Countries invol-ved in EUSpec can obtain some financial support according to the COST rules.

Detailed information:
EUSpec.sciencesconf.org

Registration:
Deadline 8th of May, No fee, max. 40 participants

Invited Speakers:
Maurizio Benfatto (LNF-INFN, Frascati, Italy)
Calogero Natoli (LNF-INFN, Frascati, Italy)
Andrea Di Cicco (Universita di Camerino, Italy)
Didier Sébilleau (IPR, Rennes, France)
Keisuke Hatada (IPR, Rennes, France)
Hubert Ebert (LMU, Munich, Germany)
Jan Minar (LMU, Munich Germany)
Ondrej Sipr (Inst. Phys. ASCR, Prague, Czech Repub.)
Peter Krüger (Chiba University, Chiba, Japan)
Anna Taranukhina (SFedU, Rostov on Don, Russia)

Additional trainers for code practice:
Elisabetta Pace (LNF-INFN, Frascati, Italy) for MXAN
Fabio Iesari (Universita di Camerino, Italy) for GNXAS
Akihiro Koide (Chiba University, Chiba, Japan) for FPMS and MCMS
Thomas Jaouen (University of Fribourg, Switzerland) for MsSpec

Computational codes within EUSpec

A central part of EUSPec are computational codes for spectroscopy. Here the authors provide brief descriptions of the functionality and method of their code. The codes presented in this issue are subject of the upcoming EUSpec training school in Rennes (page 2). More information on all EUSpec related codes can be found at http://www.euspec.eu

FPMS

Keisuke Hatada (Institut de Physique de Rennes, Université de Rennes-1, France)

Method: FPMS code is based on the Full Potential Multiple Scattering (FPMS) theory in real space [1-3] beyond Muffin-Tin (MT) approximation that forms the shape of potential as sphere and uses spherical average inside the sphere (See left panel of Fig. 2). The main feature of FPMS theory is that it does not expand Volonoi shaped potentials by spherical Harmonics. It is known that the expansion is not converged numerically which is so-called Gibbs phenomena. Instead, FPMS does not expand the potential but rather only the solution of local Schroedinger equation which converges uniformely. Treatment of full potential is useful for low dimensional systems, diamond structure, layered system and surface in which MT approximation fails.

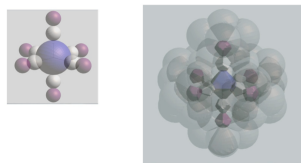In Fig. 3 Carbon K-edge XANES (X-ray Absorption Near Edge Structure) spectra for graphene are shown. [4] SCF charge density is taken from VASP [5] calculation. The pola-rization angle between graphene sheet and the electric field is 74 degrees, so that the polarization is almost perpendicular. Hedin-Lundqvist potential which is energy dependent is used as an optical potential. Because of particular structure of graphene, the convergence of cluster size is slow and the diameter becomes 60 Å (about half day of calculation with 24 CPUs for about 300 energy points). We can see significant improvement by FPMS from the MT approximation.

Features: Main application of the code is XANES. It also calculates projected DOS. With a help of small program it calculates also Resonant X-ray elastic Scattering. FPMS integrates a part of ES2MS [6] (a delivalable of WG4 of EUSpec) which is an interface to use a charge density and potential from electronic structure codes, so far only for VASP.

FPMS is cooperated with MXAN [8], so-called "FP-MXAN", to perform structure fitting for XANES spectrum without MT approximation. FPMS has an option to print out T-matirx for MsSpec code, so that one can perform full potential calculation for photo-electron diffraction.

Requirements: The code runs on Linux, Windows and Mac. The prepared executable is provided only for serial mode, no additional pro-grams or libraries are re-quired. While the parallel ver-sion must be compiled by users on their own platform. For the compilation, one needs Fortran 2003 compilers, OpenGL, MPI and LAPACK & BLAS.
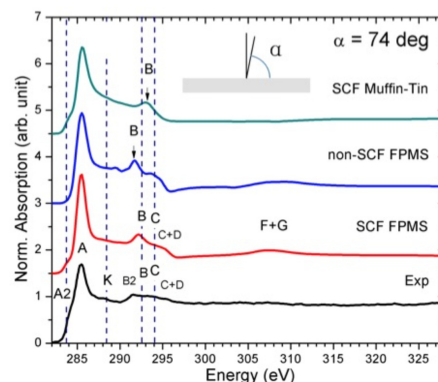

Figure 3: C K-edge XANES of gra-phene with 60 Å diameter cluster. α is the angle between the graphene sheet and the electric field.

Figure 2: Images of scatterers of $Fe(CN)_6$ for MT (left) and full potential (right)

[1] K. Hatada, K. Hayakawa, M. Benfatto and C. R. Natoli, Phys. Rev. B **76**, 060102(R) (2007)
[2] K. Hatada, K. Hayakawa, M. Benfatto and C. R. Natoli, J. Phys.: Cond. Matt. **21**, 104206 (2009)
[3] K. Hatada, K. Hayakawa, M. Benfatto and C. R. Natoli, J. Phys.: Cond. Matt. **22**, 185501 (2010)
[4] J. Xu, P. Krüger, C. R. Natoli, K. Hayakawa, Z. Wu and K. Hatada, Phys. Rev. B **92**, 125408 (2015)
[5] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999)
[6] J. Xu, C. R. Natoli, P. Kruger, K. Hayakawa, D. Sebilleau, L. Song and K. Hatada, Comp. Phys. Comm. **203**, 331 (2016)
[7] K. Hayakawa, K. Hatada, P. D'Angelo, S. Della Longa and M. Benfatto, AIP Conf. Proc. **882**, 111 (2007)
[8] D. Sébilleau, C. R. Natoli, G. M. Gavaza, H. Zhao, F. Da Pieve and K. Hatada, Comp. Phys. Comm. **182**, 2567 (2011)

MXAN

M. Benfatto and E. Pace (Laboratori Nazionali di Frascati, INFN, Frascati, Italy)

The low-energy part of an X-ray Absorption Spectrum (XAS), the so-called XANES energy region, is of great interest since it is extremely sensitive to the structural details of the absorbing site (overall symmetry, distances and bond angles). In principle, an almost complete recovery of the geometrical structure within 6-7 Å from the absorbing site can be achieved from the experimental data, bonds and angles can be obtained with atomic resolution. Experimental data can come from sample in any thermodynamic conditions.

The XANES region has also the advantage that the effects of the atomic thermal disorder are limited,

because the Debye-Waller-like term is almost independent of temperature at low energies. In fact, any multiple-scattering (MS) signal of order n can be written as a sine function whose arguments contain the term kR_{tot}, where R_{tot} is the total length of the n-order MS path. Consequently the associated total Debye-Waller factor has terms like $exp(-k^2\sigma^2)$, which gives the strongest contribution to the Debye-Waller factor and is almost equal to unity at low k values.

The quantitative analysis of the full XAS spectrum, including the edge, is a difficult problem that requires adequate treatments of the potential and time-consuming algorithms in order to calculate the absorbing cross section. Because of these difficulties, analyses of the XANES spectra are done in most of the cases only on qualitative grounds: either by comparison with model compounds or as an aid for EXAFS studies.

Few years ago a new method, called MXAN, has been proposed in the literature for performing a quantitative analysis of the XANES energy range, i.e. from the edge up to 200 eV. This method is based on a comparison between experimental data and many theoretical spectra calculated in the framework of the full MS approach, i.e. the scattering path operator is calculated exactly, without any series expansion. Starting from a putative geometrical configuration of the absorbing site, MXAN is able to reach best-fit conditions in reasonable time by the minimization in the parameter space of a square residual function. The calculations are performed in the energy space without involving any Fourier-transform algorithm; polarized spectra can be easily analyzed because the photo-absorption cross section is calculated with the full MS approach.

MXAN is based on the muffin-tin approximation for the shape of the potential and on the concept of quasi-particle complex potential, this last by using a suitable approximation of the self-energy of the excited photoelectron. The effects of non-MT corrections on the MXAN structural fitting are in general very weak, resulting in a systematic errors in the bond-length distances of the order of ± 0.01 Å. This result is not surprising because it is possible to demonstrate that the absorption cross section can be written as the sum of the MT-calculated cross section and other terms containing all of the non-MT corrections. These corrections depend on the system and go to zero as the energy increases.

The real part of the self-energy is calculated either by the X-α approximation or by using the Hedin-Lundqvist (HL) potential. To avoid over damping of the complex part of the HL potential at low energies in the case of covalent molecular systems, the MXAN method can alternatively account for all the inelastic processes by a convolution with a broadening Lorentzian function that has an energy-dependent width of the form $\Gamma(E) = \Gamma c + \Gamma mfp(E)$. The constant part Γc accounts for the core-hole lifetime while the energy-dependent term

represents all the intrinsic and extrinsic inelastic processes, its shape follows the universal functional form of the mean free path in solids.

In the last years this method has been successfully applied to a big variety of data and samples, from metallo-protein to time-dependent XAS data of meta-stable state living few hundred of femtoseconds.

GNXAS

Andrea Di Cicco (Sezione di Fisica Scuola di Scienze e Tecnologie Università di Camerino, Italy)

The GNXAS package is and advanced software for EXAFS data analysis based on multiple-scattering (MS) calculations and a rigorous fitting procedure of the raw experimental data.

Main features: Model structure analysis through n-body expansion, phase shifts calculation in the muffin-tin approximation using complex energy-dependent potentials. Calculation of n-body MS signals associated with two, three, and four atom configurations using advanced algorithms.

Advanced fitting procedure of raw absorption data allowing for multiple-edge structural refinement and rigorous statistical analysis. Inclusion of complex background multi-electron excitation features.

Modelling of the pair and higher-order distribution functions, including non Gaussian models and extremal cases, adapted for disordered systems (liquid, glasses, etc.).

Full modularity than makes easy to interface parts of the GNXAS software with other available software and extensions. GNXAS provides a flexible scientific tool for EXAFS data analysis where the user has access to every stage of the calculation. GNXAS is not a black box.

Software extensions: The GNXAS suite of programs include several software tools (readout of outputs, visualization, contour plots), data manipulation and sample optimization routines, deconvolution and handling of pair distribution functions. The full GNXAS release provides a complete data-analysis package.

The extended package, available upon request, may also include additional programs for performance of Reverse Monte Carlo structural refinement and for combined x-ray diffraction data-analysis.

Platforms: GNXAS is presently available in form of executable files for current distributions of Linux, Windows, and Mac. An user-friendly python visual interface has been also developed and will be soon available.

Website and documentation: Updated information and distribution of executables can be found at the gnxas.unicam.it website. Handbooks containing full documentation are available in form of printed books (2009) and can be requested on-line.

Authors and reference papers: The software was

originally conceived and written mainly by A. Filipponi and A. Di Cicco. The phase shift calculation program was written by C. R. Natoli and T. A. Tyson. Several other scientists have been involved in the development of GNXAS, all acknowledged in the website.

Reference papers:
A. Filipponi, A. Di Cicco, T. A. Tyson, and C.R. Natoli, , Solid State Commun. **78**, 265 (1991).
A. Filipponi, A. Di Cicco and C. R. Natoli,, Phys. Rev. B **52**, 15122 (1995).
Published handbooks:
"GNXAS: a software package for advanced EXAFS multiple-scattering calculations and data-analysis", A. Filipponi and A. Di Cicco, TASK Quarterly 4, 575-669 (2000). GNXAS. Extended suite of programs for advanced x-ray absorption data-analysis: methodology and practice., Editor A. Di Cicco, TASK publishing July 2009, ISBN 978-83-908112-8-4. [124 pages].

MCMS - the Multi-Channel Multiple Scattering code
Peter Krüger, Chiba University, Japan,
pkruger@chiba-u.jp
The MCMS code implements the Multi-Channel Multiple Scattering method [1,2] for the calculation of near-edge X-ray absorption spectra of condensed matter and molecules. It features a full multiple scattering calculation on a finite cluster of atoms in the muffin-tin approximation. In MCMS, final state correlation effects are taken into account by replacing the single-particle T-matrix of the core-hole site, by a multichannel T-matrix, corresponding to a correlated particle-hole wave function. In this way, long-range band structure effects and strong particle-hole multiplet coupling are treated on an equal footing. This makes MCMS a powerful method for L-edge spectra of light transition elements, where the independent particle theory completely fails.

The computational cost is only a few times larger than a standard (single-electron) multiple scattering calculation. This is achieved through an exact partitioning of the multichannel multiple scattering matrix between the correlated absorber atom and the scattering response of the uncorrelated cluster without absorber.

For the computation of the real-space multiple scattering matrix, some routines of the CONTINUUM code by C. R. Natoli were adapted. The scattering phase shifts and atomic matrix elements are computed from atomic potentials that need to be provided for each species.

Potentials generated with the LMTO-ASA (Linear Muffin-Tin Orbital-Atomic-Sphere Approximation) code are most convenient, but any other muffin-tin potential in two-column format can be used, too. Empty spheres can be included for open structures. The multichannel T-matrix is computed using the variational R-matrix method. Core-hole screening is taken into account by replacing the monopole term of the particle-hole interaction by a mixture of the screened an unscreeened core-hole potential. The relative weights of the two parts is currently treated as an adjustable parameter.

[1] P. Krüger and C. R. Natoli, Phys. Rev. B, **70**, 245120 (2004).
[2] P. Krüger, Phys. Rev. B **81**, 125121 (2010).

Editorial Board