Final Whole Action Meeting in Lisbon

EUSpec COST ACTION MP1306

Modern Tools for Spectroscopy on Advanced Materials

18th - 22nd February 2018

Campus da Caparica, Portugal

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FOREWORD

This book contains the final program and the abstracts of the Final Whole Action Meeting in Lisbon of the **EUSpec COST ACTION MP1306-Modern Tools for Spectroscopy on Advanced Materials,** which is a network for gathering activities in theoretical spectroscopy to offer high level support for complex spectroscopy experiments within academic, applied and industrial research. Therefore, it is expected that the presentations summarize the work developed within the scope of this Action as well as the main conclusions achieved. This meeting was sponsored by COST and Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Portugal. The Conference Program includes oral presentations and posters. We are proud to announce that the program further includes also a plenary keynote lecture, given by Ana Maria Botelho do Rego (Instituto Superior Técnico, Universidade de Lisboa, Portugal)

Conferences are also meeting places where collaboration projects can emerge from social contacts amongst the participants. Therefore, in order to promote the development of research networks there will be a Social Dinner in the evening of 20th February 2018.

We would like to express our thanks to all participants, all members of the Program Committee and to the secretariat.

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VENUE

Venue

Room 202, Building IV (E.IV), Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Campus Caparica, Portugal

PROGRAM

Monday 19th February 2018

Venue: Room 202, Building IV (E.IV)

9:00-9:15	**Reception**
9:15-9:30	**Opening Ceremony**
Session A	**Chair: *Krisztian Palotas***
9:30- 10:30	Ana Maria Botelho do Rego *X-ray photoelectron spectroscopy: a powerful tool for characterization*
10:30-11:00	**Coffee Break & Poster Session**
11:00 -11:45	Anna Taranukhina *Quantum-Chemical and Multiple Scattering Calculations of X-Ray Emission and Absorption: Correspondence between Green's Function Singularities, Molecular Orbital Energies, and Spectra Features.*
11:45-12:30	Lars G.M. Pettersson *Modeling X-Ray Emission Spectroscopy of Hydrogen-Bonded Systems with a Semi-Classical Kramers-Heisenberg Approach*
12:30-14:00	**Lunch Break**
Session B	**Chair: *Lars G.M. Pettersson***
14:00- 14:45	Jan Minar *One step model of ARPES: Photoemission response of Fe-pnictides*
14:45-15:30	Krisztian Palotas *High-resolution tunneling spin transport on a magnetic skyrmion*
15:30 -16:00	**Coffee Break & Poster Session**
16:00-16:45	Gonçalo Barreto *Impedance spectroscopy as water pollutants detector*

Tuesday 20th February 2018

Venue: Room 202, Building IV (E.IV)

Session C	**Chair: *Ondrej Sipr***
9:00- 9:45	Keisuke Hatada *New features of ES2MS package*
9:45-10:30	Martin Lueders *The Electronic Structure Common Data Format*
10:30-11:00	**Coffee Break & Poster Session**
11:00 -11:45	Alexander Soldatov *Combination of Supercomputer Modelling and Machine Learning Algorithms for the Analysis of XANES Big Data.*
11:45-12:30	Rostislav Medlín *Ti doped ZnO Thin Films: Fabrication, Structure, Phase transitions and Properties*
12:30-14:00	**Lunch Break**
Session D	**Chair: *Keisuke Hatada***
14:00- 14:45	Ondrej Sipr *Broadening calculated spectra by introducing complex energy: possible artefacts close to the edge*
14:45-15:30	Didier Sébilleau *Fitting calculations to experiment: A 1001 ways to compare two curves*
15:30 -16:00	**Coffee Break & Poster Session**
16:00-16:45	Vera Quatero *X-ray absorption spectroscopy study of CuO at high pressure: the first binary multiferroic at room temperature*
19:30-22:30	**Social Dinner**

Wednesday 21st February 2018

Venue: Room 202, Building IV (E.IV)

Session E	**Chair: *Jan Minar***
9:00- 9:45	Hubert Ebert *Theoretical description of ultrafast laser-induced demagnetization monitored by photo-emission using the non-equilibrium Green function formalism*
9:45-10:30	Roberto Grunnella *Activity of the time resolved spectroscopies working group in EUSPEC*
10:30-11:00	**Coffee Break & Poster Session**
11:00 -11:45	Ana Ferraria *XPS application to the study of carbon allotropes*
11:45-12:30	Telma Marques *Study of the effect on DNA multilayer films when submitted to UV radiation*
12:30-14:00	**Lunch Break**
Session F	**Chair: *Roberto Grunella***
14:00- 14:45	Akhiro Koide Analysis of K-edge XMCD for CrO2 as a light element magnetic material
14:45-15:30	Nadja Doslic Photoinduced Dynamics of Small Organic Compounds: Achievements and Challenges
15:30 -16:00	**Coffee Break & Poster Session**
16:00-16:45	Alberto Marmodoro Towards an approximated description of X-ray absorption under electric field within a NEGF-KKR framework
16:45-17:30	Filipa Pires Investigation of the protective role of EGCG against oxidative stress induced by ultraviolet radiation by spectroscopic techniques
17:30-17:45	D. Sebilleau/H. Ebert End of Meeting

Thursday 22st February 2018

Venue: Room 113, Building IV (E.IV)

9:00-10:30	MC Meeting
10:30 -11:00	**Coffee Break**
11:00-12:30	MC Meeting (continuation) & Departure

ABSTRACTS
Oral Contributions

X-ray photoelectron spectroscopy: a powerful tool for characterization

Ana Maria B. Rego
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X-ray photoelectron spectroscopy (XPS) is widely used for characterizing materials from the extreme surface to a depth around 10 nm. Its importance is outstanding for a large number of domains ranging from the fundamental Physical Chemistry to applied fields dealing with catalysis, corrosion, biocompatibility, etc.

In this talk, basic principles are revisited to emphasize the information which can be extracted from photoelectron regions, Auger regions, energy loss regions, valence bands and even from charging effects. Each aspect will be illustrated with results from the group.

Acknowledgements

Author would like to thank NATO for funding through the SfP984842 project and Fundação para a Ciência e a Tecnologia (FCT), Portugal, for funding the project UID/NAN/50024/2013.

Monday, 19 February 2018, 9:30

Quantum-Chemical and Multiple Scattering Calculations of X-Ray Emission and Absorption: Correspondence between Green's Function Singularities, Molecular Orbital Energies and Spectra Features

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Quantum-chemical methods are widely applied to both the determination of the electronic and atomic structures of metal complexes and calculations of various X–ray spectroscopic response functions. In many cases, energies and characteristics of molecular orbitals (MOs) can be used for evaluation of X-ray transition energies and theoretical simulation of XES and XANES reproducing the shape of experimental spectra reasonably well. However, traditional quantum-chemical methods have severe limitation regarding its applicability to calculations of strongly delocalized electronic states in the continuum. By contrast, the multiple scattering (MS) method allows calculations of XAS within practically unlimited energy ranges. Moreover, MS method in the Green's function (GF) formalism allows both occupied and unoccupied electronic states to be considered on the same footing. When using MT-approximation, an essential point is the choice of the MT potential outside the system under study. In the case of free clusters simulating bulk materials, MS method usually uses so-called extended continuum approximation (ECA) and MT-zero as a free parameter. For small molecules, the spherically symmetrical potential outside a surrounding sphere can be successfully used. The situation is different for large and, especially, elongated molecules and complexes. On the one hand, an outer sphere has a big volume, on the other hand the MT-zero should be chosen deep enough to avoid sharp discontinuities of the potential at the MT spheres. These two factors often cause an appearance of "extraneous" bound states which hybridize with "true" MOs. To exclude them, the ECA is also used, although discrete stationary states cannot actually exist in the energy range between the MT-zero and the vacuum level. One can assume that the "true" discrete stationary states originated from MOs in this range transform to the quasi-stationary (or resonance) states, whereas "extraneous" states (as well as Rydberg ones not observed in hard XAS of polyatomic systems) disappear. To verify the above assumption and to answer the question to what extent MS method using the ECA is capable of describing both XAS and XES of low-symmetry complexes where, for instance, the *p-d* mixing effect occurs, we calculated XES and XAS for the $Mn_2(CO)_{10}$ complex within the quantum-chemical method based on DFT and the MS method used ECA. It is shown that both DFT and MS methods allow calculations of XES and MnK XAS in agreement with one another and with experiment. It is revealed a one-to-one correspondence between MOs originated from well-localized atomic orbitals obtained within DFT and resonance states caused by poles of the GF calculated within MS method. Moreover, the real parts of the pole energies are close to the energies of corresponding MOs. A procedure developed for the numerical determination of the pole parameters in the lower semiplane of the second sheet of the complex energy plane allows one to distinguish a group of poles close to the real axis. These poles completely define the XES fine structure in C$K\alpha$, O$K\alpha$, Mn$L\alpha$, and Mn$K\beta_5$ spectra as well as the Mn K edge XANES. The XAS fine structure above the narrow low-energy peaks is also dominantly governed by contributions from poles, but these poles lie farther from the real axis than those corresponding to the MOs.

Monday, 19 February, 11:00

Modeling X-Ray Emission Spectroscopy of Hydrogen-Bonded Systems with a Semi-Classical Kramers-Heisenberg Approach

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The oxygen 1s core-hole life-time is long enough (~3.6 fs) that significant vibrational excitations take place in the internal OH bonds that the core-excited oxygen participates in. This results in significant life-time vibrational interference1,2 or dynamical effects that redistribute intensity in the computed spectrum. We include these effects in a semi-classical approximation to the Kramers-Heisenberg formula by running classical core-hole-induced dynamics where it is essential to sample the zero-point quantum probability distributions of momenta and initial OH positions3. We have recently performed simulations of liquid methanol4 and ethanol5 in good agreement with experiment. Here I will show how different aspects of H-bonding, initial conditions and, in the case of ethanol, also the internal conformation affect the computed spectrum. Extending to water we need significantly more trajectories since two OH groups must be sampled. I will discuss preliminary results from a search for structural criteria on simulated water that should be fulfilled in order to reproduce both x-ray absorption and emission spectra as well as the O-O radial distribution function of liquid water. In that case we employ our SpecSwap-RMC6,7 multiple-data fitting technique.

[1] Gel'mukhanov, F. K., Mazalov, L. N. & Kondratenko, A. V. A theory of vibrational structure in the X-ray spectra of molecules Chem. Phys. Lett. 46, 133, (1977).
[2] Ljungberg, M. P., Pettersson, L. G. M. & Nilsson, A. Vibrational interference effects in x-ray emission of a model water dimer: implications for the interpretation of the liquid spectrum J. Chem. Phys. 134, 044513 (2011).
[3] Ljungberg, M. P., Nilsson, A. & Pettersson, L. G. M. Semi-classical description of nuclear dynamics in x-ray emission of water. Phys. Rev. B 82, 245115 (2010).
[4] Ljungberg, M. P., Zhovtobriukh, I., Takahashi, O. & Pettersson, L. G. M. Core-hole-induced dynamical effects in the x-ray emission spectrum of liquid methanol. J. Chem. Phys. 146, 134506, (2017).
[5] Takahashi, O., Ljungberg, M. P. & Pettersson, L. G. M. X-ray Emission Spectrum of Liquid Ethanol – Origin of Split Peaks. J. Phys. Chem. B 121, 11163 (2017).
[6] Leetmaa, M., Wikfeldt, K. T. & Pettersson, L. G. M. SpecSwap-RMC: A novel reverse Monte Carlo approach using a discrete configuration space and pre-computed properties. J. Phys.: Cond. Mat. 22, 135001, (2010). (https://github.com/leetmaa/SpecSwap-RMC)
[7] Wikfeldt, K. T., Leetmaa, M., Mace, A., Nilsson, A. & Pettersson, L. G. M. Oxygen-oxygen correlations in liquid water; addressing the discrepancy between diffraction and EXAFS using a novel multiple –data set fitting technique. J. Chem. Phys. 132, 104513 (2010).

Monday, 19 February 2018, 11:45

One step model of ARPES: Photoemission response of Fe-pnictides

Ján Minár
University of West Bohemia, Pilsen, Czech Republic

In this presentation we will show an application of one-step model of photoemission to the various aspects of the photoemission response of Fe-pnictides. At the beginning a brief introduction to the theory of angle-resolved photoemission spectroscopy (ARPES) of solids is given with an emphasis on the so-called one-step-model of photoemission that describes excitation, transport to the surface and the escape to the vacuum in a coherent way. This is followed by a short description of the main features of an implementation of the one-step-model within the Munich SPR-KKR program package [1]. This method we applied recently to study the anisotropic electronic structure of antiferromagnetic BaFe2As2 and Ba(Fe1−xCox)2As2 as seen by ARPES [2]. To conclude, we were successful in reproducing the strong in-plane anisotropy of BaFe2As2 and its behavior under substitution in very good agreement with experiment using ARPES calculations. These calculations allow even predictions on possible surface terminations. In addition Ba1-xKxFe2 As2 have been investigated both theoretically and experimentally. Our results explain the previously obscured origins of all salient features of the ARPES response of this paradigm pnictide compound and reveal the origin of the Lifshitz transition. Comparison of calculated ARPES spectra with the underlying DMFT band structure shows an important impact of final state effects on the evaluation of the effective mass. Because this effect is more pronounced for low photoexcitation energies, soft-X-ray ARPES delivers more accurate values of the mass enhancement due to a sharp definition of the 3D electron momentum.

[1] H. Ebert et al., The munich SPR-KKR package, version 7.5, http://ebert.cup.lmu.de/SPRKKR (2008).
[2] Derondeau et al., PhysRev B.**93**, 144513 (2016)
[3] Derondeau et al., arXiv: 1606.08977
[4] Zabolotnyy, V. B. et al. Nature **457,** 569 (2009)

Monday, 19 February 2018, 14:00

High-resolution tunneling spin transport on a magnetic skyrmion

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Spin-polarized scanning tunneling microscopy (SP-STM) demonstrated the creation and annihilation of individual magnetic skyrmions [1] that is promising for future technological use. However, the detailed microscopic mechanisms for these processes are presently unknown. In our work the tunneling spin transport of a magnetic skyrmion is theoretically investigated in SP-STM. The spin-polarized charge current [2] and tunneling spin transport vector quantities, the longitudinal spin current and the spin transfer torque are calculated in high spatial resolution above the complex magnetic texture for the first time using a simple electron tunneling theory. Beside analyzing the vector spin transport characteristics, connections between conventional charge current SP-STM image contrasts and the magnitudes of the spin transport vectors are demonstrated.

[1] N. Romming et al., Science 341, 636 (2013).
[2] K. Palotás et al., Phys. Rev. B 96, 024410 (2017).

Monday, 19 February 2018, 14:45

Impedance spectroscopy as water pollutants detector

G. Magalhães-Mota, P.A. Ribeiro and M. Raposo
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The detection of pollutants such as triclosan in the environment is a major issue, particularly in water supplies, water courses and aquifers, which are known to be mainly contaminated by pesticides, industrial products and emergent pharmaceuticals and personal care products (PPCPs). No commercial sensors for monitoring and detecting these pollutants have been developed so far. In this regard, the electronic tongue concept, based on AC impedance measurements, can be a valuable tool towards contaminants probing. Even so, this possibility presents difficulties, namely on the AC impedance spectra interpretation and on the application of mathematical methods which allow finding classification patterns with consequent contaminant detection.

[1] WHO, Guidelines for Drinking Water Quality, 3rd ed., World Health Organization, 2003.
[2] G. Stevens, M. Mascarenhas, and C. Mathers, "Global health risks: Progress and challenges," Bulletin of the World Health Organization, vol. 87, no. 9, p. 646, 2009.
[3] C. G. Daughton and T. A. Ternes, "Pharmaceuticals and personal care products in the environment: Agents of subtle change?," Environ Health Perspect.107(Suppl 6): 907–938, 1999.
[4] M. Albareda-Sirvent, A. Merko ̧ci, and S. Alegret, "Pesticide determination in tap water and juice samples using disposable amperometric biosensors made using thick-film technology,"Analytica Chimica Acta, vol. 442,no. 1, pp. 35–44, 2001.

Monday, 19 February 2018, 16:00

New features of ES2MS package

Keisuke Hatada[1], Naoki Komiya[2], Fukiko Ota[2], Kaori Niki[2], Xu Junqing[3],
Peter Krüger[2], Ján Minár[4], Hubert Ebert[5], Calogero R. Natoli[6], and Didier Sébilleau[7]

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We present an interface package, called ES2MS[1], for passing self-consistent charge density and potential from Electronic Structure (ES) codes To Multiple Scattering (MS) codes. MS theory is based on the partitioning of the space by atomic-size scattering sites, so that the code provides the charge densities and potentials for each scattering site. For projector augmented wave codes, such as VASP [2], the interface solves Poisson equation to construct the all-electron potential on the radial mesh which is used to solve the transition operators (T-matrix) and Green's functions in MS codes. Recently we have further developed the interface [3] for Gaussian09 [4] and SPR-KKR [5]. In the case of Gaussian 09, the Poisson equation is solved by a recurrence relation based on the set of Gaussian basis. We show the algorithm of the interface and the examples.

References

1. J. Xu, C. R. Natoli, P. Krüger, K. Hayakawa, D. Sébilleau, L. Song, K. Hatada, *Comput. Phys. Commun.* **203**, 331 (2016).
2. G. Kresse, D. Joubert, *Phys. Rev. B* **59**, 1758 (1999).
3. N. Komiya, K. Hatada, F. Ota, P. Krüger, T. Fuijikawa, K. Niki, J. Electron Spectrosc. Related Phenom. **220**, 21 (2017).
4. M.J. Frisch *et al.*, Gaussian09 Revision E.01, Gaussian Inc. Wallingford CT (2009).
5. H. Ebert *et al.*, The Munich SPR-KKR package version 7.7.0 (http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR) (2017).

Tuesday, 20 February 2018, 9:00

The Electronic Structure Common Data Format (ESCDF)

Micael Oliveira, Yann Pouillon, **Martin Lueders**
STFC Daresbury Laboratory, UK

One of the main goals of the Working Group 4 was Interoperability of codes: for instance, it should be possible to use the results of an ab initio calculation without great difficulties in another code to calculate specific spectroscopic properties. This goal is not new, and there have been previous efforts to achieve this. The most advanced was the ESCDF format, which is now further developed under the umbrella of the CECAM Electronic Structure Library (ELS) activity. I will report on the latest developments and the current status of the format specifications and the library.

Tuesday, 20 February 2018, 9:45

Combination of Supercomputer Modelling and Machine Learning Algorithms for the Analysis of XANES Big Data

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World progress in the development and use of new advanced nanostructured materials is significantly constrained by limitations in the capabilities of existing non-destructive techniques for precise determination of the parameters of local atomic and electronic structures for the materials without long-range order in the arrangement of atoms. Serious challenges for modern materials science and high technologies are requests to ensure, for example, a picometer accuracy in determining interatomic distances in materials without long-range order in the arrangement of atoms, and the non- destructive nature of such a technique and the possibility of using it in-situ and even "operando" (that is, directly in the process of technologically important processes under real technological conditions). To solve such problems, large scale research facilities that provide the use of super-high-intensity radiation beams for the implementation of a wide range of research methods have recently been successfully used: synchrotron research centers and most recently - free-electron X-ray lasers. It should be noted that such a distinctive feature of studies carried out using these kind of large scale research facilities as an extremely large amount of experimental data (Big Data) leads to the fact that the results obtained during just a few days, have to be processed by standard methods for years. The complexity of the problem also lies in the fact that although, in principle, the fine structure of the X-ray absorption spectra contains information on the 3D local atomic structure of the material, XANES is not direct method for measuring the parameters of the local atomic and electronic structures, and analysis of each spectrum requires carrying out for its interpretation very complicated computations using high-performance supercomputers. Moreover, the complexity of the problem lies in the fact that, at the time of carrying out theoretical calculations for different types of XANES edges and types of materials, it is optimal to use completely different approaches, and the elements of their unification are absent nowadays. Therefore, we attracted artificial intelligence technologies (machine learning algorithms) to develop a non-destructive X-ray spectroscopic technique for characterizing the parameters of the three-dimensional local atomic structure of advanced materials without long-range order in the arrangement of atoms based on the supercomputer theoretical analysis of XANES spectroscopy data on the basis of FitIt [http://www.nano.sfedu.ru/fitit/] approach developed in our group previously.

Tuesday, 20 February 2018, 11:00

Ti doped ZnO Thin Films: Fabrication, Structure, Phase transitions and Properties

Medlin R. [1], Minar J.[1], Sutta P.[1], Khan W.[1], Sipr O.1, Novak P.[1], Netrvalova M.[1], Alarab F.[2], Hricovini K.[2], Nemsak S.[3]

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ZnO is a wide used ferroelectric material with a variety of applications. When ZnO is doped by the appropriate transition metal elements, physical properties of the material can be significantly modified [1,2]. Here we present a comprehensive study based on a combination of XRD, XPS, HRTEM and EELS to investigate the structural and electronic properties of Ti-doped ZnO. ZnO:Ti thin films were prepared by RF reactive magnetron co-sputtering in Ar/O2 atmosphere from pure Zinc and Titanium targets (99.99%).

Tuesday, 20 February 2018, 11:45

Broadening calculated spectra by introducing complex energy: possible artefacts close to the edge

Ondřej Šipr
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Before being compared to the experiment, the raw calculated XANES has to be modified to account for the finite core hole lifetime. Conventionally, it is done by convoluting the calculated spectrum with a Lorentzian. For multiple-scattering methods, there is another possibility: to add a small imaginary part to the energy. This results in spectra which are smoother from the beginning. If the cut-off of the spectra below the Fermi level EF is neglected, calculating XAS on the energy grid with an imaginary component Im(E) is fully equivalent to convoluting the spectrum with a Lorentzian whose FWHM is Gamma = 2*Im(E). The influence of the cut-off on the broadening via the imaginary energy component is negligible high above the edge. However, the situation may be different at the very edge, where neglecting the cut-off below EF might be a too crude approximation. As a case study, we focus on the K edge and L2,3 edge XAS and x-ray magnetic circular dichroism (XMCD) of Fe. We find that for energies high above the edge there is practically no difference in the final spectra, no matter which broadening procedure has been applied. At the very edge, however, there are differences. They stem from the fact that if too much weight is put on broadening by the imaginary energy component, there is a sharp cut-off of the spectra at EF, resulting in too sharp features at the edge. The situation is especially instructive for the L3 XMCD peak. Here a well-distinguished but in fact spurious fine structure appears on its low-energy side unless most of the broadening is done by means of Lorentzian convolution.

Tuesday, 20 February 2018, 14:00

Fitting calculations to experiment: A 1001 ways to compare two curves

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Comparing a calculation to an experimental curve is one of the m Key issues when modelling a spectroscopy. In photoemission and related spectroscopies, R-factors are generally used to this purpose. However, it was realized some time ago that in the course of a structure optimization process, two different R-factors could lead to two different final structure. We propose here an approach combining methods from very different areas of science and pre-processing of the data to tackle the problem. The resulting approach has been implemented into a computer code which will be presented.

Tuesday, 20 February 2018, 14:45

X-ray absorption spectroscopy study of CuO at high pressure: the first binary multiferroic at room temperature.

V. Cuartero[1], M. El Idrissi[1,2], V. Monteseguro[1], O. Mathon[1], and A. Sanson[2]
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CuO has renewed the interest of condensed matter community in the last years due to the recent discovery of multiferroicity (MF) at room temperature (RT) and high pressure (~4 GPa) [1] The origin of MF under these conditions is proposed to be the large super-exchange correlations, *J*, specially the second-neighbor interaction of the edge-sharing chains. [2] An anomaly on the dielectric constant is found around 4.4 GPa and ferroelectricity is proposed to be correlated with strong dynamic O-ion displacements. The macroscopic response of the system appears then to be closely linked to its local structural and electronic properties. We have recently performed an X-ray absorption spectroscopy experiment on BM23 beamline at the ESRF on CuO at high pressure up to 17 GPa. The Cu K-edge X-ray absorption near edge structure (XANES) spectra are shown in fig 1 (a), and two clear features can be distinguished on the pre-edge region (**A**) and at the edge (**B**). **A** peak is normally ascribed to quadrupole transitions to empty *d* states [3], and it does not show any evolution along the whole pressure range; however **B** structure mean position changes with P as the chemical shift does (fig. 1 (b)). **B** feature is normally ascribed to electronic $1s \rightarrow 4p_{xy}$ transitions accompanied by charge transfer effects from the ligand (O) to the metal. The evolution of the Cu-O distances' was obtained from the analysis of the extended X-ray absorption fine structure (EXAFS) spectra. The results are shown on figure 1 (c), which indicates that the Cu-O shorter distances barely change below 6 GPa, but a contraction of the Cu-O distances takes place above 6 GPa, concomitant to a change on the tendency on the chemical shift evolution. The Cu-O long distance is highly reduced along the whole pressure range. Our results demonstrate that above the critical pressure of 6 GPa there is a combined effect of first neighbours distances contraction which favours charge transfer in between the metal and the ligand, which can enhance magnetic correlations.

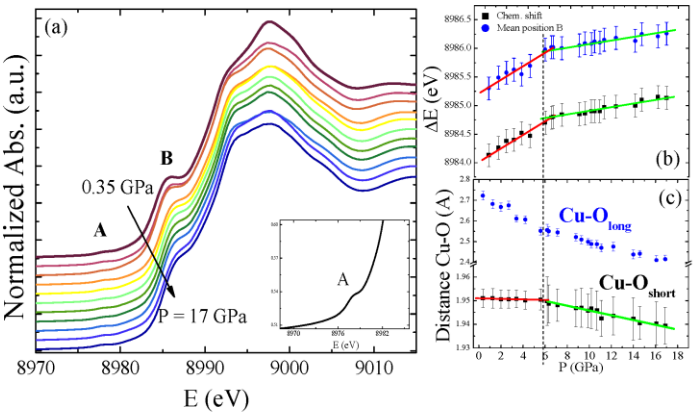

Figure 1: (a) XANES spectra shifted in vertical scale normalized to the jump at different pressure points. (b) Pressure evolution of the chemical shift and (c) first shell distances Cu-O.

[1] R. Jana et al., Sci. Rep. **6**, 31610 (2016).
[2] X. Rocquefelte et al., Nat. Commun. **4**, 2511 (2013).
[3] O. Sipr et al., J. Synchrotron Rad. **8**, 235 (2001).

Tuesday, 20 February 2018, 16:00

Theoretical description of ultrafast laser-induced demagnetization monitored by photo-emission using the non-equilibrium Green function formalism

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Most theoretical schemes to describe ultrafast laser-induced demagnetization of solids are working on a model level using input parameters that might be provided by electronic structure calculations. Only recently [1] an approach based on time-dependent density functional theory (TD-DFT) was presented that allows to calculate the time evolution of the magnetisation due to a laser pulse in a parameter-free way. The applicability of the approach was demonstrated for the elemental ferromagnets but also for Heusler alloys [2]. As an alternative we suggest to use the Keldysh non-equilibrium Green function formalism that offers a number of advantages when dealing with the dynamics of an electron system under the influence of an external perturbation. A corresponding formal basis has been worked out by us that allows in particular to describe the time evolution of the electronic system of a magnetic solid under the influence of a laser-field of arbitrary shape and intensity [3] in terms of the so-called double-time dependent lesser Green function $G^<(r,r',t,t')$. As has been shown, $G^<(r,r',t,t')$ can be calculated on the basis of a Dyson equation from the retarded Green function of the unperturbed system that in turn is obtained in a very flexible and efficient way using the multiple scattering or KKR formalism. The previous TD-DFT based work demonstrated that spin-orbit coupling plays a central role for ultrafast demagnetisation. To account for this, our fully relativistic approach is based on the Dirac equation. Using a combination of local spin-density approximation (LSDA) and dynamical mean field theory (DMFT) as a basis for the underlying electronic structure calculations allows an adequate treatment of correlation effects in narrow band systems that are represented by a corresponding complex and energy-dependent self-energy. The present approach also allows to include a double time-dependent self-energy within the calculations. This in principle allows to account for dynamical correlation effects but also for damping or relaxation effects due to electron-phonon coupling or other mechanisms. An interesting feature of our approach is that it can be combined in a direct way with the calculation of spectroscopic properties as required when dealing with pump-probe experiments [4]. This is demonstrated by results from a study on two-photon photo emission from ferromagnetic Fe (100).

[1] K. Krieger, J. K. Dewhurst, P. Elliott, S. Sharma, E. K. U. Gross, J. Chem. Theo. Comp., 11, 4870 (2015).
[2] P. Elliott, T. Müller, J. K. Dewhurst, S. Sharma, and E. K. U. Gross, Sci. Rep., 6, 38911 (2016).
[3] J. Braun, R. Rausch, M. Potthoff , J. Minar and H. Ebert, Phys. Rev. B 91, 035119 (2016).
[4] J. Braun, R. Rausch, M. Potthoff and H. Ebert, Phys. Rev. B 94, 125128 (2016).

Wednesday, 21 February 2018, 9:00

Activity of the time resolved spectroscopies working group in EUSPEC

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The COST action EUSPEC (http:\\www.euspec.eu) has one main mission: to disseminate and promote the strong advancements in the field of modern quantum mechanics to quantitatively describe atomic and condensed matter spectroscopies. Many important developments during the last two decades allow a more and more improved treatment e.g. for nano-systems, oxides or organic solids. An important example is the demanding description of time-resolved spectroscopy experiments. In this last case a still pioneering approach is necessary because of the lack of a fully comprehensive theory able to give a one-for-all solution to the challenging problems under study because of the intertwining of the expectation values of the physical observables essentially in non-equilibrium condition of matter. It is nevertheless difficult to ignore that in these fields there will be the most appealing advancements of the science from the smallest scale to the largest scale problems like in geophysical or astrophysical science. Many interesting examples of this activity will be reported and possible future development.

Wednesday, 21 February 2018, 9:45

XPS application to the study of carbon allotropes

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X-ray photoelectron spectroscopy (XPS) is a surface specific technique of analysis used to study very different systems, such as carbonaceous nanostructures, like graphene or onion-like carbon.

Context: Graphene and its derivative N-graphene have attracted an exceptional interest due to their unique chemical and physical properties. Nanosheets in the form of free-standing graphene flakes with just a few atomic monolayers find applications where an alternative to supported (on solid surfaces) graphene is needed. While in supported-graphene only one surface is available, free-standing graphene has the advantage of having both free surfaces and at least three open edges that can effectively be utilized [1]. Onion-Like Carbon (OLC) has been extensively studied due to its electronic and self-lubricating properties, which may be interestingly explored at larger scales by dispersing these carbon nanostructures in metallic matrices. Diamond nanoparticles can be successfully dispersed by attrition milling and a similar processing route can be devised for OLC [P.A. Carvalho *et al.*, work in progress].

Aim of the presentation: Among the battery of analytical techniques, XPS can help to evaluate the nanostructures quality, namely by quantifying the sp^2/sp^3 carbon ratio and/or the doping efficiency. Another useful parameter is the one obtained from the 1st derivative of the C KLL Auger structure, called the D parameter, which is the energy difference between absolute maximum and minimum. The question raised at each moment is: *does the result of your data treatment really describe your sample or what you expect it to be?*

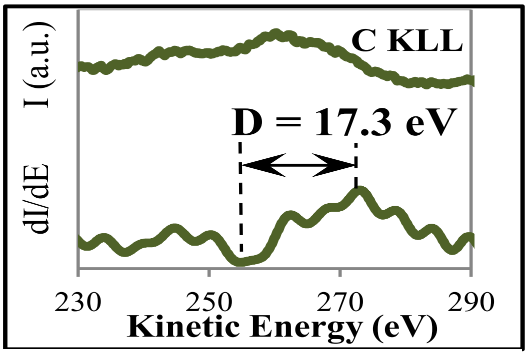

Figure 1. C KLL and 1st derivative of graphene.

Acknowledgements

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[1] “Towards large-scale in free-standing graphene and N-graphene sheets”, E. Tatarova et al., Scientific Reports, 7 (2017) Article number: 10175 (16 pages).

Wednesday, 21 February 2018, 11:00

Study of the effect on DNA multilayer films when submitted to UV radiation

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Ultra-thin films of biomolecules have crescent technological relevance due to their increasing applications in the fields of optical and electronic devices, biochips and biomaterials, sensors, molecular electronic devices, and for studies of the effect of radiation on biological molecules. Layer-by-Layer (LbL) film deposition technique is a unique tool used for the fabrication of mono and multilayered ultra-thin films of biomolecules owing to its cost effectiveness and simplicity in fabrication and allowing to obtain well controlled biological samples in an environment close to that of the cell . DNA is a long biopolymer whose monomers are nucleotides formed by a nitrogenous base (adenine, cytosine, guanine, or thymine), a pentose and at least one phosphate group [1]. On the basis of hydrogen bonding properties of the DNA base pairs, oligonucleotide probes were recently designed to detect tumour genes and various biosensors were also proposed. Thin organic films with a supra-molecular architecture in which DNA is oriented or embedded are of special interest, mainly in the development of biological sensors [2,3] including work on nanoparticles [4]. The induced damage on biological systems by electromagnetic radiation are due to the energy transfer into the medium with absorption of the radiation [1,5], and are characterized by progressive formation of events which differ according to a time scale leading ultimately to biological damage. When a cell is irradiated, two types of changes can occur, directly on the cellular component molecules or indirectly on water molecules, causing water-derived radicals. Radicals react with nearby molecules in a very short time, resulting in breakage of chemical bonds or oxidation of the affected molecules. The major effect in cells is DNA breaks [1,4]. In nucleic acids, changes are essentially loss or damage of bases, thymine dimmers formation, single or double strand breaks and also DNA-protein dimmers formation [4]. The main goal of this work is develop and characterize nanostructured films of DNA and study of the effect of UV radiation in DNA films and in DNA aqueous solutions with and without methylene blue (MB)-a photosensitizer. LbL films of DNA and DNA and DNA+MB solutions were irradiated with UV radiation (254 nm). The damage caused by the radiation in these samples was characterized by UV-Vis spectroscopy in the 200–800nm wavelength range. This study points out that MB has DNA protective action while the presence of water potentiates the degradation of DNA.

[1] P. Gomes, PhD Dissertation, FCT/UNL (2014);
[2] H. Su, K. M.R. Kallury, M. Thompson, A. Roach, Anal.Chem. 66, 769 (1994);
[3] X.H. Xu, H.C. Yang, T.E. Mallouk, A.J. Bard, J.Am.Chem.Soc. 116, 8386 (1994);
[4] C. Kielbassa, I. Roza, B. Epe, Carcinogenesis, 18, 811 (1997).
[5] J.E. Moulder, Power Lines, Cancer FAQ's, in Electromagnetic Fields and Human Health.

Wednesday, 21 February 2018, 11:45

Analysis of *K* edge XMCD for CrO_2 as a light element magnetic material

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The X-ray magnetic circular dichroism (XMCD) spectra have been used in order to obtain local information of the magnetic properties on absorbing atoms. Although the $L_{2,3}$ edge XMCD has been ex useful by the aid of the sum-rule analysis for the spin and orbital moments of *d* orbitals, the *K* edge XMCD has attracted an attention to extract an information in light element magnetic materials, such as graphene on magnetic substrates. From a view point of experiments, the *K* edge XMCD of light elements is measured by the same way as the $L_{2,3}$ edge XMCD of 3*d* transition metals. However, this similarity may make misleading. In terms of the spin orbit interaction (SOI), the SOI on 2*p* core states of the absorbing atom is only important for $L_{2,3}$ edge XMCD. On the other hand, there is no SOI on 1*s* state. This means that the SOI on unoccupied *p* states is important for the K-edge XMCD. A question is whether the SOI at the absorbing atom is also important for the *K* edge XMCD as the case of the $L_{2,3}$ edges or not.

To investigate the statement, we calculated oxygen K edge XMCD for CrO_2 as a prototype of light element magnetic materials. The calculated spectra were obtained by using a multiple scattering theory taking the first perturbed SOI into account in a frame of the relativistic correction on the non-relativistic Green's function [1-4]. This perturbation scheme enables us to represent the XMCD spectra by sum of the contribution of each site SOI. The site-resolved XMCD analysis shows that the nearest neighbour Cr ions have the dominant contribution to the oxygen *K* edge XMCD for CrO_2. The total XMCD spectra has same energy dependence of the orbital-momentum density. Moreover, the calculated XMCD spectra for a diatomic system composed by only Cr and O atoms clearly show that strong XMCD peaks are originated from Cr-d orbitals. We concluded that the absorbing light element just borrows not only the spin but also orbital moments of the surrounding magnetic ions by the hybridization. This differs from the scenario of the $L_{2,3}$ edge XMCD.

[1] C. Brouder, M. Alouani and K. H. Bennemann, *Phys. Rev. B* **54** (1996) 10.

[2] T. Fujikawa and S. Nagamatsu, *J. Electron Spectrosc. Relat. Phenom.* **129** (2003) 55.

[3] A. Koide, K. Nki, S. Seiji and T. Fujikawa, *J. Phys. Conf. Ser.* **712** (2016) 012010.

[4] A. Koide and T. Yokoyama, *Phys. Rev. B* **96** (2017) 144419.

Wednesday, 21 February 2018, 14:00

Photoinduced Dynamics of Small Organic Compounds: Achievements and Challenges

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Time-resolved photoelectron spectroscopy is a natural way to follow the ultrafast dynamics of photoexcited molecular species. In particular, valence photoelectron spectra are directly informative of the electronic structure of the investigated species and can reveal variations in response to photoexcitation. However, a proper understanding the transformations that a photoexcited system undergoes in order to dispose of the excess energy is possible only through a synergistic combination of theoretical and experimental research.

Here, we will focus on the photoinduced dynamics of small organic molecules such as pyrrole[1], furan[2] and acetylacetone[3] and discuss the different computational approaches that we are using to characterize their dynamics in detail.

[1] M. Sapunar *et al.* Phys. Chem. Chem. Phys. **2015**, *17,* 19012.
[2] A. Ponzi *et al.* J. Chem. Phys. **2016**, *144*, 084307.
[3] R. J. Squibb *et al.* Nat. Commun. **2018**, *9,* 63

Wednesday, 21 February 2018, 14:45

Towards an approximated description of X-ray absorption under electric field within a NEGF-KKR framework

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"Bidimensional heterostructures composed of magnetic and non-magnetic materials allow to investigate how spin polarization effects do not cease abruptly at the interface, but extend across it and give rise to a variety of phenomena, that are typically controlled by the details of composition and geometry. Recent experiments [1-2] have furthermore explored how this situation is changed by application of an electric field that drives a steady flux of carriers through the subsystems, and thus go well beyond a static ground state situation. We consider in particular X-ray absorption (XAS) and magnetic circular dichroism (XMCD) [3] measurements which can provide element-resolved insight on spin accumulation and its dependence on the direction and magnitude of the supplied, external stimulus on top of static, proximity induced influences. This setup is investigated within the spin-polarized relativistic multiple scattering framework (SPRKKR) which makes use of recent developments [4-5] for the non-equilibrium Green function (NEGF) description of realistic materials, suitable for parameters -free spectroscopy simulations.

[1] R.Kukreja, S.Bonetti, Z.Chen, D.Backes, Y.Acremann, J.Katine, A.D.Jent, H.A.Dürr, H.Ohldag, and J.Stöhr, "X-Ray Detection of Transient Magnetic Moments Induced by a Spin Current in Cu", Phys.Rev.Lett. 115,096601 (2015)
[2] G.van der Laan, "X Rays Expose Transient Spins", Physics 8, 83(2015)
[3] H.Ebert, "Magneto-optical effects in transition metal systems", Rep.Prog.Phys.59, 1665-1735, 1996
[4] S.Achilles, M.Czerner, J.Henk, I.Mertig and C.Heiliger, "Nonequilibrium Green's functions and Korringa-Kohn-Rostoker method: Open planar junctions", Phys.Rev.B 88, 125411 (2013)
[5] M.Ogura and H.Akai, "Schottky Junctions Studied Using Korringa,Kohn,Rostoker Nonequilibrium Green's Function Method", Journal Phys. Soc. Japan 85, 104715 (2016)

Wednesday, 21 February 2018, 16:00

Investigation of the protective role of EGCG against oxidative stress induced by ultraviolet radiation by spectroscopic techniques

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The number of skin cancer cases increases worldwide due to an extreme and unprotected exposure to ultraviolet radiation, including sunlight and tanning beds, dying in average one person every hour by melanoma. [1] Natural compounds as the epigallocatechin-3-gallate (EGCG), found in the green tea, are strong antioxidants that scavenge the reactive oxygen species coming from the ultraviolet radiation, preventing the oxidation reactions induced by these radicals in the biomolecules. In addition, several studies highlighted the fact that EGCG interacts with intracellular receptors involved in signaling transduction pathways, controlling cellular events as cell cycle arrest, cell proliferation and apoptosis.[2,3] In this work, we analyzed the protective role of EGCG incorporated on liposomes of the dimyristoylphosphatidylcholine (DMPC) in presence of ultraviolet radiation by UV-visible and infrared spectroscopies. Experimental and molecular simulations showed that after penetrating the bilayer, the EGCG stays below the phosphate groups of DMPC establishing H-bonds with oxygen lipid atoms. Our results showed that the damage induced by radiation on DMPC phospholipids is much less in the presence of EGCG.

[1]Cancer Facts and Figures 2017. American Cancer Society, http://www.cancer.org/acs/groups/content/@editorial/documents/document/acspc-048738.pdf. Accessed January 19, 2018.

[2] Zhang, J., Lei, Z., Huang, Z., Zhang, X., Zhou, Y., Luo, Z., Chen, X. (2016). Epigallocatechin-3-gallate (EGCG) suppresses melanoma cell growth and metastasis by targeting TRAF6 activity. Oncotarget,7(48), 79557.

[3] Braicu, C., Mehterov, N., Vladimirov, B., Sarafian, V., Nabavi, S. M., Atanasov, A. G., Berindan-Neagoe, I. (2017). Nutrigenomics in cancer: Revisiting the effects of natural compounds. In Seminars in cancer biology. Academic Press

Wednesday, 21 February 2018, 16:45

ABSTRACTS
Poster Contributions

XPS/UPS as an effective method to study the band alignment in Fe/2D Solid/Silicon heterostructure

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The control of interface resistance is one of the key parameter for semiconductor based spintronic devices [1]. Despite the all development of oxide tunnel barrier, notably MgO, this control is hardly achieved with conventional oxide based barriers due to deposition-induced interface states and associated Fermi level pinning. 2D crystals (graphene, h-BN, MoS_2 …) have therefore been seen as an alternative to design new heterostructure for improved spin injection into semiconductor [2,3]. In fact, due to the weak Van der Waals interaction between 2D solids and silicon, interface states are strongly reduced. We studied by X-ray photoemission spectroscopy (XPS) the band alignment and interface chemistry of iron (Fe)-Graphene (G)-hydrogen-passivated silicon (Si:H). We found that silicon is always close to flat band conditions, indicating that Fermi Level is unpinned on the semiconductor side of the G/Si(100):H interface. Iron deposition onto G/Si induced little band bending. This band bending is, moreover, strongly reduced compared to Fe/Si contact. We also studied the impact of iron on G and observed that the metal deposition induced doping of the latter. Moreover, as is shown the figure 1, the C1s and Si2p level movement are the same. This comportment is observed for p and n silicon for all dopant concentration.

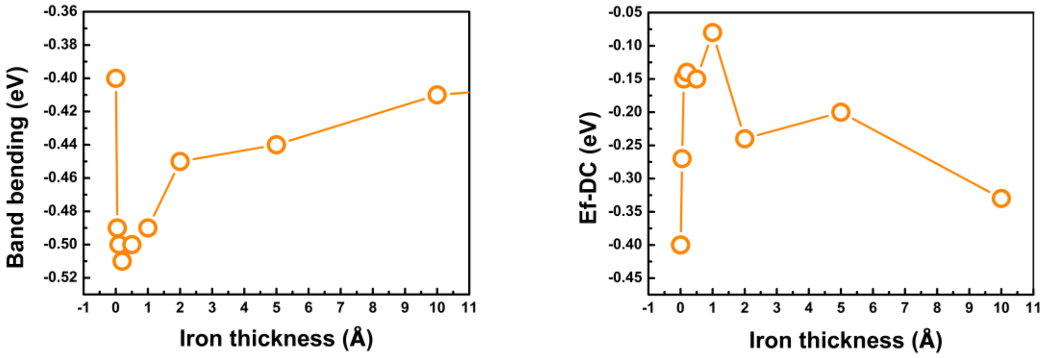

Figure 1. Silicon band bending (left) and graphene Fermi level position against Dirac point (left) as a function of iron deposited thickness.

[1] A. Fert and H.Jaffrès, Phys. Rev. B 64, 1 (2001).
[2] O. M. J. van't Erve, A L. Friedman, E. Cobas, C. H. Li, J. T. Robinson, and B. T. Jonker, Nat. Nanotechnol. 7, 737 (2012).
[3] J.-C Le Breton, S. Tricot, G. Delhaye, B. Lépine, P. Turban, and P. Schieffer, Appl. Phys. Lett. 051601, (2016).

Coffee Breaks

Development and characterization of a custom made Argon Plasma Jet Device for medical applications

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Cold atmospheric pressure plasmas (CAPs) are a specific type of non-thermal plasmas that offer the possibility to operate without the necessity of vacuum systems [1]. Recent progress in CAPs showed that these plasmas appear to be a good alternative to common treatments for cancer, such as radiation therapy and chemotherapy which frequently leads to accidental cell death, because CAPs exposure selectively kill cancer cells without harming normal surrounding cells [2]. However, the mechanisms of interaction between cells and plasma are still unclear. In order to better understand this relationship we engineered an argon plasma jet. This device consists of a hand-held principal unit (Figure 1) composed by a borosilicate capillary with an outer diameter of 6.93 mm and an inner diameter of 4.94 mm, with a pin-type electrode in its center (2 mm diameter) and a copper ring around it. The copper electrode is connected to a custom made DC power supply (2.5 mA, 20 kV). The plasma steam is produced from the top of the pin-type electrode and expands to the surrounding air outside the borosilicate tube. Preliminary plasma treatments have been done in order to study the influence of different working parameters such as gap and plasma exposure time. In order to evaluate the effects of the performed treatments, cell viability have been assessed using resazurin assay. In order to characterize the plasma effluent and determine which species are present in the produced plasma some preliminary studies of Optical Emission Spectroscopy (OES) were performed using a fiber optic (FC-UV600-2, Avantes) coupled to a spectrometer (AvaSpec-3648-USB2 7.0, Avantes). This work is supported by Fundação para a Ciência e a Tecnologia (FCT), within the Radiation Biology and Biophysics Doctoral Training Programme (RaBBiT, PD/00193/2012), through the scholarship grant number PD/BD/114444/2016 (S. Pereira) and the project UID/FIS/00068/2013 (CEFITEC).

[1] E. Stoffels, Y. Sakiyama, D. B. Graves, *IEEE Transactions on Plasma Science*, 2008
[2] C. Hoffmann, C. Berganza, J. Zhang, Medical gas research, 2013

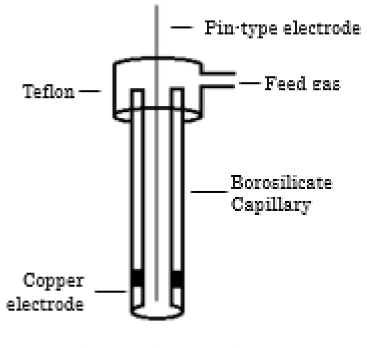

Figure 1. Schematic of the argon plasma jet.

Using Fluorescence Spectroscopy to follow Mesenchymal Stem Cells Differentiation into Keratinocytes by an Enzyme activity Approach

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The epidermis, the outermost layer of the skin, is responsible for the coating and protection of our body. It consists of keratinocytes arranged in multilayers, which constantly renew through four weeks and then are eliminated in the desquamation, an event that requires the participation of epidermal tissue kallikreins (KLK). Several approaches have been proposed to study skin biology and keratinocytes differentiation. In this context, mesenchymal stem cells (MSC) emerge as a promising alternative and have been used in both research investigation and regenerative medicine. The aim this work was to follow the differentiation process of MSC into keratinocytes by KLK activity detection using fluorescence spectroscopy. The method is based on Förster resonance energy transfer (FRET) from KLK synthetic substrates, specifically designed for this assay. The differentiation of MSC into keratinocytes was induced by culturing cells in a medium for keratinocyte development (KSFM) supplemented with 2.5 ng/ml epidermal growth factor and 1.8 mM $CaCl_2$. Cells cultivated DMEM containing fetal bovine serum were used as controls. Cultures were evaluated on days 1, 3, 7, 11, 14, 17 and 23, based on the KLK5, 6 and 7 activity upon the substrates Abz-GFSPFRSSRQ-EDDnp, Abz-AFRFSQ-EDDnp and Abz-KLYSSKQ-EDDnp,FRET, respectively. Cell morphology was also monitored at these time points. Data showed higher KLK5, 6 and 7 activity in cell lysates of KSFM-cultivated cultures at 14th and 23rd days, in comparison to day 1 of control. In combination with morphology analysis and expression of epidermal markers, these data indicate that MSC are able to differentiate into keratinocytes similarly to that occurs in the human epidermis. Thus, KLK activity detection using fluorescence spectroscopy seemed to be a good procedure for the monitoring of this differentiation process, representing a highly sensitive, low cost and low time-consuming approach, which could be also useful in other protocols developed for the evaluation of stem cells commitment and differentiation into the keratinocyte lineage.

Coffee Breaks

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