OFERTA DE UNA BECA FPI

(FORMACIÓN DE PERSONAL INVESTIGADOR)

Características:

-Beneficiarios: Licenciados en Física o Química
-- Duración: 48 meses
- Dotación económica: ~1.100 € mensuales
- Finalidad: Formación en proyecto de investigación y realización de tesis doctoral

Datos del Proyecto:

- Referencia: MAT2008-06542-C04-01

Título: NEw TOols for addressing the Size-scale cHange In MAgnetic materials: -selective spectroscopies and related magnetometries. (NETOSHIMA)

INVESTIGADOR PRINCIPAL: JESUS CHABOY NALDA
ORGANISMO: CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS
CENTRO: INSTITUTO DE CIENCIA DE MATERIALES DE ARAGON (ICMA)

Temas de Investigación: **Magnetismo y espectroscopia de absorción de rayos-x**

PERFIL de las BECAS

PERFIL I Desarrollo (experimental) de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

PERFIL II Desarrollo (computacional) de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

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- Finalidad principal: Formación en proyecto de investigación financiado por el Plan Nacional de I+D+I y realización de tesis doctoral.

Tema de Investigación:

Espectroscopía de Absorción de Rayos-X (XAS, XANES, EXAFS, XMCD)

Magnetismo

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Resumen del Proyecto.

Este proyecto se centra en el el estudio de materiales magnéticos funcionales y nanoestructurados haciendo hincapié en la relación entre las propiedades macroscópicas y la microestructura, así como en sus posibles aplicaciones tecnológicas. Uno de los pilares del presente proyecto es el Desarrollo y mejora de nuevas técnicas de caracterización (XAS y XMCD) y su aplicación a la caracterización estructural, electrónica y magnética de materiales. Se prestará especial atención al estudio de la dependencia de las propiedades físicas con la naturaleza nanocristalina de nuevos materiales nanoestructurados y nanopartículas para el que la utilización de las citadas técnicas es particularmente relevante. Planteamos el estudio de diferentes materiales en los que la reducción de tamaño ocasiona una drástica modificación de sus propiedades magnéticas.

PERFIL de las BECAS

PERFIL I

Desarrollo (experimental) de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

PERFIL II

Desarrollo (computacional) de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

PERFIL I

Desarrollo de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

(Development of advanced characterization tools).

Core level spectroscopies emerge as outstanding tools to study magnetism by incorporating its characteristic element specificity. In particular, both x-ray absorption spectroscopy (XAS) and its related magnetic evolution X-ray Magnetic Circular Dichroism (XMCD) have demonstrated in the last years their powerful capabilities to get the aforesaid characterization. This has been quite notorious in the case of the XMCD technique which becomes in recent years an outstanding tool to study Magnetism. Its element specificity, inherent to a core-level spectroscopy, combined with the application of magneto–optical sum rules allows quantitative magnetic measurements at the atomic level. However, despite these capabilities are now incorporated as a standard tool to study the localised magnetism in many systems, the application of XMCD to the study of the conduction band magnetism is not so straightforward. This is the reason why most XMCD work is devoted to the soft x-ray energy range, $L_{2,3}$-edges of transition metals and $M_{4,5}$ edges of rare-earth metals. Indeed, while the capabilities of XMCD are squeezed in the case of localised states carrying a magnetic moment (f-states of Lanthanides and Actinides ($M_{4,5}$-edges), d-states of transition metals ($L_{2,3}$)), the same does not hold when the delocalised states are being probed. This is the case of the conduction band 4p states of transition metals and the 5d states of rare-earths, whose magnetic moments are induced by the hybridisation with the localised d- and f-states, respectively. Moreover, the materials are extremely sensitive to the surface effects at these absorption edges. Consequently the magnetic response of the bulk material to the XMCD can be strongly affected by the surface, which exhibits a quite different magnetic behaviour. In addition, recent attempts of increasing the biocompatibility of magnetic nanoparticles suggest to use a capping of noble metals as Au and Pt. Unfortunately, the magnetic properties of these heavy elements has to be determined by using XMCD in the hard x-ray region which implies a dramatic change of the probing depth. As a consequence, the magnetic properties of the different components of the nanomaterial cannot be obtained at the same experimental conditions.

By these reasons it is necessary to develop new experimental methods to obtain the magnetic characterization of complex magnetic systems by using hard x-ray XMCD, especially regarding the delocalised states. In this way the surface effects are avoided by increasing the sampling depth and then XMCD becomes a real BULK probe. Moreover, the flexibility of the sample environment allows performing these studies upon extreme conditions of temperature, applied magnetic field and applied pressure. We plan to concentrate our efforts into applying the XMCD to the study of the conduction band magnetism. To this respect, we are performing a feasibility study of the possibility of measuring XMCD at SpLine (the Spanish CRG (BM25) beamline) at ESRF by using a quarter wave plate.

PERFIL II

Desarrollo (computacional) de técnicas de caracterización magnética avanzadas basadas en la espectroscopia de absorción de rayos-x.

(Computational Development)

X-ray absorption spectroscopy (XAS) has proven to be an outstanding structural tool by allowing the determination of the local environment around a selected atomic species in a great variety of systems. At present, reliable structural parameters are commonly derived from the analysis of the extended x-ray absorption fine structure (EXAFS) region of the spectrum. However, the same does not hold for the near-edge part of the absorption spectrum (XANES) despite its higher sensitivity to the bonding geometry due to the absence of an exact treatment of i) the disorder or vibration effects, ii) realistic charge densities, among others, which make the ab-initio computation of XANES spectra no so straightforward as the EXAFS one. We plan to offer new challenges into the *ab-initio* modelization of XANES by developing computer codes within both the one-electron and multi-channel multiple-scattering (MS) theory and by using new models based on a non-muffin-tin approach, looking for the fully development of XANES as a real structural probe. Formalisms for the computations will be developed and implemented in software packages by using analytical calculations and numerical simulations by means of atomic multiplets and many-body cluster calculations.
The main aim of this project to improve the theoretical computation of XANES. This is the first step prior to extend the range of applicability of XANES analysis to complex systems. Most computational codes developed to date are based on the one-electron multiple-scattering (MS) theory and by using the muffin-tin approximation in which the potential is spherically averaged inside the atomic spheres and fixed constant between them. Despite its simplicity the cluster approach got success into reproducing many different spectra. More recently, models based on a non-muffin-tin approach or in the multi-channel MS theory offers new challenges into the *ab-initio* modelization of XANES. Despite the above progresses several topics remain open. One of them is the type of the exchange-correlation potential (ECP) used into the construction of the scattering potential. The energy dependent Hedin-Lundqvist (HL) complex potential, in which the imaginary part accounts for the damping of the excited photoelectron, is the most widely used into *ab-initio* XANES calculations. However, it has been reported that in several cases the energy dependent Dirac-Hara (DH) exchange potential shows the best agreement to the experimental data. Thus, the election of the ECP is not free of controversy and its choice becomes one the most important steps into obtaining a good reproduction of the experimental spectra. Therefore, further theoretical work is still needed to get the fully development of XANES as a real structural probe. To this respect we plan as a main objective of the project improve the XANES computation by using in particular self-consistent-field (SCF) methods to describe the final state potential, including spin-polarized computations. In addition, we plan to built–up an interface to perform computations using DOS results obtained from electronic and band calculations. In this way we extend the XANES computations to the XMCD case. Finally, we plan to apply the "non-muffin-tin" approach to the case of new nanostructurated and nanoparticle materials.