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**Department or Institution involved** 



# <u>Chemical speciation using conventional and syncrotron radiation techniques applied to the</u> <u>research fields of food, biomedicine and environment</u>

#### **Topic description**

The proposed research line is focused to develop innovative technologies to characterize the chemical forms of target elements and to apply related properties on the fields of environment, food and medicine. Applications will be developed to treat polluted systems and to create new products for medical and agro-food sectors. This general objective is based on chemical speciation using conventional indirect and direct research methodologies (e.g. synchrotron and hyperspectral techniques).

In the case of environmental applications, speciation methodologies will focus on relevant chemical forms of nanostructured sorbent materials to treat contaminated systems.

In the case of agro-food sector, applications will be addressed in two different ways: 1) to identify biomarkers for food traceability and 2) to develop and characterize functional foods.

In the case of medical applications, speciation studies will be addressed to control de development of biomaterials on the area known as "human rocks", e.g, dental tissues and kidney stones. Such control will help the development of dental care materials and preventive treatment of urological lithiasis.

For these various applications, we will address advances in synchrotron radiation techniques EXAFS (Extended X-ray Absorption Fine Structure), XANES (X-Ray Absorption Near Edge Spectroscopy) 2-XANES (micro-X-Ray Absorption Near Edge Spectroscopy), TRS (Time Resolve Spectroscopy) XRF (X-Ray Fluorescence ) and Quick-EXAFS. Moreover, the Hyperspectral Imaging (HSI) will contribute to not only complement techniques based on synchrotron but also bring to market the application of methods derived from the direct investigation of speciation, e.g, robust classification of kidney stones.

On the other hand, indirect Speciation methods, including the identification and distribution of chemical forms, contribute to validate the direct spectroscopic methodologies.

The successful development of these methods requires the application of specific analytical software such as for the analysis and classification of spectroscopic data. In this sense, data analysis tools employed jointly developed with Synchrotron ALBA, an institution having a

current strong collaboration with us by developing national and international research projects.

The results derived from developed methodologies will lead to the implementation of chemical speciation, particularly through new products and biomaterials, and technologies for the treatment of polluted environmental systems. To achieve this, there will be three main activities. I) innovative processes for the treatment of soil / contaminated water, including efficient systems of adsorption (synthetic bio-sorbents). II) Robust methodology for the characterization and development of biomedical products, including dental materials (e.g, remineralizing toothpaste) and urological stones (e.g, friendly method for diagnosis). III) New products for the food industry, including functional foods (e.g, foods fortified with selenium) and methods for food traceability (e.g, traceability of Iberian and Italian hams). The validation of the products of the project will be carried out either by implementing in real environments, comparison with conventional processes and the application of reference materials.

#### Project supervisor & hosting group

Prof. Manuel Valiente.

• The group of separation techniques GTS is part of the Department of Chemistry at the Universitat Autonoma de Barcelona (UAB), located in Bellaterra (Barcelona). The GTS is linked to the master's degrees and doctoral programs of the the Department of Chemistry at UAB. The current staff of the group is composed of 18 members, one full Professor (Dr. Manuel Valiente), one Titular Professor (Dr. Cristina Palet), one Associate Professor (Dr. Montserrat López-Mesas), a Project Manager (Dr. Gustavo Pérez), a Research Support and Quality Manager (Dr. Montserrat Resina), an administrative (Maria Dolors Mir), two postdoctoral and 11 PhD students, the latter bear responsibility for the functioning and operation of scientific equipment, which guarantee service offering analysis proposed by the center following the established quality criteria. There are responsible technicians for in charge of ICP-MS, an official HPLC, GC-MS, CZE and FP-XRF equipment. Moreover it is necessary to mention that the group has a technical responsibility to implement the Quality ISO-9001 in our laboratories. This implies the need for training of all members of the group in the corresponding Quality System. The intense training capabilities developed by GTS are reflected by the presentation of 40 doctoral theses since 1996, 12 presented in the period 2009-2015, 46 supervised master degrees since 1996.

The hosting group is widely recognized for its activities in the area of Chemical Speciation and related Technology transfer.

The main relevant projects associated with data science are:

 Reference.GA645024. Title: NANOREMOVAS: ADVANCED MULTIFUNCTIONAL NANOSTRUCTURED MATERIALS APPLIED TO REMOVE ARSENIC IN ARGENTINIAN GROUNDWATER. Funding agency. Research Executive Agency. Call. H2020-MSCA-RISE-2014. Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/01/2015-31/12/208. Final funding. 369.000 €. Participation: Coordinator

- Reference. GA609550.Title: FOSTERING PARTNERSHIPS FOR THE IMPLEMENTATION OF BEST AVAILABLE TECHNOLOGIES FOR WATER TREATMENT & MANAGEMENT IN THE MEDITERRANEAN Funding agency. Research Executive Agency. Call. FP7 INCO.2013-9.1. Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/10/2013-30/09/2016. Final funding. 157.095 € Participation: Coordinator
- Reference. SOE3/P2/F591. Title. OBSERVATOIRE DE RECHERCHE SUR LA QUALITÉ DE L'ENVIRONNEMENT DU GRAND SUD-OUEST EUROPÉEN. INTERREG IVB. Funding agency. Sociedad Gestora del Programa Interreg Espacio Sudoeste Europeo Call. INTERREG IVB Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/11/2013-31/12/2014. Final funding. 1.264.162 € Participation: Research Partner (PI)
- Reference. CTM2012-30970 Title. EVOLUCION TECNOLOGICA DE LA ESPECIACION QUIMICA. TECNOLOGIA QUIMICA Y DEL SINCROTRON PARA LA CARACTERIZACION Y DESARROLLO DE SISTEMAS MEDIOAMBIENTALES Y BIOMATERIALES. Funding agency. Ministerio de Economía y Competitividad. Call. CALLS DEL PLAN NACIONAL DE I+D. Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/01/2012-31/12/2015. Final funding. 191.880 € Participation: Principal Investigator
- Reference. GA295031. Title. CHARACTERIZATION AND SUSTAINABLE USE OF EGYPTIAN DEGRADED SOILS. SUDSOE. Funding agency. Research Executive Agency Call. FP7-INCO-2011-6-ERAWIDE. Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/01/2012-31/12/2014. Final funding. 499.194 € Participation: Principal Investigator
- Reference GA295197 Title. EULANETWORK IN CERAMIC MATERIALS WITH ENVIRONMENTAL AND INDUSTRIAL APPLICATIONS. EULANETCERMAT. Funding agency. Research Executive Agency Call. FP7-MSCA-IRSES-2010. Name of main researcher: Jose Luis Briansó. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date 01/10/2012-30/09/2016. Final funding. 552.300 €. Participation: Investigator
- Reference. GA245843. Title. NETWORK IN SOLID WASTE AND WATER TREATMENT BETWEEN EUROPE AND SOUTHMEDITERRANEAN COUNTRIES (SOWAEUMED). Funding agency. Research Executive Agency. Call. FP7-REGIONS-2009-2. Name of main researcher: Manuel Valiente. Affilitation entity: Universidad Autónoma de Barcelona. Start and end date. 01/01/2009-30/11/2012. Final funding. 267.400 €. Participation: Coordinator

Another very important aspect is the fact that members of the GTS have made during the last period 2009-2015 intense activity within the various synchrotron radiation facilities scattered throughout Europe and the United States, where we had a remarkable success. The estimated funding received was about € 186,860. On the other hand, we must highlight that the research group has a scientific collaborator at ALBA synchrotron, the Interim Associate Professor Montserrat Lopez Mesas. On the other hand, former members of the GTS center, such as Dr. Martha Avila, who is conducting his post-doctoral research at the facilities of the ALBA synchrotron.

#### Planned secondments

The planned secondments to be agreed with the candidate could be carried out through the various external organizations having collaboration with our centre GTS in the framework of different projects. Preferentially with those highlighted in bold.

- Synchrotrons ESRF (Grenoble, France), HASYLAB (Hamburg, Germany) and SSRL (Stanford, USA), CELLS ALBA (Barcelona, Spain), SOLEIL (Paris, France) for direct speciation techniques applied to environmental samples and biomaterials. Project CHEMSYNCHRO.
- Laboratory of Inorganic and Analytical Chemistry Bio Environment, in collaboration with Professor Olivier Donard for the development of new methodologies based on conventional speciation (indirect) determination of organic and inorganic pollutants in samples of biota. Project ORQUE-SUDOE
- Functional Materials Division of KTH Royal Institute of Technology (Stockholm, Sweden) for the implementation of advanced nanotechnology-based adsorbents for arsenic speciation as polluting industrial effluents. Project NANOREMOVAS.
- ALBA Synchrotron "In-House Collaboration" by the analysis of biomaterials through the technique of FT-IR microscopy. Project CHEMSYNCHRO
- Karolinska Institute. Stockholm (Sweden)
- Department of Geological and Environmental Sciences at Stanford University (USA) to direct speciation techniques based on synchrotron radiation applied to biological and environmental samples.
- Università di Roma La Sapienza, Rome (Italy) for the application of NIR-hyperspectral imaging technique for the characterization of kidney stones based on speciation and differentiation based on food terroir through the chemical speciation of elements such as Fe and Zn. Project CHEMSYNCHRO
- Masaryk University of Brno (Czech Republic). Collaboration with Professor Josef Havel. Knowledge of the operation of the foundation and operation of the software required to work with Artificial Neural Networks applied to the chemical speciation in food. Project SUDSOE
- University at Buffalo School of Dental Medicine (New York, USA), collaboration with Prof. Carlos Muñoz, to develop new nanostructured materials based on chemical speciation for implementation in biomaterials used in dental hygiene . Project CHEMSYNCHRO
- UT Southwestern Medical Center (Texas, USA), in collaboration with Prof. Orson Moe, the development of new methodologies for predicting risk litogen based on a better characterization applying the chemical speciation. Project CHEMSYNCHRO
- Stone University Center Universitätsklinikum Bonn, University of Bonn with Prof. Prof. Roswitha Siena. Collaboration in the study of kidney stones aimed at the establishment and verification of a new methodology for classification of kidney stones bounce and be applied routinely to study promoters and inhibitors of kidney stones in foods. Project CHEMSYNCHRO

- Manresa Technology Centre (CTM), Dr. And Prof. Miquel Rovira Juan Pablo in the development of membrane systems for industrial applications. CHEMSYNCHRO project.
- Leitat Technology Centre (Spain) with Dr. Dr. David lover and Mirko Faccini to develop new nanostructured materials for the treatment of contaminated effluents based on the chemical speciation. DISMEC project.
- Università degli Studi di Udine (Italy) with Prof. Marilena Tolazzi to study the thermodynamic aspects of the formation of complexes between metals and sulfur ligands on cyclic compounds.
- Hospital Clinic Barcelona. Urological Service.

In addition to several departments within UAB such us Geology, Vegetal Physiology, Edaphology, etc....

## Candidate's profile

### Required:

•The applicant must have a doctorate in Chemistry, Physics, Material Science, or related disciplines.

- Previous experience in chemical speciation or related studies with synchrotron techniques using some of the techniques such as EXAFS (Extended X-Ray Absorption Fine Structure), XANES (X-Ray Absorption Near Edge Spectroscopy), D-XANES (micro-X-Ray Absorption Near Edge Spectroscopy), TRS (Time Resoleu Spectroscopy), XRF (X-Ray Fluorescence) and Quick-EXAFS. The candidate must demonstrate capabilities to spread out scientific research activities conducted as a GTS-UAB member in different areas, through publication in international peer reviewed journals and presentations at conferences or exhibitions of international relevance.Additional valuable experience
- In chemical separation techniques and some analytical instrumentation (e.g. UV-Vis and FT-IR spectrometry, together with chromatographic analytical set-ups such as HPLC and GC coupled with different detectors (i.e. UV-Visible and mass detectors), and some knowledge of atomic spectroscopy techniques, such as ICP-OES and ICP-MS).
- Experience and capabilities for the systematic search of public and private funding sources, particularly detection of opportunities to participate in consortia and European networks (e.g. Info Days brokerage or events related to the presentation of programs of projects, activities and research clusters partners). Managing skills for the preparation of project proposals for national and regional competitive bidding with the active participation of companies to promote an efficient technology transfer.
- Good interpersonal skills and capabilities to work in a multicultural environment, with high capacity for team coordination, detection of needs and supporting the co-workers as well as to work independently. Having the necessary aptitude to motivate the staff members and create a pleasant atmosphere.
- Communication ability is essential for teamwork. Therefore, a good level of English both written and spoken is mandatory (minimum C level). The working language at GTS-UAB is English.

- Experience working under Quality Assurance System, e.g, ISO 9001, ISO 17025, GLP or a similar quality control tool. Used to deal with internal and external audits, with knowledge about laboratory requirements, measurement standards, evaluation of uncertainty of measurement and any documentation related to the laboratory management and quality system.
- Experience on the establishment of cooperation agreements / contracts for research and technology transfer with private companies, based on the experience of the GTS in different research areas covering environment, biomaterials, energy and food.
- Dissemination skills for the participation in the various activities organized by the UAB Research Park and TECNIO mainly attending trade fairs and brokerage events related technology offer proposed by the researchers of the research group, to carry out the corresponding dissemination and technology transfer activity.

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