

Crystallographers in Spain

Continued from Volume 18, Number 3

COMPILED BY M. MARTINEZ-RIPOLL

Crystallographers in Spain belong to one or more of the following organizations: the European Crystallographic Association (ECA) and the Group for Crystallography and Crystal Growth (GE3C), a group associated with the Spanish Royal Society of Chemistry (RSEQ) and the Spanish Royal Society of Physics (RSEF). Other Spanish associations related to Crystallography, include the Spanish Association of Synchrotron Users (AUSE, <http://bit.ly/c1S3j7>) and the Spanish Association for Neutron Techniques (SETN, <http://bit.ly/a15Ana>). The Spanish Committee of Crystallography is the official Spanish representative to the IUCr.

Teams of Spanish crystallographers are concentrated in the regions described below:

An updated list of groups in Spain can also be found in at www.xtal.iqfr.csic.es/Cristalografia/ (in Spanish and English).

1. Galicia

Galicia is an Autonomous Community in northwestern Spain with an ancient Celtic culture (5th Century BC). It became a Roman province (Gallaecia) in 197 BC, one of the first Catholic kingdoms in 449.

The Grupo de Investigación de Química Molecular y Estructural (GIQIMO), at the U. of Santiago de Compostela, was developed by A. Castiñeiras (qiaco1@usc.es) in 1980 after his stay at the Dept. of Crystallography & Structural Biology of the Spanish National Research Council (CSIC) in Madrid (see below, #9). Their research concerns magnetic materials, bioinorganic chemistry, structural chemistry, crystal engineering, and supramolecular structures (<http://bit.ly/aeHKbf>).



The GIQIMO group.

At the U. of Santiago de Compostela the research team of A. Llamas (antonio.llamas@usc.es) engages in research projects in Inorganic, Organic and Biochemistry and is developing macromolecular crystallographic research on adenovirus proteins, viral fibers, dehydroquinase-inhibitor drug complexes and cyclic peptides (GramS analogs), (<http://bit.ly/cGJa6X>). The Universities of Vigo and Coruña maintain X-ray diffraction equipment as general service units for their universities (<http://bit.ly/eVsMxW> and



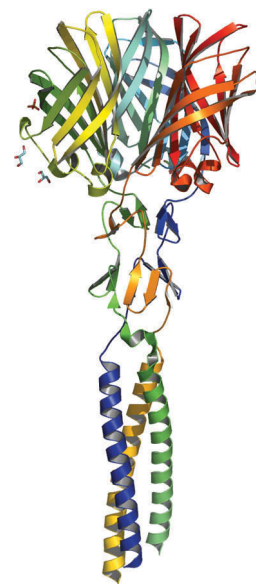
Crystallography groups in Spain. Orange circles show their approximate location. Numbers mean regional references only used in the text.

<http://bit.ly/9zwfIV>, respectively).

2. Asturias

Asturias, on the north coast of Spain facing the Cantabrian Sea, has been occupied by humans since the Lower Paleolithic era. It has cave paintings and megaliths from the Bronze Age. There were Celtic inhabitants in the Iron Age, Romans from 29 to 19 BC, Visigoths from the 6th to the 8th century and then the Moors invaded. The lands along the northern coast were never fully part of Islamic Spain and became a refuge for Christian nobles. In 722, a *de facto* independent kingdom was established, the Regnum Asturum, which was to become the cradle of the incipient Reconquest.

The Dept. of Physical Chemistry at the U. of Oviedo has one of the most active Spanish crystallographic teams in Asturias. It was established in the 80's by F. Beltrán and S. García-Granda (sgg@uniovi.es) for study of molecular structure and properties, automatic determination, QSAR and QSPR modeling, and chemical crystallography. S. García Granda, is currently the President of the European Crystallographic Association (ECA), (<http://bit.ly/9viBu4>). The Group on Crystal Growth and Experimental Aquatic Geochemistry, at Oviedo U. is a multi-departmental team supported by the European Commission to study the dissolution and precipitation rates of solid solutions. Groups from six European countries participate in this project. The Spanish team is headed by M. Prieto (mprieto@geol.uniovi.es) (<http://bit.ly/anZmfz>). In the Dept of Physics of Oviedo U., J.A. Blanco (jabr@uniovi.es) and P. Gorria (pgorria@uniovi.es) study magnetic materials with



C-terminal fragment of avian reovirus σ C fiber protein

neutron diffraction.

3. Cantabria

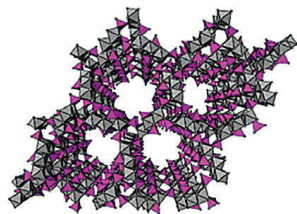
Cantabria is one of the richest regions in the world in archaeological sites from the Upper Paleolithic period. Paintings in the cave of Altamira, date from 16,000 BC.

In 1974 the magnetic materials group of Cantabria U. headed by J. C. Gómez Sal (jose.gomezsal@unican.es), published the first magnetic structure from Spain and developed collaborations with the neutron and X-ray communities at the ILL. The activities of the group, with J.R. Fernandez (jesus.rodriquez@unican.es) and L. F. Barquín (barquinl@unican.es) include crystallization, crystal and magnetic structures and small angle diffraction of metals and nanocrystals (<http://bit.ly/ceXijZ>). In the High Pressure and Spectroscopy Group, F. Rodriguez (fernando.rodriquez@unican.es) examines the structures of insulators under extreme conditions (<http://bit.ly/b0j7BK>).

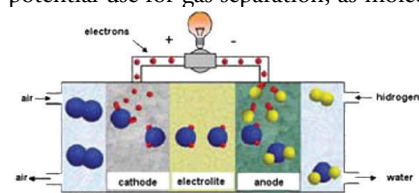
4. The Basque Country

The Basque Country in the western Pyrenees spans the border between France and Spain. Although little is known about the pre-history of the Basques, several Basque archaeological sites provide evidence for continuity from Aurignacian times to the Iron Age. Some of the same people appear to have continued to inhabit the area for thirty millennia.

The Dept. of Mineralogy and Petrology of the U. of the Basque Country (UPV/EHU <http://bit.ly/92zVzg>), is headed by K. Urtiaga (karmele.urtiaga@ehu.es), and M. I. Arriortua (maribel.arriortua@ehu.es) is currently Director of the General Services for Research of the UPV/EHU for the entire university (<http://bit.ly/cFitTW>). Research targets are multifunctional systems for environmental and energy applications including zeotypic materials. Microporous inorganic frameworks that can bind organic molecules are being studied for potential use for gas separation, as molecular sieves or in catalytic



Structural porosity in arsenates of transition metals with organic molecule and ammonium cations.



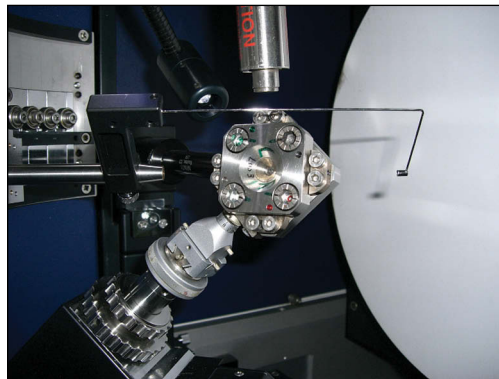
Scheme of a Solid Oxide Fuel Cell.

processes. The group is also attempting to optimize the performance of solid oxide fuel cells (SOFC) *via* their full characterization before, during, and after operation.

The long term goals are to achieve cost effective processing techniques, reduce operating temperatures and find inexpensive stable and durable materials.

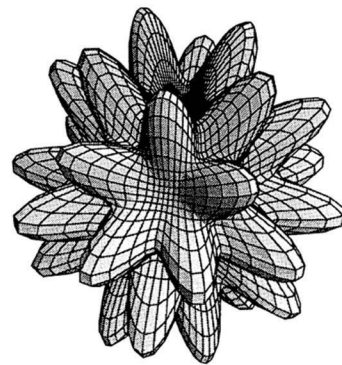
The Dept. of Inorganic Chemistry (UPV/EHU) directed by P. Román (pascual.roman@ehu.es) has three major projects on two campuses. Lamellar and tubular magneto-resistant phosphate transition metals, mixed oxides of technological interest and molecular magnetic materials, are being studied by T. Rojo (teo.rojo@ehu.es); the chemistry of polyoxometalates and organic-inorganic hybrid systems is led by J.M. Gutiérrez-Zorrilla (juanma.zorrilla@ehu.es); and studies of the magnetic behavior of polynuclear complexes with polyfunctional organic ligands, are co-directed by P. Román (pascual.roman@ehu.es) and A. Luque (antonio.luque@ehu.es) (www.ehu.es/qi/).

The Group of Structural and Dynamical Properties of Sol-



The Ahsbahs-type diamond cell mounted in Bilbao on the IPDS-2T diffractometer (STOE & Cie GmbH, Darmstadt, Germany).

ids, headed by J.M. Pérez-Mato (wmpemam@lg.ehu.es) at the Dept. of Condensed Matter Physics of the Basque Country U. (UPV/EHU) in Bilbao, (I. Aramburu, M.I. Aroyo, L. Elcoro, I. Etxebarria, K. Friese, A. Grzechnik, J. Igartua, G. Madariaga and F.J. Zúñiga) focuses on structural and lattice dynamics of functional materials, phase transitions in inorganic and molecular crystals, mathematical crystallography, nonconventional crystallographic methods, thermal properties, aperiodic crystals, high-pressure crystallography and *ab-initio* studies of ferroic materials.



Three-dimensional atomic domain describing the atomic positions of a subset of atoms of an icosahedral quasicrystal, within a 6-D super-space refined model.

The UPV/EHU was founded in 1969, as a result of the teaching skills and the contagious scientific enthusiasm of J. Eugenio Iglesias. His students F. Javier Zúñiga and J.M. Perez-Mato, joined the Physics Dept. to form the nucleus of the group that studied phase transitions, incommensurate phases and aperiodic crystals. In 1991 the group organized an “International workshop on methods of structural analysis of modulated structures and quasicrystals” in Lekeitio (Spain) which influenced the development of the field. The team of physicists had a natural affinity for studies of structural thermal behavior and methods of analysis of aperiodic crystals. Recently, scientists with mineralogical and chemical backgrounds (K. Friese, A. Grzechnik) have joined the group, fostering multidisciplinary work.

The Bilbao Crystallographic Server (www.cryst.ehu.es/), directed by M.I. Aroyo, provides free online access to crystallographic databases, computer tools and programs for crystallogra-



bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country.]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]



Sections	Space Groups Retrieval Tools
Retrieval Tools	GENPOS Generators and General Positions of Space Groups
Group-Subgroup	WYCKPOS Wyckoff Positions of Space Groups
Representations	HKLCND Reflection conditions of Space Groups
Solid State	MAXSUB Maximal Subgroups of Space Groups
Structure Utilities	SERIES Series of Maximal Isomorphic Subgroups of Space Groups
Subperiodic	WYCKSETS Equivalent Sets of Wyckoff Positions
ICSDB	NORMALIZER Normalizers of Space Groups
Contact us	KVEC The k-vector types and Brillouin zones of Space Groups
About us	SYMMETRY OPERATIONS Geometric interpretation of matrix column representations of symmetry operations

Heading of the Bilbao Crystallographic Server, a popular webpage with online computer tools for crystallographic analysis

phers and materials scientists. An international school on the use and applications of this server was organized in 2009. A database of incommensurate structures is being reorganized by G. Madariaga.

The Magnetism and Magnetic Materials Group (UPV/EHU), headed by J.M. Barandiaran García (manub@we.lc.ehu.es), works on nanocrystalline structures and crystallization processes (<http://bit.ly/cetJqA>). The Biophysics Unit, a joint center of UPV/EHU and the CSIC, headed by F.M. Goñi (felix.goni@ehu.es), was created in 1999 and studies mainly biological membranes. The crystallography group headed by D. Guérin (gbxguxxd@lg.ehu.es) conducts research on membrane protein crystallization, crystallization in lipidic mesophases and virus crystallography (www.unidaddebiofisica.org/).

The Center for Cooperative Research in Biosciences (CIC bioGUNE), headed by J.M. Mato, is a non-profit biomedical research organization founded in 2002 by the Dept. of Industry of the Basque Government and opened in 2005 (www.cicbiogune.com). The Structural Biology Unit at the CIC bioGUNE is composed of four groups. The group headed by A. Martínez de la Cruz (amartinez@cicbiogune.es) focuses on cystathionine β -synthase domains and is part of the Spanish Ion Channel Initiative, a multidisciplinary cooperative headed by A.F. Montiel from the U. Miguel Hernández in Elche, Spain. A group headed by L. Malinina (lucy@cicbiogune.es) is focused on protein complexes with RNA and lipids related to neurodegenerative diseases. The leader of the third group is A. Hierro Ayuela (ahierro@cicbiogune.es), whose research interest is intracellular trafficking processes. N.G.A. Abrescia (nabrescia@cicbiogune.es) leads the fourth group using crystallography to study virus assembly mechanisms and archaeal transcription machinery (<http://bit.ly/a4DTF4>).

5. Navarre

In 824, Íñigo Arista was chosen King of Pamplona, laying a foundation for the Kingdom of Navarre, which at its zenith covered the area of the present-day Navarre, the Basque country, La Rioja, and parts of modern Cantabria, Castile, León, and Aragon. The army of Navarre fought in the battle of Las Navas de Tolosa in 1212, after which the Muslim conquests on the Iberian Peninsula were slowly reduced to a small territory in the south. In 1515, Navarre south of the Pyrenees was absorbed into the Kingdom of Spain and Navarre north of the Pyrenees came under French rule.

In the Dept. of Physics of the Public U. of Navarre, V. Recarte (recarte@unavarra.es) and I.P. de Landazabal (ipzlanda@unavarra.es) study structural transformations and magnetic properties of ferromagnetic alloys with shape memory, as part of the Physical Properties and Applications of Material Group (<http://bit.ly/bfT7fT>).

6. Castile and León

Ferdinand III of Castile, later canonized, united the Crowns of Castile and Leon in 1231. The medieval Cortes of León is one of the earliest ancestors of Europe's parliaments. The Cortes of León of 1188, called by Alfonso IX, is one of the earliest documented gatherings of the estates in which commoners of the cities and towns are represented beside the clergy and nobility as counselors to the monarch.

Macromolecular crystallography in the vast region of Castile and León is represented by the Structural Biology Group at the Cancer Research Center (CIC), coordinated by both the U. of Salamanca and the Spanish National Research Council (CSIC). The group was established in 2003, when J.M. de Pereda (pereda@usal.es) joined the CIC after post-doc training in Leicester, UK and San Diego, CA. The group applies protein crystallography to study cell-adhesion and signaling proteins, such as the integ-



From left to right, J.M. de Pereda, E. Ortega, N. Alonso and M. Gómez

rin family of receptors. Since this is the first laboratory devoted to macromolecular crystallography in the Castile and León region, the training of young students and collaboration with local non-crystallography laboratories are two major aims of the group (<http://xtal.cicancer.org>).

Three universities in the Castile and León region have service units for X-ray diffraction studies. U. of Salamanca, directed by F. Sanz (sdrayosxr@usal.es), (<http://bit.ly/b1W7Ov>); the U. of Burgos headed by J.J. Delgado (jdelgado@ubu.es), (<http://bit.ly/bmx8aB>); and U. of Valladolid, headed by F. Rull (rull@fmc.uva.es).

7. La Rioja

La Rioja is known for its wonderful wines. The Oja river ("rio") that flows through this region gives the name to this province. The U. of La Rioja, has a central diffraction unit run by J. Berenguer

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8. Aragon

Saragossa is the capital of Aragon in northeastern Spain. James I the Conqueror was the King of Aragon, Count of Barcelona, and Lord of Montpellier from 1213 to 1276. After the marriage of Isabella I of Castile and Ferdinand II of Aragon at the end of the Fifteenth Century there was a dynastic union of both crowns and most other kingdoms in Spain. Aragon remained a separate kingdom, with its own laws and institutions, until 1707. At that point Philip V, the first Bourbon king of Spain, consolidated Spain into a more centralized state.

Crystallographic research in this region is to be found in four different groups, three of them belonging to the Inst. of Material Sciences of Aragon, a joint center between the U. of Saragossa and the CSIC, and one involving only the university.

The Preparation, Properties and Molecular Solid Transformations Group, headed by L. Falvello (falvello@unizar.es) concerns the preparation and characterization of molecular solids, their properties, dynamical behavior and transformations. (<http://bit.ly/aDVwIv>).

The Coordination Chemistry and Homogeneous Catalysis Dept. of F.J. Lahoz emphasizes coordination chemistry of platinum metal complexes, mainly of Rh, Ir, Ru and Os, organometallic reactivity, and in homogeneous catalysis, (lahoz@unizar.es), <http://bit.ly/ayrYhD>.



From left to right: Larry Falvello, Milagros Tomás and Francisco Martínez.

The Dept. of Physics of Condensed Matter is headed by J. Campo (javier.campo@unizar.es), coordinator of the Spanish Collaborating Research Group at ILL and president of the Spanish Association for Neutron Techniques (SETN), and focuses on molecule based magnets, neutron scattering and magnetic chirality, (<http://bit.ly/bXfx5u>).

At the Inst. for Biocomputation and Physics of Complex Systems (BIFI) of the U. of Zaragoza, crystallographers R. Hurtado (rhurtado@bifi.es) and M. Martínez (mmartinez@unizar.es) conducts research in biological systems (<http://bifi.es>).

9. Catalonia

Catalonia has three official languages Catalan, Spanish and Aranese. Catalonia was colonized by ancient Greeks and Carthaginians. After the defeat of Carthage by Rome, it became a part of the Roman Empire. Catalonia came under Visigothic rule for four centuries and in the eighth century it came under Moorish control. After the defeat of Emir Abdul Rahman Al Ghafiqi's troops at Tours in 732, the Franks conquered the former Visigoth states. In 795 Charlemagne created the Marca Hispanica, a buffer zone of small kingdoms between the Moors and the Frankish Kingdom where the Catalan culture developed. The counts of Barcelona were Frankish vassals. In 989, Catalonia declared its independence. In 1137, a Count of Barcelona married Queen Petronila of Aragon, establishing the dynastic union of the County of Barcelona with the Kingdom of Aragon that was to create the Crown of Aragon. Catalonia became a maritime power, helping to expand the Crown into the Kingdom of Valencia, the Balearic Islands, and ultimately even Sardinia, Sicily, Corsica, Naples, Athens, the Canary Islands

and America.

The Dept. of Structural Biology of the Inst. for Molecular Biology of Barcelona, of the CSIC, includes six crystallography laboratories. At the Laboratory of Structural Biology of proteins, nucleic acids and their complexes, a team headed by M. Coll (mcoll@ibmb.csic.es), study systems related to horizontal gene transfer, DNA translocation and packaging DNA in viral capsids. (<http://bit.ly/bPCp5E>). I. Fita (ifrcr@ibmb.csic.es) leads the Laboratory for Structural Biology of Oxidative Stress Systems (<http://bit.ly/ak4m0F>). The focus of the Proteolysis Lab, led by F. X. Gomis-Rüth (xgrcri@ibmb.csic.es), is elucidating molecular mechanisms of action of proteolytic enzymes, and how bacteria overcome host defenses (<http://bit.ly/a0K3uU>). M. Solá (msvcri@ibmb.csic.es) leads efforts of the Laboratory of Structural Biology of Organelle Macromolecules to determine structure-function relationships of macromolecules and processes found only in organelles and not in other cellular compartments (<http://bit.ly/9UIJkE>). The Laboratory of Crystallographic Methods, led by I. Usón (iufcri@ibmb.csic.es), develops improved methods for macromolecular crystallography, (exploiting experimental data and chemical knowledge, deriving general methods to tackle twinning, pseudo-symmetry, anisotropic diffraction, lack of completeness and resolution; ab initio macromolecular phasing at medium resolution, (implemented in their program ARCIMBOLDO); and development of methods exploiting parallel computing in supercomputers and grids (<http://bit.ly/aMWbJA>). The laboratory of Structural virology and large biological complexes, headed by N. Verdaguier (nvmcri@ibmb.csic.es), is focused on the structural and functional characterization of different processes in the biological cycle of RNA viruses (<http://bit.ly/bp7ihg>).

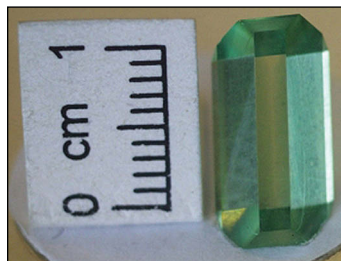
The Dept. of Crystallography of the Inst. of Materials Science of Barcelona (CSIC) is headed by E. Molins (elies@icmab.es). Crystallographic methodology for single crystal and powder diffraction data is developed by J. Rius (jordi.rius@icmab.es) and C. Miravittles (carles.miravittles@icmab.es); electron-density studies of hydrogen bonds and the relationship between their topology and energy (E. Molins and I. Mata, imata@icmab.es); and magnetic nanoparticles research and crystal engineering of pharmaceutical materials (A. Roig, roig@icmab.es) (<http://bit.ly/aJrQHZ>). In the Dept of Magnetic Materials and Functional Oxides, headed by J. L. Garcia-Muñoz (garcia.munoz@icmab.es), high precision neutron and X-ray diffraction techniques are combined with experimental and theoretical symmetry analyses (<http://bit.ly/9Wtw9z>). There is additional Crystallographic Research in the Dept of Solid State Chemistry, (N. Casañ, nieves@icmab.es) (<http://bit.ly/dq4vtd>).

In the Dept. of Crystallography, Mineralogy and Mineral Depos-



From left to right, Elies Molins, Jordi Rius, Carlos Frontera, Carlos Miravittles, Amparo Fuertes, Xavier Torrelles, Anna Roig and Judith Oró-Solé at the Institute of Material Sciences of Barcelona.

its at the U. of Barcelona S. Galí (gali@ub.edu) and M.À. Cuevas pursue crystallographic studies (mcuevasdiartel@ub.edu) (www.ub.es/cmdm/). In the Biological Macromolecules Group headed by Lourdes Campos at the Polytechnic U. of Catalonia (lourdes.campos@upc.edu),



A single crystal for photonic technology.

DNA structure and its interactions with drugs, ions and proteins is under study (<http://bit.ly/c53Ep0>). FICMA (the group of Physics and Crystallography of Materials) an interdisciplinary research group headed by F. Díaz and M. Aguiló (aguilo@quimica.urv.es) at the U. Rovira i Virgili, located in Tarragona focuses on the synthesis and structural characterization of new materials for laser and photonic technology and development of optics and photonic devices (<http://bit.ly/a4e1jA>). Crystallographic work done at the Inst. of Chemical Research of Catalonia (ICIQ) is done under supervision of J. Benet (jbenet@iciq.es), (<http://bit.ly/avdERB>). Crystallography carried out at the Crystallography and Mineralogy Unit of the Dept. of Geology of the Autonomous U. of Barcelona is the responsibility of J.F. Piniella (juan.piniella@uab.es) (<http://bit.ly/9buGXE>).

10. Madrid

Madrid, the capital of Spain, is located at the center of the Iberian Peninsula on the Castilian Central Plateau. This region has been populated since the Lower-Paleolithic period. During the Roman Empire it was crossed by two important Roman roads. During the period of the Visigothic Kingdom it was one of the least-populated regions of Al-Andalus, until the 11th century when the Muslim governors created a defensive system of fortresses all across the region with which they tried to stop the advance of the Christian Kingdoms of the north. The fortress city of Mayrit (Madrid) was built around 870 AD as a walled precinct for a military and religious community. In 1083, King Alfonso VI of Castile conquered the city of Madrid. It was under the reign of Charles III (1716-1788) that Spain began to be recognized as a nation rather than a collection of kingdoms and territories. He created a National Anthem, a flag, and a capital city with the construction of a coherent network of roads converging on Madrid.

The region of Madrid has, together with the region of Catalonia, the most crystallographic research groups in Spain. They are located in Madrid and its surroundings including the city of Alcalá de Henares, where Miguel de Cervantes was born. The following departments or crystallography groups are found in Madrid City.

The Dept. of Crystallography and Structural Biology is located in Madrid, in one of the oldest and most beautiful buildings belonging to the CSIC, the Inst. of Physical-Chemistry "Rocasolano". The building was financed by the International Educational Board of the Rockefeller Junior Foundation in 1932 and housed the Inst.



"The Rockefeller", nickname for the Institute of Physical Chemistry "Rocasolano", one of the research Institutes of the CSIC, the Spanish National Research Council.



Several members of the Department of Crystallography and Structural Biology, "at low temperature".

Nacional de Física y Química (The National Inst. for Physics and Chemistry) which played a major role in the development of physical-chemistry in Spain. Its library is one of the best in its field, with many complete collections of journals, some of which date from the 19th century.

In 1925, B. Cabrera (1878-1945) and his pupil J. Palacios (1891-1970) were responsible for the creation of one of the first Spanish groups of modern crystallography. The department became one of the most important places in Spain to learn crystallography. Today it is one of the best equipped laboratories in Spain, offering wet laboratories and dedicated facilities for protein production, protein characterization, protein crystallization, X-ray diffraction and computing.

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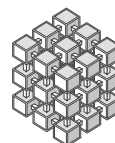
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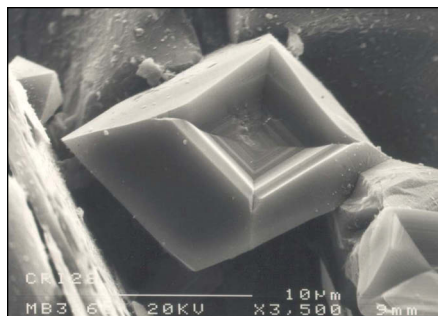
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The department head, A. Albert (xalbert@iqfr.csic.es), is leading a group studying Cellular Stress Response, J. Sanz (xjulia@iqfr.csic.es) and her group are specialists on Carbohydrate Active Enzymes; J.A. Hermoso (xjuan@iqfr.csic.es) is the leader of a group aimed at understanding host-pathogen interactions and new targets to combat antibiotic resistant bacteria (<http://bit.ly/9m9vs3>); J.M. Mancheño (xjosemi@iqfr.csic.es) is heading projects on Enzymes from Lactic Acid Bacteria, and L. Infantes (xlourdes@iqfr.csic.es) is a specialist on molecular docking. These young crystallographers form a dynamic group and one of the most important pillars of structural biology in Spain, M. Martínez-Ripoll (xmartin@iqfr.csic.es) is a bridge between the previous and the current generations (www.xtal.iqfr.csic.es/). In addition, the department houses the National Associated Centre to the Cambridge Crystallographic Data Center CCDC, distributing free of charge sublicenses of CSD for all academic institutions in Spain and Latin-American countries. The department also maintains a webpage, in English and Spanish, dedicated to teaching and attracting students to the magical world of crystallography: (<http://bit.ly/c8cHaM>).

Also in Madrid, and belonging to the CSIC, is the Group of Structural Biology of Proteins which forms a part of the Dept. of Chemical and Physical Biology at the Centre of Biological Research (Centro de Investigaciones Biológicas). The group is headed by G. Giménez, and the research is carried out in three laboratories whose principal investigators are A. Romero (romero@cib.csic.es), C. Vega (cvega@cib.csic.es) and F. Tórner (cftorner@cib.csic.es), <http://bit.ly/8Zsp5p>.

The National Center for Cancer Research (Centro de Investigaciones Oncológicas, CNIO, in Madrid) has three groups of crystallographers. The Macromolecular Crystallography Group, headed by G. Montoya (gmontoya@cnio.es) is focused on macromolecules involved in oncogenic processes, (<http://bit.ly/dDdLH>); the Cell Signalling and Adhesion Group, headed by D. Lietha (dlietha@cnio.es) probes the mechanisms that regulate focal adhesion kinase at atomic resolution (<http://bit.ly/cZn2d8>); and S. Ramón (sramon@cnio.es) leads the Structural Basis of Genome Integrity Group, deciphering the structure of the RAG1/2 protein assembly and its regulatory mechanisms and determining the role recombina- nase in lymphoid cancer (<http://bit.ly/dwOC7r>).

The Dept. of Crystallography and Mineralogy (in the Faculty of Geology) at the U. Complutense of Madrid began in 1956. At that time J.L. Amorós began research on crystal growth and analysis of inorganic and organic materials. Current research involves crystal



Villiaumite (NaF) crystals

growth of mineral phases and inorganic compounds at low- and high-temperature, growth mechanisms of solid solutions from aqueous solutions, diffusing-reacting systems, gemology, epitaxial growth on mineral surfaces, selective

chiral symmetry breaking during crystallization and characterization of geomaterials and other inorganic compounds. The department, currently headed by J.F. Barrenechea, has over twenty researchers (barrene@geo.ucm.es), (<http://bit.ly/avBUbn>).

In the Dept. of Inorganic Chemistry I at the U. Complutense, C. Otero (carlos1@quim.ucm.es) leads microstructural characterization of non-molecular crystals with commensurate and/or

incommensurate modulated structures, (<http://bit.ly/aALUdM>). The U. Complutense also maintains a General X-ray Diffraction Unit (<http://bit.ly/9dXuUc>).

The U. Nacional de Educación a Distancia, (UNED) in Madrid together with the Dept. of Geological Engineering of the Polytechnic U. of Madrid offers a web based course on crystallography for spanish speaking mineralogists known as Cristamine, (<http://bit.ly/djXrDb>).

At the Autonomous U. of Madrid (AUM) 15 km to north of the city crystallography groups are found in several departments and research Institutes of CSIC. The Dept. of Macromolecular Structures

at the National Center of Biotechnology (CNB), a joint center between the Spanish National Research Council (CSIC) and the AUM includes two groups. The Cell-cell and virus-cell interactions group, headed by J. Casanovas (jcasanovas@cnb.csic.es), focuses



J.M. Casanovas' team at the CNB.

on receptor-ligand recognition and receptors of the immune system that have been subverted by viruses to enter host cells (<http://bit.ly/9tex0T>) and the group headed by M.J. van Raaij (markvan-raaij@gmail.com) dedicated to the structural biology of viral fibres.

At the Material Physics Dept. of the AUM, the recently established Crystal Growth Laboratory lead by E. Diéguez (ernesto.dieguez@uam.es) participates in national and international projects aimed at crystallizing CdTe and related candidates for gamma-ray detectors for cardio-vascular and thyroidal imaging (<http://bit.ly/bqaKu9>).

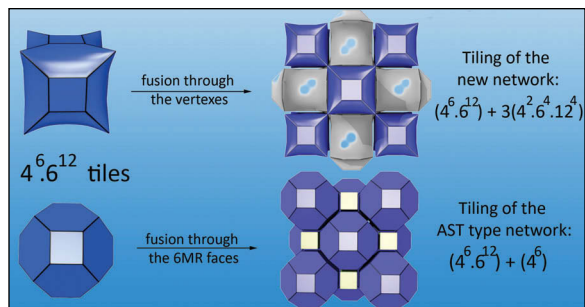


The team of the Crystal Growth Laboratory.

The Dept. of New Architectures in Materials Chemistry, belonging to the Inst. of Material Sciences of Madrid (CSIC) and located on the AUM campus, is lead by E. Gutiérrez-Puebla (egutierrez@icmm.csic.es) and Á. Monge (amonge@icmm.csic.es), who work on the design, synthesis and structure determination of new micro and nano-porous materials with multifunctional properties (sorption, heterogeneous catalysis, conductivity, and optics) and the synthesis of aromatic systems with electro-optic properties, (<http://bit.ly/bGyavs>). In the Dept. of Energy, Environment and Sustainable Technologies at the same Inst. of Material Sciences of Madrid, J.H. Velasco (hernandez-velasco@hmi.de) and J.A. Alonso (ja.alonso@icmm.csic.es) work on new materials using both X-ray and neutron powder diffractometry, and A. Landa (landa@icmm.csic.es) and P. Herrero (pherrero@icmm.csic.es) are active in electron diffraction.



Crystallographers at the Department of New Architectures in Materials Chemistry.



Similarity between MOF and zeolite cages.

In 1990 P. Gómez-Sal (pilar.gomez@uah.es) founded the Structural Chemistry Group in the Dept. of Inorganic Chemistry of the U. of Alcalá where the current activities of A. Martín M.E.G. Mosquera, and others include the synthesis and single crystal study of organometallic compounds, dendrimers, organometallic polymers and metal-organic frameworks.



The team of the Structural Chemistry Group at the University of Alcalá.

11. Castile-La Mancha

Although La Mancha is a windswept, battered plateau, it remains a symbol of the Spanish culture with its sunflowers, mushrooms, olive trees, windmills and Manchego cheese. Castile-La Mancha traces back to the Muslim Taifa of Toledo, which was taken by Alfonso VI from the Muslims in 1085. The Battle of Las Navas de Tolosa (1212) hastened the decline of the Almohad Dynasty. Four centuries later, in 1605, Cervantes' Don Quixote gave the world a lasting picture of La Mancha.

Crystallographic activity is found in several groups belonging to the Dept. of Inorganic Chemistry of the U. of Castile-La Mancha, but mainly in the Group of Organometallic Chemistry and Catalysis, where the crystallographic work is headed by M.I. López (mabel.lopez@uclm.es) (<http://bit.ly/csPCpp>).

12. Valencia

James I of Aragon led colonization of the Islamic taifas with Aragonese and Catalan people in 1208 and founded the Kingdom of Valencia in 1238. In 1707, King Philip V of Spain subordinated the Kingdom of Valencia, and the counties of the former Crown of Aragon.

The Molecular Science Inst. of U. of Valencia has two very active

research groups (<http://bit.ly/b9NRfN>, <http://bit.ly/cgTST8>) working on structural chemistry, but the crystallographic work is made by other Spanish laboratories. The Dept of Geology of the U. of Valencia has a group lead by J.M. Amigó (jose.m.amigo@uv.es) working on crystallography and mineralogy. (<http://bit.ly/9rL2wp>). In the Dept. of Inorganic Chemistry, three dimensional structures of organometallic compounds, are determined by M. Sanau (mercedes.sanau@uv.es). The Organic Crystal Engineering Group, in the Dept. of Organic Chemistry, headed by C. Rodríguez de Arellano (Carmen.Ramirezdearellano@uv.es), pursues structural studies of organometallic organofluorine compounds and modified peptides (<http://bit.ly/aKG5dP>).

In the Dept. of Inorganic and Organic Chemistry of the U. Jaime I in Castellón de la Plana (north of Valencia), Vicente Esteve (estevv@qio.uji.es) conducts powder diffraction analysis. The Molecular Materials research group of this university, headed by Rosa Llusar (Rosa.Llusar@qfa.uji.es) of the Dept. of Chemistry, Physics and Analytics, is active in single crystal diffractometry using the equipment of a general service unit of this university (<http://bit.ly/bXZQNt>).



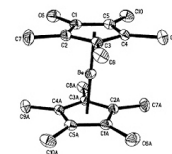
The team of Rosa Llusar at the University Jaime I.

Macromolecular crystallography is conducted at the CSIC Inst. of Biomedicine in Valencia. In its Dept. of Genomics and Proteomics, crystallographic work is focused on the characterization of signal transduction mechanisms (<http://bit.ly/aqdxN6>). V. Rubio (rubio@ibv.csic.es) head of the Structural Enzymopathology Unit promoted the use of crystallography in this institute; A. Marina (amarina@ibv.csic.es) is the leader of the Crystallography of Macromolecules Unit, and J. Bravo (jbravo@ibv.csic.es) is the leader of the Signal Transduction Unit.

13. Andalusia

Andalusia, the second largest Autonomous Community of Spain, occupies the south-east corner of the Iberian Peninsula. Andalusia was the center of power in medieval Muslim-dominated Iberia. Besides Muslim or "Moorish" influences, the region's culture has been influenced by Iberians, Carthaginians, Greeks, Romans, Vandals, and Visigoths, who preceded the Muslims, Castilian and other Christian North Iberian groups. Andalusia also had a relatively large Sephardic-Jewish population. Many cultural characteristics that are internationally seen as "typically Spanish" are largely of Andalusian origin.

In Seville, the capital city, crystallographic activity is found in the Inst of Material Science, a joint research centre between the U. of Seville and the CSIC, where M.J. Dianez (dianez@us.es), A. Justo (jjusto@icmse.csic.es), A. Criado (criado@us.es) and M.D. Estrada



A metal stabilized by CP's.



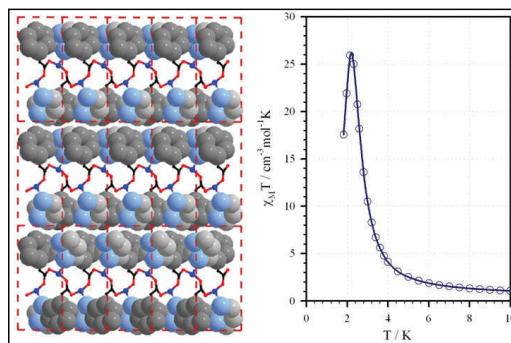
LEC: Crystallization under diffusion-controlled mass transport.

industrial crystallization, non-linear systems and pattern formation, biomineralization and biomimetic materials. They are also known for their technological products, including the “Granada crystallization box”, an Advanced Protein Crystallization Facility, used in ESA’s and NASA’s spaceships; J. García Ruiz is the principal investigator of a joint project, The Spanish Factory of Crystallization (<http://lafactoria.lec.csic.es/lafactoria/>) formed by nine Spanish groups to create an integrated platform for research and services in crystallography. Garcia Ruiz is also leading the “Master and PhD in Crystallography and Crystallization” teaching program a unique training opportunity for young investigators (<http://lec.ugr.es/> and <http://lafactoria.lec.csic.es/mcc>).

Cadiz, the oldest continuously-inhabited city in the Iberian Peninsula and possibly of all south-western Europe, has a general service diffraction unit headed by P. Valerga (pedro.valerga@uca.es).

(estrada@us.es) provide crystallographic capabilities (<http://bit.ly/bB9uHg>). At the U. of Malaga, M.A.G. Aranda (g_aranda@uma.es) leads a group in the Dept. of Inorganic Chemistry, Crystallography and Mineralogy, working with inorganic solids with unusual conducting, magnetic or structural properties (<http://bit.ly/afe1Ls>).

Granada, the city of “La Alhambra”, located near to the highest peak in the Iberian Peninsula, Mulhacén (3,479 m), has two teams working in crystallography. At the U. of Granada, the crystallographic work done at the Coordination Chemistry and Structural Analysis group is led by D. Martín (jdmartin@ugr.es). The Laboratory for Crystallographic Studies (LEC) a joint Inst. of the CSIC and the U. of Granada, headed by J.M. García Ruiz (juanma.garciaruiz@gmail.com), is a group known for their expertise in nucleation and crystal growth,



Metamagnetism in hydrophobically induced carboxylate (phenylmalonate)-bridged copper (II) layers.

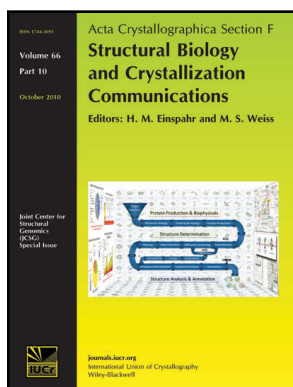
At the U. of Almeria, A. Cámara (acamara@ual.es) leads a group of macromolecular crystallographers in the Dept. of Physical-Chemistry, Biochemistry and Inorganic Chemistry analysing polyproline recognition domains and their interaction with ligands (<http://bit.ly/aMZDUJ>).

14. Canary Islands

The Canary Islands are a Spanish archipelago of seven islands, located just off the northwest coast of mainland Africa, 100 km west of the border between Morocco and the Western Sahara. In the Dept. of Fundamental Physics II of the U. of La Laguna (Tenerife), powder and single-crystal services are provided by J.G. Platas (jplatas@ull.es), who also shares with C.G. Silgo (csilgo@ull.es), a crystallographic research team (<http://bit.ly/dC1OEH>). The Laboratory of X-ray and Molecular Materials, also at the U. of La Laguna, studies multi-functional magnetic molecular materials, seeks new applications for this type of materials, conducts synthesis of new ligands, coordination chemistry of selected carboxylates, systematic synthesis for crystal engineering and preparation of precursors for magnetism. The group leader is C. Ruiz-Pérez. Neutron and Synchrotron data complement X-ray diffraction techniques (caruiz@ull.es) (<http://bit.ly/97zxMa>).

We all kindly invite you to participate in IUCr2011.

Acta Crystallographica Section F showcases structural genomics publications



The application of high-throughput methods to structural biology has generated an abundance of new macromolecular structures. In order to help ease the resultant publication backlog, *Acta Crystallographica Section F* now offers a special publication strategy to showcase these structures and the experiments upon which they are based. The first example was published in December 2009 and contained eight papers from the RIKEN-UK structural genomics consortium in a **special section** of the journal.

More recently (October 2010), the journal published a **special issue** that focuses exclusively on 35 structures, grouped into context, from the Protein Structure Initiative Joint Center for Structural Genomics. The issue, which is open access, is available from <http://journals.iucr.org/f/issues/2010/10/00/issconts.html>. This milestone publication has been enthusiastically welcomed by the community, and new requests and proposals for further special issues and special sections are under consideration.

For more information, please contact the Editors, Howard Einspahr (hmeinspahr@yahoo.com) or Manfred Weiss (msweiss@helmholtz-berlin.de).

