

Two members of the IQCC edit a Wiley book on spin states in chemistry with contributions from eminent scholars from all over the world

This week a new book on “Spin states in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity” has been published. The book is a recollection of a number of contributions from frontline eminent researchers from all over the world, and is the first textbook that deals entirely with spin states. The book has been published by Wiley, one of the most renowned publishers in scientific books in the world, after a preparation of more than two years.



Professors Miquel Costas and Marcel Swart proudly show the product of two years of intense labor

The concept of spin states is a relatively new topic in chemistry, which because of its complexity has been largely ignored in the scientific community and only in the past decade has gained recognition. “In part this is due to the problems of properly describing the electronic structure of transition-metal complexes by computational chemistry”, explains Prof. Swart. “Another issue is the enormous reactivity of these complexes”, adds Prof. Costas, “which makes that it is difficult to characterize them in full detail.” Therefore, a combination of a variety of techniques (both computational and experimental) is needed, for which collaborations between different research groups with their own expertise would be helpful. This has led to the construction of intense international networks through a number of European networks, such as the European Cooperation in Science and Technology (COST) and the international training network (ITN) programs. Both of these programs in which the *Institut de Química Computacional i Catàlisi* (IQCC) of the University of Girona participates are funded through the EU’s Horizon2020 framework.

“Putting together the book was made easy because of these networks”, explains Swart, “because it made it easy to identify the experts for a certain topic and ask them to contribute. In this way, we have been able to target a large number of frontline researchers to ask to share their expertise with a book chapter. To our

surprise, almost all happily agreed to do so.” The result is a book of 472 pages with a total of 17 chapters that treat a wide range of subjects, which all deal with spin states. The book is a recollection of introductory chapters with descriptions of the methods that are used for these systems, followed by more specific chapters that deal with specific aspects and/or reactions and/or systems. In the end it has parts that are targeted at starting researchers in the field, while others are clearly for advanced researchers. “Obviously, it is this overall view of spin states that makes this book a real contribution to the field, and we hope that it could be used as reference material in undergraduate and Master courses in chemistry and life sciences,” explains Costas.

Related to putting together the book is the organization of the 2016 edition of the Girona Seminar, a bi-annual conference series held in Girona in April, which has as topic “Predictive Catalysis: Transition-Metal Reactivity by Design”. Costas explains: “We have been able to put together an interesting line-up of plenary and keynote speakers, both from Europe and the USA, whose expertise is in line with the topic of the book. In fact, several of the speakers have contributed to the book, for which we are very grateful”. This has also led to the recognition by one of the most prominent journals in the scientific literature, *Nature Chemistry*, that will be supporting the Girona Seminar conference by providing awards for the best contributions by young researchers. “We are very happy and proud of this recognition, and are looking forward to a very interesting meeting in April”.

Prof. Marcel Swart obtained his PhD in Groningen (NL) with a study on copper proteins (Sept. 2002). He works since 2006 at the IQCC (Univ. Girona), and was promoted to ICREA Research Professor in Sept. 2009. He has published over 120 papers, formed part of tribunals for Masters and PhD ceremonies, formed part of evaluation committees for ANEP, and as reviewer for >30 journals and (inter)national science organizations (ANEP, NWO, FWO, SNF, Prace). He has received funding from (inter)national science organizations and companies, organized a CECAM/ESF Workshop (Zaragoza, 2012), is Chair of a COST Action (CM1305, ECOSTBio), is Editor of a Wiley-book on "Spin states in Biochemistry and Inorganic Chemistry" (2015), is the main organizer for the Girona Seminar 2016 and is Associate Editor for RSC Advances. He was awarded the Young Scientist Excellence Award 2005, the MGMS Silver Jubilee Prize 2012, supervised two PhD theses with Premi Extraordinari, and in Oct. 2014 was selected as member of the Young Academy of Europe.

Prof. Miquel Costas is professor of inorganic chemistry at the University of Girona, member of the Department of Chemistry and of the Institute of Computational Chemistry and Catalysis. He earned his doctorate at the University of Girona in 1999, and after a post-doctoral stay at the University of Minnesota became a professor at the University of Girona in 2003. He has published over one hundred articles in the field of biologically inspired inorganic chemistry and catalysis. He has been visiting professor at Carnegie University in Pittsburg and at the Debye Institute for Catalysis at the University of Utrecht. He has been awarded ICREA Academy Awards in 2009 and 2014, and the prize for research excellence of the Spanish Royal Society of Chemistry in 2014.

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