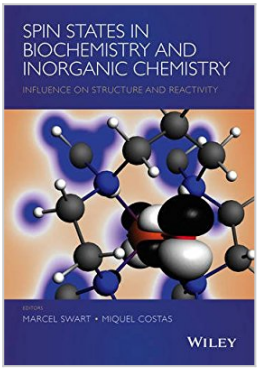

Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity

By Marcel Swart, Miquel Costas

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It has long been recognized that metal spin states play a central role in the reactivity of important biomolecules, in industrial catalysis and in spin crossover compounds. As the fields of inorganic chemistry and catalysis move towards the use of cheap, non-toxic first row transition metals, it is essential to understand the important role of spin states in influencing molecular structure, bonding and reactivity.

Spin States in Biochemistry and Inorganic Chemistry provides a complete picture on the importance of spin states for reactivity in biochemistry and inorganic chemistry, presenting both theoretical and experimental perspectives. The successes and pitfalls of theoretical methods such as DFT, ligand-field theory and coupled cluster theory are discussed, and these methods are applied in studies throughout the book. Important spectroscopic techniques to determine spin states in transition metal complexes and proteins are explained, and the use of NMR for the analysis of spin densities is described.

Topics covered include:

- DFT and ab initio wavefunction approaches to spin states
- Experimental techniques for determining spin states
- Molecular discovery in spin crossover
- Multiple spin state scenarios in organometallic reactivity and gas phase reactions
- Transition-metal complexes involving redox non-innocent ligands
- Polynuclear iron sulfur clusters
- Molecular magnetism
- NMR analysis of spin densities

This book is a valuable reference for researchers working in bioinorganic and inorganic chemistry, computational chemistry, organometallic chemistry, catalysis, spin-crossover materials, materials science, biophysics and pharmaceutical chemistry.

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Editorial Review

Review
"Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity, edited by Marcel Swart and Miquel Costas is impressive testimony to the advances in theory, computations, and experiment, especially regarding transition metals in recent years, and a revealing look at how much remains to be developed....The authors provide detailed comparison of various computational methods with each other and with experimental data in many cases. Each chapter is an extensively referenced focused review article. Chapters 1-3 emphasize computational methods....No single monograph can encompass a topic as broad as the title of this book, which is almost the entire chemistry of the periodic table. However, for the selected topics, the volume provides a very valuable concise snapshot of the field.Computational chemistry for compounds of CHNO have advanced to the point that many experimentalists can routinely apply standard methods in Gaussian and other such programs with confidence, guided only by the state of the art described in other publications. This book shows that in spite of enormous effort related to transition metal energy states and spin states, even the expert computational chemists need to proceed with caution and compare many functionals"- **(Gareth Eaton- December 2016)**

From the Back Cover

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About the Author

Prof. Dr. Marcel Swart, Universitat de Girona, Spain
Marcel Swart is ICREA Research Professor in the Institute of Computational Chemistry Catalysis at the Universitat de Girona, Spain. He is a computational/theoretical chemist working in the field of (bio)chemistry and biomedicine. He has published >100 papers in peer-reviewed scientific journals and has an h-index of 26. He was awarded the Young Scientist 2005 award by ICCMSE (International Conference of Computational Methods in Sciences and Engineering), and was selected as one of the promising young inorganic chemists of "The next generation" that were invited to contribute to a special issue of Inorganica Chimica Acta in 2007, and to a special issue of Polyhedron in 2010.
In 2012, he was awarded the MGMS Silver Jubilee Prize "for his development of new computational chemistry programs, design of new research tools and application to (bio)chemical systems that are highly relevant for society and science." In September 2012 he organized a CECAM/ESF Workshop on "Spin states in biochemistry and inorganic chemistry", highlighted in Nature Chem. 2013, 5, 7-9.

Prof. Dr. Miquel Costas, Universitat de Girona, Spain
Miquel Costas became Professor Titular at the University of Girona in 2003. He has published over 70 papers in international journals that have received over 3470 citations. His research interests involve the study of transition metal complexes involved in challenging oxidative transformations, including functionalization of C-H bonds and water oxidation. These systems commonly operate in multistate reactivity scenarios, implicating multiple spin states.

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