

Books

M. Swart and M. Costas (Eds.)

Spin states in biochemistry and inorganic chemistry: Influence on Structure and Reactivity, Wiley, **2015**

www.marcelswart.eu/books/

M. Swart

"Density Functional Theory Applied To Copper Proteins"

PhD-thesis, **2002**, September 10, Rijksuniversiteit Groningen

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Book chapters

M. Swart

"Quantum-mechanics approaches in bioinorganic chemistry: targeting the oxidation state"

In "Advances in Computational Bioinorganics: From Description to Prediction", J.D. Marechal (Ed.), Wiley, **202x**;

accepted

A.C. Castro and M. Swart

"Recent advances in computational NMR spectrum prediction"

In "Computational Techniques for Analytical Chemistry and Bioanalysis", P.B. Wilson, M. Grootveld (Eds.), Royal

Society of Chemistry, **2021**; Ch. 2, p. 41-68

M. Swart

"Dealing with spin states in computational organometallic catalysis"

In "New Directions in the Modeling of Organometallic Reactions", A. Lledos, G. Ujaque (Eds.), Springer, **2020**;

(Topics in Organometallic Chemistry Vol. 67); p. 191-226

M. Gruden, W.R. Browne, M. Swart, C. Duboc

"Computational vs. experimental spectroscopy for transition-metals"

In "Transition metals in coordination environments: computational chemistry and catalysis viewpoints", E.

Broclawik, T. Borowski, M. Radon (Eds.), Springer, **2019**; Ch. 6, 161-183

C. Daul, M. Zlatar, M. Gruden-Pavlovic and M. Swart

"Application of Density Functional and Density Functional Based Ligand Field Theory to Spin States"

In "Spin states in biochemistry and inorganic chemistry: Influence on Structure and Reactivity", M. Swart, M. Costas

(Eds.), Wiley, **2015**; Ch. 2, 7-34

M. Garcia-Borràs, S. Osuna, J.M. Luis, M. Swart and M. Solà

"Understanding the Exohedral Functionalization of Endohedral Metallofullerenes"

In "Exotic Properties of Carbon Nanomatter", M.V. Putz, O. Ori (Eds.), Springer Verlag, Berlin-London-New York,

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S. Osuna, M. Swart and M. Solà

"The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective"

Book chapter in "Carbon Bonding and Structures: Advances in Physics and Chemistry", Putz M.V. (Editor),

Springer Verlag, Berlin-London-New York, **2011**, ISBN: 978-94-007-1732-9, Ch. 4, pp. 57-78

M. Swart, M. Güell and M. Solà

"Accurate description of spin states and its implications for catalysis"

Book chapter in "Quantum Biochemistry: Electronic structure and biological activity"; Matta, C.F. (Ed.); Wiley,

2010, Vol. 2, Ch. 19, p. 551-583

M. Swart, M. Solà and F.M. Bickelhaupt

"Constraining optimized exchange"

Book chapter in "Handbook of Computational Chemistry Research"; C.T. Collett, C.D. Robson (Ed.); Nova Science,

2010, p. 97-125

P. Th. van Duijnen, M. Swart and L. Jensen

"The Discrete Reaction Field approach for calculating solvent effects"

Book chapter in "Solvation effects on molecules and biomolecules: Computational methods and applications",

Springer series "Challenges and Advances in Computational Chemistry and Physics", Ed. S. Canuto, **2008**, p. 39-102

P.Th. van Duijnen, M. Swart and F.C. Grozema

“QM/MM calculation of (hyper-)polarizabilities with the Direct Reaction Field approach”

ACS Symposium Series, **1999**, 712, 220-232

Popular science/dissemination articles

M. Swart, S. Osuna, M. Garcia-Borràs, J.M. Luis and M. Solà

“Regioselectividad en fullerenos, una visión computacional”

An. Quím **2013**, 109, 11-19

M. Swart, M. Solà, S. Osuna and J. Poater

“Metales, disolventes, proteínas: la importancia del entorno químico”

LifeSciencesLab **2009**, 5, 50-53