EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

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COST Action no. CM1305

ECOSTBio

Explicit Control Over Spin-states in Technology and Biochemistry

2014 | 2018

Objectives

- Establish a European network of researchers in (bio)chemistry which is dedicated to the understanding and application of spin-states in technological and biological applications
- Setting up a SPINSTATE database with well-characterized transition-metal complexes with known spin ground-state, providing both experimental and computational data
- Design and development of new computational methods
- Characterize spin-state properties of transition-metal complexes to be included in the database, for providing reliable reference data to compare new methods with
- Explicit control of spin states of transition-metal compounds through rational design of ligand coordination

Main Achievements

- Collaboration between experimental and theoretical groups: based on theory, proven by experiment
- Sharing of know-how and research facilities
- Creation of an accessible on-line database for the scientific community
- Formation of young scientists through courses

Chemistry and Molecular Sciences and Technologies (CMST)

Participating countries

AT, BE, CH, CZ, DE, DK, ES, FR, GR, HU, IE, IL, NL, NO, PL, PT, RO, RS, SE, SI, SK, UK

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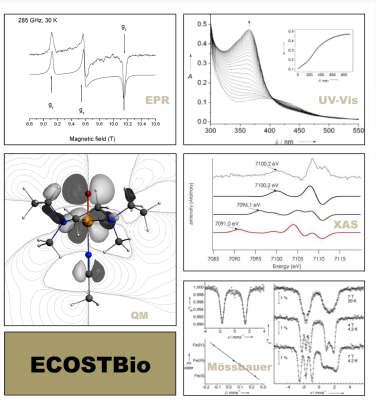

Together we're strong: experiment needs theory, theory needs experiment

COST is supported by the EU RTD Framework Programme

ESF provides the COST Office through a European Commission contract

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Working Group activities

WG1 – SPINSTATE database

- Creation of an online and freely accessible SPINSTATE database
- Well-characterized transition-metal complexes with known spin ground-state
- Filled with both experimental and computational data

WG2 – Enzymatic spin states

- Obtain profound understanding of interplay of spin state and reactivity in metal-containing enzymes
- Explore how this can be tuned to increase selectivity and/or catalytic activity

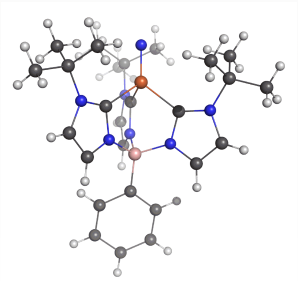
WG3 – Spin crossover

- Understand the detailed nature of cooperativity in Spin Crossover
- Explore novel metal-ligand combinations for new SCO species

WG4 – Biomimetic spin states

- Explicit control of spin states of high-valent metal-oxo or imido compounds
- Rational design of ligand coordination around the metal
- Establishment of the correlation between spin state and reactivity

Industry participation



Synthesis, Structure, and Reactivity of an Iron(V) Nitride
(K. Meyer, Friedrich-Alexander Universität Erlangen-Nürnberg, and co-workers)

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