

Program of Krakow Meeting

September 8 – 9, Faculty of Chemistry, Jagiellonian University in Krakow

Wednesday, September 7

16:00-21:00 ECOSTBio Registration (Hotel Ibis, lobby)

Thursday, September 8

08:30-08:55 ECOSTBio Registration (Faculty of Chemistry, ground floor)

Session 1 (Lecture Hall, 2nd floor)

Chair: Grace Morgan

- 09:00-09:40 **Marcel Swart**
Spinning around in transition-metal chemistry
- 09:40-10:00 Andrew Atkins
Assessment of functional and wave function method dependence on the intersystem crossing dynamics of CH₂S
- 10:00-10:20 Quan Phung
Density matrix renormalization group for transition metal complexes: does it work?
- 10:20-10:50 Coffee

Session 2 (Lecture Hall, 2nd floor)

Chair: Rob Deeth

- 10:50-11:30 **Stefan Grimme**
Simplified quantum chemical methods for consistent structures, energies, and electronic spectra of large systems.
- 11:30-12:10 **Wesley Browne**
Connecting microscopic and macroscopic mechanisms – an experimentalists perspective on the role of theory in understanding reaction mechanisms
- 12:10-12:30 Balazs Pinter
Guiding principles for controlling the redox potential of ligand-centered electron transfer processes.
- 12:30-12:50 Panel discussion
- 12:50-13:00 Closing of CTTC7 conference
- 13:00-15:00 Lunch

Session 3 (Lecture Hall, 2nd floor)

Chair: Maja Gruden

- 15.00-15:20 Grace Morgan
Ordering Phenomena and Photophysical Properties of Manganese(III) and Iron(III) Spin State Switches.
- 15:20-15.50 **Roman Boca**
Solid state cooperativeness in spin crossover systems.
- 15.50-16:30 WG1: Database discussion
- 16:30-17.00 Coffee
- 17.00-18:30 Poster Session (+ pica-pica)
- 19:15-20.00 Walking to restaurant
- 20.00-23.00 Conference dinner (ZaKładka Food & Wine, ul. Józefińska 2)

Friday, September 9

Session 4 (Lecture Hall, 2nd floor)

Chair: Jalila Simaan

- 09.00-09:30 **Rudi van Eldik**
Spin-state tuning of Fe(III) complexes in solution. Effect of non-innocent ligands and hydrostatic pressure.
- 09:30-09:50 Rubén Solorzano
Novel (coordination) polymer nanoparticles for advanced theranostics.
- 09.50-10:10 Paulo Martinho
Polymorphism in tridentate Fe(III) spin crossover compounds: transition temperatures and cooperativity.
- 10.10-10.30 Carlo Albero Gaggioli
Ligand effect on the oxidative addition of O₂ on Lau(I)-H complexes.
- 10:30-11.00 Panel discussion
- 11:00-11:30 Coffee

Session 5 (Computer Labs 114 & 114A, 1st floor)

- 11.30-13:00 Moisés Àlvarez (Davide Angelone, Marcel Swart)
SPINSTATE Database – practical training iochem-bd
- 13.00-15.00 Lunch

Session 6 (Lecture Hall, 2nd floor)

Chair: John McGrady

- 15.00-15:30 **Piotr Pietrzyk**
Open-shell binding of small molecules to nickel sites in ZSM-5 zeolite – role of the spin density flow pathways
- 15:30-15:50 Leon Freitag
Novel multiconfigurational methods for large molecules: application to spin-crossover compounds.
- 15.50-16:10 Vera Krewald
Electronic structure analysis of transition metal dimers for dinitrogen photocleavage
- 16:10-16:40 Coffee

Session 7 (Lecture Hall, 2nd floor)

Chair: Jeremy Harvey

- 16.40-17:00 Jean-Noël Rebilly
A supramolecular mimic of the regulation step of Fe-monooxygenases: allosteric modulation of Fe(III)-OOH and Fe(IV)-oxo formation by guest binding in a heterodinuclear Zn(II)-Fe(II) calix[6]arene-based funnel complex.
- 17.00-17:30 **Dimitrios Pantazis**
The mechanism of biological water oxidation: insights from spectroscopy-oriented quantum chemistry.
- 17.30-17:50 Panel discussion
- 17:50-18:00 Closing