

## Programme of Prague Meeting

IOCB, Lecture Hall

### Wednesay April 13

- 8.30-9.00 Registration  
9.00-9.20 Opening of the meeting (Chair and Local Organizers)
- 9.20-10.00 **E. Solomon**  
*Structure/Function Correlations over Non-Heme Iron Enzymes.*
- 10.00-10.20 **B. Champagne**  
*Second-order nonlinear optical (NLO) molecular switches: from conventional to transition metal containing compounds.*
- 10.20-10.40 **Q. Phung**  
*Density matrix renormalization group (DMRG) study of spin-state energetics of iron-oxo porphyrins.*
- 10.40-11.10 Coffee
- 11.10-11.30 **S. Bonnet**  
*Stabilization of the low-spin state in a mononuclear iron(II) complex and high-temperature cooperative spin crossover mediated by hydrogen bonding.*
- 11.30-11.50 **R. Herchel**  
*Iron(III) spin crossover compounds with schiff-base ligands.*
- 11.50-12.20 **F. Neese**  
*Spin States and Molecular Magnetism.*
- 12.20-14.00 Light lunch
- 14.00-14.30 **M. Gruden**  
*Density functional approximations for spin-state chemistry*
- 14.30-14.50 **T. Corona**  
*Characterization and reactivity studies of A terminal copper-nitrene species.*
- 14:50-15.10 **B. Sarkar**  
*Click-derived tripodal ligands for spin crossover and bond activation reactions.*
- 15:10-15.30 **D. Brazzolotto**  
*Dioxygen activation and catalytic reduction by a thiolate-bridged dimanganese(II) complex with a pendant thiol.*
- 15:30-15:50 **C. de Graaf**  
*Managing the computational chemistry big data problem: the ioChem-BD platform.*
- 15.50-16.30 Database discussion  
16.30-17.15 Discussion time WGs  
17.15-18.30 Poster session (+ pica pica)

## Thursday April 14

- 9.00-9.40 **L. Que Jr.**  
*The Amazing High-Valent Iron-Oxo Reaction Landscape*
- 9.40-10.00 E. Andris  
*Reactivity of stereoisomeric iron(IV) complexes with a different spin state studied in the gas phase.*
- 10.00-10.20 C. Enachescu  
*Matrix-assisted relaxation in Fe(phen)<sub>2</sub>(NCS)<sub>2</sub> spin-crossover microparticles: theoretical and experimental investigations.*
- 10.20-10.40 A. R. McDonald  
*Nickel(III)-oxygen adducts that oxidize inert hydrocarbons.*
- 10.40-11.10 Coffee + Group Picture
- 11.10-11.30 M. Radoń  
*Accurate spin-state energetics of Fe(III) and Ru(III) aquo complexes evidence significant solvation effects.*
- 11.30-11.50 M.C. Kafentzi  
*Heterometallic Nickel-Copper dioxygen complexes: electronic structure and reactivity.*
- 11.50-12.20 **P. Maldivi**  
*Quantum chemical analysis of iron complexes highly active in H abstraction and nitrene insertion reactions.*
- 12.20-14.00 Light lunch
- 14.00-14.40 **A. Borovik**  
*A Bioinspired Approach to Synthetic Iron and Manganese Complexes with Oxido and Hydroxido Ligands.*
- 14.40-15.00 S. DeVisser  
*Quantum mechanics/molecular mechanics studies of cytochrome P450 peroxygenases for the biosynthesis of biofuels.*
- 15.00-15.20 J. Klein  
*The aqueous chemistry of the [Fe<sup>IV</sup>(O)TMC)]<sup>2+</sup> complex: determining the pK<sub>a</sub> of an aqua ligand bound to an Fe<sup>IV</sup>=O unit.*
- 15.20-15.40 A. Kochem  
*Polynuclear methane monooxygenase bioinspired copper complexes.*
- 15.40-16.00 R. Travieso-Puente  
*Reversible spin state changes in a tetrahedral iron complex with redox-active formazanate ligands.*
- 16.00-16.30 **K. Pierloot**  
*Describing oxygen atom transfer with DFT and multiconfigurational methods.*
- 16.35-18.00 MC meeting

## Friday April 15

- 9.00-9.40 **K. Bren**  
*Effects of Heme Conformation on Spin State, Spin Distribution, and Electron Transfer in Cytochromes*
- 9.40-10.00 P. Weinberger  
*Variable temperature ATR-IR spectroscopy as a valuable tool for the in situ spin state detection of iron(II) spin crossover complexes.*
- 10.00-10.20 D. Luneau  
*Valence tautomerism in 2D manganese-nitronyl nitroxide radical systems.*
- 10.20-10.40 P. Kyritsis  
*Mononuclear single molecule magnets: the case of manganese(III), Iron(II) and Cobalt(II) complexes bearing imidodiphosphinato chelating ligands.*
- 10.40-11.10 Coffee
- 11.10-11.30 G. La Penna  
*Reactive oxygen species and the Cu[Amyloid-Beta] complex.*
- 11.30-11.50 H. J. Krüger  
*Intermediate-spin state in six-coordinate iron complexes with a pseudo-octahedral coordination environment.*
- 11.50-12.20 **K. Meyer**  
*Uranium-mediated electrocatalytic H<sub>2</sub> production from water*
- 12.20-14.00 Light lunch