Programme of Prague Meeting

IOCB, Lecture Hall

Wednesday 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)
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:00-09:40</td>
<td>L. Que Jr.</td>
<td><em>The Amazing High-Valent Iron-Oxo Reaction Landscape</em></td>
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<tr>
<td>09:40-10:00</td>
<td>E. Andris</td>
<td>Reactivity of stereoisomeric iron(IV) complexes with a different spin state studied in the gas phase.</td>
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<tr>
<td>10:00-10:20</td>
<td>C. Enachescu</td>
<td><em>Matrix-assisted relaxation in Fe(phen)$_2$(NCS)$_2$ spin-crossover microparticles: theoretical and experimental investigations.</em></td>
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<tr>
<td>10:20-10:40</td>
<td>A. R. McDonald</td>
<td>Nickel(III)-oxygen adducts that oxidize inert hydrocarbons.</td>
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<td>10:40-11:10</td>
<td>Coffee + Group Picture</td>
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<tr>
<td>11:10-11:30</td>
<td>M. Radoń</td>
<td>Accurate spin-state energetics of Fe(III) and Ru(III) aquo complexes evidence significant solvation effects.</td>
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<td>11:30-11:50</td>
<td>M.C. Kafentzi</td>
<td><em>Heterometallic Nickel-Copper dioxygen complexes: electronic structure and reactivity.</em></td>
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<td>11:50-12:20</td>
<td>P. Maldívi</td>
<td>Quantum chemical analysis of iron complexes highly active in H abstraction and nitrene insertion reactions.</td>
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<td>12:20-14:00</td>
<td>Light lunch</td>
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<tr>
<td>14:00-14:40</td>
<td>A. Borovik</td>
<td>A Bioinspired Approach to Synthetic Iron and Manganese Complexes with Oxido and Hydroxido Ligands.</td>
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<tr>
<td>14:40-15:00</td>
<td>S. DeVisser</td>
<td>Quantum mechanics/molecular mechanics studies of cytochrome P450 peroxygenases for the biosynthesis of biofuels.</td>
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<td>15:00-15:20</td>
<td>J. Klein</td>
<td><em>The aqueous chemistry of the [Fe$^{IV}$(O)TMC]$^{2+}$ complex: determining the pK$_a$ of an aqua ligand bound to an Fe$^{IV}$=O unit.</em></td>
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<td>15:40-16:00</td>
<td>R. Travieso-Puente</td>
<td>Reversible spin state changes in a tetrahedral iron complex with redox-active formazanate ligands.</td>
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<td>16:00-16:30</td>
<td>K. Pierloot</td>
<td>Describing oxygen atom transfer with DFT and multiconfigurational methods.</td>
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<td>16:35-18:00</td>
<td>MC meeting</td>
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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 nitrooxide 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**  

11.50-12.20  **K. Meyer**  
*Uranium-mediated electrocatalytic H₂ production from water*

12.20-14.00  Light lunch