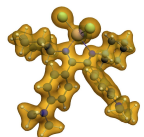


Monday, 24.08.2015

University of Belgrade-Faculty of Chemistry/Lecture room-first floor (Studentski trg 12-16)

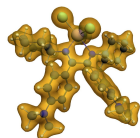
8:30-9:00	Registration
9:00-9:20	Opening of the workshop (Chair and Local Organizer)
9:20-10:00	Grace Morgan , University College Dublin, Ireland <i>Optical and Thermal Spin State Switching in Iron(III) and Manganese(III) Spin Crossover Complexes</i>
10:00-10:20	Adam Stepniewski , Institute of Catalysis PAS, Poland <i>Spin states of cobalt active sites in zeolites and their influence on the ability of Co centers to activate NO ligand (DFT periodic modeling).</i>
10:20-10:40	Christine McKenzie , University of Southern Denmark, Denmark <i>Halogen Bonding Stabilizes a catalytically competent Fe(III)OIPh species</i>
10:40-11:10	Coffee break
11:10-11:30	Ivan Salitros , Slovak University of Technology, Slovakia <i>Thermal and Photoinduced Spin Crossover in Iron(II)-Bis(Pyrazol-1-yl)Pyridine Mono- and Polynuclear Complexes</i>
11:30-11:50	Deborah Brazzolotto , DCM, France <i>Ni-Fe complexes mimicking the active site of Ni-Fe Hydrogenase.</i>
11:50-12:10	Matthew Quesne , Polish Academy of Science, Poland <i>Utilizing QM/MM techniques in the study of enzyme catalyses reaction mechanisms</i>
12:10-14:00	Lunch (Club Restaurant Teatroteka, Gospodar Jevremova 19)
14:00-14:40	Leticia Gonzalez , University of Vienna, Austria <i>Shining light on transition metal complexes -- Challenges for theory.</i>
14:40-15:00	Marc-Etienne Moret , Utrecht University, Netherlands <i>Hemilabile behavior of a Diphosphine-Ketone Ligand with Mid-to-Late First-Row Transition Metals</i>
15:00-15:20	Wesley Browne , University of Groningen, Netherlands <i>Determining redox potentials of iron complexes - does spin state matter?</i>
15:20-16:10	Database Discussion
16:10-17:00	WGs discussions
17:00-19:00	Poster session / "Pica Pica"
20:00-23:30	Conference dinner (Restaurant Boat Serena)



Tuesday, 25.08.2015

University of Belgrade-Faculty of Chemistry/Lecture room-first floor (Studentski trg 12-16)

- 9:00-9:40 **Malcolm Halcrow**, University of Leeds, United Kingdom
Structure: function relationships in molecular spin-crossover compounds
- 9:40-10:00 **Alex Domingo**, KU Leuven, Belgium
Tuning the spin crossover phenomenon through fine control of nitrogen positions on imidazol-diazine Fe(II) complexes
- 10:00-10:20 **Xenia Engelmann**, Humboldt-University Berlin, Germany
Heterobimetallic Transition-metal dioxygen complexes - Electronic structure and reactivity
- 10:20-10:40 **Laurentiu Stoleriu**, Alexandru Ioan Cuza University, Romania
Study of cluster evolution in 3D spin crossover compounds in the framework of an elastic model.
- 10:40-11:10 Coffee break and group picture
- 11:10-11:30 **Dominique Mandon**, CNRS, France
Insights in the reaction of O₂ with Fe(II) complexes with sterically hindered tripods: spectroscopic detection of a ferric-superoxide adduct
- 11:30-11:50 **Carlo Alberto Gaggioli**, University of Perugia, Italy
O₂ insertion into a gold-hydride bond: mechanistic theoretical study.
- 11:50-12:10 **Aniko Labas**, Budapest Uni. of Tech. and Eco, Hungary
QM, MD and QM/MM modeling of nitric oxide binding to myoglobin.
- 12:10-14:00 Lunch (Club Restaurant Teatroteka, Gospodar Jevremova 19)
- 14:00-14:40 **Matthias Stein**, Max Planck Institute Magdeburg, Germany
Hydrogen Conversion by Earth-Abundant Catalysts.
- 14:40-15:00 **Dijana Zilic**, Ruder Boskovic Institute, Croatia
Magnetic properties of transition metal complexes and organic radicals studied by ESR spectroscopy
- 15:00-15:20 **Inés Monte Pérez**, Humboldt University Berlin, Germany
Study of Reactive Intermediates of Late-Transition-Metal Compounds with Oxidizing Agents in C-H Bond Activation
- 15:20-15:40 **Stepan Stepanovic**, University of Belgrade, Serbia
The role of spin states in catalytic mechanism of the intra- and extradiol cleavage of catechols by O₂.
- 15:40-16:00 **Kasper Kepp**, DTU, Denmark
On the spin state balance in coordination chemistry
- 16:00-18:00 MC meeting



Monday, 24.08.2015

University of Belgrade-Faculty of Chemistry/Lecture room-first floor (Studentski trg 12-16)

17:00-19:00 **Poster session / "Pica Pica"**

1 Yiannis Sanakis	Spin Relaxation in Mononuclear S=2 FeII Complexes	Y. Sanakis, I. Govor, M. Pissas, E. Devlin, R. Raptis
2 Cristian Enachescu	Spin crossover microparticles in surfactants	C. Enachescu, M.L. Boillot
3 Polydoros C. Ioannou	Ni(II) complexes with (P,P) ligands	P. C. Ioannou, Konstantina Stergiou, Ioanni
4 Despoina Chriti	METATHESIS POLYMERIZATION REACTIONS INDUCED BY DIT	G. Raptopoulos, M. Pitsikalis, P. Paraskevopoulou
5 Alena Packova	Mononuclear Co(II) Single Molecule Magnet showing	R. Boca
6 Andrew J. Atkins	Benchmarking TD-DFT Calculations for $[\text{Ru}(\text{bpy})_3]^{2+}$	A. J. Atkins, L. Freitag, L. Gonzalez
7 Ljubica Andjelkovic	Spin states of hepta coordinated complexes	Lj. Andjelkovic, M. Zlatar, M. Gruden
8 Filip Vlahovic	DFT study of spin states in scorpionate complexes	F. Vlahovic, M. Peric, M. Gruden
9 Quan Phung	Spin state energetics in first row transition metal complexes: Role of 3s3p correlation	Q. Phung, A. D. Toro and K. Pierloot
10 Barbora Brachnakova	MAGNETISM OF SCHIFF BASE IRON(III) COMPLEXES	B. Brachnakova, I. Å ALITOÅ
11 Claire Deville	O ₂ Activation and Double C-H Oxidation by a Mononuclear Manganese(II) Complex	C. Deville, S. K. Padamati, J. Sundberg, V. McKee, W. R. Browne, C. J. McKenzie
12 Vibe Jakobsen	Solid State MAS ¹³ C NMR Chemical Shifts In Bio-mimetic Cu(I/II) Compounds	V. Jakobsen, J. Sundberg, V. McKee, U. Gro Nielsen, and C. J. McKenzie