



Program Tuesday 13/01/2015
Amphithéâtre Gastaut, Jardin du Pharo

- 9:00-9:40 The Molecular & Electronic Structure of High-Valent Nitrido Complexes of Manganese, Iron, and Cobalt
Karsten Meyer
- 9:40-10:00 Understanding the outer-valence electronic structure of metal-organic compounds with density functional theory and many-body perturbation theory.
L. Kronik
- 10:00-10:20 Binuclear copper active site: tyrosinase vs. pMMO.
C. Belle, H. Jamet, M. Orio, R. Hardré, B. Faure, J. Simaan, M. Réglie
- 10:20-10:40 Magnetostructural correlations in tetrahedral $[M(II)\{(E)P\text{r}_2\text{N}\}_2]$, $M = \text{Fe, Co, Ni}$; $E = \text{S, Se}$, and octahedral $[\text{Mn(III)}\{(OPPh_2)(OPPh_2)N\}_3]$ or $\text{trans-}[\text{Ni(II)}\{(OPPh_2)(E)P\text{r}_2\text{N}\}_2(\text{sol})_2]$, $E = \text{S, Se}$; $\text{sol} = \text{dmf, thf, dmsO}$, complexes.
P. Kyrtsis
- 10:40-11:10 Coffee break and group picture
- 11:10-11:30 Nitrene radicals' in the coordination sphere of cobalt complexes - characterization and reactivity.
M. Goswami, B. de Bruin, S. DeBeer, K. Ray
- 11:30-11:50 Fe(II) spin crossover complexes: Using 1-substituted tetrazole ligands to tune the spin transition properties.
D. Müller, C. Knoll, M. Reissner, G. Giester, P. Weinberger
- 11:50-12:10 Spectroscopy-constrained modelling of metalloenzymes.
D. A. Pantazis
- 12:10-12:30 On line monitoring of reaction intermediates and their kinetics using MS.
J. Roithová
- 12:30-14:00 Lunch (New Hotel of Marseille)
- 14:00-14:40 Spin states of myoglobin. Insights from QM/MM and MD.
J. Harvey
- 14:40-15:00 Non-empirical prediction of the photophysical and magnetic properties of systems with open d- and f-shells.
C. A. Daul
- 15:00-15:20 O_2 activation by Mn thiolate complexes.
M. Gennari, D. Brazzolotto, C. Duboc
- 15:20-15:40 Spin-crossover in cobalt(II) complexes as a means of switching organic ligands from a closed-shell to an open-shell state.
R. Dolai, M. Graf, H.-J. Krüger
- 15:40-16:00 An ionizable active-site tryptophan imparts catalase activity to a peroxidase core.
P. Vidossich, X. Carpena, P. Loewen, I. Fita, C. Rovira
- 16:00-18:00 MC meeting