Sixth scientific workshop: Lisboa, March 30-31, 2017

Organizers: Dr. Ricardo Louro (Univ. Nova de Lisboa), Dr. Paulo Martinho (Univ. Lisboa)

With support from **Portuguese Society of Chemistry**

SOCIEDADE PORTUGUESA DE QUÍMICA

International Invited Experts

- **Patrick Holland (Yale)**

Keynote speakers

- **Elvira Fortunato (Lisboa)**
- **Christian Limberg (Humboldt Univ. Berlin)**
- **Jalila Simaan (CNRS & Marseille)**

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time	*item*
Wednesday March 29	
all day	Europe: Travel to Lisboa
20.00-23.30	Carcavelos city center: Informal dinner

Thursday March 30

Scientific sessions (Hotel Riviera)

08.30-09.00	Registration
Session Chair: Peter Weinberger	
09.00-09.15	Opening of the workshop
09.15-09.55	**Keynote lecture: E. Fortunato**
09.55-10.15	Scientific talk: P. Comba
10.15-10.35	Scientific talk: M. Srnec
10.35-10.40	GROUP PICTURE
10.40-11.10	Coffee + Poster session
11.10-11.30	Scientific talk: J. McGrady
11.30-11.50	Scientific talk: M. Cimpoesu
11.50-12.10	Scientific talk: S. Suarez
12.10-12.30	Scientific talk: Y. Garcia
12.30-14.30	Light lunch

Session Chair: Hans-Jörg Krüger	
14.30-15.10	**Keynote lecture: C. Limberg**
15.10-15.30	Scientific talk: M. Orio
15.30-15.50	Scientific talk: D. de Sousa
15.50-16.10	Scientific talk: M. Feldt
16.10-17.20	Coffee + Poster session
17.20-17.40	Scientific talk: J. Isaac
17.40-18.00	Scientific talk: M. Melchor
20.00-23.30	Hotel Riviera: Conference dinner

Friday March 31

08.30-09.10	**Keynote lecture: J. Simaan**
09.10-09.30	Scientific talk: B. Le Guennic
09.30-09.50	Scientific talk: M. Halcrow
09.50-10.10	Scientific talk: E. Fournier
10.10-10.40	Coffee + Poster session
10.40-11.00	Scientific talk: A. Carvalho
11.00-11.20	Scientific talk: M. Zlatar
11.20-11.40	Scientific talk: M. Desage-El Murr
11.40-12.00	Scientific talk: M. Sensi
12.00-12.20	Scientific talk: M. Ahlquist
12.20-14.20	Light lunch

Session Chair: Carole Duboc

14.20-15.10	**Invited lecture: P. Holland**
15.10-15.20	Closing of the workshop
15.20-15.55	WG meetings
16.00-17.30	MC meeting
20.00-23.30	Carcavelos city center: Informal dinner

Saturday April 1

all day	Europe: Travel back home

A GLIMPSE INTO THE LIGAND FIELD THEORY FROM DENSITY FUNCTIONAL PERSPECTIVE

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Electronic structure of transition metal complexes are commonly rationalized within the Ligand Field Theory (LFT). For example, the combination of the LF splitting and the pairing energy determines spin-state preferences of a complex.[1] In LFT the Hamiltonian is parameterized in terms of one-electron (LF) parameters and two-electron repulsion integrals (Racaha's parameters) within the manifold of d-electrons. These parameters are determined from a fit to some experimental spectrum. The main drawback of LFT is its empirical nature, thus being limited to a description of the data, and predictions are often restricted to a chemical intuition. To overcome this, hybrid methodology, which combines a multideterminant DFT-based method with LFT, so called LF-DFT, has been developed.[2] At the same time, LF-DFT successfully tackles many shortcomings of standard DFT, including orbital degeneracy and excited states. It works by evaluating DFT energies of all the Slater determinants arising from a d^n configuration of the transition-metal ion in the environment of coordinating ligands using Kohn−Sham orbitals. This set of energies is then analyzed within a LF model to obtain variationally the energy and wave function of the ground and excited states. In doing so, both dynamical correlation (via exchange-correlation energy) and non-dynamical correlation (via LF CI) are considered. The quality of the LF-DFT for the calculations of d-d transitions is comparable to the high-level *ab initio* calculations, and in some cases, e.g. $[CrF_6]^{3-}$, $[MnF_6]^{2-}$, $[Mn(H_2O)_6]^{2+}$, $[Fe(H_2O)_6]^{3+}$ even outshines them.[1,3] One of the main strengths of LF-DFT is accurate prediction of magnitude and sign of the Zero-Field Splitting (ZFS) parameters,[4-6] as well as the orientation of the principal magnetic axes.[4] In addition, we can pin-point the excitations that control the sign and magnitude of the ZFS parameters.[4-6] Therefore, with a help from DFT based LF theory we can, hopefully, find a way to control the magnetic properties of transition metal complexes.

References:
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2) M. Atanasov, C.A. Daul, C. Rauzy, Chem. Phys. Lett. **2003**, 367, 737.
3) F. Vlahovic, Marko Peric, M. Gruden-Pavlovic, M. Zlatar, J. Chem. Phys. **2015**, 142, 214111.
4) M. Zlatar, M. Gruden, O. Y. Vassilyeva, E. A. Buvaylo, A. N. Ponomarev, S. A. Zvyagin, J. Wosnitza, J. Krzystek, P. Garcia-Fernandez, C. Duboc, Inorg. Chem. **2016,** 55, 1192
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