

Collaborative CSC-Bordeaux University (France) program

Doctoral School of the Chemical Sciences (ED n°40)

PhD topic proposed by Dr. Hab. Rodolphe Clérac (CNRS Research Director), clerac@crpp-bordeaux.cnrs.fr

Research team: « Molecular Materials & Magnetism » at Centre de Recherche Paul Pascal (CRPP, Pessac); <https://m3.crpp.cnrs.fr/>

Project Title: New Single-Molecule Magnets and Single-Chain Magnets Based On Redox-Active Ligands

The miniaturization of electronic components is a major challenge. In computer sciences, it is expected by 2019 that Moore's law will not be able to be respected with classical "top-down" strategies for miniaturization (photolithography...). New approaches and new techniques need to be developed. For data storage and information processing, a potential solution to this large problem can come in the form of single-molecule magnets (SMMs) or single chain magnets (SCMs) as these materials show appealing and potentially useful properties at the molecular scale. Their ability to store information at a nanometric scale makes them ideal candidates for future information storage devices as they offer a potentially much higher information storage density. In addition, their quantum properties can also be used as "qubit" for future quantum computers.

The research project aims at the synthesis, the study and the functionalization of new redox-active SMMs or SCMs with enhanced properties, through a rational design of the molecular components. The redox activity will be provided either by the metal centers or the bridging ligand, or both. This will allow us to tune and sometimes to enhance significantly the magnetic properties of the resulting molecular architectures, with the goal of making molecular magnets with higher operating temperatures [1-5], which is a long-standing challenge in this research area and a requirement for industrial applications.

The first step for this project will be to make a new class of ligand specially designed i) to act as a redox-active bridge between the metallic spin carriers with the possibility of being stabilized in a radical form (see the example of a nickel dinuclear complex in the Figure), ii) to increase dramatically the magnetic interactions between the spin carriers, iii) to stabilize delocalized mixed valence states to promote interesting electronic, optical and improved magnetic properties [1-5].

Initially bimetallic "prototype" systems will be synthesized by reaction of the bridging ligand with "capped" metal centers. This will allow us to undertake complete magnetic and electronic

studies of both the metal centers and ligand within the complex. Further polynuclear complexes as potential SMMs as well as one dimensional coordination networks with potential SCM properties will be synthesized using dinuclear compounds as building blocks (see figure), with a better understanding of their behavior. All these new potential enhanced SMMs/SCMs will be fully characterized and investigated.

The achievement of this innovative and ambitious research should have a strong impact in the molecular magnetism community, and could contribute to the next generation of some basic components of computers. See the recent published papers from our group:

[1] *Angew. Chem. Int. Ed.*, **2018**, *57*, 7841; [2] *Nature Chemistry*, **2018**, *10*, 1056; [3] *J. Am. Chem. Soc.*, **2019**, *141*, 7721; [4] *Chem. Commun.*, **2020**, *52*, 4906; [5] *Science*, **2020**, Vol. *370*, Issue 6516, 587.

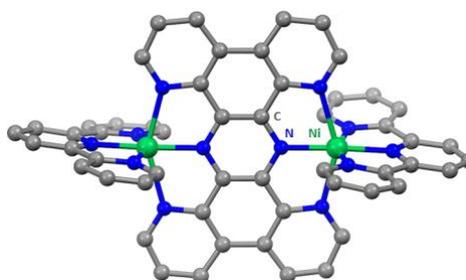


Figure Crystal structure of the cationic complex $[\text{Ni}_2(\text{tphz})(\text{tpy})_2]^{4+}$ using the redox-active tetrapyrrophenazine (tphz) bridging ligand.[3]

Personal qualifications and skills for the applicants: Good knowledge of, and experience with preparative coordination and/or solid-state inorganic chemistry is mandatory. Experience with X-ray crystallography is an advantage. Fluency and clarity in spoken as well as written English is essential.

Short CV: [Rodolphe Clérac](#), born in 1971 in Versailles (France), received his education in Physical-Chemistry at the University of Bordeaux 1, France. His Ph.D. work was devoted to the physical properties of molecular antiferromagnetic materials under the supervision of Prof. C. Coulon (in 1997). After short post-doctoral stay in the group of Prof. O. Kahn (ICMCB, Bordeaux), he joined in 1998 Prof. K. R. Dunbar's group at Michigan State University (East Lansing, Michigan, USA) and worked on the magnetic properties of coordination chemistry based materials. In 1999, he moved with Prof. K. R. Dunbar's group to Texas A&M University (College Station, Texas, USA) where he collaborated with Prof. F.A. Cotton on the magnetic properties of metal-metal bonded complexes. He joined the University of Bordeaux 1 in 2000, as associate professor, then in 2008 became full CNRS researcher and in 2013 was promoted CNRS Research Director. He was elected in 2019 at the European Academy of Sciences, became in 2014 a distinguished fellow of the French Chemical Society and received various awards including in 2017 the France-Berkeley Fund Award, in 2014 the National Chinese Award of the "1000 Talents Program" and in 2009 the Young Researcher award of the Physical Chemistry Division of the French Chemical Society. Since 2000, Dr. R. Clérac has developed at the Centre de Recherche Paul Pascal (CNRS) a research group on "molecular materials & magnetism" interested in the synthesis and physical studies of molecular materials (that is currently composed of 1 Professor, 1 Assistant Professor, 3 CNRS researchers, 1 Assistant Engineer, 1 Post-docs, 5 PhD students). The main subjects currently developed in his group deal with (i) macroconjugated polyaromatic molecules, (ii) molecule-based magnets, (iii) switchable paramagnetic complexes, and (iv) magnetic and/or electro-active solutions and liquid-crystals. In this research field, he has published ca. 510 articles with ca. 22600 citations and has an h factor of 78. During his career, Dr. R. Clérac has trained 31 postdocs, 25 PhD students (including 3 Chinese PhD students), 22 Master students, 48 visiting PhD students (for short training period) and 24 undergraduate students. Importantly Dr. R. Clérac has also developed a scientific network of active collaborations across the globe with currently 79 research teams in 27 different countries.

History of Rodolphe Clérac collaborations with Chinese institutions:

- **Collaborations with 11 Chinese research groups (29 joined publications since 2010):** Prof. E. Wang & Prof. Y.-G. Li, Liaoning Normal University, Jilin University, Changchun; Prof. G. Wu & Prof. S. Qiu, Jilin University, Changchun; Prof. J. Tang, Chinese Academy of Sciences, Changchun; Dr. G.-F. Xu, Tianjin University of Commerce, Tianjin; Prof. D. Li, Central China Normal University, Wuhan; Prof. Z. Xu, City University of Hong Kong, Kowloon, Hong Kong; Prof. D. Xue, Dalian University of Technology, Dalian; Prof. D.-Z. Liao, Nankai University, Tianjin; Prof. X.-M. Zhang, Shanxi Normal University, Linfen; Prof. L. Zhang, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian; Prof. X. Bao, Nanjing University of Science and Technology, Nanjing; Prof. M.-L. Tong & Dr. J.-L. Liu, Sun Yat-Sen University, Guangzhou.
- **17 talks given in China since 2010, including 5 invited conferences.**
- **2 major awards in relation with Chinese organizations:** June 2008: Distinguished Visiting Professor at Northeast Normal University, Changchun; 2014: National Chinese Award of the "1000 Talents Program" at Central China Normal University, Wuhan.
- **14 invitations in China:** **2019:** Nanjing University of Science and Technology, Nanjing University; **2018:** Sun Yat-Sen University, Southern University of Science & Technology Shenzhen; **2017:** Frontier Institute of Science and Technology Xi'an Jiaotong University; **2016:** Nanjing University of Science and Technology, Nanjing University, Nankai University, Peking University & Sun Yat-Sen University; **2015** and **2013:** Central China Normal University, Wuhan; **2010:** Nanjing University; Peking University.
- **5 Chinese professors invited since 2010 in my laboratory, as well as 9 Chinese students (Master & PhD students and postdoc fellows)**