PhD position | Quantum chemical inspection and magnetic measurements of organolanthanide Single Molecule Magnets

Contract	Fully funded 3-year PhD position starting October 2024
Institution	Institut des Sciences Chimiques de Rennes (ISCR)
Supervisors	Dr. Boris LE GUENNIC, Pr. Olivier CADOR
Contact	Dr. Boris LE GUENNIC, Email: boris.leguennic@univ-rennes.fr

A full-time 3-year PhD position is available in the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR) under the supervision of Dr. Boris Le Guennic and Pr. Olivier Cador. The position is for three years starting October 2024 and fully funded by the French Research National Agency (ANR). The project is dedicated to the simulation, using quantum chemistry approaches, and advanced magnetometry investigations of organolanthanide Single Molecule Magnets.

Organolanthanide chemistry has become a booming research field over the last 25 years. In particular, over the last years, tremendous advances have been made in the field of single-molecule magnets (SMMs),[1] triggered by the 2017 ground-breaking discovery of the first lanthanide-based SMM with magnetic hysteresis close to liquid nitrogen temperature, i.e. $[Dy(Cp^{ttt})_2][BAr_4]$.[2] Since then, many other carbon-based mono- and di-anionic ligand types have been successfully investigated, leading to the best performing sandwich complex $[DyCp^*(C_5iPr_5)][BAr_4]$.[3]

Within this context, and in close collaboration with our experimental partners, the PhD candidate will concentrate on the proper description of the electronic structure of the target complexes (**Figure 1**) using state-of the art ab-initio wavefunction based quantum chemical approaches. A close look at spin-phonons interactions will be also necessary fo a complete picture.[4] Moreover, as the impact of pressure on the electronic and magnetic properties will also be investigated, the PhD candidate will also investigate geometries under hydrostatic pressure using DFT with periodic boundary conditions.

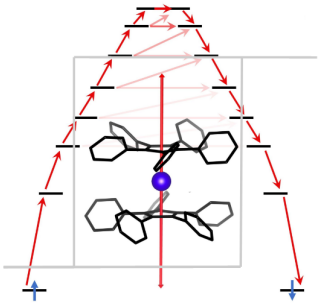


Figure 1 | Example of predicted SMM properties for the hypothetical $[Dy(C_5Ph_5)_2]^+$.

Due to the extreme sensibility of the targeted complexes, the second challenge of this PhD will concern their proper magnetic investigations based on magnetometry. In more details, the static and dynamic magnetization needs to be carried out in inert atmosphere and in controlling the thermal stability of the materials. The complete magnetic characterization will then be confronted with the results of the quantum chemical calculations.

References

[1] (a) Woodruff, D. N.; Winpenny, R. E. P.; Layfield, R. A. *Chem. Rev.* **2013**, *113*, 5110; (b) Zhu, Z.; Guo, M.; Li, X.-L.; Tang, J. *Coord. Chem. Rev.* **2019**, *378*, 350.

[2] (a) Goodwin, C. A. P.; Ortu, F.; Reta, D.; Chilton, N. F.; Mills, D. P. *Nature* **2017**, *548*, 439; (b) Guo, F.-S.; Day, B. M.; Chen, Y.-C.; Tong, M.-L.; Mansikkamäki, A.; Layfield, R. A. *Angew. Chem. Int. Ed.* **2017**, *56*, 11445.

[3] Guo, F.-S.; Day, B. M.; Chen, Y.-C.; Tong, M.-L.; Mansikkamäki, A.; Layfield, R. A. *Science* **2018**, *362*, 1400.

[4] (a) Mondal, S.; Lunghi, A. *J. Am. Chem. Soc.* **2022**, *144*, 22965. (b) Staab, J. K.; Chilton, N. F. *J. Chem. Theory Comput.* **2022**, *18*, 6588.

Related references

[1] Moutet, J.; Schleinitz, J.; La Droitte, L.; Tricoire, M.; Pointillart, F.; Gendron, F.; Simler, T.; Clavaguéra, C.; Le Guennic, B.; Cador, O.; Nocton, G. *Angew. Chem. Int. Ed.* **2021**, *60*, 6042 HAL

[2] Korzynski, M. D.; Bernhardt, M.; Romankov, V.; Dreiser, J.; Matmon, G.; Pointillart, F.; Le Guennic, B.; Cador, O.; Copéret, C. *Chem. Sci.* **2022**, *13*, 10574 HAL

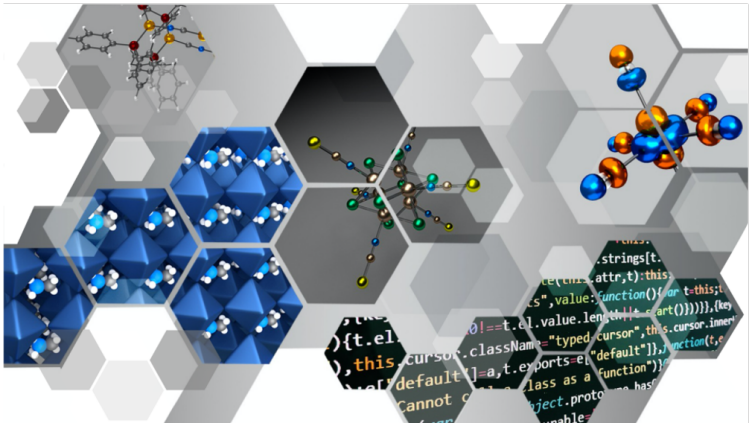
[3] Pointillart, F.; Flores Gonzalez, J.; Douib, H.; Montigaud, V.; McMonagle, C. J.; Le Guennic, B.; Cador, O.; Pinkowicz, D.; Probert, M. R. *Chem. Eur. J.* **2023**, *29*, e202300445 HAL

[4] Wang, H.; Zhu, Z.; La Droitte, L.; Liao, W.; Cador, O.; Le Guennic, B.; Tang, J. *Chem. Sci.* **2023**, *14*, 7208 HAL

Profile of the candidate | A degree in Chemistry or Physics is required. Solid background in at least one of the following topics is expected: molecular quantum chemistry (theory and/or practice), theoretical spectroscopy, crystal-field theory. The successful candidate should be highly motivated and eager to learn and apply advanced modelling concepts. Scientific programming and communication skills and the ability to work in close collaboration with other theoreticians and experimentalists will be a plus.

The CTI team | The PhD student will work in the the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR). The CTI team gathers computational chemists and physicists (15 permanent staff members, approx. 15 students and postdocs) with complementary skills, working with a broad set of quantum chemical tools, ranging from high precision ab initio wave function-based calculations to fast semi-empirical methods.

CTI team members are interested in diverse type of systems, including molecular species, bulk materials and surfaces, mainly of high experimental and societal interest. The CTI team provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as regularly receiving internationally-recognized visitors. The quantum chemistry codes necessary for the project are available together with considerable local, national and European computing resources.



Inquiries | Potential candidates should contact by email Dr. Boris Le Guennic with an up-to-date CV and a motivation letter.