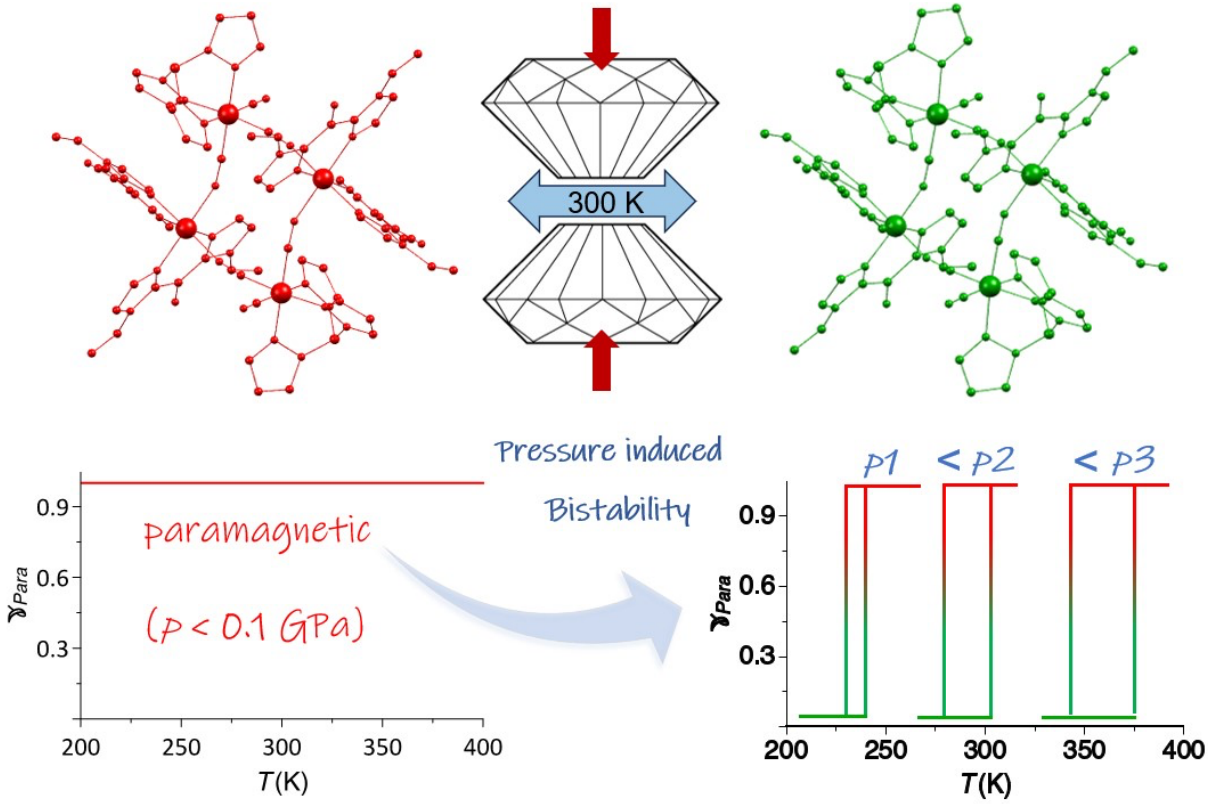
Pressure-Sensitive Molecular Switches

Our group is working on the design of molecular switches showing controllable electron-transfer (ET) under external stimuli (temperature, light, electric field). These molecules could find potential application as memory device or sensor. Since few years, we have used an almost unexplored stimulus, hydrostatic pressure, on a family of tetranuclear square complexes of general formula $\{[Fe(Tp)(CN)_3]_2[Co(vbik)_2]_2\}\cdot(A)_2$ where Tp is a tris(pyrazolyl)borate ligand, vbik - bis(vinylimidazolyl)ketone, A – a mono-charged anion (figure below). At ambient pressure, this complex is in a paramagnetic state, Fe^{III}_{LS}-Co^{II}_{HS}, but the application of an external pressure converts this compound into a switch, showing a bistability domain of controlled width (see figure). We have rationalized the unusual pressure-induced ET of one square complex by high-pressure X-ray diffraction on single crystal and developed a promising approach for probing the fundamental aspects of molecular switching. This thesis is aimed to demonstrate the versatility of this approach by applying it to other related molecular systems.



The recruited PhD candidate will work for enlarging the family of pressure-sensible molecular materials based on square complexes. This can be achieved by adequate substitution of the ligands on both Co and Fe sites. He/She will start by the synthesis of new functionalized bis(imidazolyl)ketone ligands (^{R}bik) bearing aryl group and then the square complexes $\{[Fe(Tp)(CN)_3]_2[Co(^Rbik)_2]_2\}\cdot(A)_2$. Parallelly, he/she will use the functionalized tris(pyrazolyl)methane (^{R}Tpm) ligands to obtain neutral $\{[Fe(^RTpm)(CN)_3]_2[Co(L)_2]_2\}$ complexes without any counterions in the crystal structure. The PhD candidate will carry out the characterizations of the prepared compounds by means of electrochemical, NMR and spectroscopic techniques as well as by magnetic measurements. Selected compounds will be analyzed by advanced high-pressure (HP) magnetic characterizations and HP-Raman, HP-SC-XRD analysis in the frame of our established local and national collaborations.

Funding source and thesis duration

Ministry of higher education and research of French government, 36 months from October 2024.

Application deadline

27th April 2024.

Profile and skills required

We are looking for a young scientist having a master degree in molecular chemistry with skills in organic or inorganic synthesis and characterization of molecular compounds. The PhD candidate must have good knowledge in inorganic chemistry. Basic knowledge in magnetic materials would be a plus but is not mandatory. The success of this project will depend on the PhD candidate ability to acquire knowledge in several different fields of research and to adapt to different learning environments.

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