Theoretical Control and Modeling of Bistability in Molecular Switches with Experimental Insights

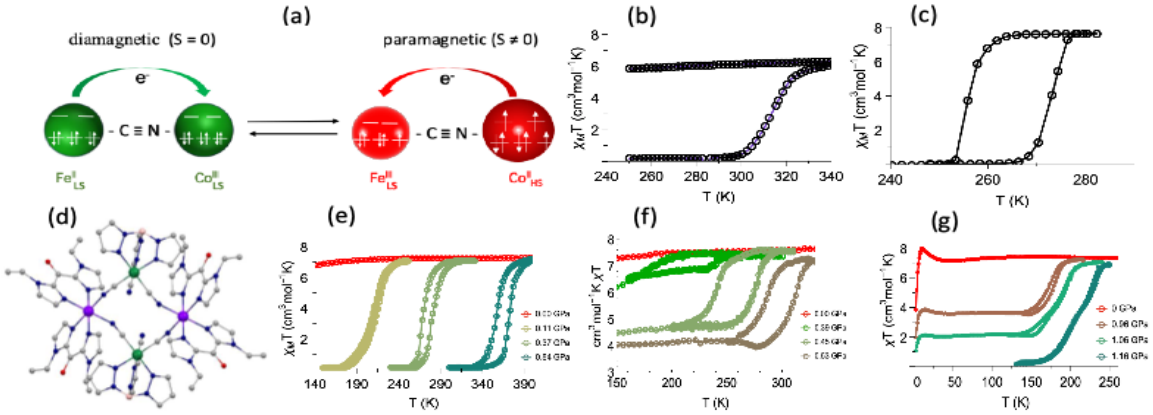
General Information

- Work location : Sorbonne University Abu Dhabi (SUAD), Abu Dhabi, United Arab Emirates, Institut parisien de chimie moléculaire (IPCM), Paris, France
- Type of contract: PhD fixed-term contract, fully funded by Sorbonne University Abu Dhabi
- Contract duration: 36 months
- Tentative start date of the PhD: November 10 2025
- CN Section: 28 – Dense matter and materials

Context and Goal

Magnetic molecular switches are bistable compounds which can change their electronic configuration upon external stimuli such as light, temperature and pressure. The control of this bistability is crucial for the potential applications of molecular switches as sensors, electronic devices and solid refrigerants. On one hand, the team in Abu Dhabi has strong expertise in numerical simulation of spin transition systems, particularly in understanding the interplay between elasticity, nucleation dynamics, and cooperative effects in spin transition materials. Their research integrates microscopic modeling, Monte Carlo simulations, and heat diffusion approaches to explore how external stimuli excitation influence the structural and magnetic bistability of molecular systems.[1-4] On the other side, the team in Paris is skilled in designing cyanide-bridged Fe_2Co_2 square complexes that exhibit controllable electron transfer - coupled spin transition (ETCST). These complexes bears the general formula: $\{[Fe(^{R1}Tp)(CN)_3]_2[Co(^{R2}bik)_2]_2\}\cdot(A)_2$ (where A stands for the counter-anion, ^{R1}Tp represents tris(pyrazol-1-yl)borate derivatives and ^{R2}bik, bis(vinylimmidazole-2-yl)ketone derivatives).[5] The change in ligand's substituents or counter-anion can modify the crystal packing, thus influencing the supramolecular interactions and the core structure of the complexes. This leads to a diversity in ETCST process (see figure below).[5-7] The combined expertise of both teams will allow us to refine the design of new switchable materials, optimize their cooperative response under external stimuli, and develop predictive strategies for tailoring bistability in molecular-based electronic and magnetic devices.

The recruited PhD candidate will develop new computational approaches, guided by the expertise of the SUAD team, to simulate the spin-state bistability of cyanide-bridged Fe_2Co_2 complexes, based on the experimental results recently obtained by the Sorbonne Paris team. In the second phase of the project, the candidate will join the team in SU Paris to perform experimental work, including the synthesis of new FeCo complexes, guided by the theoretical results obtained during the initial phase.



Various thermally activated ETCST behaviors of $\{[Fe(^{R1}Tp)(CN)_3]_2[Co(^{R2}bik)_2]_2\}\cdot(A)_2\cdot S$ square complexes with and without pressure application. (a) Schema of ETCST. (b) Thermal ETCST of **1** (R_1 = H, R_2 = vinyl, A = PF_6^- and S = nH2O·mMeOH) under ambient pressure. (c) Cooperative thermal ETCST of **3** (R_1 = H, R_2 = vinyl, A = ClO_4^- and S = $2CNCH_3$) under ambient pressure. (d) Molecular structure of **2** (R_1 = H, R_2 = vinyl, A = BF_4^- and S = 2 MeOH). (e) Thermal ETCST of **2** under various pressures. (f) Thermal ETCST of **3** (R_1 = H, R_2 = vinyl, A = PF_6^- and S = 2MeOH) under different pressures. (g) Thermal ETCST of **4** (R_1 = 2 methyl, R_2 = 2 methyl, A = BF_4^- and S = 2MeOH) under different pressures.

Profile and skills required

We are looking for a highly motivated student with a master's degree in physical chemistry, physics, or materials science who is eager to work at the intersection of experiments and simulations.

Contacts:
Ahmed Slimani: Ahmed.Slimani@sorbonne.ae ; Yanling Li : yanling.li@sorbonne-universite.fr

References

1. A. Slimani *et al, Physical Review B, **2015**, 92, 014111*
2. A. Slimani *et al, Physical Review B, **2023**, 108, 064107*
3. A. Slimani *et al, Physical Review B, **2017**, 108, 174104*
4. A. Slimani *et al, Phys. Chem. Chem. Phys., **2018**, 20, 28583-28591*
5. Y. Li *et al*, *Angewandte Chemie*, **2020**, 132 (39), pp. 17425-17429
6. B. Xu *et al*, *Chemistry of Materials*, **2024**, 53(29), pp. 8990-9001
7. B. Xu *et al*, *Inorganic Chemistry frontier*, **2024**,12, pp. 744-756