Photoactive Derivatives of Cu(I) Ion for Reversible Energy Storage

General Context. The preparation of new molecular materials enabling the capture and reversible storage of chemical and solar energy is crucial to promote the transition to a sustainable economy. In the current context, it is essential to define synthesis methods that are simple, cost-effective, and based on metals being both low in toxicity and widely available on a global scale. In this regard, Cu(I)-based compounds offer promising prospects not only due to the low cost and abundance of copper but also to the diverse structural and photoactive properties that these complexes exhibit.

Project. This work will focus on the preparation and the study of the solid-state photoactive and thermal properties of novel polymetallic Cu(I) molecular assemblies. These derivatives will enable the molecular-scale storage of chemical and/or light energy through reversible coordination bond formations or photochemical reactions, allowing the subsequent release of energy. Based on synthetic approaches mastered in the group,[1] that are straightforward to implement, Cu(I) based derivatives with tunable molecular architectures and properties will be prepared. The newly prepared compounds, before and after energy captation, will be characterized using various techniques such as powder and single-crystal X-ray diffraction, NMR, UV-Vis, and IR spectroscopy. The temperature-dependent photophysical properties (emission spectra, quantum yield measurements, and excited-state lifetimes) of the emissive materials obtained will be studied in the solid state, allowing to elucidate the electronic structure of the synthesized species in both their ground and excited states. Extensive thermogravimetric analysis measurements will be carried out to quantify the amounts of energy stored and to study and rationalize the reversibility of the energy storage processus.

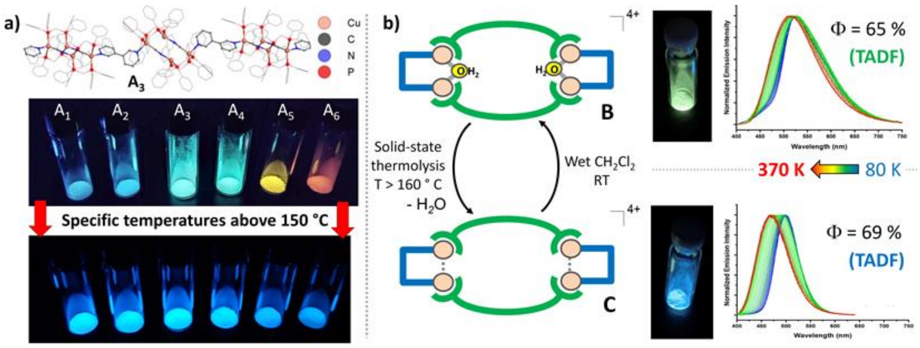

Figure: a) examples of solid-state thermal transitions of the luminescence of the 1D-CPs **A_{1-6}**,[1a] b) luminescent metallacycle **B** bearing a bridging aqua ligand and solid-state thermal transition towards the metallacycle **C** [1b].

The candidate will join the INSA component of the Solid State Chemistry and Materials team at the Institute of Chemical Sciences of Rennes (https://iscr-csm.insa-rennes.fr/members/). As part of this work, the recruited student will be actively involved in ongoing collaborations within our research group (with possible mobility), particularly with the groups of Professor Dr. Manfred Scheer at the University of Regensburg in Germany and Professor Leonard MacGillivray at the University of Sherbrooke in Canada.

Candidate's profile. Skills in synthetic molecular chemistry as well as in classical analytical techniques (NMR, UV-vis, IR, etc.) are requested. A strong interest in solid-state characterization such as X-ray crystal structure resolution and solid-state photophysical studies is also required. Skills in shaping molecular materials in polymer matrices would be appreciated, as well as good knowledge in English.

Contact (for more information and application procedure).
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[1] Lescop et al. a) *Adv. Opt. Mat.*, **2024**, *20*, 2400347; b) *Angew. Chem. Int. Ed.*, **2024**, e202413151; c) Acc. *Chem. Res.* **2017**, *50*, 885. *J. Am. Chem. Soc.*, **2018**, *140*, 12521.