



## PhD position in Grenoble

### Heterometallic sulfide clusters for small molecules activation

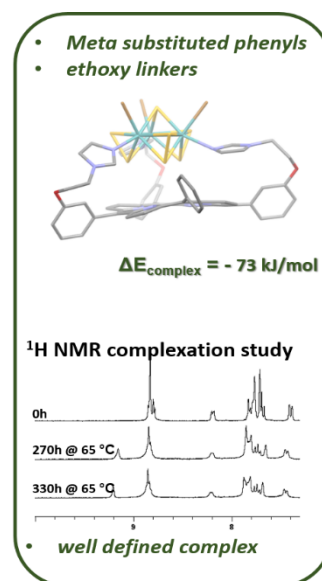
**Organization:** Laboratoire Chimie et Biologie des Métaux (LCBM, UMR 5249 CEA-CNRS-UGA)

**Project Leaders:** Matthieu Koepf and Vincent Artero

#### Project Description:

##### Project summary:

The development of strategies for the activation and conversion of small molecules ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{N}_2$ ) into basic chemicals feedstock ( $\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{NH}_3$ ) is of particular interest for the transition towards more sustainable economy. In stark contrast with the demanding thermochemical processes currently used in the industry, such as the Haber-Bosch and Fisher-Tropsch processes for the reduction of  $\text{N}_2$  into  $\text{NH}_3$  and alkanes synthesis from  $\text{CO}$ , respectively, some living organisms offer examples of fascinating biological pathways supporting related transformations by the use of specialized biocatalysts. One family of enzyme, the Nitrogenases, is particularly intriguing. It is known to drive the reduction of  $\text{N}_2$  into  $\text{NH}_3$  in vivo, via controlled proton and electron transfers, and has been shown to support the unexpected reduction of carbon oxides ( $\text{CO}_2$ ,  $\text{CO}$ ) into low-mass alkane/alkene derivatives ( $\text{CH}_4$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$ ...) in vitro when treated with strong chemical reductants. This remarkable activity is promoted by unusual (hetero)metallic sulfides cofactors of the general formula  $[\text{MFe}_7\text{S}_9\text{C}]$  ( $\text{M} = \text{Mo}$ ,  $\text{V}$ ,  $\text{Fe}$ ) and has driven the preparation of a variety of bio-inspired metal-sulfide clusters. Remarkably, synthetically accessible  $[\text{Fe}_4\text{S}_4(\text{SR})_4]$ ,  $[\text{Mo}_2\text{Fe}_6\text{S}_8(\text{SR})_9]$ , and  $[\text{Mo}_3\text{FeS}_4(\text{Cp})^*_3]$  cores appear to support related activities leading to the reduction of  $\text{N}_2$  and  $\text{CO}/\text{CO}_2$  under controlled conditions. In this project, we aim to investigate the ability of advanced synthetic ligand frameworks to stabilize and tune the reactivity of  $[\text{MMo}_3\text{S}_4]$  ( $\text{M} = \text{none}$ ,  $\text{Mo}$ ,  $\text{Ni}$ ) clusters towards nitrogenase substrates.



**Methods and Materials:** synthetic organic chemistry, coordination chemistry, physical organic chemistry, analytical chemistry, electrochemistry.

**Requirements:** strong interest in molecular chemistry and electrochemistry, solid experience in coordination chemistry/synthetic organic chemistry, good knowledge of the usual spectroscopic and electrochemical analytical methods.

**Application Process:** Interested candidates should submit their CV, motivation letter, copies of academic transcripts, degrees, and names and contact information of two references to Matthieu Koepf (matthieu.koepf@cea.fr). **APPLICATION DEADLINE: application will be considered until the position is filled (latest 1st of June 2023)**