

# Understanding dioxygen activation by manganese complexes using mass spectrometry and DFT calculations (ManOx)

PhD Grant (3 years) in mass spectrometry and organometallic chemistry

Funding: ANR JCJC ManOx  
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## Scientific context and objectives

Dioxygen activation by transition metals plays a key role in both biological and chemical processes. Indeed, oxygen is cheap and environmentally friendly as an oxidant used in chemical synthesis. In addition, oxygen activation is also linked to innovations in energy production in H<sub>2</sub>/O<sub>2</sub> fuel cells. Despite decades of research, a rapid, robust, inexpensive and efficient catalyst able to activate oxygen remains undiscovered.

Understanding the oxygen activation mechanism and the characterization of reaction intermediates is therefore essential.

The main challenging objective of this project is **the generation and the identification of manganese-O<sub>2</sub> species by mass spectrometry** with the aim of explaining how O<sub>2</sub> activation by manganese species occurs and to unravel connections between the different Mn-O<sub>2</sub> intermediates. The characterization of Mn-O<sub>2</sub> adducts and the **determination of their kinetic and thermodynamic parameters** will be realized by ion-molecule reaction or (photo)dissociation in the gas phase using advanced mass spectrometric techniques.

## Applicant profile

The candidate should have a background in organic/organometallic chemistry. Previous experience in mass spectrometry would be highly appreciated but not necessarily required. Applicants should provide evidence of academic performance, excellent English writing and communication skills, and a taste for multidisciplinary teamwork. The candidate must also be motivated to work on scientifically difficult problems and have the desire to set up new experiments.

## Documents for application

Please submit your application in English, including a cover letter describing your motivations, a curriculum vita, and two reference letters.