

## Investigating Homo- and Heterometallic dimers by Resonance X ray Emission Spectroscopy

Rebeca Gomez Castillo

PhD Student at Max Planck Institute CEC, Germany.

Inorganic Spectroscopy Department. Prof. Serena DeBeer's group.

The binuclear iron site in class Ia ribonucleotide reductase catalyzes the formation of deoxyribonucleotides from ribonucleotides, an essential step in the synthesis of DNA<sup>1</sup>. The ribonucleotide reductase from *Chlamydia trachomatis* (Ct) **CtR2** loads one Mn and one Fe atom in the active site. While the protein can be reconstituted with two irons or two manganese, the optimal reactivity is only achieved when the active site contains both FeMn in a 1:1 ratio<sup>2</sup>. Does metal-metal bonding play a role in the stability/reactivity of these active sites?

Resonance XES has been proposed in this work to study Charge Transfer interactions between a series of model FeMn complexes with known crystal structures, revealing intriguing results when resonantly exciting in both pre-edge and CT regions.

A systematic Mn and Fe K $\beta$  Resonant Emission X-ray Spectroscopy (RXES) study was conducted at the Cornell High Energy Synchrotron Source on a series of synthetic model complexes  $[(\text{ttacn})_2\text{M}(\text{III})(-\text{O})(\mu\text{-OAc})_2\text{M}(\text{III})]^{2+}$ . We were able to monitor how the K- $\beta$  emission changes as the excitation energy moves through the 1) 1s to 3d pre-edge transitions, 2) the higher energy pre-edge transitions that have been assigned as metal-to-metal charge transfer (MMCT), and 3) the continuum. Results show a strong dependence of the resonant emission on the excitation energy and suggest that K $\beta$  RXES at incident energies above the pre edge region is likely ascribed to a MMCT/LMCT event.