Dithiolene Containing Peptides: Synthesis and Characterisation of their Molybdenum Complexes.

The industrial revolution has increased the atmospheric concentration of CO_2 , which makes it a major concern for the environment. The abundance of this polluting gas can be tackled in a useful manner by CO_2 valorization, that is its conversion to high value-added chemicals and fuels. This valorization can be the basis of a greener and more sustainable chemical industry. However, the thermodynamic and kinetic stability of CO_2 makes its activation a challenging task. Formate dehydrogenases are enzymes present in Nature which have a Mo or W metal center in their active site bound to two pyranopterin guanosine dinucleotide units, known as the molybdenum cofactor (Moco). These enzymes can reversibly convert formate to CO_2 and thus, they have attracted a lot of interest in recent years. Many research groups have tried to develop biomimetic and bioinspired models of these enzymes, but only a few are hardly functional. Our aim is to develop a new generation of bioinspired Mo complexes by incorporating dithiolene units in peptides and studying their structures, properties and reactivities using both experimental and theoretical approaches. We will explore the capabilities of these Mo complexes to behave as active electrocatalysts for mediating CO_2 reduction.

