

## Plan Overview

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*A Data Management Plan created using DMPTool*

**Title:** FROM SINGLE ATOM TO SUPPORTED NANOPARTICLES CATALYSTS: THE USE OF METAL COMPLEXES TO PRODUCE A NEW CLASS OF CATALYSTS FOR METHANE AND CO<sub>2</sub>

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**Template:** UNICAMP-GENERICICO: Aplicável a todas as áreas

### Project abstract:

This post-doctorate project aims to produce a new class of catalysts by using metal complexes of interest for methane and CO<sub>2</sub> conversion. In the first part of this project, we will use metal complexes of Ni, Fe, Cu and Au that are commercially available or that can be synthesized by well-established routes, such as (cyclohexadiene) iron tricarbonyl. This will allow us to focus on the parameters that determine the successful anchoring and dispersion of the metal complexes on different supports, depending on the target reaction (zeolite; MgAl<sub>2</sub>O<sub>4</sub>, SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub> and CeO<sub>2</sub>). Characterization techniques such as DRIFTS, XPS and state of art HAADF-STEM with aberration corrector will be used. The catalysts will be submitted to heating treatments, to decompose the metal complexes, and we will study the parameters that determine the metal species that are formed, targeting to tune from single atom to homogenous nanoparticles (<3 nm in diameter). Besides parameters such as nature of the support, pre-treatments (reducing/oxidizing), heating protocol and atmosphere during to promote the metal complex decomposition, we expect that the nature of the ligands will also contribute to the species that are formed since they will tune the overall interaction with the support. The most promising materials will be tested in the reactions involving CO<sub>2</sub> and CH<sub>4</sub> conversion, in collaboration with

other members of this thematic project, and their performance will be correlated to their structural and electronic properties. One important aspect will be the stability of the catalysts under reaction conditions and we will perform a detail characterization of the catalysts post-reaction. According to the results, the second part of this project will involve the synthesis of new bimetallic complexes, specially targeting to produce bimetallic supported catalysts

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## FROM SINGLE ATOM TO SUPPORTED NANOPARTICLES CATALYSTS: THE USE OF METAL COMPLEXES TO PRODUCE A NEW CLASS OF CATALYSTS FOR METHANE AND CO<sub>2</sub>

DADOS DE CARACTERIZAÇÃO E ATIVIDADE CATALÍTICA DE MATERIAIS CONTANDO NANOPARTÍCULAS OU ÁTOMOS ISOLADOS PREPARADOS A PARTIR DA HETEROGENEIZAÇÃO E DECOMPOSIÇÃO TÉRMICA DE COMPLEXOS METÁLICOS CONTENDO DERIVADOS DE LIGANTES SALEN.

DUBLIN CORE - TÍTULO, AUTOR, COLABORADORES, PALAVRAS-CHAVE, RESUMO, FORMATO, LÍNGUA, AGÊNCIA FINANCIADORA, NÚMERO DO PROJETO, LOCALIZAÇÃO.

OS DADOS NÃO ESTÃO SUJEITOS À NENHUMA RESTRIÇÃO ÉTICAS OU LEGAIS.

OS DADOS ESTARÃO SOB LICENÇA CC\_BY.

TEXTUAIS (.DOC), DADOS DE CARACTERIZAÇÃO (RMN, FTIR, DRX, TEM, XAS, ETC) SERÃO CONVERTIDOS EM .TXT OU IMAGENS .TIFF. EM CASOS ESPECÍFICOS DE DADOS COM SOFTWARE EXCLUSIVO, SERÁ FEITA A INDICAÇÃO DO MESMO.

DURANTE A VIGÊNCIA, OS DADOS SERÃO MANTIDOS NO GOOGLE DRIVE DO PESQUISADOR. AO TÉRMINO DA VIGÊNCIA, OS DADOS CONTINUARÃO NO GOOGLE DRIVE DO PESQUISADOR POR TEMPO NÃO INFERIOR À 10 ANOS, E SERÃO TAMBÉM DEPOSITADOS NO REPOSITÓRIO DA UNICAMP, SEGUINDO AS POLÍTICAS DE PRESERVAÇÃO, BACK-UP E ARQUIVAMENTO.

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