CELSA
Central Europe Leuven Strategic Alliance

CELSA - Collaborative research project - Application form - COVER PAGE

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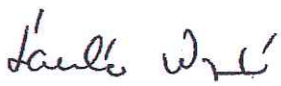
Signature: 

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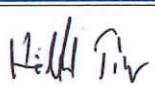
Signature: 

4. Non confidential and public friendly summary (max. 2000 characters)

Project title: Copper clusters as model catalysts for carbon dioxide hydrogenation to methanol

Summary:

Carbon capture and utilization is a promising strategy to avoid CO_2 release in the atmosphere. Industrially, CO_2 is converted to the alternative fuel methanol using as catalyst a mixture of Cu, ZnO and Al_2O_3 nanoparticles. Despite the industrial importance, the nature of the active centers and the working principle of the catalyst are not fully understood on an atomistic level. This lack of knowledge hampers the development of a more effective catalyst that allows hydrogenating CO_2 to methanol at lower temperatures, thereby reducing the energy input and the cost of the process.

In this collaborative research project, we model the active sites of the catalyst by pure and zinc doped copper clusters, either isolated in the gas phase or deposited on an alumina support. The objectives of this novel approach are to measure, with atomic precision, the cluster size dependence of elementary reaction steps and to investigate the role of zinc as promotor element. In a first step, the active sites and the binding configuration of CO_2 and H_2 on isolated pure and Zn-doped copper clusters will be identified. Next, the reaction rates for the adsorption of either CO_2 or H_2 and for the co-adsorption of both molecules on the isolated clusters will be measured. Last, the role of the alumina support on the hydrogenation of CO_2 will be studied for soft-landed clusters. The experimental characterization (Leuven) is complemented with first principles modelling (Budapest) to obtain insight into the structural and electronic effects of the reaction steps.

The project will yield a thorough understanding of the CO_2 hydrogenation, which eventually will allow for the design of an improved catalyst. The project also will strengthen the collaboration between the KU Leuven and the Budapest University of Technology and Economics and will lay the foundations for joint European project applications that make use of clusters as model systems for heterogeneous catalysis.

5. List 5 key words

carbon fixation, gas phase reactivity, clusters of atoms, heterogeneous catalysis,
density functional theory calculations