MAX-PLANCK-GESELLSCHAFT
Fritz-Haber-Institut

NOMAD
NOVEL MATERIALS DISCOVERY

iqtc
Institut de Química Teòrica
i Computacional

Storage, release and conversion of CO_2 to valuable chemicals and fuels

The NOMAD CoE provides a huge amount of computational data already available at the repository and also offers to perform new high-quality calculations for materials where important information is missing in the database. Here, we are carefully listening to suggestions from our industrial colleagues. A particular example where interest from various industrial partners has arisen includes the storage, release and conversion of CO_2 towards the creation of valuable chemical and fuels such as methanol or syngas and this is being developed jointly by the groups at the Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB) and the group of the Theory Department at the Fritz-Häber Institut of the Max Planck Society in Berlin.

In the case of CO_2 conversion, interest has been also shown from I-deals, a company coordinating the Methanol fuel from CO_2 (MefCO2) project aiming at developing an innovative green chemical production technology which contributes significantly to the moreEuropean objectives of decreasing CO_2 emissions and increasing renewable energy usage. This project has a budget of over 11 Million Euros and, with an execution period of four years, it is scheduled to be completed towards the end of 2018. In this sense, I-deals and the different MefCO2 partners, especially those involved with the computational assisted design of catalysts for CO_2 activation are impressed by results at hand involving CO_2 sequestration and activation by transition metal carbides [1] and from computational and experimental studies showing excellent CO_2 conversion to methanol on Cu supported on MoC [2] and on Mo_2C [3]. This adds one more family to the already large class of materials which are proposed or used for carbon storage and sequestration (CSS) involving zeolites, activated carbons, calcium oxides, hydrotalcites, organic–inorganic hybrids, and metal-organic frameworks [4] and show the need for a more systematic study.

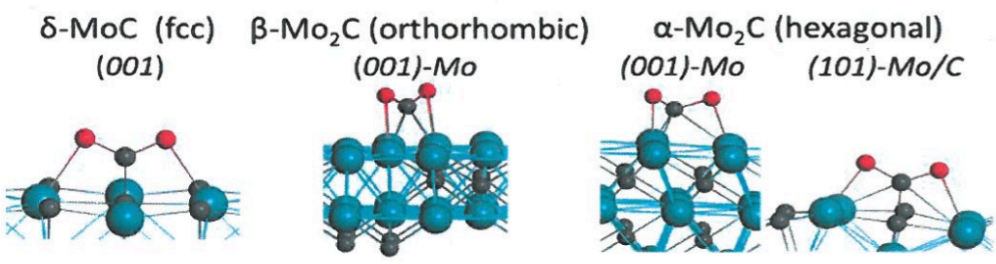

Figure 1.- Molecular structure of CO2 adsorbed on MoC and Mo2C surfaces, the bent OCO angle is a clear indication of activation which is confirmed by theoretical analsysis and experiments on model systems.

I-deals and the Department of Catalysis and Chemical Reaction Engineering (DCCRE) of the National Institute of Chemistry of Slovenia would like to know more about the result of NOMAD on-going high-throughput calculations aimed at rationalizing the available information available from computational studies that is already present at the NOMAD repository. Yet, the amount of information is too large and, at the same time, incomplete with many systems lacking. This part of NOMAD aims at applying big-data analytics techniques and machine learning algorithms using biased results some of which are now being obtained. From the calculations descriptors will be obtained to be included in the machine learning protocols which will hopefully propose new and better materials for CCS, activation and conversion. Both, I-deals and DCCRE will be glad to have access to this results which indeed may help to make progress on the MefCO2 project itself.

[1] "**Transition Metal Carbides as Novel Materials for CO_2 Capture, Storage, and Activation**", Ch. Kunkel, F. Viñes, F. Illas, Energy Environ. Sci., 9 (2016) 141-144

[2] "**Highly Active Au/δ-MoC and Cu/δ-MoC Catalysts for the Conversion of CO_2: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability**" S. Posada, P. Ramírez, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez, J. Am. Chem. Soc., 138 (2016) 8269-8278

[3] **The Conversion of CO_2 to Methanol on orthorhombic β-Mo_2C and Cu/β-Mo_2C Catalysts: Mechanism for Admetal Induced Change in the Selectivity and Activity**", S. Posada, P. Ramírez, R. Gutiérrez, D. Stacchiola, F. Viñes, P. Liu, F. Illas, and J. A. Rodriguez, Catal. Sci. Technol., 6 (2016) 6766-6777

[4] "**Adsorbent Materials for Carbon Dioxide Capture from Large Anthropogenic Point Sources**", S. Choi, J. H. Drese, C. W. Jones, ChemSusChem 2 (2009) 796