Storage, release and conversion of CO₂ 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 CO₂ 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-Háber Institut of the Max Planck Society in Berlin.

In the case of CO₂ conversion, interest has been also shown from I-deals, a company coordinating the Methanol fuel from CO₂ (MefCO2) project aiming at developing an innovative green chemical production technology which contributes significantly to the more European objectives of decreasing CO₂ 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 CO₂ activation are impressed by results at hand involving CO₂ sequestration and activation by transition metal carbides [1] and from computational and experimental studies showing excellent CO₂ conversion to methanol on Cu supported on MoC [2] and on Mo₂C [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.
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.


