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Process-informed design of tailor-made sorbent materials for energy efficient carbon capture (PrISMa)

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Abstract

Carbon Capture, Utilization and Storage (CCUS) is a key technology for achieving the global emissions reduction targets because of its role in power and industrial decarbonization. Together with bioenergy, CCUS can achieve negative emissions to remove CO_2 from the atmosphere. Decarbonisation from a variety of industrial emission sectors highlights a marked need for capture technologies that can be optimized for different sources of CO_2 and integrated in an equally diverse range of applications of captured CO_2 as a feedstock. At high TRLs, there are substantial efforts focusing on optimizing a single particular carbon capture technology (e.g. amine-based capture) for a single typical stationary source (e.g., coal-fired power plants). However, significant gains in energy efficiency and other economic benefits can be obtained if we tailor make a capture technology for a particular CO_2 source (e.g., waste incineration, coal combustion, cement manufacture) and a particular CO_2 destination, such as utilization or transport via pipeline, or ship to permanent storage. Such tailoring requires a systematic view of separation methodologies, microscopic processes, and engineering design.

Recent work has shown that sorbent-based capture technologies have the potential to significantly reduce effective price of carbon, i.e., reduce the energy penalty (OPEX) and/or equipment costs (CAPEX) when compared with state-of-the art amine-based solvent capture processes.[1] In parallel, there has been a remarkable scientific development in the synthesis of nanoporous materials.[2] We can now tailor make materials with well-defined properties. However, promising materials must be assessed and modelled at a process level as process integration plays a key role in the energy efficiency and economics of capture processes.

This paper will present the PrISMa project (http://www.act-ccs.eu/prisma), which is an international effort that aims to accelerate the transition of energy and industrial sectors to a low-carbon economy by developing a technology platform to tailor-make cost-efficient carbon capture solutions for a range of different CO_2 sources and CO_2 use/destinations. To achieve this goal PrISMa unites the efforts of world-leading research teams from Heriot-Watt University (HWU) in the UK, École Polytechnique Fédérale de Lausanne (EPFL) in Switzerland, Lawrence

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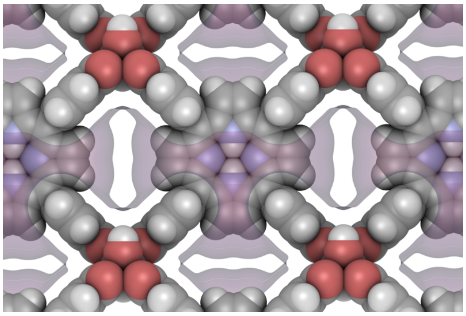

Figure 1:A molecular representation of the carbon capture material Al-PMOF (picture by Mohamad Moosavi and Kevin Jablonka; iRASPA software was used for visualisation)

Berkeley National Laboratory (LBNL) in the USA, and SINTEF Energy Research (SINTEF-ER) in Norway. These teams have the expertise to bridge the gap between molecular sciences (LBNL and EPFL) and process engineering (SINTEF-ER and HWU). The team is supported by market-leading companies and non-governmental organizations, which are committed to minimize CO_2 emissions of their industrial sectors and will provide case studies and maximise knowledge exchange and impact of PrISMa.

The PrISMa methodology starts with a high-level analysis, in terms of an effective carbon price, on how the performance of a separation process depends on the source of CO_2 and its use/destiny. This analysis is subsequently translated into key performance indicators (KPIs) that novel materials need to achieve in terms of their potential to reduce the effective carbon price in order to compete with state-of-the-art capture processes. A materials genomic approach is used to screen libraries of millions of *in silico* predicted structures to identify materials that meet the KPIs. The most promising materials will then be synthesized, characterised, and tested for their performance in a carbon capture process. For those materials that yield a significant reduction of the effective carbon price, a roadmap to bring these materials to TRL5 will be developed through case studies.

PrISMa will provide the platform needed for high-throughput screening of materials to maximise their impact, to enable the design of efficient pilot-scale test facilities with improved processes under real conditions and, to decrease the time to market of affordable, cost-competitive, low environmental impact, and resource-efficient advanced capture technologies. Through the integration of materials design and process design we aim to change the paradigm on how novel materials are developed for chemical engineering applications. Some recent results from the PriSMa collaboration involved the design of a metal organic framework that can capture CO_2 in wet flue gasses (see Figure 1).[3] As a similar approach can be developed for other separations, we expect the impact of PrISMa in terms of the potential to decrease the time to market for novel materials to go beyond carbon capture. In addition, PrISMa aims to initiate a systematic thinking about efficient solutions to mitigate CO_2 emissions from different local CO_2 sources that are optimal for a specific local setting. In such a setting the impact of PrISMa will be significant as the need for tailor-made solutions will be increasingly important if CO_2 mitigation at the local level becomes the norm.

Keywords: novel sorbent materials; carbon capture; material genomics; process design.

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