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Introduction to CO_2 capture, utilization and storage (CCUS)

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In recent years, great efforts have been devoted to limiting rising atmospheric carbon dioxide (CO_2) concentrations while meeting increasing global demand for energy. To prevent the detrimental impacts of climate change, CO_2 capture, utilization and storage (CCUS) technologies have to be implemented to reduce the cumulative amount of CO_2 in the atmosphere. CO_2 capture processes generally include adsorption, absorption, biochemical, and membrane technologies that can effectively separate CO_2 from flue gases (post-combustion), industrial processes (pre-combustion), or even the atmosphere (DOI: 10.1039/d1re00233c). In addition, how to deal with the captured CO_2 is another big issue. So far, we can convert it into useful chemicals, fuels, and polymers, or utilize it for oil extraction and alkaline industrial waste remediation, or inject it in geologic formations and oceans.

For CO_2 capture at relatively low temperatures, porous materials, such as metal–organic frameworks (MOFs), zeolite, carbon, and supported solid amines, have attracted great attention (DOI: 10.1039/d1re00214g). MOFs are a

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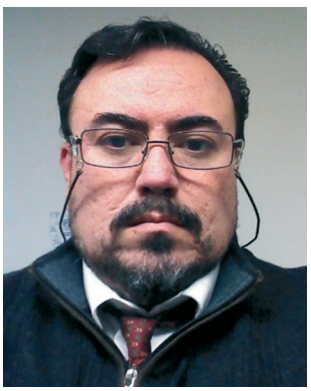


Dr. Heriberto Pfeiffer

Dr. Heriberto Pfeiffer is a member of the Materials Research Institute of the Universidad Nacional Autónoma de México, at Mexico City. His research is focused on CO_2 capture and its conversion to value added products. At the same time, he works on different catalytic processes (reforming processes, WGS, POM, NO_x sorption–reduction, etc.) as well as on the CO oxidation–chemisorption process as a possible syngas separation process. Finally, he is interested in biomass pyrolysis and decomposition for H_2 production and he has several studies on ceramic membranes for gas separation. He has published more than 155 scientific articles and several book chapters.

relatively new class of porous materials with unique structural characteristics such as high surface areas, chemical tunability and stability, and have been extensively studied as promising CO_2 capture materials. Cotlame-Salinas *et al.* (DOI: 10.1039/d0re00410c) studied the enhancement of CO_2 capture in MOFs *via* molecular confinement. They critically reviewed the most significant advances on the enhanced CO_2 uptake performance of selected MOFs with pre-adsorbed polar (water, alcohols, and amines) and non-polar (toluene and benzene) molecules, as well as some interesting findings from robust computational calculations. In addition, the preferential CO_2 adsorption sites, water stability, CO_2–MOF complex configuration, CO_2 adsorption dynamics, bonding angle, decomposition mechanism, and swing effects are also of great research interest for MOF-based CO_2 capture materials (DOI: 10.1039/d1re00090j). Paudel *et al.* (DOI: 10.1039/d0re00416b) reported that the gas interactions and diffusion mechanisms of CO_2 and CH_4 in ZIF-8 can be computationally investigated using density functional theory. Gandara-Loe *et al.* (DOI: 10.1039/d1re00034a) pointed out that MOFs are not only promising for CO_2 capture, but also offer opportunities as advanced catalysts for gas-phase CO_2 conversion.

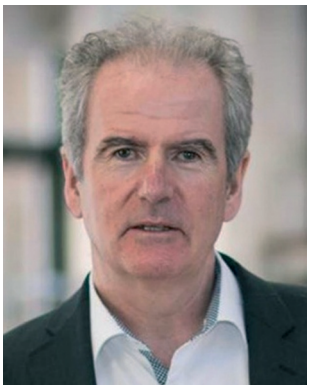
For CO_2 capture at high temperatures, various sorbents, including Li_4SiO_4, $KNaTiO_3$ and CaO, have been intensively studied. In a recent work, Blanco *et al.* (DOI: 10.1039/d1re00125f) provided a detailed study on the synthesis of Na_2TiO_3 *via* a solid-state route starting from NaOH and TiO_2. *In situ* experiments performed under different conditions revealed the occurrence of thermally-driven phase transitions derived from the structural instability of the material at high temperatures. These reactions could be differentiated from carbonation processes, allowing the proposal of a mechanism for CO_2 sorption. The obtained results could explain the abnormal dynamic thermogram displayed by Na_2TiO_3 in the presence of CO_2 within a temperature range that is of interest for practical applications and serves as a basis for evaluating the feasibility of using this material in CO_2 capture schemes. Within a similar context, Hernández-Castillo *et al.* (DOI: 10.1039/d1re00087j) reported a new approach to consecutive CO oxidation and CO_2 chemisorption using Li_2CuO_2 ceramics modified with Na and K molten salts.

In a different CO_2 separation conceptualization, dense ceramic–carbonate dual-phase membranes have been recently proposed as an alternative for pre-combustion CO_2 capture in the integrated gasification combined cycle (IGCC) process at high-temperature, where these membranes can work as reactors for H_2 production and CO_2 separation/capture. González-Varela *et al.* (DOI: 10.1039/d0re00375a) investigated the high-temperature CO_2 perm-selectivity of yttrium-doped SDC (Y-SDC) ceramic–carbonate dual-phase membranes, and revealed that the ionic conductivity of Y-SDC depends on the O_2 partial pressure and yttrium content. The CO_2 permeation flux is correlated to the ionic conductivity of Y-SDC and can be improved by tailoring the membrane microstructure.

In addition to CO_2 capture or separation, CO_2 utilization is also of great importance for carbon neutrality. To date, many technologies, including CO_2 hydrogenation, electrochemical CO_2 reduction, photochemical CO_2 reduction, bioelectrochemical CO_2 reduction, CO_2 conversion to polymers, *etc.*, have been studied. Shah *et al.* (DOI: 10.1039/

Professor Rose Amal

Professor Rose Amal is a Scientia Professor in the School of Chemical Engineering, UNSW Sydney. Her current research focuses on designing nanomaterials for solar to chemical energy conversion applications (including photo and electrocatalysis for water and air purification, water splitting and CO_2 reduction) and engineering systems for solar induced processes. Prof. Amal is a Fellow of the Australian Academy of Technological Sciences and Engineering (FTSE) and a Fellow of the Australian Academy of Science (FAA). She received the nation's top civilian honour – the Companion of the Order of Australia – as part of the 2018 Queen's Birthday Honours for her eminent service to chemical engineering, and was named 2019 NSW Scientist of the Year.



Dermot O'Hare

Dermot O'Hare is a Professor of Organometallic and Materials Chemistry in the Department of Chemistry at the University of Oxford. In addition, he is currently the Director of the SCG–Oxford Centre of Excellence for Chemistry and Associate Head for Business & Innovation in the Mathematics, Physical and Life Sciences Division. Professor O'Hare leads a multidisciplinary research team that works across broad areas of catalysis and nanomaterials. O'Hare's research is specifically targeted at finding solutions to global issues relating to energy, zero carbon and the circular economy. He has been awarded numerous awards and prizes for his creative and ground-breaking work in Inorganic Chemistry, including the Royal Society Chemistry Ludwig Mond Prize, the Royal Society Chemistry Tilden Medal and Royal Society of Chemistry Academia–Industry Prize.

d1re00150g) investigated the enhanced conversion of methane using Ni-doped $Ca_2Fe_2O_5$ oxygen carriers in chemical looping partial oxidation systems with CO_2 utilization. This work revealed that the addition of Ni as a dopant can lower the oxygen vacancy formation energy and increase the CO_2 adsorption energy, which is favorable for CO_2 activation and splitting. Jeng *et al.* (DOI: 10.1039/d0re00261e) studied the potential impacts of current densities, CO_2 feeding rates, and reaction temperatures on the single-pass conversion of CO_2 in a typical CO_2 flow electrolyzer. Fu *et al.* (DOI: 10.1039/d1re00001b) pointed out that the direct reduction of CO_2 to multi-carbon (C_{2+}) products suffers from low activity in non-alkaline electrolyte or problems with electrolyte degradation caused by carbonate formation in alkaline electrolyte. They reviewed the potential for a two-step process for CO_2 electroreduction circumventing such problems by converting CO_2 to CO (the first step) in the non-alkaline electrolyte and promoting the rate of carbon–carbon coupling for CO-to-C_{2+} conversion (the second step) in alkaline electrolytes. Metal halide perovskite materials have emerged as one of the leading candidates for CO_2 photoreduction due to their exceptional optoelectronic properties. Méndez-Galván *et al.* (DOI: 10.1039/d1re00039j) found that it is possible to create, modify, improve, and finally enhance the photocatalytic activity of metal halide perovskites to reduce atmospheric CO_2 concentrations. Some challenges must be addressed to develop this technology further, such as identifying and quantifying the other reaction products, the influence of the process parameters, and kinetics. Mo_2C/TiO_2 represents another promising catalyst with enhanced visible-light photoreduction of CO_2 to methanol (DOI: 10.1039/d0re00376j). Thatikayala *et al.* (DOI: 10.1039/d1re00166c) revealed that CO_2 can be converted into volatile fatty acids through microbial electrosynthesis (MES) in a single chamber reactor. Ozorio *et al.* (DOI: 10.1039/d1re00036e) reported that CO_2 could react with styrene oxide to cyclic organic carbonates over appropriate catalysts.

In this themed collection, we showcase the global efforts on CCUS as an issue of worldwide concern, and the diverse chemistry and engineering approaches that are being used. Herein, we would like to thank all the contributors for their nice submissions to this themed collection. We hope this successful themed collection will encourage the future expansion of this impactful research area and eventually make an impact on the goal of carbon neutrality.