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# Shedding Light on the Stakeholders’ Perspectives for Carbon Capture

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## Abstract

Reducing CO<sub>2</sub> emissions requires urgently deploying large-scale carbon capture technologies, amongst other strategies. The quest for optimum technologies is a multi-objective problem involving various stakeholders. Today’s research of these technologies follows a sequential approach, with chemists focusing first on material design and engineers subsequently seeking the optimal process. Eventually, this combination of materials and processes operates at a scale that significantly impacts the economy and the environment. Understanding these impacts requires analyzing factors such as greenhouse gas emissions over the lifetime of the capture plant, which now constitutes one of the final steps. In this work, we present the PrISMa (**P**rocess-**I**nformed design of tailor-made **S**orbent **M**aterials) platform, which seamlessly connects materials, process design, techno-economics, and life-cycle assessment. We compare over sixty case studies in which CO<sub>2</sub> is captured from different sources in five world regions with different technologies. These studies illustrate how the platform simultaneously informs all stakeholders: identifying the cheapest technology and optimal process configuration, revealing the molecular characteristics of top-performing materials, determining the best locations, and informing on environmental impacts, co-benefits, and trade-offs. Our platform brings together all stakeholders at an early stage of research, which is essential to accelerate innovations at a time this is most needed.

## Introduction

We must prepare for a Net-zero world where we cannot allow anthropogenic CO<sub>2</sub> to escape into the atmosphere.<sup>1</sup> In this world, we need to connect all kinds of sources of CO<sub>2</sub> (e.g., industries or waste incineration) with CO<sub>2</sub> sinks (e.g., geological storage or chemical industry). This requires us to identify the optimal technology to capture the CO<sub>2</sub> at the source’s conditions and deliver the CO<sub>2</sub> at the targeted sink’s specifications. Importantly, the slow implementation of carbon capture in the last decades<sup>2</sup> has taught us that the optimal capture technology for each sink and source depends on the specific social, economic,

and regional context. Thus, the CO<sub>2</sub> capture challenge cannot be expected to be solved by a “one-solution-fits-all” approach.

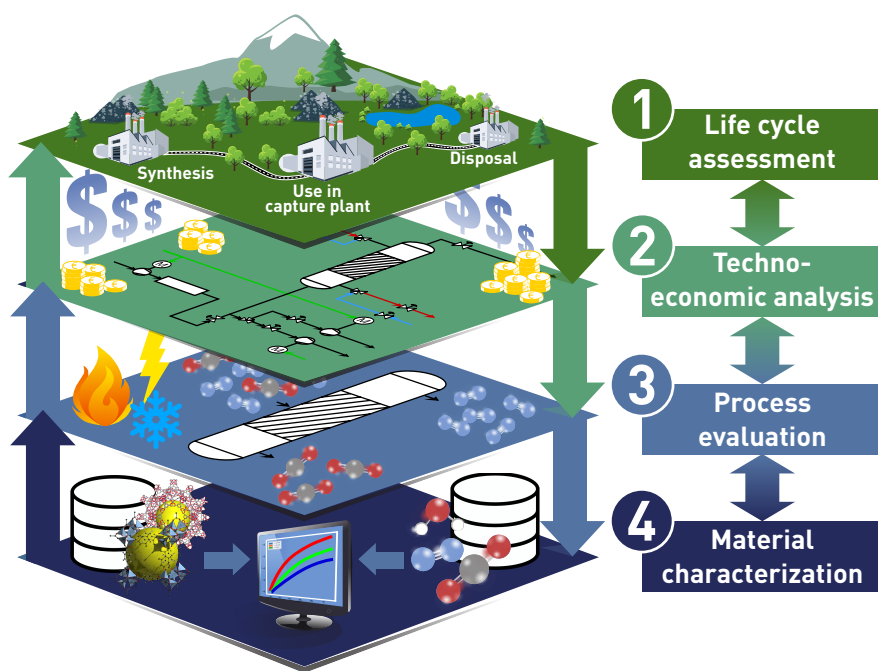
As an alternative, this work explores tailor-made capture technologies. Solid adsorbent-based carbon capture has the potential to take advantage of modern, reticular chemistry to synthesize millions of possible adsorbents.<sup>3</sup> Indeed, chemists have synthesized about 100,000 novel metal-organic frameworks (MOFs) by combining organic linkers with metal nodes.<sup>4,5</sup> Yet, to fully explore the potential of this technology, we need to go beyond the conventional sequential, time-consuming trial-and-error approach. As a first step to speed up the discovery process, computational groups started a material genomics approach.<sup>6-9</sup> Materials are generated in silicon, and molecular simulations predict the adsorption properties of these materials.<sup>6</sup> While the property predictions were sound, the impact has been limited. The main reason is that these studies assume that the performance of a material in a capture process can be evaluated with a single or a few basic material adsorption properties (e.g., Henry selectivity or CO<sub>2</sub> capacity). In practice, an optimal material depends on the specifics of the process, scale-up, location attributes, and life cycle assessment.<sup>10-17</sup> Due to a lack of such a system-level contextualization, materials discovery has often failed to engage the views of all stakeholders involved in the implementation of large-scale carbon capture technologies (see Extended Data Figure 1). To evaluate the overall performance of a material, one needs a holistic approach in which material properties are linked to the process design coupled with a techno-economic analysis. Finally, a life-cycle assessment enables assessing environmental impacts beyond climate change and ensures that we do not emit more CO<sub>2</sub>-eq. than what we produce in building and operating the capture plant over its lifetime.<sup>18</sup> The entire life cycle captures here not only the operation of the capture plant but also its construction and disposal as well as the material synthesis and disposal.

The needed reconciliation of the views of the different stakeholders motivated our PrISMa (**P**rocess-**I**nformed design of tailor-made **S**orbent **M**aterials) platform, where we seamlessly link quantum calculation, molecular simulations, process design, techno-economic analysis,

and life cycle assessment. Based on the crystal structure of a material, we evaluate its performance for a specific carbon capture process, connecting a CO<sub>2</sub> source with a CO<sub>2</sub> sink in a region of the world, using a total of 49 Key Performance Indicator (KPI).

## The PrISMa platform for carbon capture

The PrISMa platform allows for the interrogation and high-throughput screening of materials for a given carbon capture application. A carbon capture application, which we refer to as a Case Study, is defined by the CO<sub>2</sub> source, the destination of the CO<sub>2</sub> (sink), the capture technology, the available utilities, and the region of the world (see Extended Data Table 1). The platform integrates life cycle assessment, techno-economic analysis, process evaluation, and material characterization (see Figure 1).



**Figure 1** | A schematic illustration of the four layers of the PrISMa platform: linking life cycle assessment (LCA), techno-economic analysis (TEA), process evaluation, and material characterization. A detailed description of the methods used in each layer can be found in Supplementary Information Section 3.

At the Materials layer, we use available experimental data or the material's crystal struc-

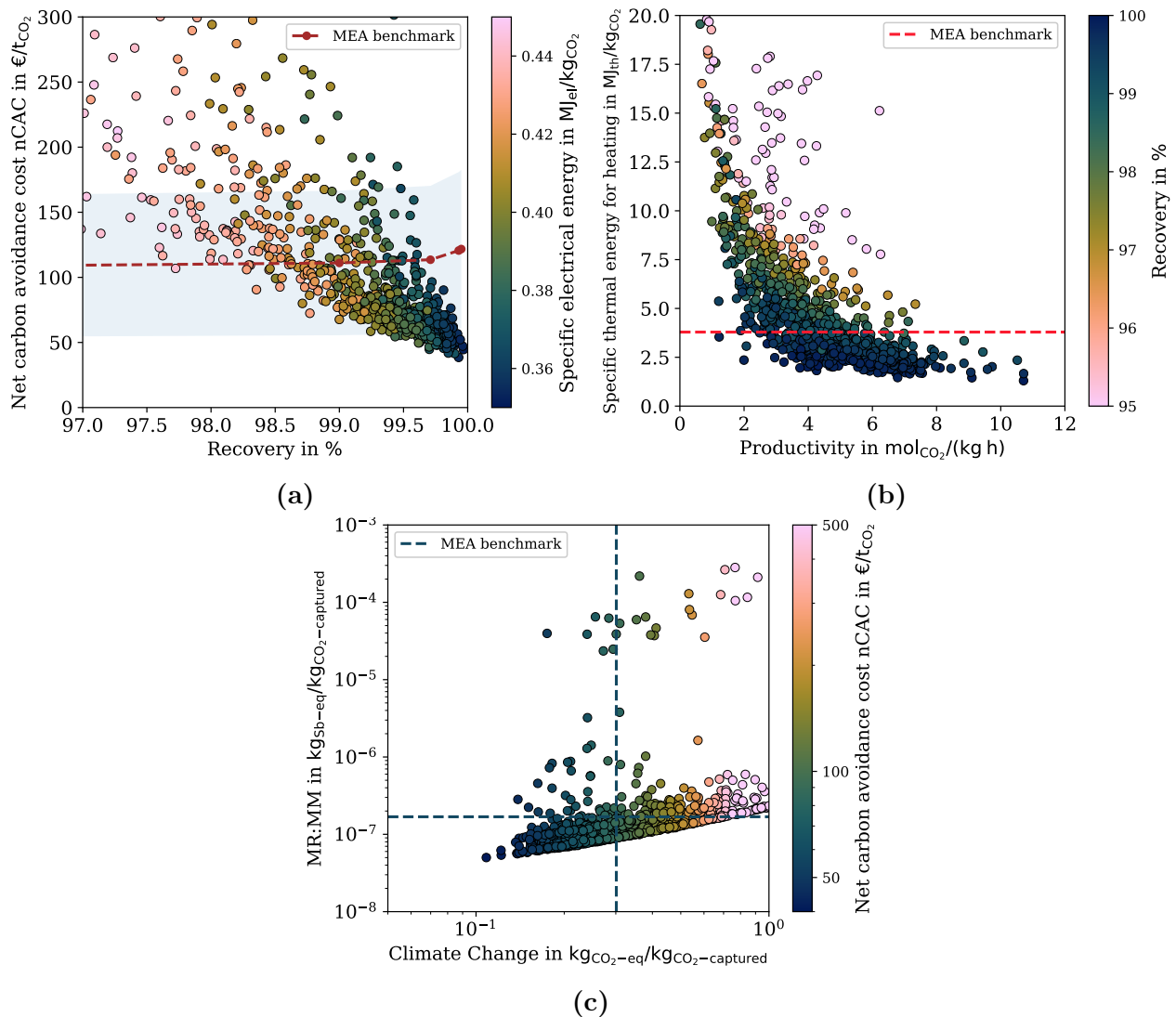
ture to predict the adsorption thermodynamics using molecular simulations. This thermodynamic data is the input for the Process layer together with process and equipment data. We compute process performance parameters at this layer, such as purity, recovery, productivity, and energy requirements. In the Techno-economic (TEA) layer, the economic and technical viability of the capture plant is assessed. Next, the Life Cycle Assessment (LCA) layer evaluates the environmental impacts of the carbon capture plant over its entire lifetime (e.g., climate change or metal resources).

## Informing stakeholders perspectives

The modular structure of the PrISMa platform enables us to consider the perspectives of the different stakeholders (see Extended Data Figure 1). We compute a list of 49 KPIs (see Supplementary Information Table S4) KPIs for any combination of source, sink, technology, utilities, and region shown in Extended Data Table 1. We carried out a Spearman analysis of KPIs in each layer of the platform to identify a set of six reference-KPIs (see Extended Data Table 2) that encapsulate the most important trends (see Extended Data Figure 2), and, in the remainder, we refer mainly to these reference KPIs. Our interactive visualization tool can access all other KPIs for all case studies and over 1000 materials.<sup>19</sup>

To illustrate the use of the platform, let us first look at one case study: capturing CO<sub>2</sub> using a temperature-swing adsorption process (TSA) from a cement plant located in the United Kingdom (UK). In this study, the captured CO<sub>2</sub> is compressed and sent for geological storage. In Figure 2, we compare the performance of the materials for some selected KPIs with the Mono-Ethanol-Amine-based (MEA) benchmark,<sup>20</sup> and we observe that many materials outperform the benchmark.

The nCAC is the KPI that quantifies the cost of avoiding emitting CO<sub>2</sub> into the atmosphere over the life cycle of the plant, and it is deemed to be the most appropriate metric to make a first selection of the most promising materials for a given application. However, it



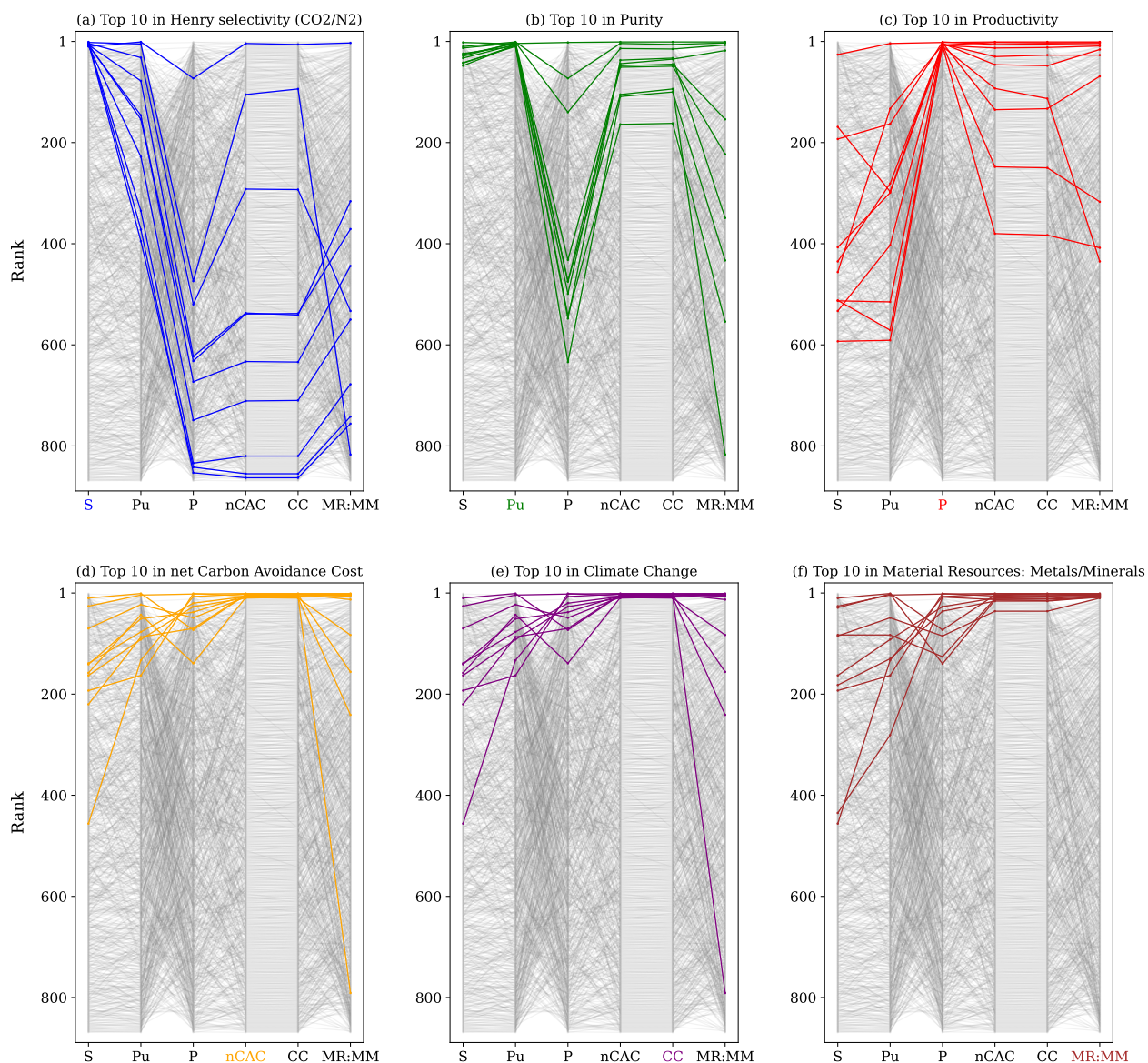
**Figure 2 | Materials performance for a TSA carbon capture process added to a cement plant in the UK:** The dotted lines show the MEA benchmark (see Supplementary Information Section 6), whereas in Figure (a), the blue shaded area gives the uncertainty. Each dot represents a material. (a) nCAC versus recovery (R) with color coding the specific electrical energy consumption, (b) Specific thermal energy consumption for heating versus productivity (P) with color coding the recovery, and (c) Material Resources: Metals/Minerals (MR:MM) versus Climate Change (CC) with color coding the nCAC. The interactive version of this graph can be found here: <https://prisma.matcloud.xyz/>.

is not the only criterion, and evaluating materials across all KPIs and from all stakeholder’s perspectives is important. For such an evaluation, we rank all materials for the reference KPIs. Figure 3 highlights the top-performing materials for a given KPI, together with how they score on the other KPIs across the different layers of the platform. The comparison of the material rankings in Figure 3 illustrates the complexity of selecting an optimal material for a given carbon capture application; the top 10 materials for a given KPI do not usually rank top for the other KPIs. The holistic PrISMa approach allows for extracting relevant information for all stakeholders.

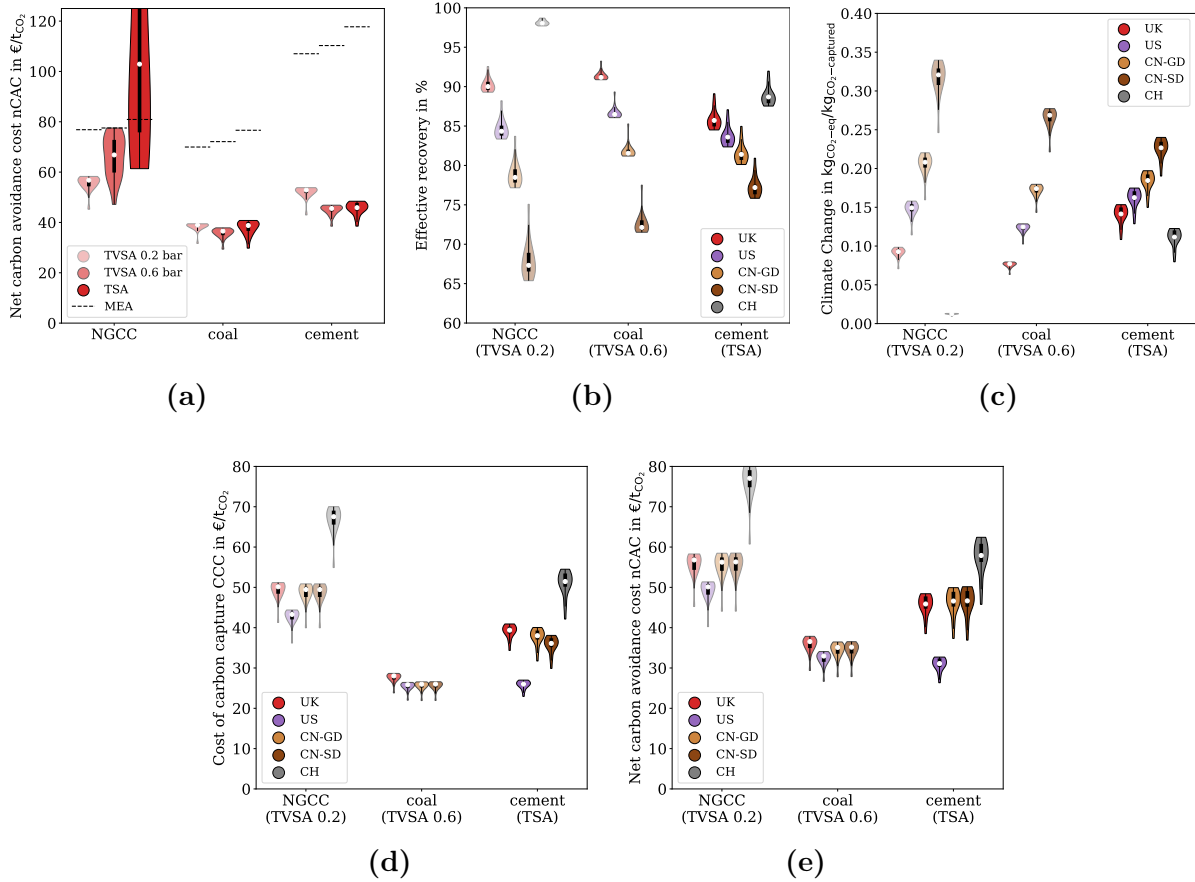
**The engineer’s perspective:** The engineer needs to identify and design the best technology option for a given separation. In Figure 4a, we compare the nCAC of the 20 top-performing materials for three process configurations, i.e., Temperature Swing Adsorption (TSA) and Temperature Vacuum Swing Adsorption (TVSA) with two vacuum levels 0.2 bar and 0.6 bar, and for three CO<sub>2</sub> sources. For cases with a low CO<sub>2</sub> concentration in the feed stream, i.e., for NGCC power plants, the vacuum step in the process configuration reduces the cost significantly. The additional vacuum in a TVSA process increases the purity of the product stream. This increase is achieved by rapidly purging the non-adsorbed gas fraction after the adsorption step, increasing the working capacity, and decreasing the CAPEX. Coal power plants still benefit from some vacuum (0.6 bar). For the most concentrated CO<sub>2</sub> stream, the cement plant, the difference between TVSA with 0.6 bar and TSA is so small that one would prefer the simpler TSA process. In the remainder, we will focus on these combinations of sources and technologies.

**The environmental manager’s perspective:** Running a carbon capture plant inherently leads to emissions of CO<sub>2</sub> and other greenhouse gasses due to energy and materials demand, and the environmental manager aims to maximize the captured CO<sub>2</sub> while simultaneously minimizing these associated CO<sub>2</sub>-eq. emissions and other possible environmental impacts.





**Figure 3 | Comparison of materials ranking for a TSA carbon capture process added to a cement plant in the UK.** Rankings according to Henry selectivity (S), purity (Pu), productivity (P), Net Carbon Avoidance Cost (nCAC), Climate Change (CC), and Material Resources: Metals/Minerals (MR:MM) for a Temperature Swing Adsorption carbon capture process added to a cement plant in the UK. In these graphs, the top-performing material is ranked number one. Colored lines represent the top 10 performers for each of the six KPIs. The same color is used to highlight the KPI of interest. Every line illustrates how the ranking of a specific material (y-axis) changes across all other KPIs (x-axis). The interactive version of this graph can be found here: <https://prisma.matcloud.xyz/>



**Figure 4 | Comparison of process configurations and regions.** Our analysis of the different stakeholders' perspectives focuses on the 20 materials with the lowest Net Carbon Avoidance Cost (nCAC). In these violin plots, the white circle gives the median, which we use as a (conservative) estimate of the performance of these materials. The bottom of the violin represents a few materials with an even better performance. The width indicates the number of structures with a particular  $y$ -value, and the thick black bar contains 50% of the structures. (a) the Net Carbon Avoidance Cost (nCAC) for depending on the technologies (temperature swing adsorption (TSA) and vacuum swing adsorption (TVSA) with two vacuum levels 0.2 bar and 0.6 bar), (b) and (c) the five regions' net recovery and Climate Change (CC), respectively. (c) Carbon Capture Cost (CCC) and (d) the Net Carbon Avoidance Cost for the five regions. The data from which these violin plots are computed are given in Supplementary Information Section 8.

From this perspective, we are interested in the net amount of CO<sub>2</sub> we capture over the plant’s lifetime. To obtain this effective recovery (see Figure 4b), we must correct the recovery obtained from the process layer for the CO<sub>2</sub>-eq. emissions associated with building and operating the carbon capture plant as calculated within the Climate Change KPI. For some materials, we find a CC > 1 (see Extended Data Figure 3a); a carbon capture process with these materials will emit more CO<sub>2</sub>-eq. over the plant’s lifetime than the total amount of CO<sub>2</sub> that is captured. Interestingly, some of these materials rank high in other KPIs, which again highlights the importance of obtaining insights into all aspects of the capture process.

Another important environmental KPI is the Material Resources: Metals/Minerals, which indicates the use of minerals and metals resources over the entire life-cycle of the plant to capture a kg of CO<sub>2</sub>. In Extended Data Figure 4, we compare the ranking of materials based on their constituent metals, focusing on several abundant metals (Mg, Zn, and Mn) and some rather rare metals (Cu, Lu, and Ag). The same metal will have a worse MR:MM ranking if more of the corresponding MOF is needed to remove a unit of CO<sub>2</sub> or if the total energy demand is higher. The abundant metals (Mg, Zn, and Mn) rank better, while the rank drops for the rather rare metals (Cu, Lu, and Ag). All metals spread across the entire materials, process, and economic KPIs rankings, which implies that the type of metal is not the sole determining factor in a capture process. So, if a MOF scores poorly on MR:MM, it may inspire chemists to explore if a similar structure could be synthesized with a more abundant metal.

The platform provides additional KPIs related to the process’s environmental impacts (see Extended Data Figure 3b). These KPIs include the impact on the ecosystem, human health, and the use of resources (land, water, materials, and energy) and allow us to flag materials that impact the environment.

**The CO<sub>2</sub> producer’s perspective:** A CO<sub>2</sub> producer aims to find the most cost-efficient capture technology to deploy in a specific plant. For example, the available utilities in the host plant can be integrated into the capture process, and the platform can guide the decision on if such an integration reduces costs.

Heat integration with the existing host plant is the default strategy for power-plant producers. In Figure S17a, we compare those cases where heat extraction from the power plant is not possible. In those cases, natural gas boilers provide the required heat for the regeneration process. We then observe that the effective recovery decreases because the climate change impact increases due to using a natural gas boiler. In Figure S17b, we also see that the use of natural gas boilers increases the nCAC because of these increased indirect emissions and the higher operating costs.

For cement producers, the available utilities at the host plant are very limited; a natural gas boiler has to be built on-site to satisfy heat energy demand. For cement, the emissions derived from the natural gas boilers are the main factor contributing to the indirect emissions from the capture plant. The cement producer could then consider how replacing such a boiler could affect the plant’s environmental footprint and at what cost. Such analysis was conducted for Switzerland, where the CO<sub>2</sub>-eq. emissions can be reduced using electric boilers instead of natural gas-fired ones. This replacement significantly reduces the Climate Change because of the low carbon intensity of the electricity grid in Switzerland, which provides the cement producer with almost 100% effective recovery in the process. This improvement comes, however, at the expense of an increase in cost by about 10 to 15 €/t<sub>CO<sub>2</sub></sub> due to the high plant operating costs in Switzerland (see Supplementary Information Section 8.2).

**The investor’s perspective:** If one needs to perform large-scale carbon capture tomorrow, the most obvious choice is the well-established MEA technology. However, our platform shows that solid sorbent-based TSA or TVSA capture processes can outperform the MEA benchmark for all case studies. The cost reductions increase with CO<sub>2</sub> concentration, and

for cement, the nCAC is almost a factor three lower than the benchmark. These conclusions should be an important incentive to invest in developing these solid-sorbent technologies.

The global nature of CO<sub>2</sub> emissions reduction will require the deployment of carbon capture plants in many parts of the world. Figure 4e gives the break-even carbon price for a given CO<sub>2</sub> source in five regions of the world using the year 2019 as a reference. This figure shows that for all three sources, the US has the lowest nCAC. In the US, the energy prices are significantly lower than in the UK and Switzerland. The prices in China are also relatively low, but the indirect emissions in China are larger than in the US.

The Carbon Capture Cost for both NGCC and cement is the highest in Switzerland, mainly due to the country’s highest capital and operating costs. In contrast, the Climate Change KPI of Switzerland is the lowest amongst all studied countries because of the very low carbon intensity of the electricity grid. Yet, such a low CC cannot compensate for these higher costs, and consequently, the nCAC is the highest of all regions.

**The chemist’s perspective:** The route from the first synthesis of a new material to its implementation into a commercial process can take many years. It is, therefore, important to provide some guidance at the very early material’s design stage on how molecular characteristics impact the material’s performance.

An interesting practical question is whether one can synthesize materials that work well for any CO<sub>2</sub> source. Extended Data Figure 5 compares the ranking of the materials based on the Net Carbon Avoidance Cost for NGCC and coal power plants and the cement plant. We observe a significant change in ranking if we go from the NGCC to the coal power plant (highlighted in the dark color coding). If we move from the coal to the cement plant, the changes in the rankings are smaller but still considerable. If the partial CO<sub>2</sub> pressure is low, materials with a high CO<sub>2</sub> Henry coefficient typically rank high, but for a source with a higher partial CO<sub>2</sub> pressure, the CO<sub>2</sub> capacity is more important.

Our platform’s rankings are based on dry flue gases (Figure 2), but we can also assess

the effect of additional components in the feed gas stream, such as water, on the plant’s performance. To assess that, we identify those materials that maintain their capacity for capturing CO<sub>2</sub> in wet flue gasses. We highlight these materials in Extended Data Figure 6; many materials that maintain their capacity to capture CO<sub>2</sub> are among the top-performing materials.

The impact of a simulation study like our high-throughput screening is limited if it cannot reflect the actual performance of the material in a real-world process. Of particular interest is the MOF CALF-20,<sup>21</sup> which is currently the first MOF employed commercially for capturing CO<sub>2</sub> from a cement plant in Canada.<sup>22</sup> Extended Data Figure 7 shows that the nCAC obtained from the experimental thermodynamic data agrees very well with our estimate predicted from the crystal structure. In addition, our estimate of the cost is very close to the 50 €/t<sub>CO<sub>2</sub></sub> by Svante Inc<sup>23</sup>. That these two independent cost estimates agree so well is an important validation of the predictive power of the platform.

One of the motivations for our platform is that over the last few years, on average, each day, one to two new MOF structures have been published for a range of different applications.<sup>24</sup> Many of these MOFs are synthesized by groups that do not have the infrastructure to evaluate their materials for carbon capture such that they, at best, measure some elementary thermodynamic properties. We envision that the crystal structure of any newly synthesized MOF is uploaded to the PrISMa platform together with adsorption data, if available. To illustrate this functionality of the platform, we uploaded the crystal structure of a novel MOF, MIP-212 (see Supplementary Information Section 5) to determine its performance potential for carbon capture from a cement plant. Interestingly, this novel material is also promising as it outperforms the MEA benchmark and can potentially reduce the cost by as much as a factor of two. Also, for this material, Extended Data Figure 7 shows that the KPIs computed with experimental thermodynamic data agree very well with those predicted from the crystal structure.

Screening over a thousand materials allows us to apply data-driven methods to identify

the molecular characteristics of the top-performing materials. We show that by retaining the descriptor related to the pore geometry (i.e., persistence images), we can accurately predict whether a material has a lower nCAC than the MEA-based benchmark and can maintain its CO<sub>2</sub> adsorption capacity in wet flue gases (see Supplementary Information Section 8.5.1). These persistence images also rank the importance of each atom in these predictions. The collection of these atoms characterizes the molecular features that define the adsorbaphore.<sup>25</sup> A common theme in the materials that outperform MEA is a geometrical rod of metal atoms (highlighted in Extended Data Figure 8). These features are often correlated with stacked delocalized systems (aromatic rings) with a separation of 6 Å to 11 Å (see also Figures S38 and S39). The structures that have a high Water resistance coefficient tend to have these aromatic rings with a specific 6 Å separation, while those materials with open metal sites (OMS) and charged anions are to be avoided. Such an adsorbaphore does not need to be realized in a MOF, which may further inspire chemists to synthesize alternative materials with similar features.

## Concluding remarks

The importance of bringing together all stakeholders at an early research stage cannot be overstated. The complexity and the scale of the CO<sub>2</sub> mitigation problem make it essential to have a mutual understanding of the impact a decision of one stakeholder has on all others. The PrISMa platform is aimed not only at providing this understanding but also at allowing a quantification of the impact of these decisions. Such a bridge between fundamental research and large-scale implementation will accelerate the speed at which innovations are successfully implemented.

For each platform layer, we have implemented models that compromise robustness (needs to work for thousands of materials) and accuracy for the available data on the materials. We then apply a systematic sensitivity analysis to improve the accuracy of our predictions.

We envision many possible extensions of our platform. CO<sub>2</sub> is seen increasingly as a carbon source for the chemical industry and for producing synthetic fuels. Hence a logical extension is to include these utilization routes of CO<sub>2</sub> as sinks. CO<sub>2</sub> from waste incineration, biogas production, and other industries are also obvious sources to add. One can add different technologies, more regions of the world, and even more stakeholders (e.g., society).<sup>26</sup>

As our platform will be made open science, it can become a reference platform for the research community, where groups can upload any newly generated or synthesized material and get prompt feedback on its performance for an increasing range of applications.

## Data availability

All the results obtained by the platform for all case studies presented in this work have been deposited on Zenodo (<https://doi.org/10.5281/zenodo.8042599>). On this website, one can also find the crystal structure (cif files) of all materials studied in this work, together with the simulated isotherms, values of the heat capacity, and data that characterize the materials.

The results of this work can also be accessed through our visualization tool on the Materials Cloud <https://prisma.matcloud.xyz/>. This tool allows users to inspect all case studies and all KPIs. In addition, the Materials Cloud provides interactive versions of the graphs presented in this work. Updates and new case studies will be made available through the Materials Cloud. This tool also allows uploading the crystal structure of novel materials to be analyzed across the various case studies.

## Code availability

The code for the analysis of the persistence images and the interactive visualisation tool can be found at <https://github.com/kjappelbaum/prisma-adosorbaphore> and [https://github.com/ElMouba/PrISMa\\_VisTool](https://github.com/ElMouba/PrISMa_VisTool), respectively.



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## Author contributions

E.M., S.M.M., K.M.J., and B.S. developed the materials layer, C.C., J.W., F.M., and S.G. developed the process layer, E.S.F., C.C., L.H., and S.G., developed the techno-economic analysis layer, and J.S. and A.B. developed the life-cycle assessment layer. E.M. and J.V.H. developed the visualization software, and the MIP-212 MOF was synthesized and characterized by G.M. and C.S. All authors contributed to analyzing the data and writing the manuscript.

## Competing interest

The authors declare no competing interests.

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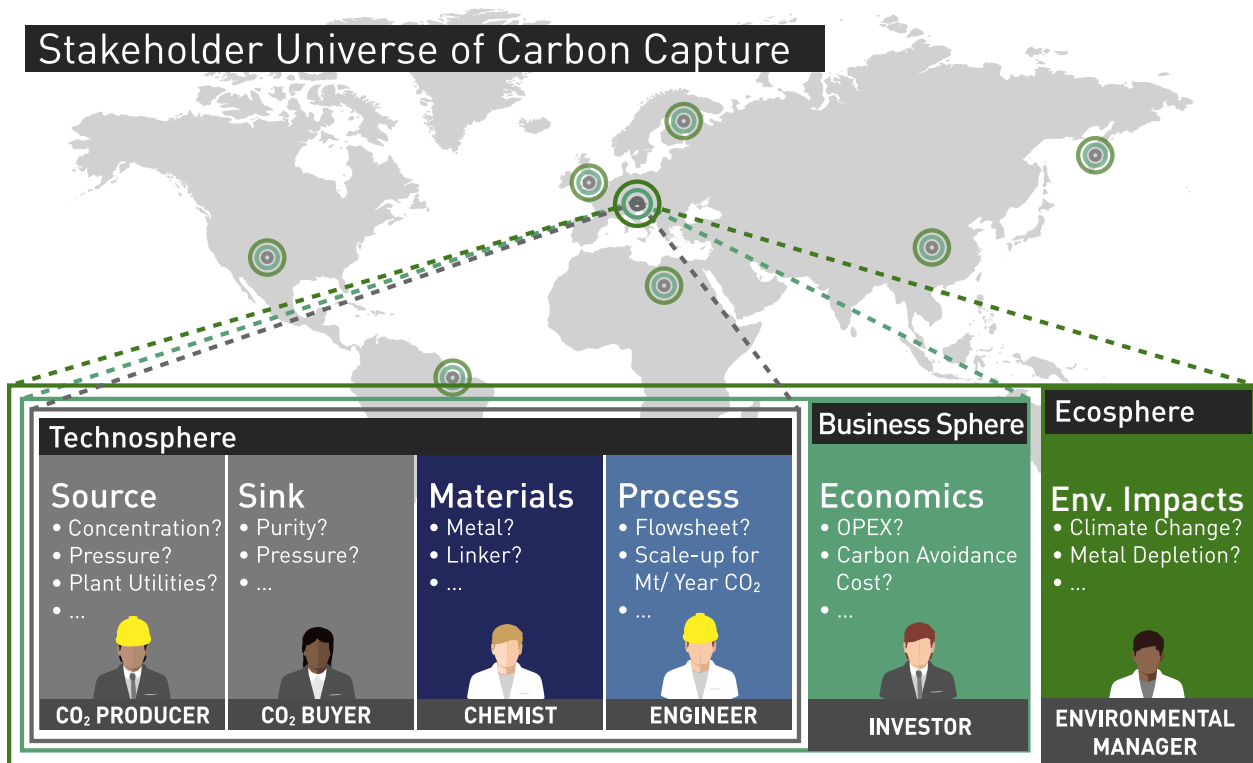
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**Extended Data Table 1 | Available case studies in the PrISMa platform.** Any source, sink, technology, utility, and region in the platform can be combined. Switzerland has no coal-fired power plants, so this combination of source and region is not considered. Three technologies are available: Temperature Swing Adsorption (TSA) and Temperature Vacuum Swing Adsorption (TVSA) with two vacuum levels, 0.2 and 0.6 bar. We have a total of 63 case studies. The complete input parameters defining these case studies are in Supplementary Information Table [S2](#).

Source	Sink	Technology	Utility	Region
NGCC	Geological storage	TSA	Natural gas boiler	UK
Coal		TVSA - 0.6 bar	Electric boiler	US
Cement		TVSA - 0.2 bar	From host plant	China (Guangdong)
				China (Shandong)
			Switzerland (CH)	

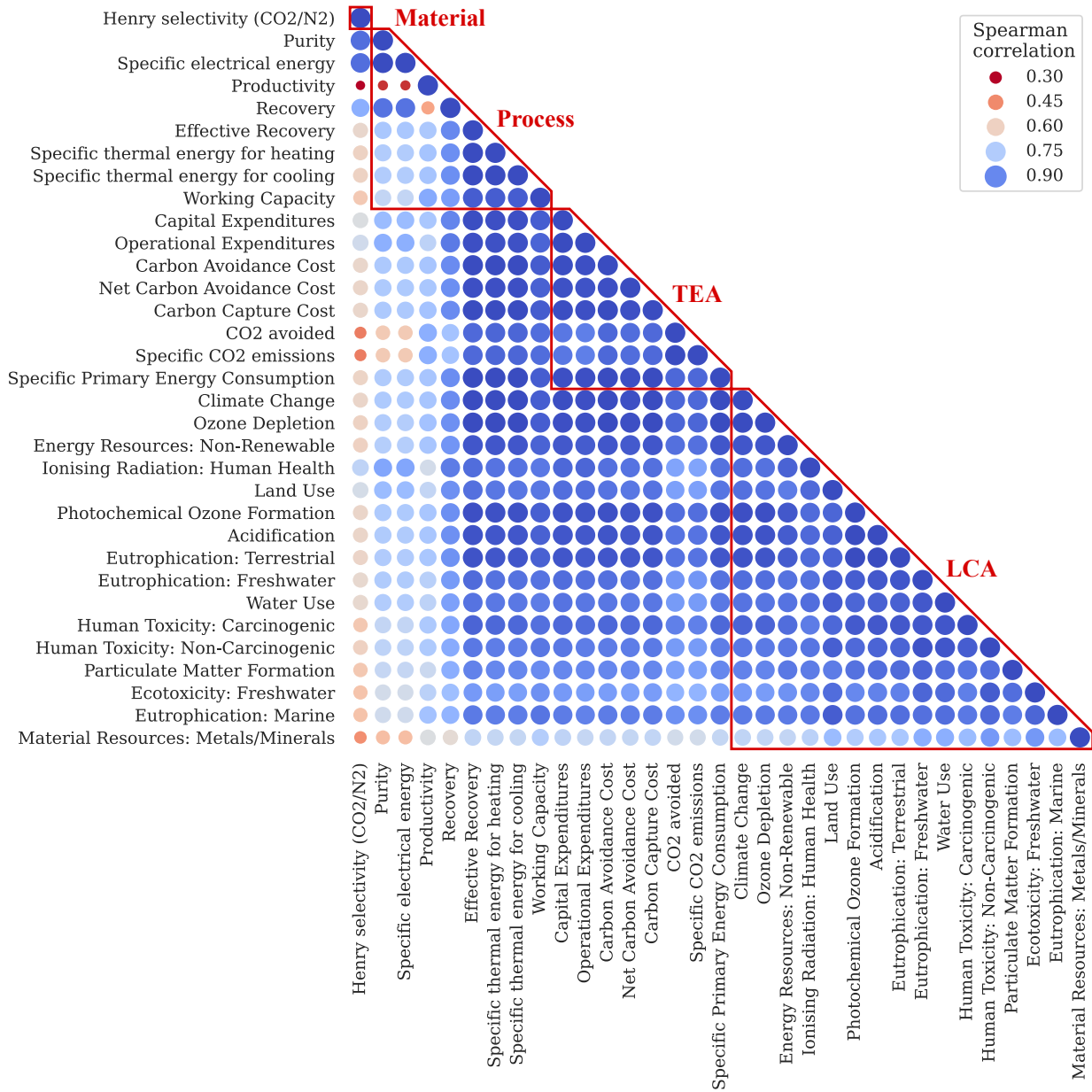
**Extended Data Table 2 | The six reference Key Performance Indicators (KPIs).** Henry selectivity (S), Purity (Pu), Productivity (P), Net Carbon Avoidance Cost (nCAC), Climate Change (CC), and Material Resources: Metals/Minerals (MR:MM). Based on Spearman analysis, we have identified six key performance indicators that describe the most important trends in each layer of the PrISMa platform (see Supplementary Information Section 7). A description of all KPIs and data generated by the platform can be found in Supplementary Information Section 4.

KPI	Description	Definition (SI)
<b>Materials layer</b>		
S	Ratio of the CO <sub>2</sub> and N <sub>2</sub> Henry's coefficients.	(4.1.2)
<b>Process layer</b>		
Pu	The molar fraction of CO <sub>2</sub> in the product stream.	(4.2.1)
P	The amount of captured CO <sub>2</sub> per kg adsorbent during a process cycle	(4.2.5)
<b>Techno-economic analysis (TEA) layer</b>		
nCAC	Quantifies the cost of avoiding emitting CO <sub>2</sub> into the atmosphere over the life cycle of the plant. For power generation case studies, the nCAC is calculated from the levelized cost of electricity and the net carbon intensity of the plant. For cement, the nCAC is calculated from the costs of carbon capture and the Climate Change (CC), as we assume that cement production is not affected by the capture plant.	(4.3.4)
<b>Life cycle assessment (LCA) layer</b>		
CC	Gives the total Global Warming Potential (GWP) due to greenhouse gas emissions from the capture process to the air and CO <sub>2</sub> uptake from the atmosphere	(4.4.1)
MR:MM	Indicates the use of non-renewable non-fossil natural resources (i.e., minerals and metals), and considers the availability of a mineral or metal on earth and the current mining rate. The use of natural resources like minerals and metals is measured using antimony (Sb) as reference material.	(4.4.2)

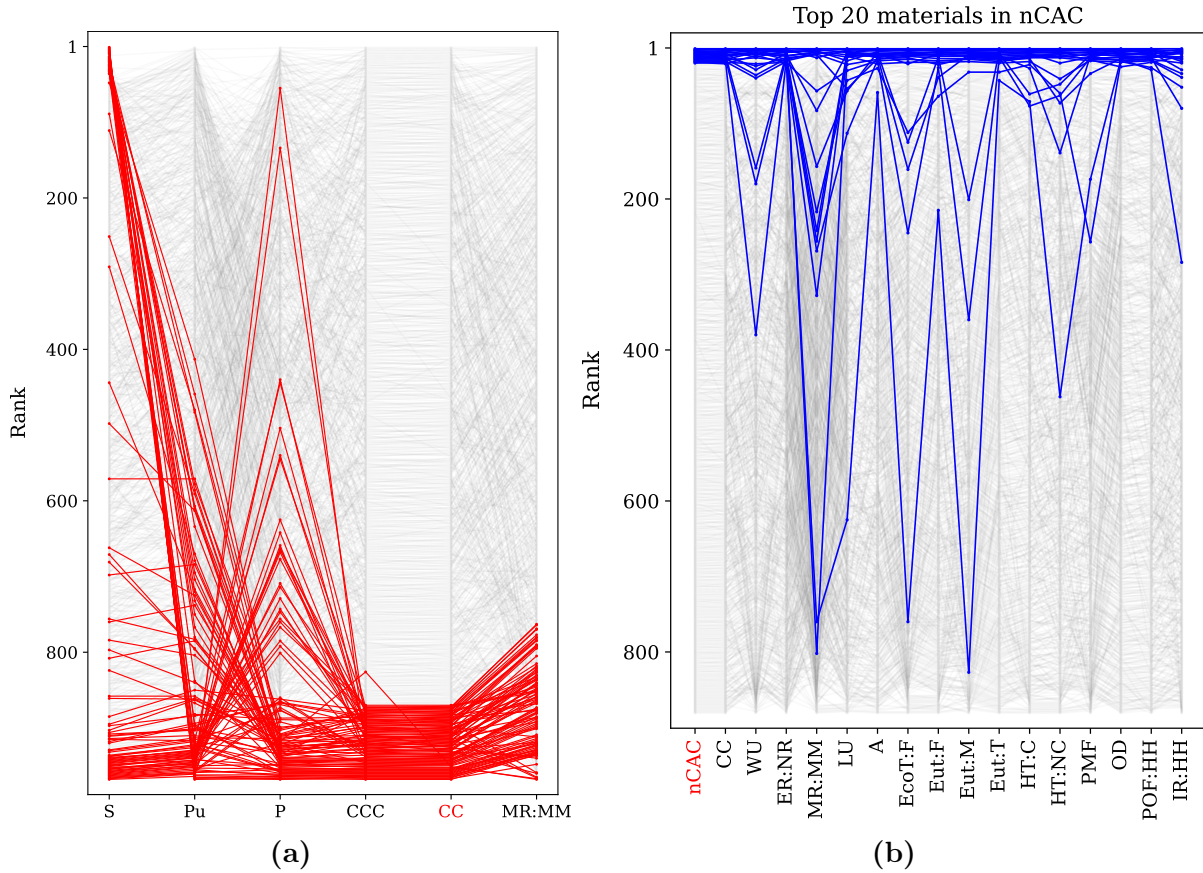


**Extended Data Figure 1 | Stakeholder universe of carbon capture.** Illustration of the perspectives the various stakeholders have on the development of a carbon capture process.

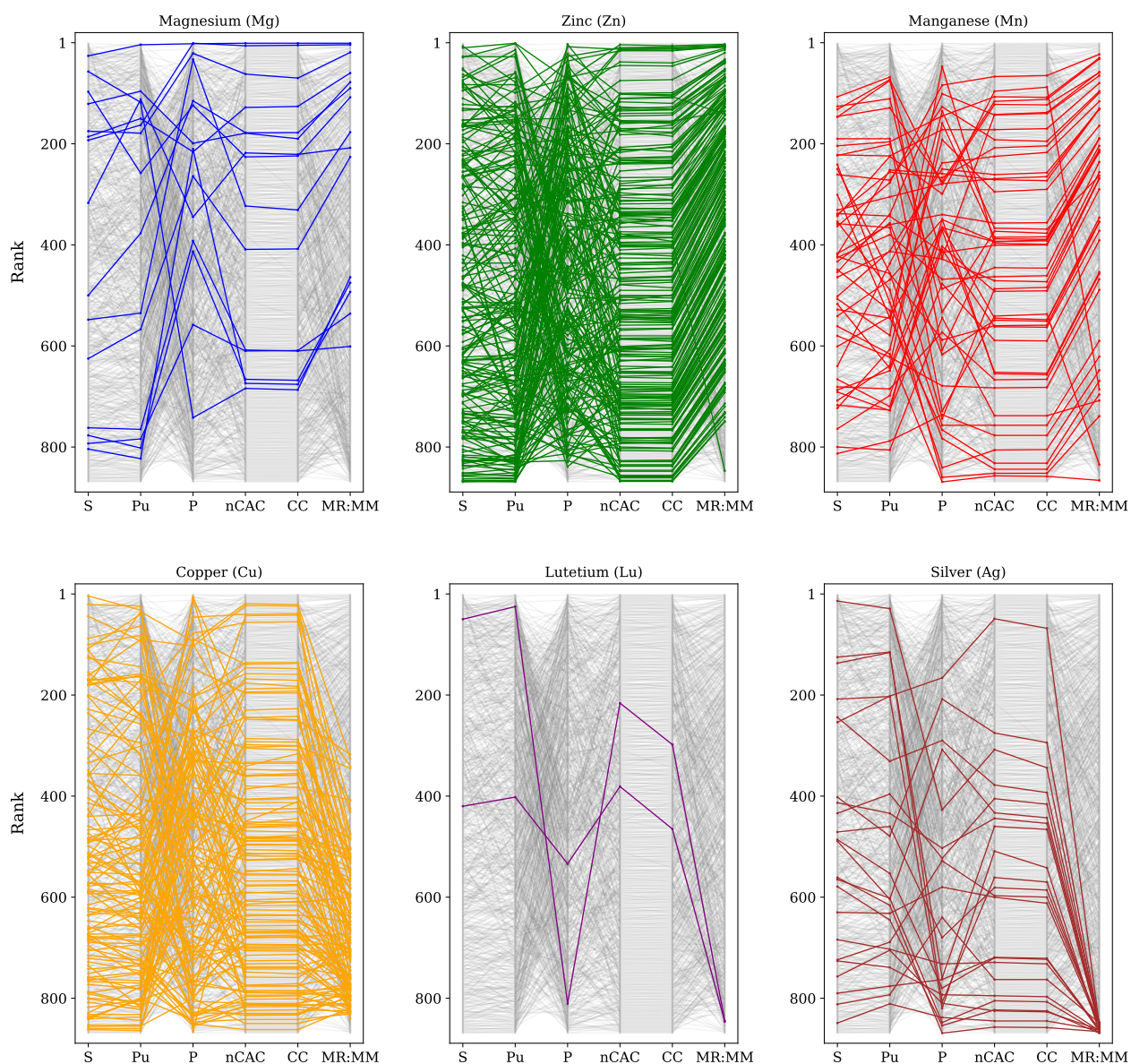




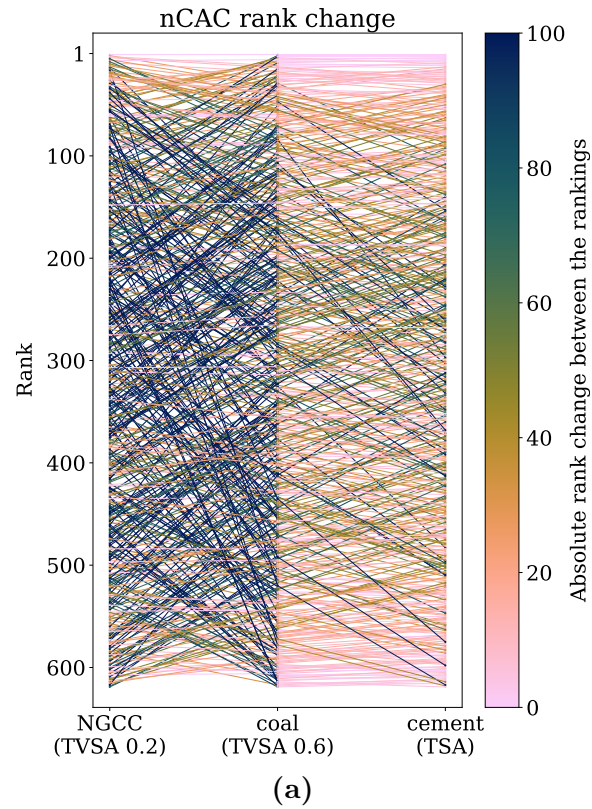
**Extended Data Figure 2| Spearman’s rank correlation matrix for the cement case in the UK with TSA process.** Spearman’s rank correlation matrix of the rankings considering one material KPI, eight process KPIs, eight TEA KPIs, and 16 LCA KPIs. A dark blue color represents very strong correlations, while dark red represents lower correlations. The size of the circle is proportional to the absolute value of the correlation. The diagonal circles in the matrix have a Spearman’s correlation coefficient of 1 since they represent the Spearman’s correlation of a KPI with itself. A more detailed description can be found in Supplementary Information Section 7.



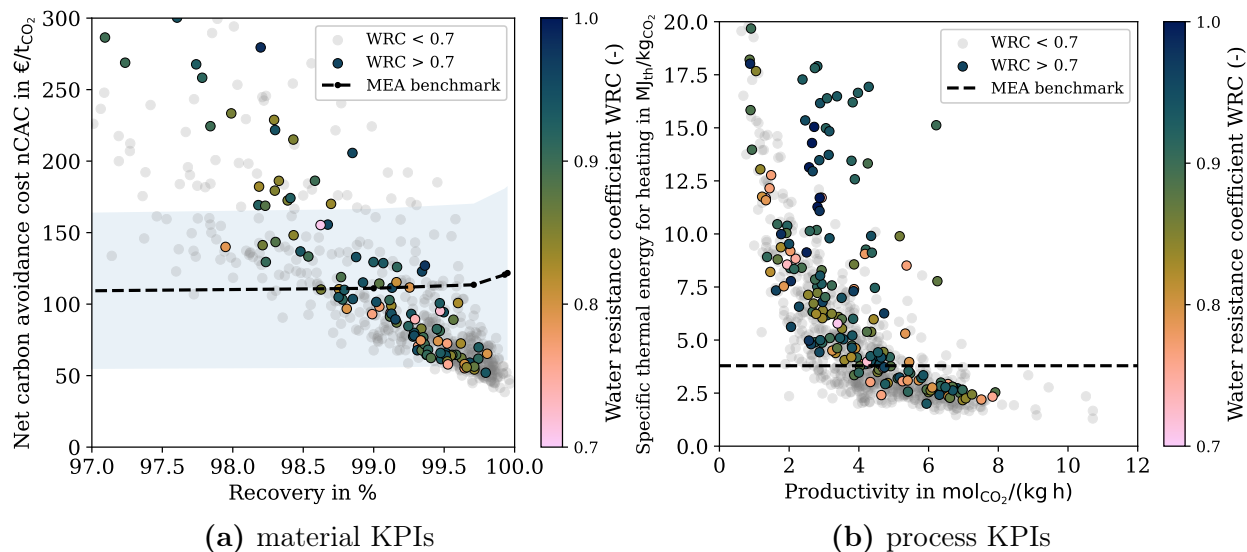
**Extended Data Figure 3 | Materials ranking for LCA-KPIs for cement in the UK with TSA process:** (a) Impact of climate change on materials ranking for materials for which more CO<sub>2</sub> is emitted than captured during the entire life cycle of the capture plant. The materials that are colored red have a Climate Change larger than 1, which implies that the total CO<sub>2</sub>-eq. emissions of the capture plant using this material are larger than the amount of CO<sub>2</sub> that is captured. Note that we changed nCAC to the Carbon Capture Cost (CCC) (see Supplementary Information Section 4.3.6) because the nCAC is not defined for these materials. (b) Material ranking for all 16 main LCA KPIs: Climate Change (CC), Water Use (WU), Energy Resources: Non-Renewable (ER:NR), Material Resources: Metals/Minerals (MR:MM), Land Use (LU), Acidification (A), Ecotoxicity: Freshwater (EcoT:F), Eutrophication: Freshwater (Eut:F), Eutrophication: Marine (Eut:M), Eutrophication: Terrestrial (Eut:T), Human Toxicity: Carcinogenic (HT:C), Human Toxicity: Non-Carcinogenic (HT:NC), Particulate Matter Formation (PMF), Ozone Depletion (OD), Photochemical Ozone Formation: Human Health (POF:HH), and Ionising Radiation: Human Health (IR:HH). The colored lines show the top 20 materials for nCAC shown in the first column (red).



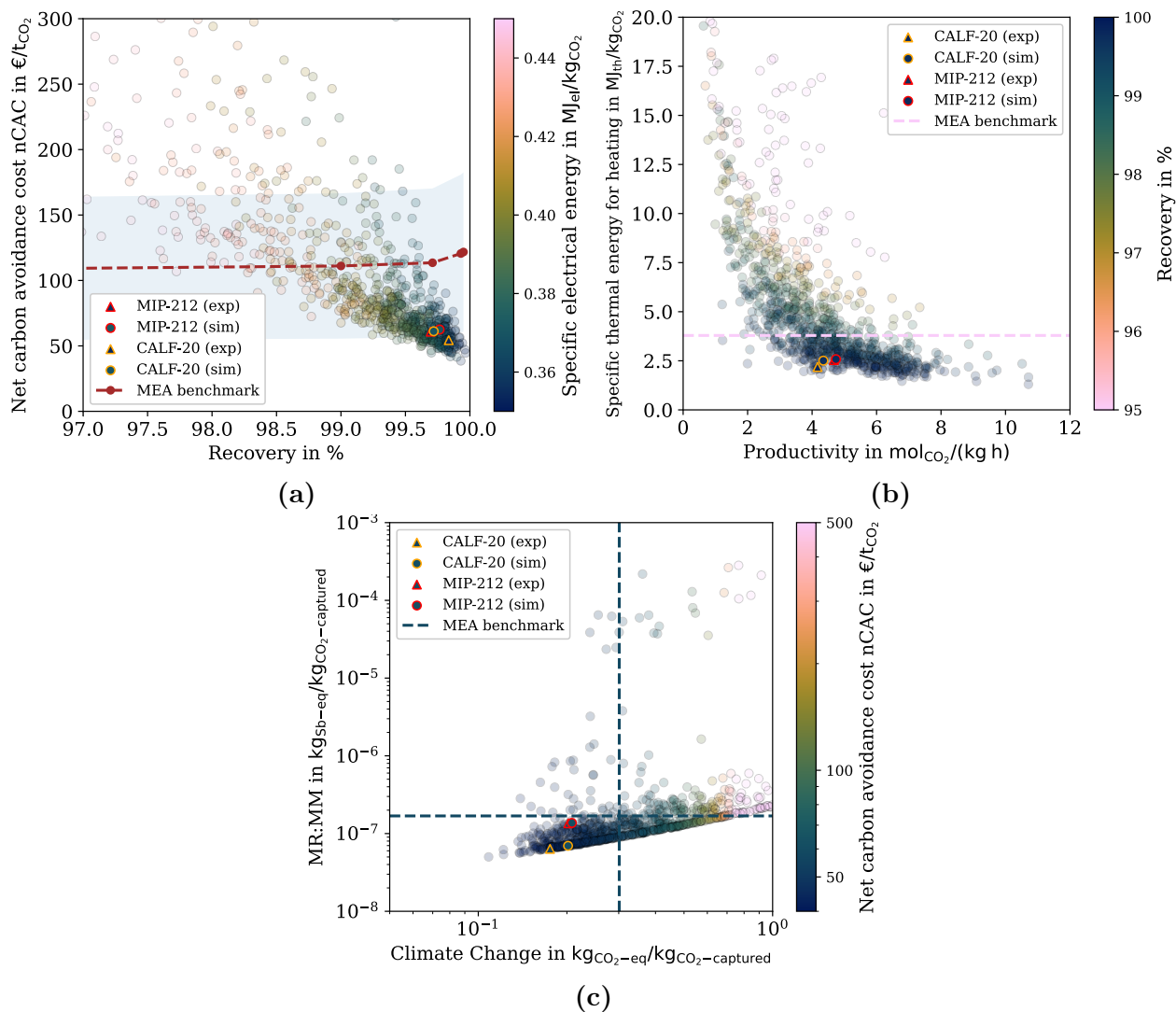
**Extended Data Figure 4 | Ranking of the two classes of metals for the cement case in the UK with TSA process.** Top: abundant metals (Mg, Zn, Mn), and Bottom: more rare metals (Cu, Lu, Ag). Some MOFs contain more than one type of metal. All these metals are considered in the KPI MR:MM and can lower the ranks significantly. A combination of two or three metals is, for example, contained in the worst-performing Manganese (Mn) materials leading to their bad performance in MR:MM compared to the other materials containing the same metal.



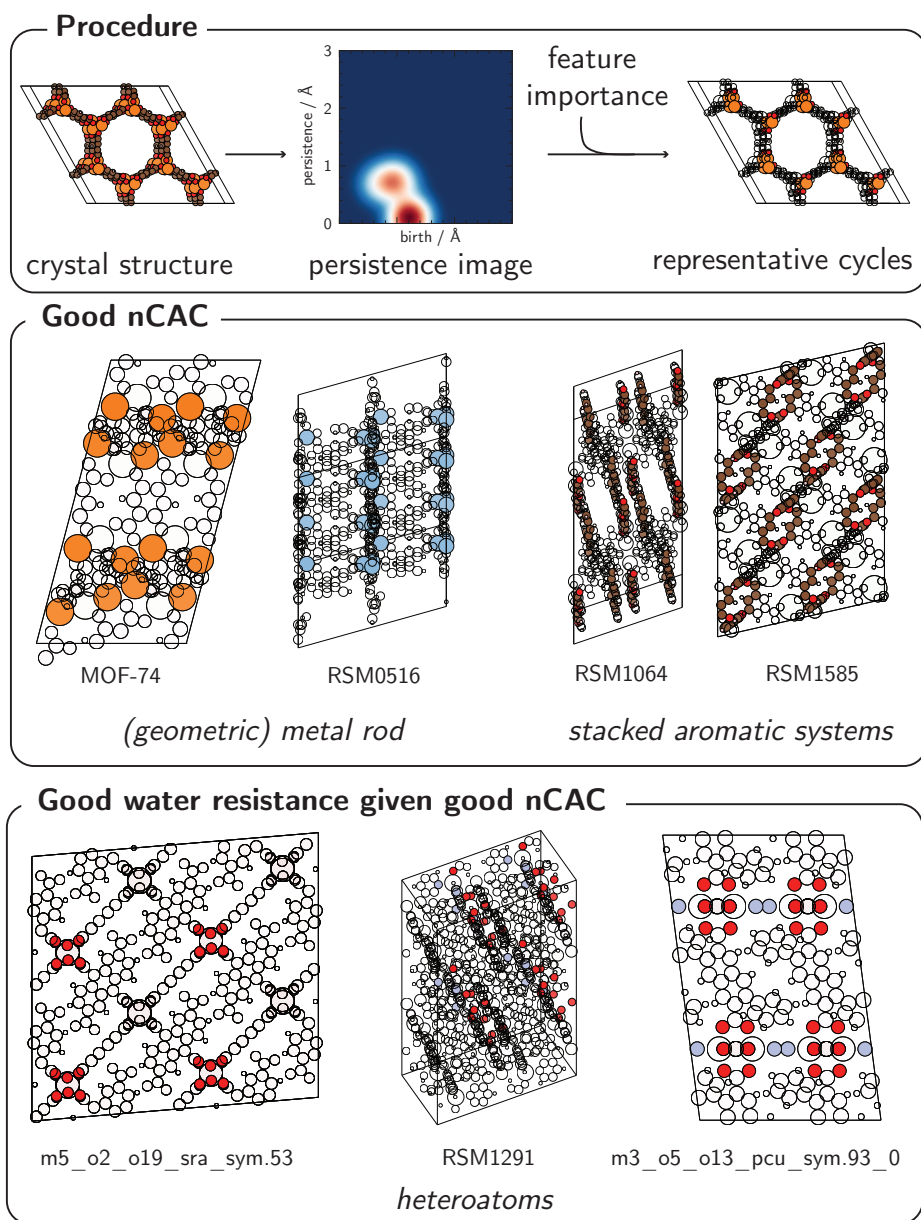
**Extended Data Figure 5 | Ranking of materials for NGCC power plant (TVSA at 0.2 bar), coal power plant (TVSA at 0.6 bar), and cement plant (TSA).** The materials are ranked according to the Net Carbon Avoidance Cost (nCAC) using the preferred technology. The color coding of the lines shows the number of ranks a material change ranking.



**Extended Data Figure 6 | Materials with a high water resistance coefficient for the cement case in the UK with TSA process.** The water resistance coefficient is defined as the ratio of the  $\text{CO}_2$  capacity in wet and dry flue gasses (see Supplementary Information Section 4.1.10). We computed the water resistance coefficient from molecular simulations at the adsorption conditions for the cement case study. The materials with a water resistance coefficient  $< 0.7$  are colored grey. Color coding is used for materials with a coefficient  $> 0.7$ . (a) gives the net carbon avoidance costs versus recovery, and (b) gives specific thermal energy versus recovery for cement in the UK.



**Extended Data Figure 7 | Materials performance for a TSA carbon capture process added to a cement plant in the UK using experimental data:** The dotted lines in these figures show the MEA benchmark, whereas in figure (a), the blue shaded area gives the uncertainty. Each dot represents a material. The triangles are the structures for which experimental property data is used directly in the platform (see Supplementary Information Section 5). (a) CAC versus recovery (R) with color coding the specific energy consumption, (b) Specific energy consumption versus productivity (P) with color coding the recovery, and (c) Material Resources: Metals/Minerals (MR:MM) versus Climate Change (CC) with color coding the nCAC.



**Extended Data Figure 8 | Identifying the adsorbaphore:** The top figures illustrate the methodology; the crystal structure is converted into a persistence image. From a model that is trained to predict whether the CAC is lower than the MEA-based benchmark, we extract the most relevant pixels of the persistence images. For the top-performing structures w.r.t. the CAC, we additionally build another model to classify them based on the water-resistance performance. We then identify representative cycles, which are collections of atoms that generate a corresponding topological feature (i.e., birth/persistence pair). The bottom figures show examples of the top-performing structures' recurring molecular features (adsorbaphores). Supplementary Information Section 8.5.1 provides more examples of these top-performing structures and it gives the details of the methods that are used.

## Acronyms

**CAC** Carbon Avoidance Cost.

**CAPEX** Capital Expenditure.

**CC** Climate Change.

**CCC** Carbon Capture Cost.

**KPI** Key Performance Indicator.

**MEA** Mono-Ethanol-Amine.

**MR:MM** Material Resources: Metals/Minerals.

**nCAC** Net Carbon Avoidance Cost.

**NGCC** Natural Gas Combined Cycle.

**PrISMa** Process-Informed design of tailor-made Sorbent Materials.

**TSA** Temperature Swing Adsorption.

**TVSA** Temperature Vacuum Swing Adsorption.

**WRC** Water resistance coefficient.