



The Best Carbon-Capture Material Does Not Exist

The rapid growth of artificial intelligence and computational materials discovery is creating vast libraries of candidate sorbents for carbon capture, but identifying a material with attractive CO₂ adsorption properties is not the same as identifying a good carbon-capture material. A sorbent's usefulness depends on how its molecular properties translate into process performance, energy consumption, cost, environmental impact, stability, and ultimately the amount of CO₂ genuinely avoided.¹

Here, we use metal–organic frameworks² as a model system to illustrate an application-driven strategy for materials discovery in which the relevant objective is defined at the level of the complete carbon-capture process rather than by a single materials descriptor. In the PrISMa framework, molecular simulations couple directly to process optimization, techno-economic analysis, and life-cycle assessment, enabling candidate materials to be ranked using metrics such as net carbon-avoidance cost.¹ This perspective fundamentally changes how large materials spaces should be explored: adsorption capacity, selectivity, or even regeneration energy alone cannot determine the optimum material, and the properties worth predicting depend on the capture application and process configuration.

Artificial intelligence can greatly accelerate this search by generating candidate materials, predicting missing properties, and replacing computationally demanding process calculations with surrogate models, but only when it is embedded within the physics and engineering of carbon capture.³ The central challenge is therefore not to discover more materials, but to discover materials that remain superior when placed inside a realistic carbon-capture system.

References

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