Using machine learning to explore the full potential of porous materials

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Advanced tools can help sift through nearly endless combinations to find materials with desired properties.

Metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs) are exciting new classes of porous materials rapidly growing in importance across several fields. Due in part to the nearly limitless possible combinations between metal or nonmetal clusters and organic linkers, these materials have wide-ranging applications in everything from gas separation to drug delivery.

However, the dizzying number of these materials introduces a unique problem: finding the right one. Gulbakan et al. discussed recent machine learning approaches that can significantly reduce computation time when searching for promising MOF or COF materials.

“The number of MOFs and COFs has increased significantly and has already reached hundreds of thousands of different porous materials,” said author Seda Keskin. “It is impossible to analyze each material individually using brute-force molecular simulations and trial-and-error experiments.”

The team focused on porous materials used for methane purification, a field that faces a complicated version of this problem due to a variety of gas mixtures and operating conditions. Despite these additional variables, machine learning-based tools could identify patterns in existing datasets and predict material properties.

“Recently, researchers have started to employ machine learning algorithms to analyze the vast amount of data generated from molecular simulations,” said Keskin. “By identifying correlations between structural features of MOFs and COFs and their separation performance, machine learning models can predict the performance of new materials with high accuracy.”

In addition, by establishing relationships between structure and function, these machine learning models can help researchers better understand the underlying mechanisms of these interactions.

Thanks to these tools, the authors look forward to a future where the boundless possibilities of MOF and COF materials can be more thoroughly explored.