Unlocking membrane-based He/H_2 separation with AI

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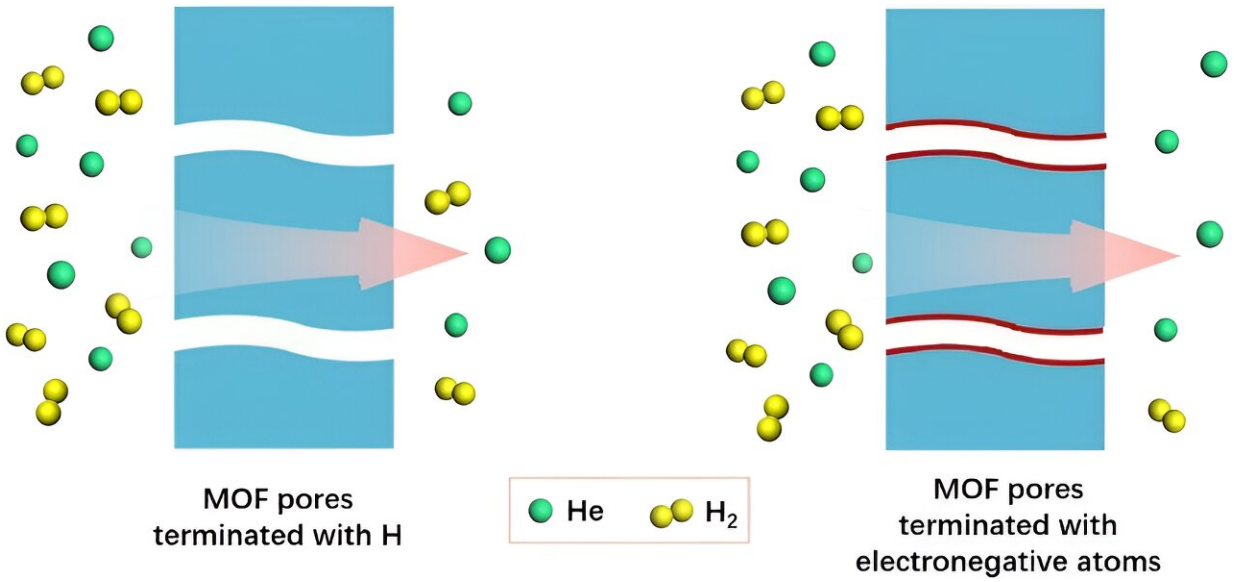

How the separation performance enhanced. Credit: Zhang. S. et al.

Technological advancement and data proliferation have deemed artificial intelligence (AI)-driven innovation as a growth opportunity for the development of breakthrough materials for special applications, especially in the field of gas separation. One of the main challenges associated with this process is the extremely close kinetic diameters of the two gas molecules, resulting in low membrane selectivity.

In a study published in *Green Chemical Engineering*, a group of

researchers from China came up with a novel approach to explore materials with enhanced helium extraction efficiency—with the aid of AI.

In particular, the researchers investigated structure-performance relationships, elucidated separation mechanisms and identified crucial factors influencing the separation performance to design metal-organic framework (MOF)-based membranes. The pore limiting diameter (PLD) and void fraction (φ) were revealed as the most important physical features for determining the membrane selectivity and He permeability, respectively.

"Traditional material development faces constraints, but AI is revolutionizing the field," says Zhengqing Zhang, lead investigator of the study "Our approach not only reveals hidden mechanisms but also uncovers new insights."

The team hopes that their results will encourage scientists to continue investigating the intersection of AI and material science, opening doors to unprecedented technological advancements.

More information: Shitong Zhang et al, Machine learning aided investigation on the structure-performance correlation of MOF for membrane-based He/H_2 separation, *Green Chemical Engineering* (2024). DOI: 10.1016/j.gce.2024.01.005

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