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Unlocking membrane-based He/H2 separation with AI

USA, April 9, 2024 /EINPresswire.com/ -- Researchers found that the electronegative atoms on the pore surfaces can enhance the gas separation by a combination of machine learning and multiscale simulation. This approach not only provides valuable theoretical guidelines but also accelerates the development of novel MOF membranes aimed at efficient separation of He/H2.

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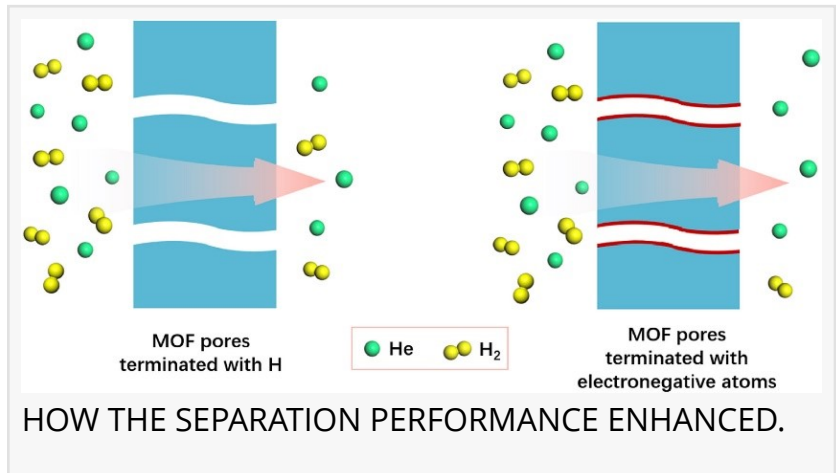
Technological advancement and data proliferation have deemed artificial intelligence (AI)-driven innovation as growth opportunity to the development of breakthrough materials for special applications, especially in the field of gas separation. One of the main challenges associated with this process is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

In a study (https://doi.org/10.1016/j.gce.2024.01.005) published in the KeAi 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 would encourage scientists to continue investigating the intersection of AI and material science, opening doors to unprecedented technological

advancements.

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