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Propane/Propylene Separation via Molecular Dynamics Simulations in Metal-Organic Frameworks.

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Propylene is crucial for the petrochemical industry, and most studies focus on separating it from propane. However, current methods for obtaining pure propylene require complex, energy-intensive desorption processes using propylene-selective porous materials. A more efficient approach is to develop an adsorbent that prefers propane, allowing for one-step high-purity propylene production, reducing energy consumption and the need for large amounts of adsorbent. To find suitable materials, the CoRE MOF database is used, employing molecular dynamics simulations in identifying materials with strong potential for propane/propylene separation. The top 5 MOFs for propane and propylene separation are identified, with carbonyl groups found to significantly enhance separation. Additionally, a machine learning model is used to predict self-diffusion values, showing good agreement with molecular dynamics simulation data.

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