Contribution ID: **135** Type: **Lightning Talk (short presentation on 2nd day, max. 5 minutes, max. 2 slides)**

Xylene isomers' separation: A computational investigation via molecular dynamics and grand-canonical Monte Carlo simulations.

Thursday, September 26, 2024 10:05 AM (5 minutes)

This study presents a computational investigation of the separation of xylene isomers, with a particular focus on the selective isolation of para-xylene. The separation of xylene isomers is a challenging process due to their similar physical properties, which necessitates the use of energy-intensive and complex separation techniques. To address these challenges, we employed a dual approach combining molecular dynamics (MD) simulations and grand-canonical Monte Carlo (GCMC) simulations. The Computation-Ready Experimental Metal-Organic Framework (CoRE MOF) 2019 database served as the foundation for our computational screening, allowing us to identify promising materials for xylene isomer separation based on diffusion and adsorption characteristics. Our findings highlight specific metal-organic frameworks (MOFs) that exhibit superior selectivity and capacity for para-xylene, offering valuable insights into the design of efficient separation processes for industrial applications.

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