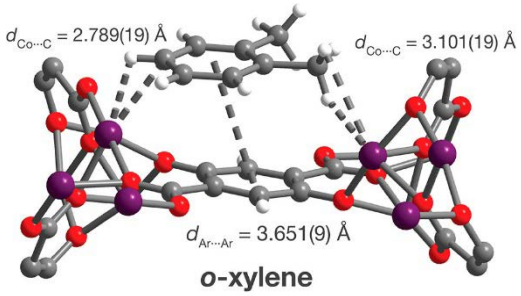
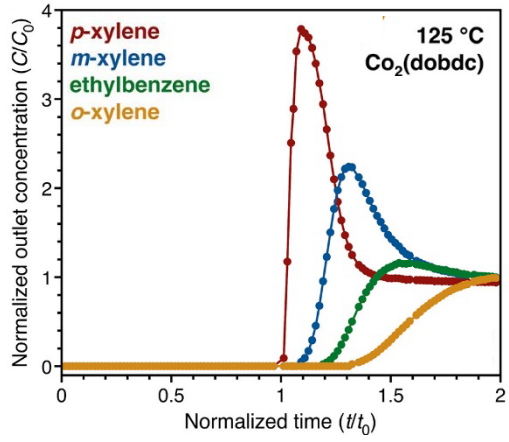
# Separation of Xylene Isomers through Multiple Metal Site Interactions in Metal–Organic Frameworks

## Multi-metal site interactions




**(Top)** Single crystal structure of *o*-xylene binding in $Co_2$(dobdc) **(Bottom)** Multi-component vapor breakthrough measurement in $Co_2$(dobdc).

## Scientific Achievement

**Two adjacent Co(II) metal centers in a metal–organic framework effectively separate molecules by using both metal sites to synergistically bind guest molecules**

## Significance and Impact

**This method allows for separation of all four industrially relevant xylene isomers in a multi-component mixture, and can be used to design new hydrocarbon isomer separation adsorbents**

## Research Details

- Vapor breakthrough measurements and multi-component solution phase adsorption measurements show ability of $Co_2$(dobdc) to separate four $C_8$ alkylaromatic isomers
- Single crystal X-ray diffraction reveals unique interaction of one molecule binding to two metal sites, serving as the basis for selective adsorption
- Framework flexing to accommodate higher capacities of xylenes was also experimentally observed in a $M_2$(dobdc) analogue for the first time


Gonzalez, M. I.; Kapelewski, M. T.; Bloch, E. D.; Milner, P. J.; Reed, D. A.; Hudson, M. R.; Mason, J. A.; Barin, G.; Brown, C. M.; Long, J. R. *J. Am. Chem. Soc.* **2018**, *140*, 3412-3422



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