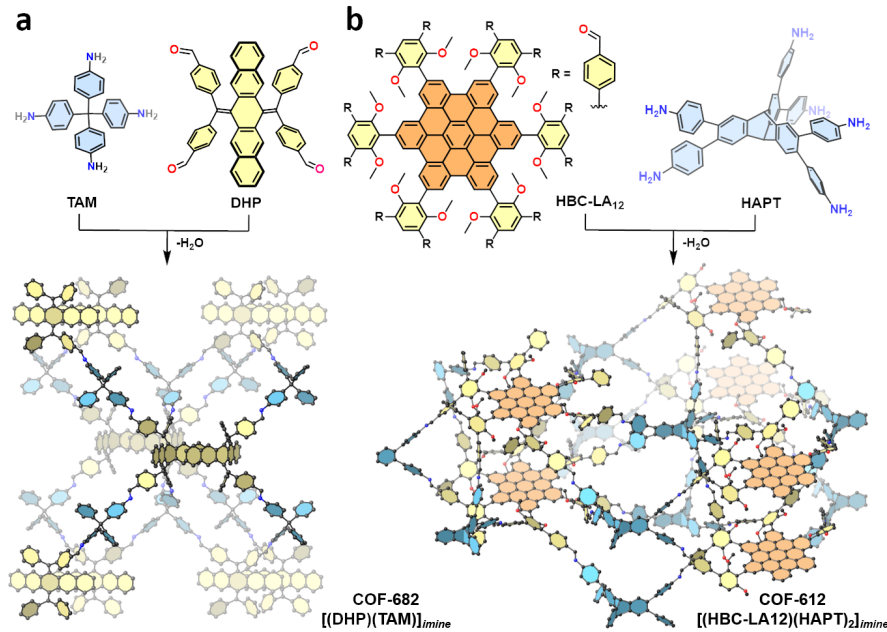


X-ray Data and Simulations Explore Porous Polymer Framework



To create COF-682 (a) and COF-612 (b), specifically shaped molecular building blocks are chemically linked together. COF-682 is built from smaller, V-shaped units, while COF-612 incorporates much larger, flatter building blocks. Researchers found that these differences in size combined with the shape of their molecular components give each framework different properties and dynamics.

F. Tavani, S. Mirzaei, J. Yin, Y. H. Lin, C. Myers, C. H. Lin, A. M. M. Abeykoon, S. J. L. Billinge, O. M. Yaghi, "Local Structure and Dynamics of Three-Dimensional Covalent Organic Frameworks" *Journal American Chemical Society* (2026). <https://doi.org/10.1021/jacs.6c17514>

Scientific Achievement

Scientists use X-ray pair distribution function (PDF) data and machine-learning-assisted molecular dynamics simulations to reveal the local structure and dynamics of 3D covalent organic frameworks (COFs).

Significance and Impact

Because framework dynamics influence material properties, understanding and controlling flexibility could help researchers design COFs with specific functions and applications.

Research Details

- PDF measurements at NSLS-II and machine-learning-assisted molecular dynamics simulations helped probe the local atomic structure and dynamics of COFs, including flexibility and disorder
- Scientists studied two 3D COFs, COF-682 and COF-612, and found that differences structure led to different degrees and types of flexibility.
- Tunable COFs show promise in applications like gas storage, chemical separation, catalysis, and more.