Crystallography Beyond Structure in Metal–Organic Frameworks

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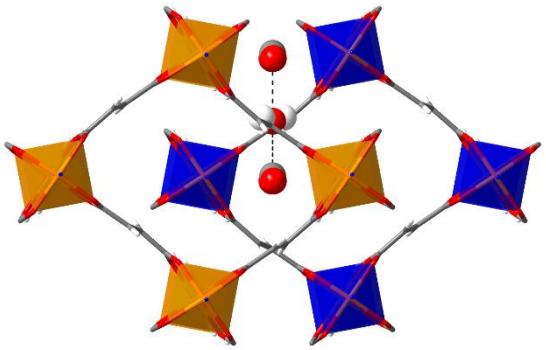
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Modern crystallography has made remarkable advances in probing materials beyond static structures, including in situ and time-resolved investigations. However, functional porous materials such as metal–organic frameworks (MOFs) still challenge our ability to fully capture structure–property relationships, as their behavior arises from dynamic processes, local heterogeneities, and subtle structural rearrangements.

In this keynote, I will show how an integrated crystallographic approach, combining variable-environment powder X-ray diffraction with complementary spectroscopic techniques, enables direct insight into these complexities. By probing materials under working conditions, we can simultaneously access long-range structural evolution and local electronic changes.

Selected examples will demonstrate how this strategy allows us to: (i) identify transient and preferential adsorption sites; (ii) elucidate the role of defects and coordinatively unsaturated metal centers; and (iii) extract thermodynamic and structural information directly from diffraction data.

Taken together, these examples show how crystallographic methods can directly link structural evolution to functional behavior in MOFs, providing a practical basis for understanding and designing responsive porous materials.



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