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Strategies for the Design of Functional MOFs: Addressing Energy-intensive Separations

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Metal Organic Frameworks (MOFs) are a promising class of crystalline solid-state materials amenable to tailoring their porosity and functionality towards various applications. MOF reticular chemistry using the Molecular Building Block (MBB) approach offers potential to construct robust made-to-order MOFs, where desired structural and geometrical information are incorporated into the building blocks prior to the assembly process.

We will discuss two recently implemented conceptual approaches facilitating the design and deliberate construction of metal–organic frameworks (MOFs), namely supermolecular building block (SBB) and supermolecular building layer (SBL) approaches. Additionally, the concept of net-coded building units (net-cBUs), where precise embedded geometrical information codes uniquely and matchlessly a selected net, as a compelling route for the rational design of MOFs will be presented.

Our progress in the development of functional metal-organic frameworks (MOFs) to address some energy-intensive separations will be discussed. Namely, the successful practice of reticular chemistry affording the fabrication of various stable MOFs with controlled pore-aperture size and allowing effective separation of various gas or vapors pairs.

Keywords: Design of MOFs, Topology, Molecular building block (MBB) approach