Novel design strategy advances discovery of metal-organic frameworks

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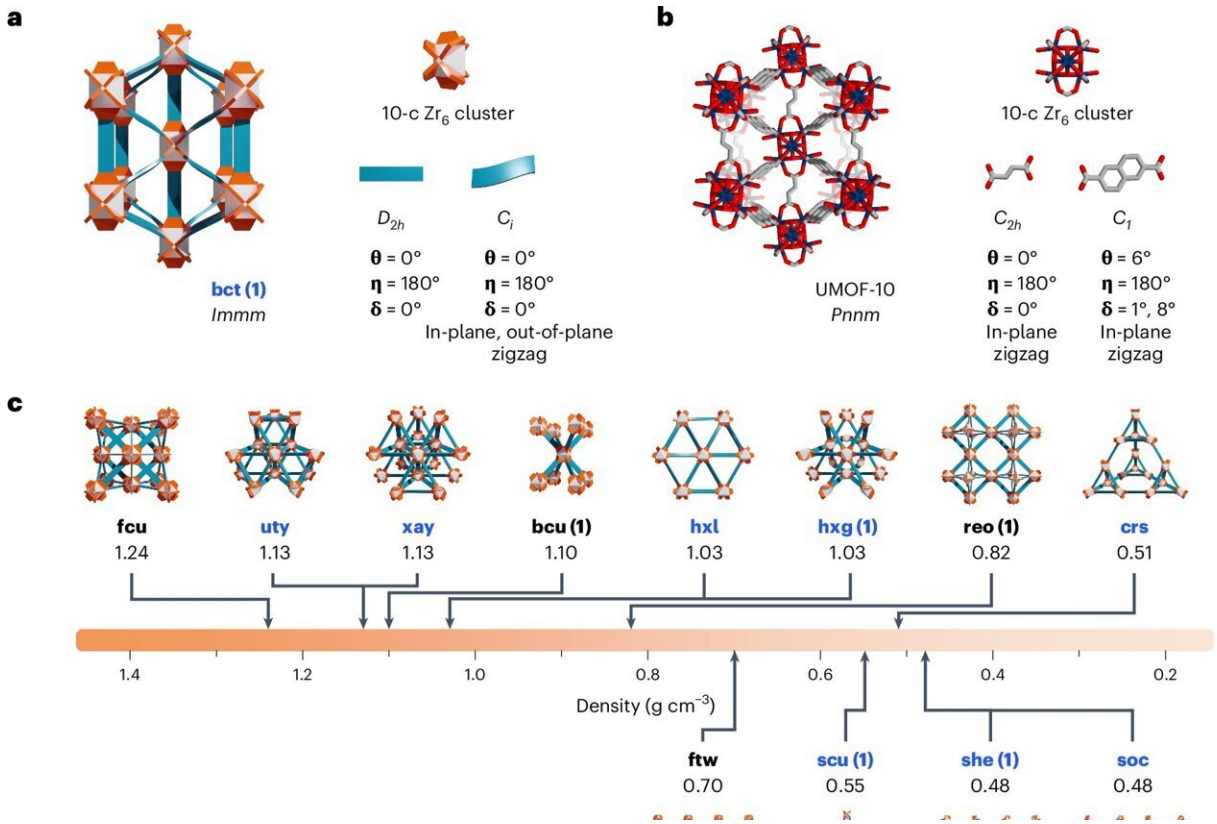

Discovery of new Zr_6-based MOFs with bct (1) and scu (1) configurations. Credit: *Nature Synthesis* (2024). DOI: 10.1038/s44160-024-00638-x

An innovative strategy, known as the "Up-Down Approach," has the potential to dramatically accelerate the creation of metal-organic

frameworks (MOFs). The paper is published in the journal *Nature Synthesis*.

The research team, led by Professor Wonyoung Choe at Ulsan National Institute of Science and Technology (UNIST), South Korea, has developed a novel strategy for designing MOFs. MOFs, which consist of metal clusters and organic molecules, are emerging as crucial materials for various applications, including carbon dioxide capture, storage, and catalysis.

Their primary advantage lies in their customizable structure, which enables the creation of materials with tailored properties.

Traditionally, MOFs have been designed using either a bottom-up or top-down approach. The bottom-up approach begins by selecting the metal clusters and organic ligands, followed by the exploration of potential structures. In contrast, the top-down approach begins with a desired structure and identifies the appropriate components to achieve the target structure.

The Up-Down Approach merges these methodologies, facilitating a broader exploration of structures based on metal clusters before selecting suitable organic ligands. This approach overcomes the limitations of traditional methods, which are often constrained by predefined components and structural restrictions.

By enabling new combinations of diverse elements, the Up-Down Approach opens new avenues for discovering novel structures that were previously inaccessible.

By applying this strategy, the team identified 26 new zirconium-based MOFs, which are renowned for their high chemical stability. They successfully synthesized two of these new structures, demonstrating the

effectiveness of the Up-Down Approach.

Additionally, the team employed a "Ribbon Representation" to visualize the precise geometric features of organic ligands, further enhancing the accuracy and efficiency of the design process.

Jiyeon Kim, the first author of the study, stated, "The Up-Down Approach provides a powerful tool for rapidly exploring and developing new materials with a range of chemical properties. This method significantly enhances the efficiency of material development research."

Co-first author Dongsik Nam added, "This research paves the way for the discovery of innovative materials that can be applied across various fields, including catalysis, gas storage, and environmental remediation."

Professor Wonyoung Choe remarked, "Our study represents a major advancement in expanding the chemical space of MOFs, significantly broadening their potential applications. We anticipate that this will mark a transformative moment in functional materials research."

More information: Jiyeon Kim et al, Up–down approach for expanding the chemical space of metal–organic frameworks, *Nature Synthesis* (2024). DOI: 10.1038/s44160-024-00638-x

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