Algorithm identifies optimal pairs for composing metal-organic frameworks

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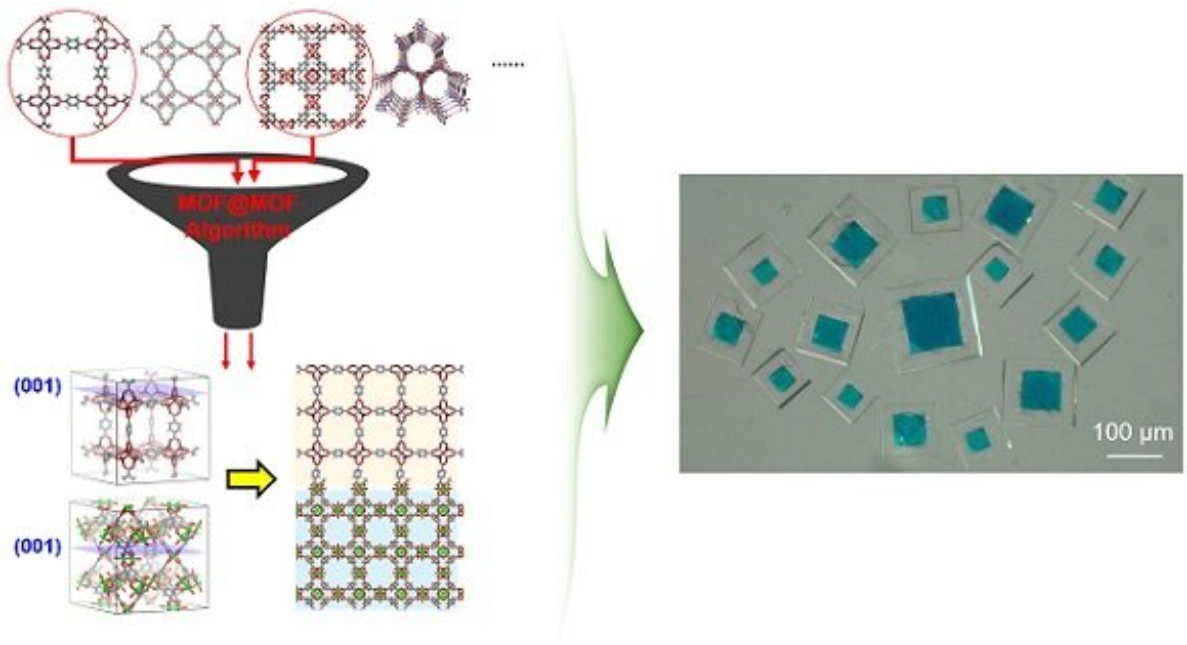

Figure: An example of a rationally synthesized MOF@MOFs (cubic HKUST-1@MOF-5). Credit: The Korea Advanced Institute of Science and Technology (KAIST)

The integration of metal-organic frameworks (MOFs) and other metal nanoparticles has increasingly led to the creation of new multifunctional materials. Many researchers have integrated MOFs with other classes of materials to produce new structures with synergetic properties.

Despite there being over 70,000 collections of synthesized MOFs that can be used as building blocks, the precise nature of the interaction and the bonding at the interface between the two materials still remains unknown. The question is how to sort out the right matching pairs out of 70,000 MOFs.

An algorithmic study published in *Nature Communications* by a KAIST research team presents a clue for finding the perfect pairs. The team, led by Professor Ji-Han Kim from the Department of Chemical and Biomolecular Engineering, developed a joint computational and experimental approach to rationally design MOF@MOFs, a composite of MOFs where an MOF is grown on a different MOF.

Professor Kim's team, in collaboration with UNIST, noted that the metal node of one MOF can coordinately bond with the linker of a different MOF and the precisely matched interface configurations at atomic and molecular levels can enhance the likelihood of synthesizing MOF@MOFs.

They screened thousands of MOFs and identified optimal MOF pairs that can seamlessly connect to one another by taking advantage of the fact that the metal node of one MOF can form coordination bonds with the linkers of the second MOF. Six pairs predicted from the computational algorithm successfully grew into single crystals.

This computational workflow can readily extend into other classes of materials and can lead to the rapid exploration of the composite MOFs arena for accelerated materials development. Even more, the workflow can enhance the likelihood of synthesizing MOF@MOFs in the form of large single crystals, and thereby demonstrated the utility of rationally designing the MOF@MOFs.

This study is the first algorithm for predicting the synthesis of composite

MOFs, to the best of their knowledge. Professor Kim said, "The number of predicted pairs can increase even more with the more general 2-D lattice matching, and it is worth investigating in the future."

More information: Ohmin Kwon et al. Computer-aided discovery of connected metal-organic frameworks, *Nature Communications* (2019). DOI: 10.1038/s41467-019-11629-4

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