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Communication

Functionality proportion and corresponding stability study of multivariate metal-organic frameworks

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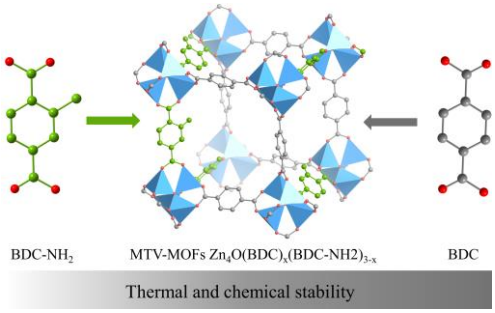
Graphical Abstract



Zn-based multivariate metal-organic frameworks (MTV-MOFs) with different functionality proportions and with different thermal and chemical stabilities can be obtained by employing the appropriate synthesis method.

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ABSTRACT

Multivariate metal-organic frameworks (MTV-MOFs) with different ratios of terephthalate (BDC) linker and amino-benzenedicarboxylate (BDC-NH_2) linker were synthesized through both direct synthesis from linker mixture and linker exchange of activated single-linker MOFs. Functionality proportion was impacted by the thermodynamics during the one-pot MOF construction, resulting in preference of BDC over BDC-NH_2 in the MTV-MOF, in agreement with the quantum mechanics calculations. The functionality difference also affects the thermodynamics in the linker exchange process, as indicated by the more effective linker exchange in BDC-NH_2-based IRMOF-3 than in BDC-based MOF-5. Furthermore, the thermal decomposition temperatures and chemical integrity upon ambient air exposure of these MOFs with variate functionalities were investigated, and it reveals that higher proportion of BDC in the MTV-MOF crystals contribute to both higher thermal and higher chemical stabilities.

The family of metal-organic frameworks (MOFs) [1-3] has greatly extended after the discovery of multivariate metal-organic frameworks (MTV-MOFs) that maintain the same topology of the crystals with multiple metal ions or organic linkers [4-6]. MTV-MOFs provide a platform to adjust the proportion of the functionalities without losing order, which makes them promising materials for gas adsorption [7] and catalysis [8-11] by providing different functionalities that could work together and complement each other.

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