A NUCLEATION MECHANISM OF ZINC-BASED MOF STRUCTURES

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Metal-organic frameworks (MOFs) are of interest due to their high porosity and are used in catalysis, gas separation, and biology [1–4]. Although numerous experimental studies have been conducted on MOF synthesis, the nucleation mechanism has not been sufficiently investigated. Therefore, in this study, we explore the nucleation processes of IRMOF-1 using reactive Molecular Dynamics simulations. The preliminary results indicated that the selected ligand (1,4-benzodicarboxylate) and the metal node (Zn₄O) preferentially combine, forming the IRMOF-1 unit cell (Fig. 1).

Figure 1. Nucleation of Mono IRMOF-1 based on Zn4O and 1-4-benzodicarboxylate

This study provides new insights into the early synthesis stages of zinc-based IRMOFs.

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