

安定な超分子集合体の合成
Synthesis of stable supramolecular assemblies

京都大学高等研究院物質—細胞統合システム拠点 古川 修平

研究成果概要

In this study, the supercomputer system at the Institute for Chemical Research, Kyoto University, was used to simulate crystal structures, structural distortions, and intermolecular interactions between discrete molecules. Metal-organic polyhedra (MOPs) were designed and linked using imidazole- or pyridine-based connectors to form either amorphous soft structures or extended 3D networks, such as metal-organic frameworks (MOFs).

For the 3D extended networks, some structures remained stable after solvent removal, while others underwent amorphization. To better understand and rationalize these behaviors, thermodynamic simulations were conducted. Additionally, interactions between purely organic moieties were analyzed to compare different imidazole- and pyridine-based linkers. These simulations were then compared with structural data from the Cambridge Structural Database.

For the amorphous structures, the organic moieties of the MOPs were modeled and segmented using Q-Chem to evaluate their contributions to non-covalent interactions. The objective was to identify the dominant intermolecular forces and pinpoint the specific locations of interacting moieties within the MOPs.

発表論文(謝辞なし)

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