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

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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）

1. “Phase-transformable metal-organic polyhedra for membrane processing and switchable gas separation”, Po-Chun Han, Chia-Hui Chuang, Shang-Wei Lin, Xiangmei Xiang, Zaoming Wang, Mako Kuzumoto, Shun Tokuda, Tomoki Tateishi, Alexandre Legrand, Min Ying Tsang, Hsiao-Ching Yang, Kevin C.-W. Wu, Kenji Urayama, Dun-Yen Kang & Shuhei Furukawa, *Nat Commun.* **2024**, 15, 9523.

2. “Pore-networked membrane using linked metal-organic polyhedra for trace-level pollutant removal and detection in environmental water”, Zaoming Wang, Idaira Pacheco-Fernández, James E. Carpenter, Takuma Aoyama, Guoji Huang, Ali Pournaghshband Isfahani, Behnam Ghalei, Easan Sivaniah, Kenji Urayama, Yamil J. Colón & Shuhei Furukawa, *Commun. Mater.* **2024**, 5 161.

3. “Frameworks Construction with Rhodium‐Organic Cuboctahedra via Rigid Linker Incorporation”, Yu-Shan Lin, Javier Lopez-Cabrelles, Chia-Her Lin, Shuhei Furukawa, *Chem Asian J.* **2025**, e202401456.