

多孔質材料における分子動力学シミュレーション
Molecular Dynamics Simulations in Porous Materials

京都大学 高等研究院 物質－細胞統合システム拠点 MezaGonzalez Brandon

Mixed-matrix membranes (MMMs), which integrate metal–organic frameworks (MOFs) with polymers, are promising candidates for selective gas separation under realistic operating conditions. However, their performance under competitive gas mixtures cannot be predicted from neat-phase properties alone and often exhibits non-linear transport behavior. The molecular-scale origin of this behavior, particularly the dynamical role of polymer–MOF interfaces, remains unresolved.

This project develops a collective-dynamics framework to elucidate gas transport mechanisms in MMMs using large-scale all-atom molecular dynamics (MD). Rather than relying on static structural descriptors, we combine time-structure independent component analysis (TICA), dynamic cross-correlation (DCC), and hidden Markov modeling (HMM) to identify long-timescale collective modes and quantify dynamical coupling between gas, polymer, and MOF phases. The goal is to establish a mechanism-level understanding of how interfacial coupling topology governs transport under both single-gas and competitive mixture conditions.

The computational results generated through this supercomputing effort are currently being consolidated into two manuscripts. The first focuses on the emergence of collective transport mechanisms and interfacial coupling topology in MMMs under single-gas and mixture conditions, collaborating with an experimental group in New Zealand. The second develops the methodological framework (TICA–DCC–HMM integration) as a generalizable approach for analyzing collective dynamics in multi-phase porous materials. Continued access to high-performance computing resources is essential to complete trajectory ensembles, finalize kinetic analyses, and ensure statistically robust results suitable for publication in high-impact journals.