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Molecular Simulation Of The Activation Of Metal Organic Frameworks

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Metal organic frameworks (MOFs) hold great promise as new, functional materials owing to their structural varieties and highly tunable chemistries. In particular, MOF-808 has been considered a next-generation filtration material due to its relatively large, micro-sized pores and potentially reactive undercoordinated metal centers. While MOFs in general have been extensively studied for several decades, much molecular-scale mechanistic detail of the activation process remains unclear. In this talk I will report on ab initio and large-scale reactive molecular dynamics calculations of the activation of MOF-808 through the removal of formate moieties on the metal sites via proton transfer dynamics.

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