Unveiling the Thermal Stability of Metal-Organic Framework Using Reactive Molecular Simulation

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Metal-organic frameworks (MOFs) are a new class of porous materials, which are composed of metal nodes connected by organic linkers. MOFs have promising applications including adsorption, membrane separation, catalysis and drug delivery. However, most of MOFs suffer from thermal stability issue, limiting their applicable working temperature. In this work, we investigated the thermal stability of the well-known MOF-5 by the mean of reactive molecular dynamic (MD) simulation. The results showed that the thermal breakdown process starts by breakage of the coordination bond that connects the metal node with the organic linker. Hence, at high temperature, the linker dynamics play essential role in depriving the stability. Such trend was also confirmed after incorporation of a methyl group on the linker. The modified structures showed high flexibility, and accordingly less thermal stability. Present work highlights the effect of temperature-induced linker dynamics on the stability of MOFs. Therefore, synthesizing MOFs using a rigid linker can improve its thermal stability and endurance for high temperature applications.