Computational-aided development of MOF water sorbents for heat reallocation

Guillaume MAURIN (ICGM, Université Montpellier CNRS, Montpellier)

Abstract

Development of thermally driven water-sorption-based technologies presents a promising eco-friendly solution to meet the exponential increase of global energy demands for applications like dehumidification, water desalination, and heating/cooling. Hydrophilicity of water adsorbents plays a pivotal role in these processes, given their operation within narrow thermodynamic windows. Metal organic frameworks (MOFs) offer exceptional tunability of porosity and chemical properties — due to the vast selection and combination of metal nodes and organic linkers — which allows for effective modification of MOF hydrophilicity by adjusting the nature, concentration and distribution of hydrophilic moieties/sites within the framework. Utilization of MOF/water working pairs has shown significant progress in adsorption-driven heat-reallocation, dehumidification, atmospheric water harvesting, and indoor moisture control systems. The quest for efficient and stable water adsorbent MOFs necessitates a thorough examination of the mechanistic behavior of water adsorption at the microscopic level before performance evaluations at system level. In this regard, molecular simulations have proven to be a powerful tool in characterizing materials, predicting equilibrium adsorption uptakes, and identifying atomically detailed adsorption mechanisms—often leading or complementing the systematic experimental evaluations at both material and system levels. This presentation will elaborate on how microscopic insights drive a rational design strategy to fine-tune hydrophilic strength, consequently adjusting the step position of water adsorption and enhancing the working capacity to improve MOF water adsorption performance. We will illustrate our approach through case studies featuring state-of-the-art MOF adsorbents.