Rational design of Metal-Organic Frameworks for the efficient capture of VOCs

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Volatile organic compounds (VOCs) are concerning atmospheric pollutants due to their impact on air quality, human health, and the environment[1]. Benzene, in particular, is known for its deleterious effects on human health, notably increasing the risk of leukemia, justifying the continuous reduction of its maximum allowable concentration. On the other hand, acetic acid plays a crucial role in preserving heritage objects exhibited in museums. It is often a byproduct of the degradation of objects made of organic materials such as paper or photographic films, thereby accelerating the deterioration process by increasing the acidity of the materials (autocatalytic hydrolysis).

To counteract the harmful effects of VOCs, a widely adopted strategy involves capturing them using adsorbents. These adsorbents must not only exhibit high adsorption capacity but also significant selectivity to maintain their effectiveness in the long term. Metal-Organic Frameworks (MOFs) stand out as an ideal family of materials for this task. These crystalline and porous hybrid solids are formed by combining metal ions or clusters with polydentate organic ligands. MOFs offer a high specific surface area and adjustable adsorption properties. By changing the metal type, functionalizing the ligands, and adjusting their length while retaining the same topological structure[2], it is possible to optimize the adsorption capacity and selectivity of these materials for the efficient capture of VOCs.

During this seminar, we will explore various approaches that combine experimentation and theoretical modeling to design selective adsorbents for capturing benzene[3,4] and acetic acid[5,6] under real conditions.

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