Nanoengineering of multivariate flexible metal-organic frameworks (flexMOFs) for separation processes: versatile experimental and theoretical approach

1. Introduction

In 1944, **Erwin Rudolf Josef Alexander Schrödinger** in his ingenious series of lectures collected in a short book "*What is the life?*", has emphasized **fundamental differences in the complexity of structures** which are subject of interest of chemists and occur in living organisms: "The arrangements of the atoms in the most vital parts of an organism and the interplay of these arrangements differ in a fundamental way from all those arrangements of atoms which physicists and chemists have hitherto made the object of their experimental and theoretical research." It is worth mentioning that one day this complexity and functionality induced by aperiodicity may be understood and introduced in flexible metal-organic frameworks (flexMOF).

By the insertion of many functional linkers in the flexMOF platform which work as a dynamic backbone, it is theoretically possible to mimic biological aperiodical dynamic "crystals" like DNA or proteins. So far, **fundamental limitations in introducing and understanding the spatial distribution of linkers in aperiodical** crystals is a hinderance in the design and development of synthesis and characterization procedures.

2. Objectives of the project

The main research objective is to work out an **experimental and theoretical protocol to produce and elucidate the spatial distribution of linkers in the multivariate flexible metal-organic** frameworks (MTV-flexMOF).

The next research objective will be **understanding untypical behavior of flexMOF and their derivatives** through the use of high/low pressure and temperature-dependent crystallography, adsorption studies and versatile *in situ* techniques during adsorption.

Understanding the heterogeneity and flexibility as well as subtle interaction between them is base for the last – most practical - research objective: **the use of MTV-flexMOFs for separation processes by building them into semipermeable membranes**.

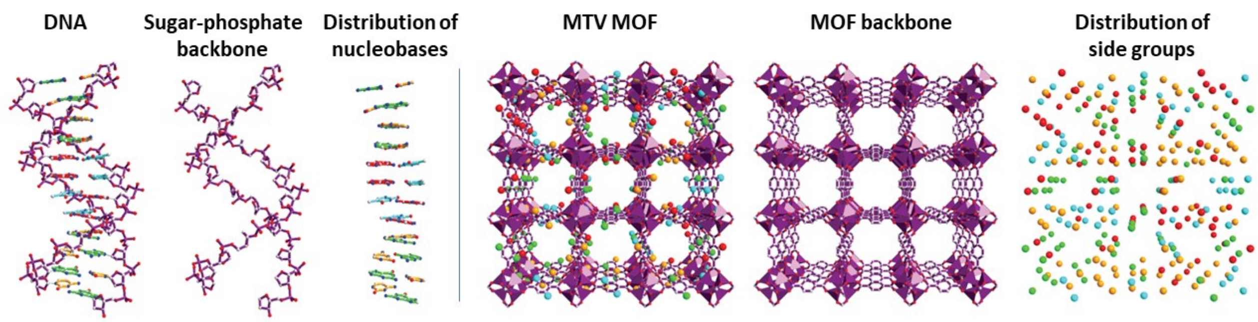

Figure 1 The comparison of the DNA molecule (left) and the MTV MOF-5 (right). Figure was adapted from the *Accounts of Chemical Research* with permission of ACS.

3. Reasons for choosing the research topic

One of the most **energy-demanding industrial processes, that emits globally 10-15% of CO_2 is the separation of similar molecules**. The rising level of CO_2 in atmosphere causes a **pressing environmental issues** such as droughts, wildfires, heat waves and flooding. MTV-flexMOFs with well-defined pore structure and intrinsic elastic behavior emerges as a **potential game changer in this application**. By introducing many different linkers into one structure and integration of MTV-flexMOFs into membranes, it is possible to **create specific interaction for very effective separation of similar molecules or carbon dioxide from exhaust fumes**.