Computational design of next generation porous materials for sensor applications

Metal organic frameworks (MOFs) are exciting new materials with a wide range of industrial applications crucial for the advancement of our society. In particular, MOFs are renowned for gas sorption, which is relevant for efficient fuel transport, and for removal of atmospheric green house gases. Further on, MOF pores come in all sorts of sizes and shapes, effectively acting as a sieve allowing certain molecules to enter, while keeping other species outside. This principle has found applications in separation of gas mixtures, water purification, as well as in sensor devices for detection of poisons, explosives and other kinds of adverse substances.

So what makes MOF applications so diverse? To understand that, we need to look into how MOF materials are constructed. As the name "metal organic framework" suggests, MOFs are modular structures constructed from metal atoms nodes connected by organic molecule linkers, which form rigid 3D porous structures (Figure 1). By combining different metals and organic linkers we can control the sizes, shapes and surface properties of MOF pores, producing materials with diverse range of properties.

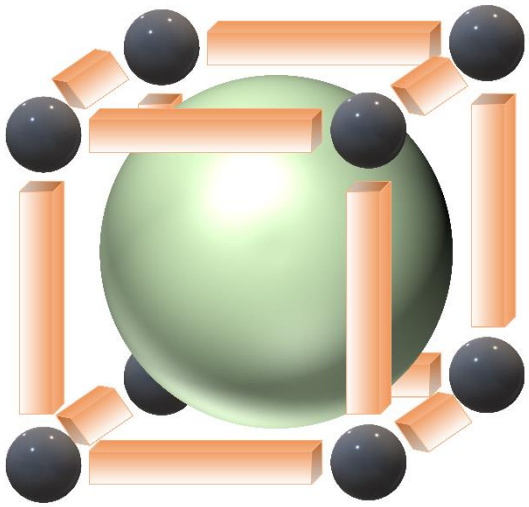

Figure 1. MOFs are porous materials built from metal nodes (grey spheres) connected by organic linkers (orange rods)

While the modularity of MOFs is the key to their success as new generation porous materials, one problem remains: how do we choose the best combination of metals and linkers to produce a material with desired properties? More often than not, this requires multiple laboratory trials, where different MOF architectures are synthesized and tested to find the material that best meets the requirements. Laboratory trials require a lot of manual work, while also producing significant amounts of chemical waste. As MOFs are to become materials driving the new green economy, we should strive to use greener techniques to develop them, in the first place.

Our plan to is to improve the efficiency of MOF design by employing computational methods. In collaboration with researchers from UK and Canada we are developing a program for building MOF structures starting from the simplest building blocks i. e. metal atoms and organic linkers. Using this procedure, we find the most probable MOF structures, and predict their properties. Our primary aim is to computationally design MOFs acting as sensors for the detection of contaminants in air and water. **With the successful development of our computational methodology, we will be able to suggest promising MOF sensor structures, for laboratory chemists to synthesize.** As a result, the effort put into experimental trials will be greatly reduced and we will be able to design new materials much more efficiently.

Our method, named *ab initio* random structure sampling (AIRSS) involves random positioning of MOF building blocks in the unit cell. These starting structures get optimized using density functional theory (DFT) calculations, leading to a MOF crystal energy landscape, which is essentially a map of structures and their associated energies. The structures predicted to have lower energies are more likely to be observed experimentally. We then perform additional calculations on the predicted MOF structures, in order to assess their mechanical stability and sensing properties. In the end we synthesize the materials experimentally and analyze their properties, in order to assess the accuracy of our computational predictions.