Adsorption is the phenomenon which has many applications in the science and technology. In particular, adsorption in porous materials can be used for applications as wide ranging as gas storage, liquid-phase sorption and separation catalysis magnetism, sensing, thin films, proton conduction, drug delivery, and many more. The MOF (metal organic framework) material is a big new group of nano-porous materials which attracts a lot of attention. One of their key advantages compared to their organic (carbons) or inorganic counterparts (zeolites, silica), is the possibility to easily tune their composition through a change of the metal and/or the organic linker. The diversity and controllable size of the organic linkers and metal clusters allow the tailoring of these structures to specific applications. In addition, some of them show the structural transformation coupled to the thermodynamic parameter as well as to the adsorption uptake. MOFs with surface areas over 6000 m^2/g have been synthesized to date and these have exhibited exceptional gas uptake.

Gas molecules typically adsorb in MOF pores, due to strong interactions with the framework. We will try to improve gas storage in MOFs by tuning gas molecule interactions with the frameworks. Very often it can be done through catenation of multiple frameworks, inclusion of unsaturated “open” metal sites in the nodes, and incorporation of various functional groups (including metal cation sites) in the organic linkers. In this project it will be done by designing the chemical composition of new structures and by imposing a mechanical stress on the MOF framework. The ability to introduce the appropriate features for specific applications, along with the huge variety of potential MOF structures, opens up the possibility to truly design MOFs for desired applications.

In this project, we propose computational studies of gas adsorption in new deformable MOFs, focusing on molecular modeling of methane, hydrogen, and carbon dioxide. Methane is a desirable fuel because it burns more cleanly than gasoline and has higher hydrogen to carbon ratio than any other hydrocarbon fuel. However, a major drawback is that the volumetric energy density of compressed methane is only one-third that of gasoline. Materials that increase the volumetric density of stored methane could help expand the role of natural gas (which is mostly methane) as a transportation fuel. To motivate research and development of methane storage materials, the Department of Energy (DOE) has set storage targets of 180 STP (standard temperature and pressure) liters of CH_4 stored per liter of storage vessel. MOFs have already been synthesized that exceed this value. Hydrogen is an attractive fuel because it has a high gravimetric energy density, it is nontoxic, and its oxidation product is water. However, the very small volumetric density of H_2 makes storage difficult and is a major hurdle for the expansion of the hydrogen economy. The DOE has established targets for hydrogen storage systems of 75 gH_2/kg and 70 g H_2/L for an entire H_2 storage system. No material has yet been synthesized that meets these criteria, although computational studies of H_2 in MOFs have proposed design strategies that could meet the gravimetric targets.

Molecular simulation has become an indispensable tool for MOF design. Simulations can provide molecular level details of chemical phenomena that cannot be viewed directly in experiments. Additionally, it is usually much simpler to construct a MOF model on the computer than it is to synthesize and characterize the material in the laboratory. Therefore, one can probe a large number of materials via simulation more easily than through experiment. After this screening procedure, the most promising structures must be verified experimentally. Such approach can accelerate the generation of new insights. Simulations have been used to assess the capabilities of MOFs design features before synthesis new MOF structures. Simulations are also useful for predicting uptake at high temperatures and pressures, which are difficult to achieve experimentally. This is particularly useful for assessing MOFs for gas storage applications, as the desired storage conditions are typically at high pressure.

For the most promising materials the verifacation experiments will be carried out, The most desirable is to effectively adsorb methane or carbon dioxide, which are the main components of biogas. Their selective sorption allow not only the possibility of storing the gas, but at the same time allow for the purification of biogas.

MOF materials are still expensive substances but their cost will be lower when the amount of the production willl increase. In the project we will be compareing the MOF properties with activated carbon which are easily available on the market.