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Computer modelling of molecular self-assembly to porous materials

Evolution has created the ultimate art of molecular engineering from “pre-fabricated” blocks which autonomously and spontaneously assemble into supramolecular complexes, such as proteins, nucleic acids and cellular structures. Synthetic molecular aggregates can be designed based on the very same mechanisms. The area of self-assembly has exploded during the last two decades along with the concept of nano fabrication of materials. Applications of new technologies based on self-assembling are entering our everyday life, e.g., non-volatile FLASH memories to digital cameras, MP3 players, mobile phones, etc.. In this project we will study a special category of molecular aggregates with large holes to be used in gas storage and separation, and as catalytic centers for chemical reactions as typical examples. These porous materials include zeolites, mesoporous materials made of silica using various self-assembling template-forming amphiphilic molecules, and a big new family of so called metal organic frameworks (MOFs). You will be using powerful computers and state-of-the-art molecular modeling tools from quantum chemistry to Molecular Dynamics and Monte Carlo simulations to build the structures in computers, investigate their stability and elastic properties, simulate their storage, separation and transport capabilities, immobilize suitable molecules in the pores to functionalize them and investigate their capability as centers in heterogeneous catalysis. You are expected to have good knowledge in physical chemistry. Good knowledge/experience in organic, inorganic, biochemistry, physics and materials science is highly meriting as well as computer science/programming or computer modeling. This project is integrated in the activities of the Berzellii Center EXSELENT (EXtremely SElective and ENanTio-selective nanoporous materials for controlled sorption and catalysis).