Molecular simulations for adsorption of light hydrocarbons in microporous materials regarding to experimental thermodesorption studies

Porous materials are solids which structure is crisscrossed by the network of channels and cages, where the guest molecules can enter (and be adsorbed). Channels of diameter less than 2 nm, which fits the size of small molecules (e.g. hydrocarbons), are called micropores. Microporous materials find many technological applications e.g. as catalysts for the production of gasoline or adsorbents allowing purification of gases and liquids. Therefore, in-depth knowledge of the adsorption properties of such materials is important.

The **main aim** of this project is application of the Monte Carlo computer calculations for modelling of adsorption of light hydrocarbons on selected microporous adsorbents in relation to experimental data obtained with the QE-TPDA (*Quasi-Equilibrated Temperature Programmed Desorption and Adsorption*) method. The molecular simulations provide detailed knowledge about the adsorption on the molecular level, and allow better understanding of this phenomena. Based on the QE-TPDA experimental profiles one can obtain a high quality adsorption isobars, i.e. the temperature dependence of the adsorption extent, for a constant pressure. This approach to the adsorption is rare but it can be a good alternative to the isothermal one.

Two classes of microporous materials were selected for the study, and their synthesis is the **additional aim** of this project. Pure Silica Zeolite frameworks, because of their intrinsic properties, such as high thermal stability, structural diversity, chemical simplicity and close relation to zeolites make them perfect candidates to be studied both experimentally and with molecular simulations. Metal-organic frameworks (MOFs) are extremely interesting due to their structural and functional customizability and because of potential applications as hydrogen and methane storage adsorbents, carbon dioxide capture materials and “fine chemistry” catalysts. Therefore advancement of the experimental technique suitable for studying their porosity seems important.