Laboratorium for Molecular Simulation

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General area(s)
Computational Chemistry, Molecular Simulations, and MOF synthesis

Research themes
The MolSim group focuses on the development and application of molecular simulation techniques to systems that are relevant for energy. Recent systems that have been studied include:

- Material for carbon capture
- Materials for methane storage
- Development of a nanoporous materials genome
- Understanding of interactions of gasses in MOFs with open metal sites

A new research theme is the synthesis of novel MOFs

Methodology of work / instrumentation
The group uses different kinds of molecular simulation techniques (molecular dynamics, Monte Carlo) and electronic structure calculations.

For the synthesis the group has a high-throughput robot.

Examples of MSc / PhD theses
- The molsim is starting July 2016