Seminar
International Graduate Research Training Group 1524:
"Self-assembled soft matter nanostructures at interfaces"
07. 07. 2011

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Towards designing micro-porous organic materials via molecular simulations

The question about designing micro-porous materials with special ability for gas adsorption has become enormously interesting since not only the environmental pollution issue by e.g. CO_2 gas has not been solved so far, but also since energy resources have started to shrink. Therefore, synthesizing and predicting adequate and smart materials for different purpose, in terms of the ability to bind CO_2 or to increase gas selectivity and catalysis property are vitally important. Finding materials appropriate to serve as an energy carrier devise with storing and releasing ability of H_2 gas, would enable this gas to be used as a clean energy resource. In this context, synthetic organic materials have been found to be promising candidates. They have molecular-scale porosity, which originates from the packing and the form of the molecule compounds. Thus the topology of the voids can range from ordered one-, two- or three-dimensional networks with complicated interconnected tunnels and cavities (cages) up to amorphous frameworks. This diversity also allows a range of flexibility of the frameworks and interactions between the pore sites and the guest molecules. By performing molecular simulations we want to understand the dynamic behaviour of the host-structure and the impact on the mobility of guest molecules. As a first step we developed a methodology for analysing the dynamic surface area, because changes in structure affect the size and geometry of the pores. Molecular Dynamic Simulations of a material with one dimensional network showed that there can be large fluctuations of the surface area such that one can assume an opening and closing of channels between different tunnels. To be able to compare simulation results with sorption experiments there is a need to close the gap between the different measurement techniques. Namely, to find an adequate definition of the pore size on the molecular level and so to define pore size distributions in simulations or predict accurate sorption isotherms. This would also help to characterize in advance designed, not yet synthesized, micro-porous materials and to propose for experimental research.