Nanomaterial Modeling

Nanomaterial Modeling

The Group of Nanomaterial Modeling, a part of the Department of Physical and Macromolecular Chemistry, focuses on the development and applications of computational methods for the investigation of physical and chemical properties of novel nanomaterials.

It employs a variety of models and methods, including *ab initio* methods for the accurate description of electronic structure as well as methods of statistical thermodynamics which allow for simulations of large molecular ensembles. In close collaboration with experimental researchers, the group's research is focused on modeling of microporous aluminosilicates, carbon nanomaterials, polymers, and metal?organic frameworks. The research topics of the group include the structure and properties of new microporous materials for adsorption and catalysis, properties of metal nanocatalysts on supports (carbon or silica) and properties of these supports, structure and properties of polymeric materials, in particular water?soluble polyelectrolytes for environmental applications. In addition to theoretical description of properties of existing materials also materials that have not been prepared yet are computationally investigated. The aim of the research is to gain an increased understanding of physical and chemical properties (including catalysis) of nanomaterials ranging from the atomic?scale up to the supramolecular level. The theoretical research carried out in close collaboration with experimental groups heads towards the synthesis of new materials with designed properties for specific applications.

Selected outputs

- Wieslaw J. Roth, Petr Nachtigall, Russell E. Morriss, Paul S. Wheatley, Valerie Seymour, Sharon E. Ashbrook, Pavla Chlubná, Lukáš Grajciar, Miroslav Položij, Zrnošt Zukal, Oleksiy Shvets, Jiří Čejka, "A family of zeolites with controlled pore size prepared using a top-down method", Nature Chemistry, **5** (2013) 628.
- Wieslaw J. Roth, Petr Nachtigall, Russell E. Morris and Jiří Čejka, "Two-dimensional zeolites: current status and perspectives", Chem. Rev., **114** (2014) 4807.
- F. Uhlík, P. Košovan, Z. Limpouchová, K. Procházka, O. V. Borisov, F. A. M. Leermakers, "Modeling of Ionization and Conformations of Starlike Weak Polyelectrolytes", Macromolecules, **47** (2014) 4004.