L27

STRUCTURE ANALYSIS BY MOLECULAR SIMULATION TECHNIQUES. CALCULATED STRUCTURES OF LAYERED SILICATES

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Welcome to the fantastic world of molecular simulations, where everything is possible, but it is very hard work to find the truth about molecular structures which, moreover, should correspond with the experimental data.

History and present

Our molecular simulations laboratory was established in 1997, when prof. Pavla Čapková obtained a developing project. Finances from this project were used for buying Octane computer (2x 150MHz MIPS R10000 processors) from Silicon Graphics and package software Cerius from MSI. An interesting fact is that Octane has been upgraded only once by two 300 MHz MIPS R12000 processors and 2GB of memory and it is still working with IRIX64 Release 6.5 operating system. Cerius^2 software has been gradually updated to Cerius^2 4.5 final version. The firm MSI was bought by Accelrys which develops their own molecular simulation program Material Studio [MS]. Cerius was incorporated into the MS as one module called Forcite. Cerius^2 hasn't been hereafter developed and updated. It is necessary to say that some special features of Cerius^2 software package haven't been incorporated into Forcite and these ones are still used in Cerius^2 as complementary features. Nevertheless, MS with its modules can cover wider area of molecular simulation problems. It is not necessary to bye the whole software package but a buyer can buy only the modules he demands. Nevertheless, the price of individual modules is higher than the price for the same module in the whole software package. First of all, a Visualiser module must be bought, that is a control interface between the user and the modules of the program. We have several modules of MS running on 8 Intel processors PC under windows 7 operating system in our laboratory, which we use for a research or teaching activities.

Software

The modules in Material Studio 5.0 used in our laboratory are Forcite, Discover, Reflex, Conformers, Blends and Synthia. There are about other 16 modules in MS. Forcite module is used for energy calculation of the system, geometry optimization, various kinds of dynamics, mechanical properties. Discover module allows a parallel computing and it is used similarly like Forcite module for energy calculations, geometry optimization, dynamics and properties analysis. Reflex module allows solving of crystal structures from powder diffraction pattern. Conformers module calculates the most probable conformation of investigated molecules. Blends module is used for mixing of various components and for description of the resultant mixture. Synthia is a module for polymer calculation. It predicts macro properties of resultant polymers on the base of knowledge of micro structure. This software is continuously updated together with the computer. Moreover the computer cluster is used for calculations in software packages like Amber, Gromacs, Gaussian, etc.

Research problems

In our laboratory molecular simulation methods were mainly used for calculation of various types of silicates intercalated with organic species like various ammonium cations [1, 2], dye cations [3-5], neutral polar molecules [6], etc. Intercalated silicates are usually in powder form. Direct diffraction methods solve the structure of these powders with difficulties. In this case, molecular simulations can significantly help us to describe the structures in detail. The similar procedures are valid for anionic clays like layered double hydroxides (LDH) with positive layer charge intercalated with benzoic acid and its derivatives [7] and porfyrin molecules [8, 9].

Other calculations were used for properties description of energetic materials. Mutual interaction between molecules and intramolecular interactions have been investigated. Dynamic calculations bring a new insight into the behaviour of energetic materials under high pressure and high temperature [10]. Calculated result like a time of decomposition or the energy release were compared with experimental results like sensitivity or detonation energy. The energy characteristics from energetic materials structures were derived and used for a possible explanation of sensitivity behaviour [11]. Other case is a dynamic calculation of the phase transition for liquid crystals or cocoa butter.

Teaching

The software for molecular simulations is also permanently used for teaching of under graduated and post graduated students. During the existence of the laboratory, 4 diploma theses (Václav Bittner, Miroslava Fraňová, Jana Čurdová, Marek Veteška) and 5 doctoral theses (Daniel Janeba, Miroslav Pospíšil, Bohdan Koudelka, Jarmila Repáková, Petr Kovář) have been defended. Miroslava Fraňová and Marek Veteška continue in the branch of the molecular simulations in their Ph.D. theses now.

A 2 hours lecture "Molecular simulations in chemical physics" and 1 hour seminar is regularly taught at the Faculty of Mathematics and Physics. The students obtain a knowledge about principles, procedures and also practical experiences with molecular calculations during seminar. This knowledge can be amplified during 4 hour practical seminar called "Computational experiments in molecular

Figures of solved structures

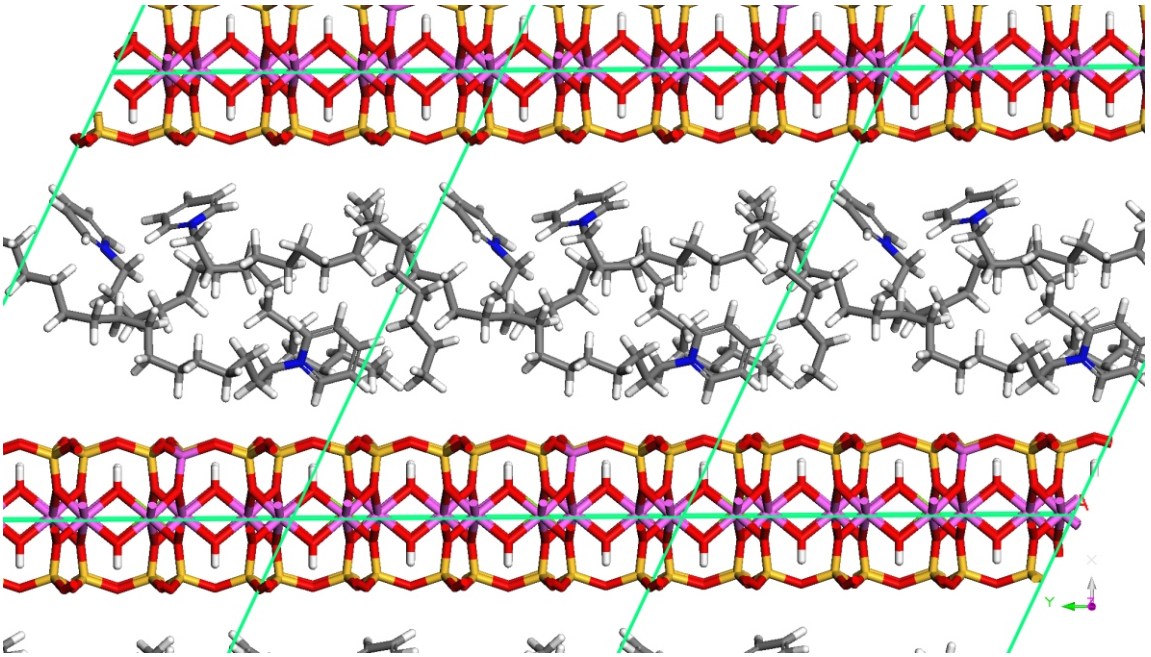

Figure 1. Montmorillonite intercalated with cetylpyridinium cations [1]. There are 3 cations per one unit cell.

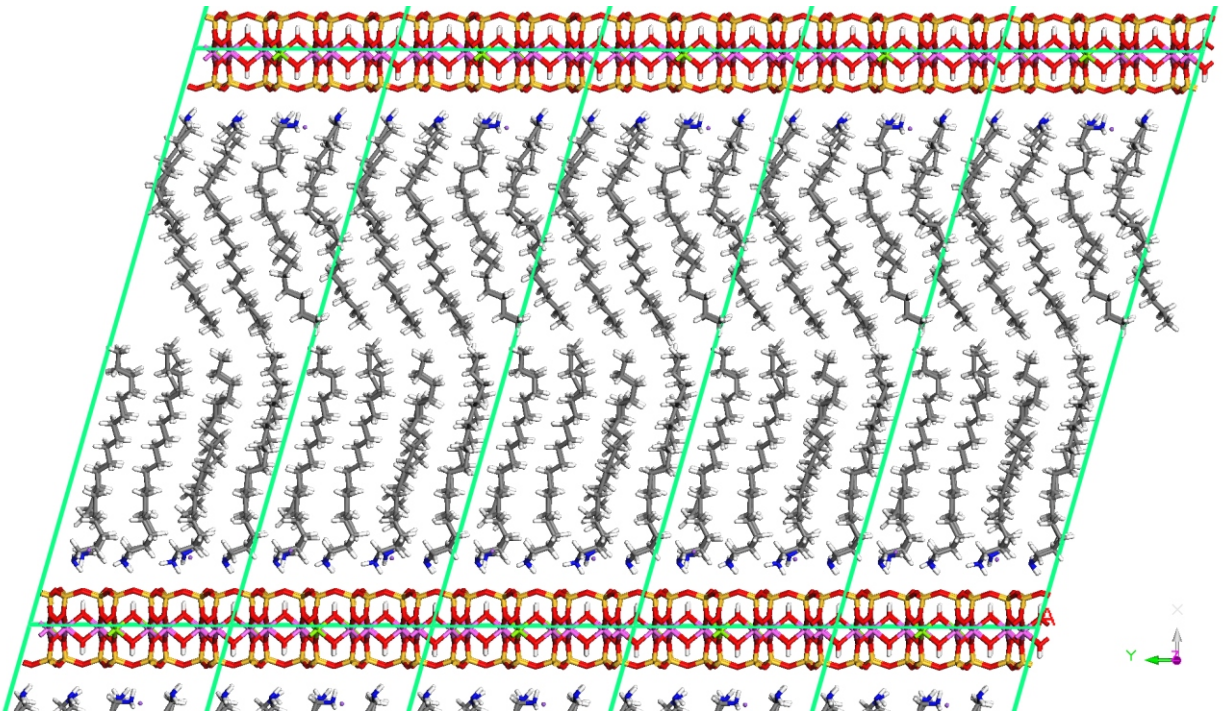

Figure 2. Montmorillonite intercalated with neutral octadecylamine molecules [6]. There is 16 octadecylamine molecules and 3 Na cations per one unit cell.

theory I and II" where simple mechanical and quantum chemical methods and empirical molecular mechanics and dynamics are taught.

Future plans

We would like to update MS software and enlarge the using of software packages installed on the computer cluster of physical section of the faculty. Moreover, we would like to increase the interconnection between classical molecular simulations and quantum calculations. We started both types of these calculation with porphyrin molecules intercalated into LDHs [9]. In the end we would like to return back to polymer calculations and we would like expand the simulations to non linear optics materials and drugs.

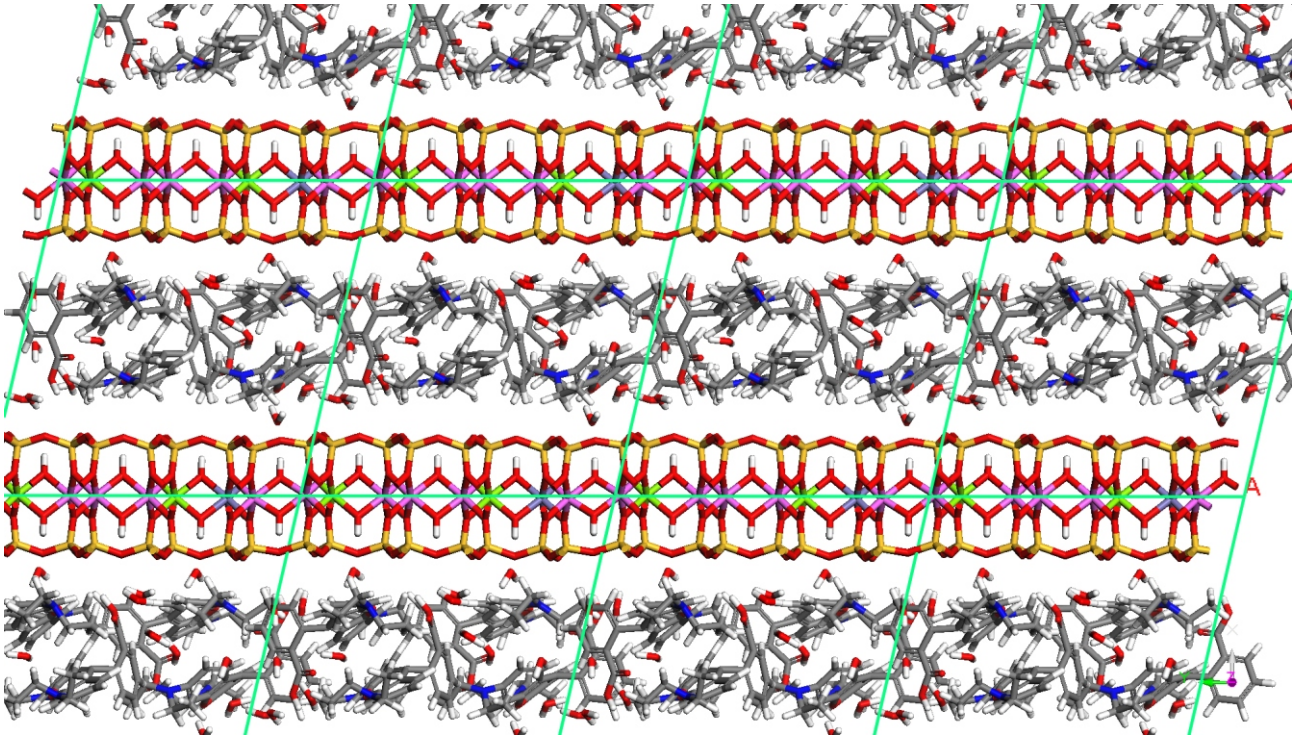

Figure 3. Montmorillonite intercalated with rhodamine B [3]. There is 2 H dimer from 2 rhodamine B molecules and 16 water molecules per one unit cell.

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