NMR-Approaches in studying dynamic molecules in porous materials

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Molecular translational dynamics in porous materials at different stages of its production or usage is one of the most basic, and also most fascinating physical phenomena. It plays a large role in applications related to long action preparations and production of different materials with given properties. Contemporary possibilities of the methods of NMR-relaxation, NMR diffusometry (pulse field gradient NMR) and methods of double-quantum-filter (DQF) NMR in a study of diffusion properties and molecular dynamics in the systems with the anisotropic properties are considered. In many cases the most focus of research is on understanding diffusion and its relation to structure and functionality in complex nanostructured materials. The work shows how the study results in information about molecular dimensions, character of limitation and the structure of the surrounding matrix. DQF NMR is applied for investigating the systems, in which there is an order (on the macro- or the micro-levels), in particular for fibres and porous systems or the systems with anisotropic motion of molecules. The results obtained reveal also the special feature of the approaches of one-dimensional and two-dimensional NMR and show examples of the work of these methods in addition to the traditional methods of single-quantum NMR-spectroscopy. The work presents the data of two-dimensional correlation NMR-spectroscopy (DD COSY) as the distributions of diffusion coefficients in two orthogonal directions on the systems with anisotropic mobility. Simulations of two-dimensional NMR-experiments have been done showing how it leads to the explanation of experimental data on the anisotropy of diffusion coefficients. These NMR-methods reveal the correlation of the diffusion motion of molecules along either collinear or orthogonal directions of applied pulse gradients of magnetic field. The results on some materials with anisotropic structure demonstrated how these methods reveal microscopic local anisotropy in the presence of global isotropy. NMR-techniques in combination with simulations give new useful links between the nanotechnology applications and chemical engineering by clarifying the relationships between structure and translational dynamics in complex materials.

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Ionic liquid assisted sonochemical synthesis of LiFeO$_4$ for ion-lithium batteries application

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Lithium-ion battery technology is a recent breakthrough in electrochemistry that has gone into commercial success. Lithium-ion batteries have the highest energy storage capacity of the rechargeable battery systems and have allowed for the powering of portable electronic devices. Large demanding applications, such electric vehicles, require significant breakthroughs in battery technology. Nanoscale materials for lithium ion storage devices are emerging as successful solutions to improve rate capability, which, in the case of lithium ion insertion batteries, focuses on anodes and cathodes. This works deals with the development of ionic liquid assisted sonochemical synthesis of LiFeO$_4$ for ion-lithium battery applications. Successful preparation conditions have been achieved whereas 1-ethyl-methyl imidazolium sulphate enhanced crystallinity and surface area of LiFePO$_4$ particles. Thermal analysis (DSC and TGA), XRD and SEM confirms thermal behavior, structure nature and morphology of prepared samples. At the present time electrochemical characterization (GITT, PITT and EIS) is being performed.

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