Title: Simulation of Spin Dynamics in Solid-State NMR using SPINEVOLUTION software
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NMR spectroscopy is a very powerful technique, one of the few capable of probing sub-nanoscale structures in disordered media and of measuring diffusion with thermodynamics parameters. It is of high interest to obtain structural information on molecules, which advance the essential insights of materials system. Our work is mainly focused on solid-state NMR spectroscopy, which is an atomic-level method to determine the chemical structure, 3D structure and dynamics of solids and semi-solids. The control of spin dynamics in solid-state NMR is the basic principles of NMR spectroscopy as applied to the wide range of solid systems. The nuclear spin interactions and the effects of magnetic fields and radiofrequency pulses on nuclear spins in solid-state NMR are the same as in liquid-state NMR spectroscopy. However, because of the orientation dependence of the nuclear spin interactions in the solid state, the majority of high-resolution solid-state NMR spectra are measured under magic-angle spinning (MAS), which has profound effects on the types of radiofrequency pulse sequences required to extract structural and dynamical information. Here, we describe some basics pulse sequences and used the Spinevolution software to simulate solid-state NMR experiments such as CW and TPPM. The SpinEvolution and SIMPSON software may be regarded as a virtual NMR spectrometer as it simulates pulse sequences, chemical exchanges, and NMR interactions. The SpinEvolution software is still about an order of magnitude more efficient than SIMPSON.

We describe the most common MAS NMR experiments and data analysis approaches for investigating biological macromolecules, organic materials and inorganic solids. Continuing development of sensitivity-enhancement NMR approaches, including ^{1}H-detected fast MAS experiments, dynamic nuclear polarization and experiments in ultra-high magnetic fields, is described. We highlight recent applications of solid-state NMR spectroscopy to biological and materials chemistry. The Primer ends with a discussion of current limitations as well as areas of development of solid-state NMR spectroscopy and points to emerging areas of applications of this sophisticated spectroscopy.

Nuclear magnetic resonance (NMR) is a powerful tool to study lithium-ion battery electrolytes.

. For this reason, we use a general simulation program for solid-state NMR spectroscopy called SIMPSON, we observe the chemical reactions and compositions of LIBs. SIMPSON may be regarded as a virtual NMR spectrometer as it simulates chemical exchanges. It is used to simulated solid-state NMR experiments. The purpose of this study is to analyze the chemical reactions as well as developing new NMR methods providing results that partially revise previous works. Our goal is to keep the cathode in the battery electrically and ionically conductive to make sure that the battery stays after many cycles.

1. Introduction and Description of NMR
2. Motivation of using Solid-State NMR
3. Description of Pulse Sequences: Spin Echo
4. Simulation of Solid-State NMR Experiments: CW, TPPM