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### **In situ NMR Methods in Catalysis | Joachim Bargon | Springer**

Lasse Greiner, Stephan Laue, Jens Wöltinger, Andreas Liese. Pages 111-124. Exploiting Nuclear Spin Polarization to Investigate Free Radical Reactions via in situ NMR

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The latter may allow a direct observation or an indirect inference from unusual phenomena occurring in the reaction products during in situ investigations of their corresponding chemical reactions. In NMR spectroscopy, for example, transient emission and enhanced absorption lines may be observed, and one is inclined to believe that there is a universal ...

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High resolution solution in situ NMR can identify/quantify soluble reaction species. • Dynamic nuclear polarization can enhance

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NMR signal by 2–3 orders of magnitude. • Optical detection makes nitrogen vacancy (NV) NMR ultrasensitive. • Developing in situ EC NV NMR will greatly help advance electrocatalysis research.

### **In situ electrochemical nuclear magnetic resonance ...**

For static equilibria, Tolstoy et al. introduced an in situ combination of UV/Vis and high-resolution solution NMR spectroscopy (UVNMR) in 2009 to achieve absolute comparability of both methods.<sup>13</sup> However, this setup cannot be applied for dynamic, light-induced (photo) chemical processes because of the hampered diffusion caused by a reflector between bulk solution for NMR spectroscopy and an aliquot for UV/Vis spectroscopy. Furthermore, an additional light source for illumination is ...

### **Combined In Situ Illumination-NMR-UV/Vis Spectroscopy:**

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**A ...**

This Account reviews the recent use of in situ solid-state NMR spectroscopy, a technique that probes local structure and dynamics, to study these devices. In situ NMR studies of lithium-ion batteries are performed on the entire battery, by using a coin cell design, a flat sealed plastic bag, or a cylindrical cell. The battery is placed inside the NMR coil, leads are connected to a potentiostat, and the NMR spectra are recorded as a function of state of charge.

### **In Situ Solid-State NMR Spectroscopy of Electrochemical**

**...**

In this work, in situ NMR is further developed to study supercapacitors comprising activated carbon electrodes and a NEMO 4 BF<sub>4</sub> in acetonitrile electrolyte. We first address some of the practical aspects associated with in situ NMR of supercapacitors, using <sup>19</sup>F NMR in this study because of the

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high sensitivity of this nucleus. We then show how this methodology can provide insight into the charge storage mechanism of supercapacitors by directly tracking changes in the amount of charge ...

### **In Situ NMR Spectroscopy of Supercapacitors: Insight into ...**

An in situ method for the preparation of N-methyleneamines has been devised by Overman and Osawa for use in condensation reactions with enolates 164 and organometallic reagents. 165 These species, with the exception of very hindered N-methyleneamines, cannot be isolated in the condensed phase because they rapidly trimerize to hexahydro-1,3,5-triazines.. In this in situ method, N ...

### **In Situ Methods - an overview | ScienceDirect Topics**

In situ speciation in solution of both inorganic and organic parts

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during hydrothermal crystallization were monitored using  $^{27}\text{Al}$  and  $^1\text{H}$  NMR spectroscopy. The nature and morphology of the various intermediate solid phases, at different reaction times, were monitored by means of ex situ powder X-ray diffraction (XRD) and scanning electron microscopy (SEM), in relation with the solution speciation.

### **In Situ NMR, Ex Situ XRD and SEM Study of the Hydrothermal ...**

The in situ MAS NMR studies of the mechanisms of zeolite catalyzed reactions are reviewed. The first part of the critical review contains brief information on the different experimental approaches used for the in situ MAS NMR studies under batch and flow conditions. In the second part, a cross reference index between the reactions studied, the catalysts used, the mechanistic information ...

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## **Impact of in situ MAS NMR techniques to the understanding ...**

In Situ NMR Studies of Lithium Ion Batteries. The Electrochemical Society Interface • Fall 2011 69. Nuclear Magnetic Resonance (NMR) is a useful tool to probe the structural changes that occur in electrode materials on electrochemical cycling. Most NMR studies of materials for lithium ion batteries have been performed ex situ: the battery is cycled to a specific state of charge, taken apart to extract a sample, and then NMR of this sample is performed.

## **In Situ NMR Studies of Lithium Ion Batteries**

In situ nuclear magnetic resonance measurements are very powerful to monitor the evolution of lithium deposits, including insight into reaction kinetics and occurring microstructures, readily distinguishable due to their characteristic  ${}^7\text{Li}$  NMR chemical shifts (note that the presence of “mossy” or “dendritic”

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microstructures is indicated by NMR signals at 260 and 270 ppm [or even higher], 14 while pristine lithium metal resonates at 240–250 ppm (see Figure 1A; Li ions trapped ...

### **Quantification of Dead Lithium via In Situ Nuclear ...**

In situ solid-state NMR probes. Automatic tuning/matching cyclor (ATMC) single-resonance NMR probe; Double-resonance  $^{19}\text{F}/^1\text{H}-\text{X}$  in situ NMR probe . In situ NMR and MRI equipment. Plastic cell capsule and (dis)assembly tool; In situ NMR setup: make commercial NMR/MRI probes “in situ” ready! User training: NMR on battery materials

### **In situ NMR/MRI - NMR Service**

In this paper, acknowledging the important potential of NMR to perform in situ characterisation and monitoring of electrochemical reactions, we address the issues that arise by introducing metallic electrodes in the proximity of the NMR

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detection region, in particular for the case when LOC devices, miniaturised NMR detectors, and small (sub- $\mu\text{L}$ ) sample quantities are involved.

### **An NMR-compatible microfluidic platform enabling in situ**

...

Herein, we demonstrate the use of nuclear magnetic resonance (NMR) spectroscopy as an in situ method for VLE measurements. The experiment is carried out entirely inside the NMR sample tube. The simultaneous measurement of liquid- and vapor-phase composition was achieved by the insertion of a sealed glass capillary into the NMR sample tube.

### **Nuclear Magnetic Resonance (NMR) Spectroscopy for the In ...**

Major conclusions: A number of methods were developed to enrich the isotope-labeled proteins inside the cells, enabling the

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in-cell NMR observation of bacterial cells as well as eukaryotic cells. In-cell NMR has been applied to various biological systems, including de novo structure determinations, protein/protein or protein/drug interactions, and monitoring of chemical reactions exerted by the endogenous enzymes.

### **In situ structural biology using in-cell NMR**

In summary, our studies have demonstrated a new method for the in situ solid state NMR studies of membrane proteins in their native environment. This approach offers an opportunity to expand the field of in situ membrane proteins structural and dynamic studies in native membranes, which can provide native conditions for the membrane proteins, including native lipid compositions and functional partners.

### **In situ $^{19}\text{F}$ NMR studies of an E. coli membrane protein**

The RF coil needs to generate an AC magnetic field ( $B_1$ ) which is

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orthogonal to static magnetic field ( $B_0$ ) generated by the magnet. The opposed-solenoid RF coil, shown as Fig. 2(a), consists of two reverse-connected solenoids, and it was applied on inside-out NMR probe for the first time in this paper. Basically,  $B_1$ , the RF magnetic field, is along the radial direction of dumbbell-shape ...

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