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Turcu; Eric Walter; Karl Mueller; *Pacific Northwest National Laboratory, Richland, WA*

The Environmental Molecular Sciences Laboratory (EMSL) is a Department of Energy national scientific user facility, located at Pacific Northwest National Laboratory. The EMSL user facility houses magnetic resonance systems for applications such as 1) ultra high-field NMR for solid-state experiments at 900, 850, 800, and 750 MHz; 2) pulsed EPR spectrometers including a high-power, high-field (95 GHz) system; 3) an ultra high-field radiological wide bore NMR with capabilities for imaging, solution, and solid-state NMR including multi-receiver spectroscopy; and 4) a 500 MHz micro-imaging spectrometer for in-vivo magnetic resonance imaging, localized NMR spectroscopy, and NMR diffusion studies. Capabilities and expertise that contribute to a problem-solving research environment in areas including materials development, catalysis, geosciences, structural biology and metabolomics will be highlighted.

Poster 115

Resource for NMR Molecular Imaging of Proteins

Christopher V. Grant; Chin H. Wu; Stanley J. Opella; *University of California San Diego, La Jolla, CA*

The developments of methods and instrumentation, and their application to membrane bound proteins will be presented. The Resource is dedicated to solid-state NMR spectroscopy for the study of protein structure and function. Recent solid-state NMR methods, applications and developments will be summarized, including solid-state NMR probes optimized for magic angle spinning and static oriented methods. The Resource for NMR Molecular Imaging of Proteins is supported by the National Institute of Biomedical Imaging and Bioengineering (P41EB002031).

EXOTICA & BEYOND, 116 - 126

Poster 116

Monitoring *in situ* Copper Electrodeposition Reaction Using NMR Unilateral

Luis Fernando Cabeça; Luiza Maria da Silva Nunes; Luiz Alberto Colnago; *EMBRAPA Instrumentation, São Carlos, Brazil*

We are showing by the first time the coupling of electrochemistry and NMR Unilateral (UNMR) spectrometer (constructed in a classical "U-shaped" geometry). The measurements provide better conditions because the electrochemical reaction takes place outside of the radio frequency (RF) coil probe. The work evaluated the potential of combination between UNMR and electrochemical to monitor in situ cooper electrodeposition. The Cu^{+2} concentrations during the reaction were calculated using CPMG decay (every ten minutes during 3 hours). As expected the Cu^{+2} concentration decrease rapidly with the electrodeposition until approximately 130 min, and then remained constant. After 3 hours reaction, 57.5% of ions in solutions were deposited on the work electrode. These results bring good prospects for monitoring electrochemical reactions in situ.

Poster 117

100x Enhancement of Hyperpolarized Xenon-129 Dissolved-phase Signal During Functional MR Studies of Fatty Tissues

Rosa Tamara Branca[1, 2]; Arjun Khanna[2]; Matthew Freeman[3]; [1]*Department of Physics and Astronomy, University of, Chapel Hill, NC;* [2]*Chemistry Department, Duke University, Durham, NC;* [3]*Department of Medical Physics, Duke University, Durham, NC*

Due to its high solubility in blood and tissue and its high sensitivity to the local environment, HP 129-Xe has long been considered a unique probe for imaging living tissues. Unfortunately, imaging results have been disappointing mainly because of the low concentration of xenon that dissolves in tissue. Here we report the first HP 129-Xe functional MR studies of fatty tissues, specifically Brown Adipose Tissue (BAT). Our studies show that HP-129Xe is highly sensitive to BAT activity during which more than a 100x enhancement of the HP 129-Xe dissolved-phase signal can been observed.

Poster 118

A Dynamical Theory of Spin Relaxation

Timothy R. Field; Alex D. Bain; *McMaster University, Hamilton, Canada*

The dynamics of a spin system is usually calculated using the density matrix. However, the usual formulation in terms of the density matrix predicts that the signal will decay to zero, and does not address the issue of individual spin dynamics. Using stochastic calculus we develop a dynamical theory of spin relaxation whose origins lie in the component spin fluctuations. This entails consideration of random pure states for individual protons, and how these pure states are correctly combined when the density matrix is formulated. Both the lattice and the spins are treated quantum mechanically. Such treatment incorporates both the processes of spin-spin and (finite temperature) spin-lattice relaxation. Our results reveal the intimate connections between spin noise and conventional spin relaxation.

Poster 119

Below Cut-off Traveling Wave NMR at 16.4T: Interference of Propagating Modes in a High Dielectric-filled Waveguide

Alexey Tonyushkin[1]; Gregor Adriany[2]; Dinesh Deelchand[2]; Michael Garwood[2]; Andrew Kiruluta[1]; [1]*MGH, Harvard Medical School, Boston, MA;* [2]*University of Minnesota Medical School, Minneapolis, MN*

At ultra-high field strength, the propagation wave vector of the excitation field can no longer be ignored as the wavelength becomes comparable to the imaging volume, particularly if the medium dielectric constant is large. Here, we present our latest developments on a traveling wave waveguide system allowing mode propagation in a 16.4 T horizontal bore NMR imaging system. The waveguide consists of a metal bore of the magnet and an acrylic tube filled with high dielectric material.

The excitation of a waveguide is achieved through a transmit-receive loop coil probe placed at one or both ends of the guide. We describe propagating mode phenomena that were observed in the dielectric and discuss the implications for ultra-high field NMR.

Poster 120

Time Domain NMR Spectroelectrochemistry: Monitoring *in situ* Copper Electrodeposition Reaction

All posters should be set up 8:00 to 9:00 am on Monday and removed at 3:45 pm on Thursday. Be sure to use the poster space number printed here. Authors of odd-numbered posters present on Monday and Wednesday. Even numbered posters present on Tuesday and Thursday.

Luis Fernando Cabeça; Luiza Maria da Silva Nunes; Paulo Falco Cobra; Luiz Alberto Colnago; *EMBRAPA Instrumentation, São Carlos, Brazil*

The combination of electrochemical (EC) and Nuclear Magnetic Resonance (NMR) has been rarely performed due to distortion of the static magnetic field (B0) homogeneity. Because of the bench top NMR (Time Domain – TDNMR) low homogeneity, the distortion caused in magnetic field by the electrodes is not critical. Therefore, the copper electrodeposition reaction can be monitored using the Carr-Purcel-Meiboom-Gill (CPMG) to measure transverse relaxation time. The results showed that Cu^{+2} concentration decreased rapidly with the electrodeposition until 100 min, and then, remained constant. After 3 hours reaction the Cu^{+2} concentration was $2x10^{-3}$ M, corresponding to 10% of the initial Cu^{+2} concentration. The measures show that EC-TDNMR combination can be very fast, simple and an efficient technique to monitor electrodeposition reaction.

Poster 121

Multiple Spin Coherences and the Time Evolution of a Magic Echo

Steven Morgan[1]; Vadim Oganesyan[2]; Gregory Boutis[1]; [1]*Brooklyn College/CUNY, Brooklyn, NY;* [2]*College of Staten Island/CUNY, Staten Island, NY*

We report on an average Hamiltonian treatment of a magic echo to second order. The degradation of time-reversal with increasing evolution time is shown theoretically and via simulation and experiment to be strongly influenced by finite pulse width effects. We investigate the spin dynamics under a magic echo sequence beyond the single-spin, single-quantum portion of the density matrix. In a sample of adamantane we observe that the evolution of multiple spin correlations following a magic echo is similar to the FID even though the overall signal amplitude decreased more than 50% for the longest magic echo measured. Additionally, the long-time portion of the coherences detected is observed to decay at the same rate for both the FID and magic echoes.

Poster 122

Methodology to Measure Temperature and Thermal Diffusivity in Intact Seeds and Seeds Inside Soils by Time Domain NMR

Maria Gabriela Aparecida Carosio[1]; Luiz Alberto Colnago[2]; [1]*Institute of Chemistry of São Carlos, São Carlos, Brazil;* [2]*EMBRAPA Instrumentation, São Carlos, Brazil*

Soil temperature is important in agriculture and affects directly the seed germination. Some seeds may survive in high temperature environment for days, but the seedling may die in few hours. Several NMR parameters are affected by temperature and can be used to monitor it. We are showing that we can use time domain NMR to measure temperature using oilseeds as a sensor. The measurement is based on the T_2 dependence of oil viscosity and temperature. Although soil type doesn't influence directly on the signal acquisition, it'll be indirectly influenced, because the seed will heat more or less depending on the soil type. This study shows it is possible to obtain information in vivo and quickly, compared with other techniques.

Poster 123

The Chemical and Structural Characterization of Soil: A Comprehensive Multiphase NMR Approach

Hussain Masoom[1]; Denis Courtier-Murias[1]; Ronald Soong[1]; Hashim Farooq[1]; Werner E. Maas[2]; Michael Fey[2]; Brian Andrew[2]; Jochem Struppe[2]; Howard Hutchins[2]; Sridevi Krishnamurthy[2]; Rajeev Kumar[3]; Martine Monette[3]; Henry J. Stronks[3]; Alan Hume[3]; Andre J Simpson[1]; [1]*University of Toronto, Scarborough, Canada;* [2]*Bruker Biospin, Billerica, MA;* [3]*Bruker Biospin Canada, Milton, ON*

Comprehensive multiphase (CMP)-NMR is useful to investigate complex environmental samples because it has the capability to study solid, liquid, and gel-phase (HR-MAS) components without sample pre-treatment. Here we have used CMP-NMR to look at the structure and chemistry of soil colloids at the water interface in whole untreated samples. 13C CP-MAS experiments on a wet and dry soil indicate that carbohydrate and aliphatic moieties are present on the surface of soils while aromatic and proteinaceous components lay buried in the solid phase and have been confirmed by 1H experiments. Additionally, more penetrating solvents and multidimensional NMR were used to characterize the various soil components, strengthening the notion that soil organic matter is made of small subunits which form supra-molecular associations.

Poster 124

Diamond Magnetometer near the Shot Noise Limit at Room Temperature

Chang Shin[1, 2]; Claudia Avalos[1, 2]; Mark Butler[1, 2]; David Trease[1, 2]; Scott Seltzer[1, 2]; Daniel Kennedy[1, 2]; J. Peter Mustonen[1, 2]; Victor Acosta[3, 4]; Dmitry Budker[3, 4]; Alexander Pines[1, 2]; Vikram Bajaj[1, 2]; [1]*Department of Chemistry, University of California, Berkeley, CA;* [2]*Materials Science Division, LBNL, Berkeley, CA;* [3]*Department of Physics, University of California, Berkeley, CA;* [4]*Nuclear Science Division, LBNL, Berkeley, CA*

The negatively charged nitrogen vacancy centers (NV–), substitutional point defects in diamond have recently been exploited in several applications including magnetometry. We operate a nitrogen vacancy (NV–) diamond magnetometer at ambient temperatures and study the dependence of its bandwidth on experimental parameters including optical and microwave excitation powers. We introduce an analytical theory that yields an explicit formula for the response of an ensemble of NV– spins to an oscillating magnetic field, such as in NMR applications. We measure a detection bandwidth of 1.6 MHz and a sensitivity of 4.6 nT/√Hz, unprecedented in a detector with this active volume and close to the photon shot noise limit of our experiment.

Poster 125

NMR of Polyoxometallates (POM): Mo132 Meets Amino-Acids

Erhard T.K. Haupt; *Department Chemistry University Hamburg, Hamburg, Germany*

Previous studies concerning the lipophilic attraction of a ball-like polyoxometallate like Mo132 loaded with aliphatic chain internal linkers (like actetates) towards molecules with intermediate aliphatic chains like hexane, hexanol....[Chem. Eur. J. 17, 9634 (2011)] are extended to more biological interesting compounds like simple amino-acids. The surprising result is, that the amino-acids interact clearly with the Mo132-molecule, but there is no contact with the internal part of the moiety. Careful NMR-studies show (CSM and DOSY) that there is a contact, but in form of a slow exchange of the