

## 2 Plenary

### I1 2D NMR Studies of Local Order, Disorder, and Dynamics in Zeolites and Layered Silicates

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Solid porous silicates often exhibit subtle combinations of short- and long-range structural order and disorder, as manifested by solid-state 1D and 2D <sup>29</sup>Si NMR and X-ray scattering measurements. Such features generally arise in the presence of organic structure-directing species that strongly interact with and direct the formation of co-assembling and/or co-crystallizing silicate networks, whose resulting structures are often difficult to establish. Heteronuclear <sup>29</sup>Si{<sup>1</sup>H} dipole-dipole couplings allow interactions between the organic structure-directing species and silicate framework moieties to be measured and their interrelationships determined. Furthermore, homonuclear <sup>29</sup>Si{<sup>29</sup>Si} scalar and dipole-dipole interactions can be used to establish the interconnectivities and local bonding environments among different sites in ordered silicate frameworks [1-4]. In combination with X-ray scattering and molecular modeling analyses, these yield new insights on the processes by which complicated silicate frameworks become ordered and provide important constraints that can be used to assess their local structures. Recent results will be presented that demonstrate the challenges involved and new opportunities available for understanding and establishing the structures of siliceous zeolites and layered silicates, including those for which scattering analyses are indeterminate.

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**I2 Restricted Diffusion of Hyperpolarized Helium-3 to Probe Lung Structure**

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Hyperpolarized helium-3 offers a high spin sensitivity, allowing the air spaces of human and animal lungs to be imaged. Our group's focus has been on diffusion MRI of the lungs, probing structural features (e.g., airway and alveolar walls) that are too small to be imaged directly. In short-range ADC measurements, the diffusion time is typically 2 ms and the gas explores regions as large as 1 mm. Thus the acinar airways, with typical radii of 0.35 mm, substantially restrict the diffusion. An early successful application has been to distinguish healthy and emphysematous lungs (and regions within lungs) by their ADC. In health, the ADC is about  $0.2 \text{ cm}^2/\text{s}$ , compared to a free gas diffusivity of  $0.88 \text{ cm}^2/\text{s}$ . In emphysema, a disease characterized by airway expansion and airway/alveolar wall destruction, the ADC climbs by as much as a factor of 3, an unambiguous discrimination between healthy and diseased lung.

The signal decay from diffusion is fundamentally inhomogeneous in lung. There are airways oriented at essentially all orientations with respect to any gradient axis, and the diffusion along the airway ( $D_L$ ) is much larger than the diffusion across the airway ( $D_T$ ). The non-exponential signal decay measured with several values of diffusion-weighting  $b$  can be fit to determine the separate values of  $D_L$  and  $D_T$ . In turn,  $D_T$  can be used to establish the mean acinar airway radius  $R$ ; the value of  $D_L$  determines the depth  $h$  that the alveoli penetrate into the airway channels. This is remarkably detailed information from a non-invasive measurement. Thus it has been named »helium-3 MRI lung morphometry«, a reference to the method it replaces: microscope examination of excised tissue.

Long-range ADC probes the motion of gas atoms over seconds and several centimeters. It uses spatial modulation of the longitudinal spin magnetization (SPAMM), or »striping«. Once the stripes are applied, the stripe amplitude decays and can be followed by repeated small-angle MR imaging. Long-range ADC is exquisitely sensitive to collateral ventilation paths, small homes in airway walls connecting one airway to its neighbor. Not surprisingly, long-range ADC is even more sensitive to emphysema than is short-range ADC. Even in normal lungs, the long-range ADC is determined primarily by collateral paths. We have computer-simulated diffusion on the airway network and find it is much too slow to explain the measured long-range ADC in normal lungs. Instead, the important paths are collaterals, as confirmed by comparing long-range ADC in species with collateral paths (man, dog) and without (pig, sheep).

**I3 Signals in Post-War Ruins, Five Orders of Magnitude and Pore Spaces Explored by Diffusion Measurement**

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The presentation strives to justify Richard Ernst's appraisal of Leipzig as the "East Pole of Magnetic Resonance". Exploiting the special conditions of an after-dinner talk, the development of Magnetic Resonance in Leipzig is correlated with its history and its international rank as a city of sciences and arts. Molecular diffusion is selected as an example for illustrating the surprises which may be generated by scientific progress. This is in particular true for diffusion in pore spaces. Diffusion studies were recognized to provide an important novel route for the structural characterization of porous materials, including a detailed monitoring of the dynamic features of the guest species accommodated by these materials. Important features of great technological relevance, which otherwise would have remained unrecognized, have thus become accessible by direct measurement. Manifold activities in the field promise a most prosperous continuation of this development into future.