THE PHYSICS COLLOQUIUM

Thursday 25 April 2024, 4:00 p.m.
Nijenborgh 4, Lecture Hall 5111.0080

Site-specific dynamic nuclear polarization in biomolecular MAS NMR

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Solid-state NMR under magic-angle spinning is an important tool in many scientific fields, including structural biology and materials science. However, NMR's inherently low sensitivity requires oftentimes long acquisition times or even renders many experiments unfeasible. Dynamic nuclear polarization can overcome this limitation by transferring much larger electron spin polarization to neighboring nuclei, thus enhancing their magnetization by up to several orders of magnitude. Typically, fast spin diffusion within the hyperpolarized 1H bath is taken advantage of in order to widely spread polarization over relatively large distances before transferring the 1H polarization to heteronuclei for detection or further evolution. This results in a fast and uniform enhancement of the whole NMR spectrum.

Interestingly, DNP also features the potential to site-specifically hyperpolarize nuclei and thus create spatial selectivity in the NMR spectrum. This is particularly useful in biomolecular MAS NMR where spectral crowding becomes a serious problem for large assemblies or complexes. In the presentation, two approaches to create site-specific DNP enhancement are introduced. (1) In site-specific direct DNP a metal ion polarizing agent is attached or bound to a biomolecule while direct DNP of heteronuclei such as 13C or 15N can yield electron–nuclear distance-dependent build-up of enhanced polarization. (2) Specific cross-relaxation enhancement by active motions under DNP (SCREAM-DNP) can provide site-specific channels for spontaneously transfer of enhanced 1H magnetization to heteronuclei in a hetNOE-type process. A detailed explanation of both mechanisms will be given and exemplary applications on proteins, nucleic acids, and ribonucleoprotein complexes presented. Effects of uniform or sparse isotope labelling on nuclear spin relaxation, diffusion, and site-specificity of DNP as well as limitations of the techniques will be discussed. In conclusion, site-specific direct DNP with metal ions can provide additional, up to long-range distance constraints for structural modeling, while SCREAM-DNP has the power to yield spatially selective NMR spectra, for example, of sought-after biomolecular interfaces.

Join us for coffee starting 3:30 p.m. Refreshments will be served after the lecture.

For more information contact the host: Patrick van der Wel (p.c.a.van.der.wel@rug.nl)
Website: http://www.rug.nl/research/vsi/colloquia/