

Seminar

Novel and augmented methods for distance estimation with magic-angle spinning solid-state NMR

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Measuring quantitative distances are important for studying the structural properties of molecules at an atomic scale. Dipole-dipole coupling encodes distance information between spin pairs. REDOR and DIPSHIFT experiments are the most preferred experiments for measuring distances between a heteronuclear spin pair in MAS solid-state NMR. But these experiments can be used only for a small range of couplings and at slow MAS frequencies. In this talk, I will discuss the latest developments we have made for measuring a wide range of couplings using REDOR over a wide range of MAS frequencies. Additionally, I will also show that REDOR and DIPSHIFT are different realisations of a same experiment and this unification comes naturally out of our modified REDOR sequence. Further, I will discuss a method to perform REDOR experiments with low radiofrequency amplitude pulses at any MAS frequency. This method extends the application of REDOR and DIPSHIFT at very fast MAS frequencies, where the radiofrequency amplitude requirement is high. These methods allow the possibility of measuring distances over a wide range of experimental conditions.

Further, we have developed a method for obtaining selective ^1H - ^1H distance restraints from a fully protonated protein. This method is intended for elucidating protein structures at MAS frequencies above 100 kHz. The method is better than traditionally used methods in terms of information content and sensitivity, while preserving the selectivity observed only from perdeuterated samples.

Friday, Jun 28th 2019

3:00 PM (Tea/Coffee at 2:30 PM)

Auditorium, TIFR-H