Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Webinar

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

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Measuring quantitative distances at an atomic scale is important for studying the structural and dynamic properties of molecules. Dipole-dipole couplings encode distance information between NMR active spin pairs. Rotational-echo double resonance (REDOR) and correlation of chemical shift and dipolar coupling (DIPSHIFT) experiments are the most preferred magic-angle spinning (MAS) solid-state NMR experiments for measuring distances between a heteronuclear spin pair. But these experiments can be used only in a limited range of coupling strength, MAS frequency and radiofrequency amplitude. I will discuss our efforts to widen these preconceived boundaries of the experiments. We also show that these two seemingly different experiments are the two different realizations of a single unified experiment.

Additionally, we also developed a novel method for obtaining selective ^{1}H-^{1}H distance restraints from a fully protonated protein. At 100 kHz MAS, this method is better than traditionally used RFDR recoupling in terms of the density of spatial restraints and sensitivity. It also provides selective correlations similar to those observed in perdeuterated samples.

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4:00 PM