MONDAY

COLLOQUIUM

From Methods to Molecules: Innovations in Solid-State NMR

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7 Jul 2025 (Monday) | 16:00 Hrs (Tea / Coffee 15:45 Hrs) | Venue: TIFRH Auditorium

Solid-state NMR (SSNMR) is exciting because it provides unique structural and dynamic insights into complex systems often inaccessible by other techniques. Positioned at the intersection of chemistry, physics, and biology, SSNMR is a powerful and versatile tool for both fundamental and applied research. In this presentation, I would summarise two key developments from our lab.

Quantifying structural information in homogeneously coupled spin systems, such as dense proton networks in solids, is challenging due to strong couplings and rapid spread of magnetisation, which reduces spatial specificity. Multispin behaviour and strong couplings violate simple two-spin models, complicating distance extraction. This difficulty is further compounded by spectral congestion from overlapping resonances, especially in uniformly protonated samples, hindering assignment and resolution of individual spins. We will discuss two-, three- and four-spin recoupling methods to estimate quantitative and qualitative distance for different applications.

Nitrogen contributes to critical structural features that profoundly influence molecular architecture, dynamics, and intermolecular recognition. Although ^{15}N NMR spectroscopy has been extensively used to investigate nitrogen environments owing to its spin-½ nature and sensitivity to structural and dynamic properties, the more abundant ^{14}N isotope (~99.6%), a spin-1 quadrupolar nucleus, has historically seen limited use due to its broader lines and lower resolution. We highlight new developments that allow rapid measurement of 2D/3D ^{14}N spectra and ^{14}N relaxation parameters in solids. The development of such techniques opens new avenues for studying nitrogen's role, intermolecular interactions, proteins and material functionality using ^{14}N ssNMR.

Finally, I will briefly discuss applications in pharmaceutical molecules and amyloids.

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