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

Colloquium

Manipulating Proton-Driven Spin Diffusion under MAS Solid-state NMR

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Proton-driven spin diffusion under MAS[1] is one of the most commonly used experiments due to its robustness and simplicity of implementation. It is mostly used in the form of the DARR experiment[2] where the protons are irradiated at the n = 1 rotary-resonance condition. Such a cw irradiation of the protons broadens the zero-quantum line and leads to faster spin diffusion over a larger range of chemical shifts especially at higher spinning frequencies. Using more complex irradiation schemes[3] one can control the chemical-shift areas where spin diffusion is driven and where it is inhibited. Such an approach allows the optimization of spin diffusion under fast MAS conditions. In this talk I will discuss two different approaches to analyze and understand such experiments and illustrate how one can design irradiation schemes that cover different chemical-shift areas. I will show examples of 13C spin diffusion and also experiments where proton spin diffusion is controlled through irradiation of the 15N spins.

References:

1. A. Kubo, C. McDowell, Spectral Spin Diffusion in Polycrystalline Solids under Magic-Angle Spinning, J. Chem. Soc. Farad. Trans. 1. 84 (1988) 3713–3730.
2. K. Takegoshi, S. Nakamura, T. Terao, C-13-H-1 dipolar-driven C-13-C-13 recoupling without C-13 rf irradiation in nuclear magnetic resonance of rotating solids, J. Chem. Phys. 118 (2003) 2325–2341.
3. J.J. Wittmann, L. Hendriks, B.H. Meier, M. Ernst, controlling spin diffusion by tailored rf-irradiation schemes, Chem. Phys. Lett. 608 (2014) 60–67.

Monday, Feb 10th 2020

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H