Tata Institute of Fundamental Research
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Seminar

Proton Line Width in MAS Solid-State NMR

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Magic-angle spinning is routinely used to average anisotropic interactions in solid-state NMR. Due to the fact, that the Hamiltonian of a strongly-coupled spin system does not commute with itself at different time points during the rotation, second-order and higher-order terms lead to a residual line broadening in the observed resonances. Additional truncation of the residual broadening due to isotropic chemical-shift differences can be observed. We analyze the residual line broadening in coupled proton spin systems based on theoretical calculations of effective Hamiltonians up to third order using Floquet theory and compare these results to numerically obtained effective Hamiltonians in small spin systems. We show that at spinning frequencies beyond 50 kHz, second-order terms dominate the residual line width leading to a $1/\omega_r$ dependence of the second moment which we use to characterize the line width. However, chemical-shift truncation leads to a partial ω_r^{-2} dependence of the line width which looks as if third-order effective Hamiltonian terms are contributing significantly. We show that second-order contributions not only broaden the line but also lead to a shift of the center of gravity of the line. Experimental data reveals such spinning-frequency dependent line shifts in proton spectra in model substances that can be explained by line shifts induced by the second-order dipolar Hamiltonian.

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05:00 PM

Auditorium, TIFR-H