Internal Webinar

Quantifying the NMR spectra of Spin I=1/2 nuclei coupled to Quadrupolar spin in solids

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Quantifying spin I=1/2 NMR spectra coupled to quadrupolar nuclei (S>1/2) remains a challenge due to complex quadrupolar interference. While high-field probes improve sensitivity, simultaneous heteronuclear dipolar and quadrupolar interactions often complicate data interpretation. Current numerical frameworks are operationally cumbersome and lack analytic insight. This work proposes a quantitative "Effective Fields" theory to describe underlying spin dynamics and deduce optimal experimental conditions. This framework quantifies spectral intensities and frequencies via allowed and forbidden transitions. Such a methodology enables more efficient iterative fitting and modelling of experimental data in complex spin systems.

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