

Theory and description of solid state nuclear magnetic resonance spectroscopy and its application.

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One of the powerful methods that allows the understanding of molecular structure and dynamics is Solid-State Nuclear Magnetic Resonance (NMR) Spectroscopy. The technique of NMR consists of applying an intense external electromagnetic field (B_0) to a non-silent NMR nucleus (with spin quantum number $I \neq 0$), which results in an alignment between nucleus's spin magnetic momentum and the external magnetic field. Low energy α state and high energy β state are separated by an energy gap (ΔE), which is eventually equivalent to the electromagnetic radiation needed for the α spin state to reach the β spin state which it's known as resonance energy $\Delta E = \gamma \frac{\hbar}{2\pi} B_0$. When the resonance condition, $\Delta E = \gamma \frac{\hbar}{2\pi} B_0 = h\nu$, is reached, then the proton spin in the α low energy state will resonate and jump or promote to the β high energy state. Our group focus is on solid-state NMR, which is a branch of NMR technique for characterizing atomic level structure in solid materials e.g. powders, single crystals and amorphous samples and tissues. The anisotropy part of many spin interactions are present in solid-state NMR, unlike in solution-state NMR where rapid tumbling motion averages out many of the spin interactions. As a result, solid-state NMR spectra are characterized by larger linewidths than in solution state NMR, which can be utilized to give quantitative information on the molecular structure, conformation and dynamics of the material. Solid-state NMR is often combined with magic angle spinning to remove anisotropic interactions and improve the resolution as well as the sensitivity of the technique. While several theories such as average Hamiltonian theory (AHT), Floquet theory, Fermi expansion, and Floquet-Magnus expansion (FME) have been used to control the spin dynamics in solid-state NMR, this poster will share some particular results on AHT and FME, which explains how periodic pulse sequences can be used to switch off or transform the symmetry of selected interactions in coupled, many-spin systems, allowing magnetic resonance spectroscopists to create effective spin Hamiltonians with a wide variety of intriguing and useful properties. Theory on pulse sequences create the possibility of manipulating spin evolution and hence magnetic resonance signals in an endless variety of ways, which can be accurately described by quantum mechanics and mathematics that lend themselves to creativity and new insights.