

Welcome Seminar

20 Novembre 2025 - h15:00
Aula A

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Ricercatore a tempo
determinato di tipo A

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Photochemically induced dynamic nuclear polarization for dye-sensitized solid-state NMR spectroscopy

Poor signal sensitivity is still one of the main barriers in cutting-edge applications of NMR spectroscopy for structural and chemical analysis. Hyperpolarization techniques can alleviate the sensitivity issue by enhancing the population imbalance between the nuclear spin states. In solids, dynamic nuclear polarization (DNP) represents today the most successful and broadly applicable protocol for the amplification of the NMR signal. In a typical DNP experiment, the sample is co-formulated with a paramagnetic species – known as the polarizing agent (PA) – that acts as a source of thermal electron spin polarization. Upon microwave irradiation at cryogenic temperatures, the large β electron spin polarization is transferred from the PA to nearby ^1H nuclei and successively, by spontaneous ^1H – ^1H spin diffusion, to the sample bulk.

Here, we show that bulk NMR hyperpolarization can also be achieved in solids by replacing the paramagnetic PAs with donor–acceptor covalent systems and by irradiating the sample with light instead of microwaves. In this case, nuclear hyperpolarization is developed via solid-state ^1H photochemically induced DNP (photo-CIDNP), which has the potential to generate polarization levels even larger than those obtained via DNP. As such, ^1H photo-CIDNP could hence be used to establish a general light-induced hyperpolarization protocol to improve the sensitivity of solid-state NMR spectroscopy beyond the DNP limit through the combined use of donor–acceptor dyes and optical irradiation of the sample.