Dynamic nuclear polarization by photo-excited electronic spins
– towards the initialization of an NMR quantum computer –

(CREST[†], Department of Chemistry, Graduate School of Science, Kyoto University[‡])
K. Takeda[‡], K. Takegoshi[‡], and T. Terao[‡]

In order to overcome the low sensitivity in nuclear magnetic resonance (NMR), dynamic nuclear polarization (DNP) is carried out in doped solids, in which large electron spin polarization of the photoexcited triplet state of the guest molecules is transferred to nuclear spins. The use of the photoexcited triplet state for DNP has the advantages such as, (a) photoexcited triplet states often exhibit tremendously large electron spin polarization, so that much higher nuclear polarization is expected, (b) when the polarization transfer is complete, the time evolution of the nuclear spin state is not disturbed by the hyperfine coupling with the electron spins, since the triplet state is allowed to decay to the ground state simply by stopping the photo-excitation.

The DNP experiments are carried out in naphthalene and *p*-terphenyl which are doped with pentacene guest molecules. It is shown that the nuclear polarization can be enhanced even in a polycrystalline sample. Possible applications as well as the effect of the scattering of the light of the excitation laser in polycrystalline materials is discussed. NMR signal enhancement is also demonstrated in spin systems of low abundance including ^{13}C as well as diluted proton spins by deuteration. Proton polarization of 0.27 is achieved in a field of 3187 G and at a temperature of 150 K, corresponding to $\sim 10^5$ enhancement of the polarization as compared to that in thermal equilibrium. For such a hyperpolarized spin system subjected to nuclear dipole-dipole interactions, peculiar asymmetry is observed in the NMR spectrum, from which the absolute sign of the dipole-dipole interaction can be determined.

In order to realize a NMR quantum computer with many qubits, initialization of a nuclear spin state is very important, since the NMR signal amplitude, which decreases exponentially with increasing the number of qubits, gets too weak to observe without any signal enhancement techniques. We believe that the present work opens the way of enhancing nuclear polarization in various situations of interest, including materials which may found to be feasible for NMR quantum computers.