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Optimization of laser-induced OH• Radical Generation in Water

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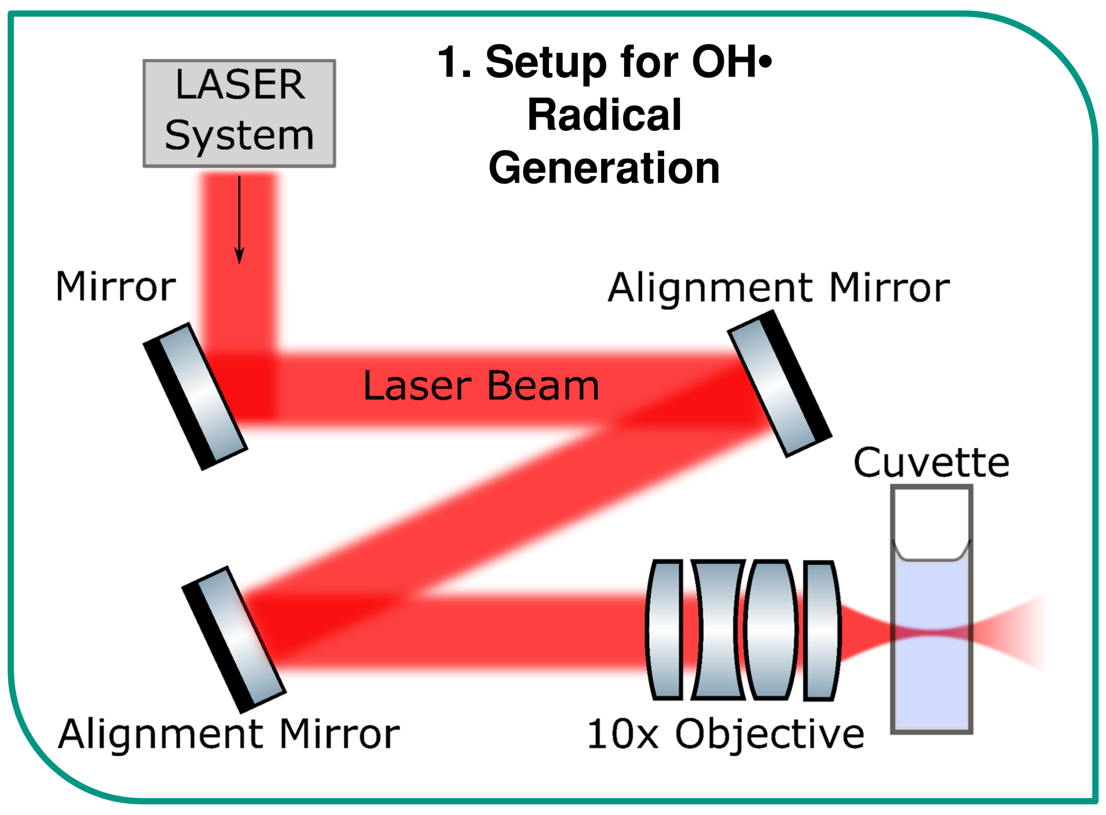
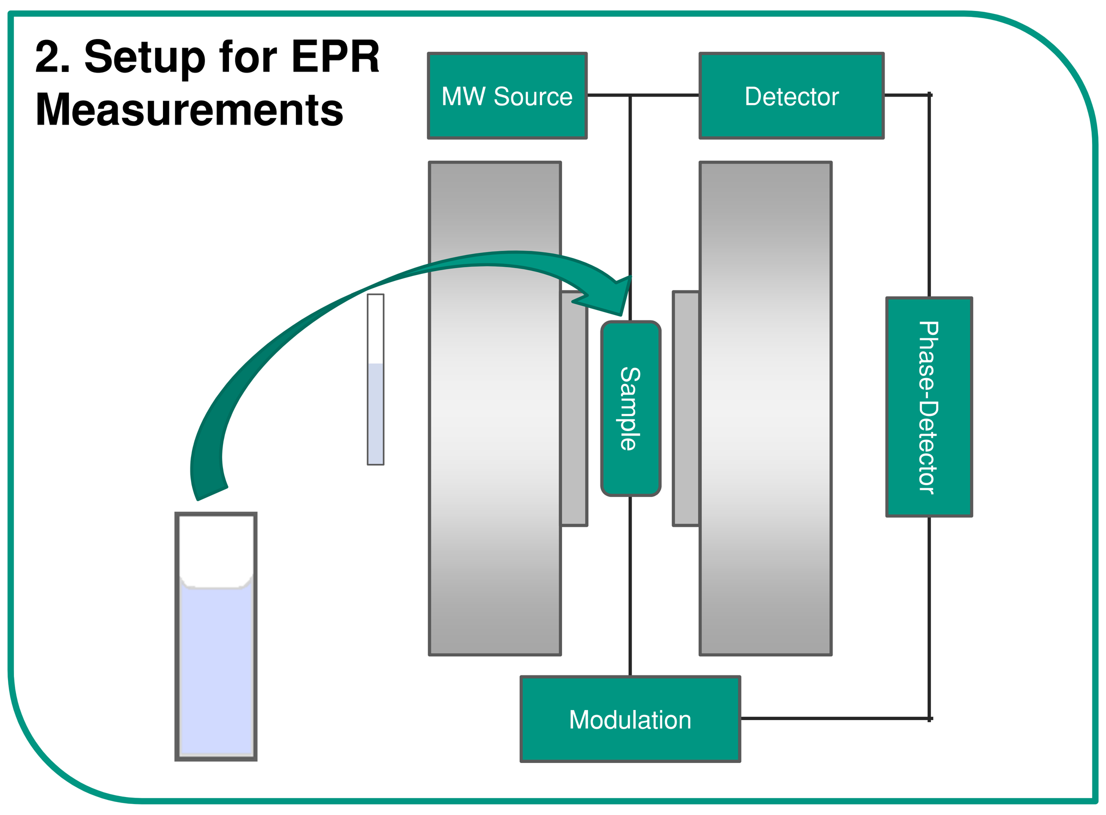
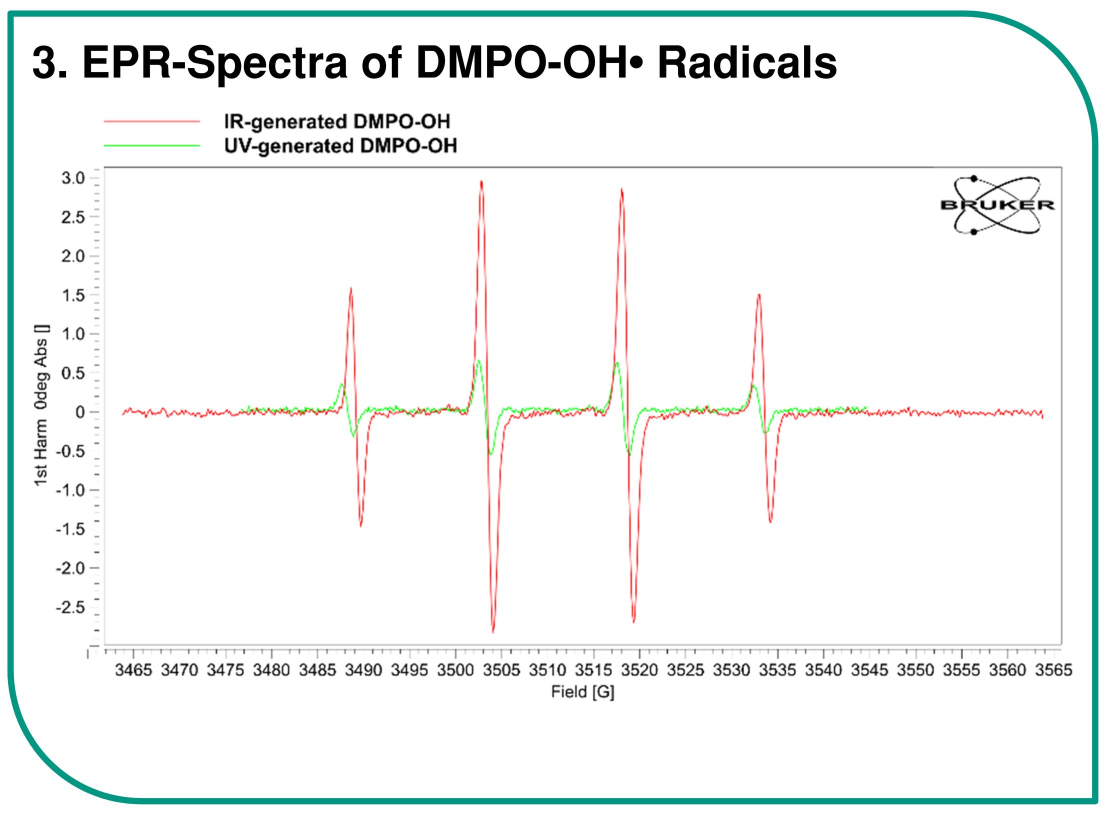
The use of radicals to transfer **spin polarization** to nuclei is an important technique to **increase the signal intensity of NMR** measurements. The generation of OH• radicals is usually done with UV irradiation of hydrogen peroxide or sonication of water among other techniques.[1] These methods require several tens of minutes and therefore suffer from the degradation of radical concentration during the generation process when spin-traps like DMPO (5,5-Dimethyl-1-pyrrolin-N-oxid) are used. Hence, the usable radical concentration is lower than the number of radicals produced during the generation process. Therefore, we investigated the **laser-induced radical generation** dependent on **pulse length** and **pulse energy**.



1. Setup for OH• Radical Generation



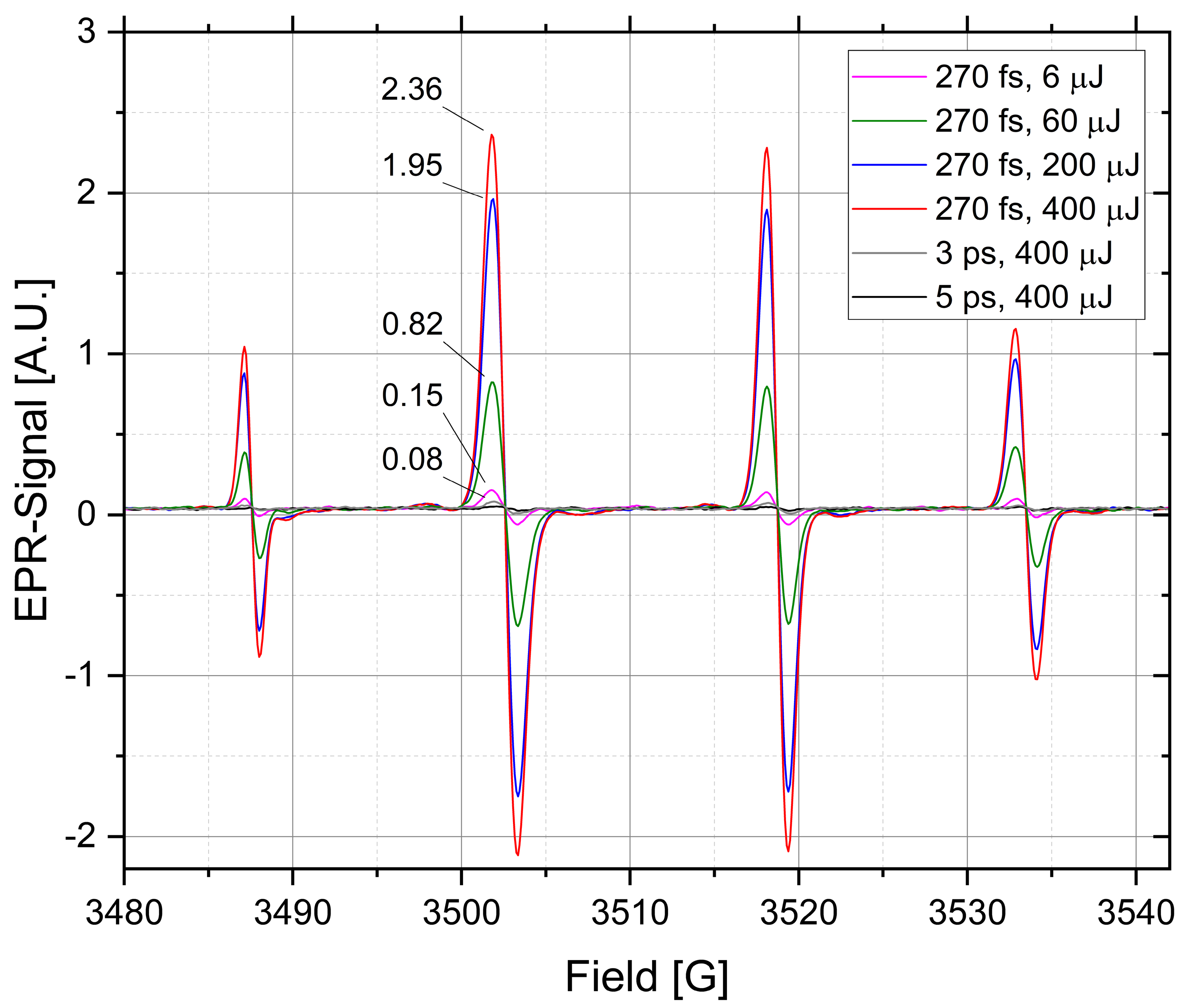
2. Setup for EPR Measurements



3. EPR-Spectra of DMPO-OH• Radicals

The influence of laser pulse length

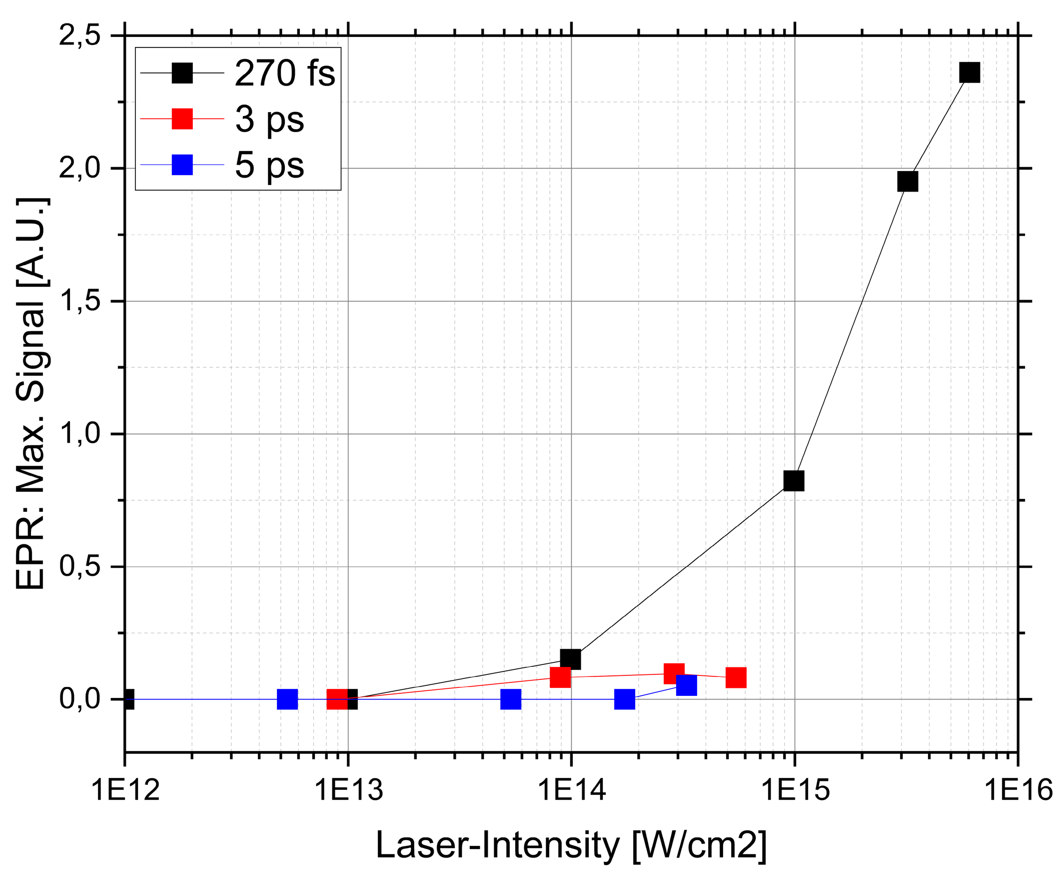
The 10 mM DMPO-water solution shows a significant increase of captured OH• radicals with increasing laser intensity. The sample solution was irradiated for 1 min, directly followed by the EPR measurement. However, significantly less radicals are produced when the pulse length is increased. At 3 ps pulse length the EPR signal intensity drop by the factor of 30. No signal can be acquired with 5 ps pulse length.



How does the plasma effect radical generation?

Even though multiphoton absorption in water starts from 10^9 W/cm^2, the EPR signal was measurable exceeding a laser intensity of 10^{13} W/cm^2. With our laser setup, a 270 fs pulse length at the highest laser intensity resulted in the highest DMPO-OH• radical concentrations. This agrees well with the plasma generation in water theory.[2] With shorter pulses more energy is transformed into the plasma – and water dissociation – compared to longer pulses. Longer pulses are more likely to heat the water instead of dissociating water molecules.

The concept of laser-induced radical generation is an attractive method for spin polarization due to its speed and the absence of additive molecules. These preliminary results lay the foundation for exploring **laser-generated radicals in the context of NMR signal hyperpolarization**.



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[2] J. Noack and A. Vogel, "Laser-induced plasma formation in water at nanosecond to femtosecond time scales: calculation of thresholds, absorption coefficients, and energy density," in IEEE Journal of Quantum Electronics, vol. 35, no. 8, pp. 1156-1167, Aug. 1999, doi:10.1109/3.777215.

KSOP Karlsruhe School of Optics & Photonics

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