

Magn. Reson. Discuss., community comment CC1
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Comment on mr-2022-8

Andriy Marko

Community comment on "The effect of spin polarization on double electron–electron resonance (DEER) spectroscopy" by Sarah R. Sweger et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2022-8-CC1>, 2022

This an interesting paper improving understanding of physical processes and interpretation of DEER measurements, which are often attempted to use for resolving important questions of structural biology. This paper goes into the analysis of the situation when DEER experiments are performed at low temperature and high magnetic fields, that is, when a significant spin polarization is present. It predicts an out-of-phase signal component of the inter-molecular contribution, which was overseen and was not analyzed in the previous work. The predicted out-of-phase inter-molecular component is used to explain qualitatively experimental data, although there is still quantitative mismatch between theory and experiment. The magnitude of the out-of-phase inter-molecular component is determined by the value of the integral (S58), the convergence of which is not straight forward and apparently, this integral relay strongly on the assumption of homogeneous and isotropic distribution of spins on long distances R in the sample. I think, some inhomogeneity or anisotropy of spin distribution can change the value of this integral significantly, perhaps much more than of the corresponding in-phase component integral. However, these are my rough estimation. Probably, some more extensive investigation/comments regarding this point would be useful in the paper or in the discussion. Anyway, apparition for an interesting work!