

Magn. Reson. Discuss., community comment CC2
<https://doi.org/10.5194/mr-2021-10-CC2>, 2021
© Author(s) 2021. This work is distributed under
the Creative Commons Attribution 4.0 License.

Comment on mr-2021-10: Code availability?

Nino Wili

Community comment on "The decay of the refocused Hahn echo in double electron–electron resonance (DEER) experiments" by Thorsten Bahrenberg et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-10-CC2>, 2021

Dear authors,

Once again, it is amazing to see that numerical simulations can be made efficient enough to treat realistic spin systems. I am glad you deposited the experimental and simulated traces on zenodo, but I was wondering where and how you will make the code and the MD coordinates available? This would help the community (or - more honestly - at least me) to apply the same simulations to other problems. For example, I would like to look at the electron coherence decay under continuous microwave irradiation.

I understand that your standards are very high, but this code would be valuable even if it is not fool-proof and documented as rigorously as "EasySpin".

Thank you and best wishes,

Nino Wili