

# Selective Excitation by Optimal Control (OC) Pulses as Alternative Approach to Conventional Solvent Suppression Methods

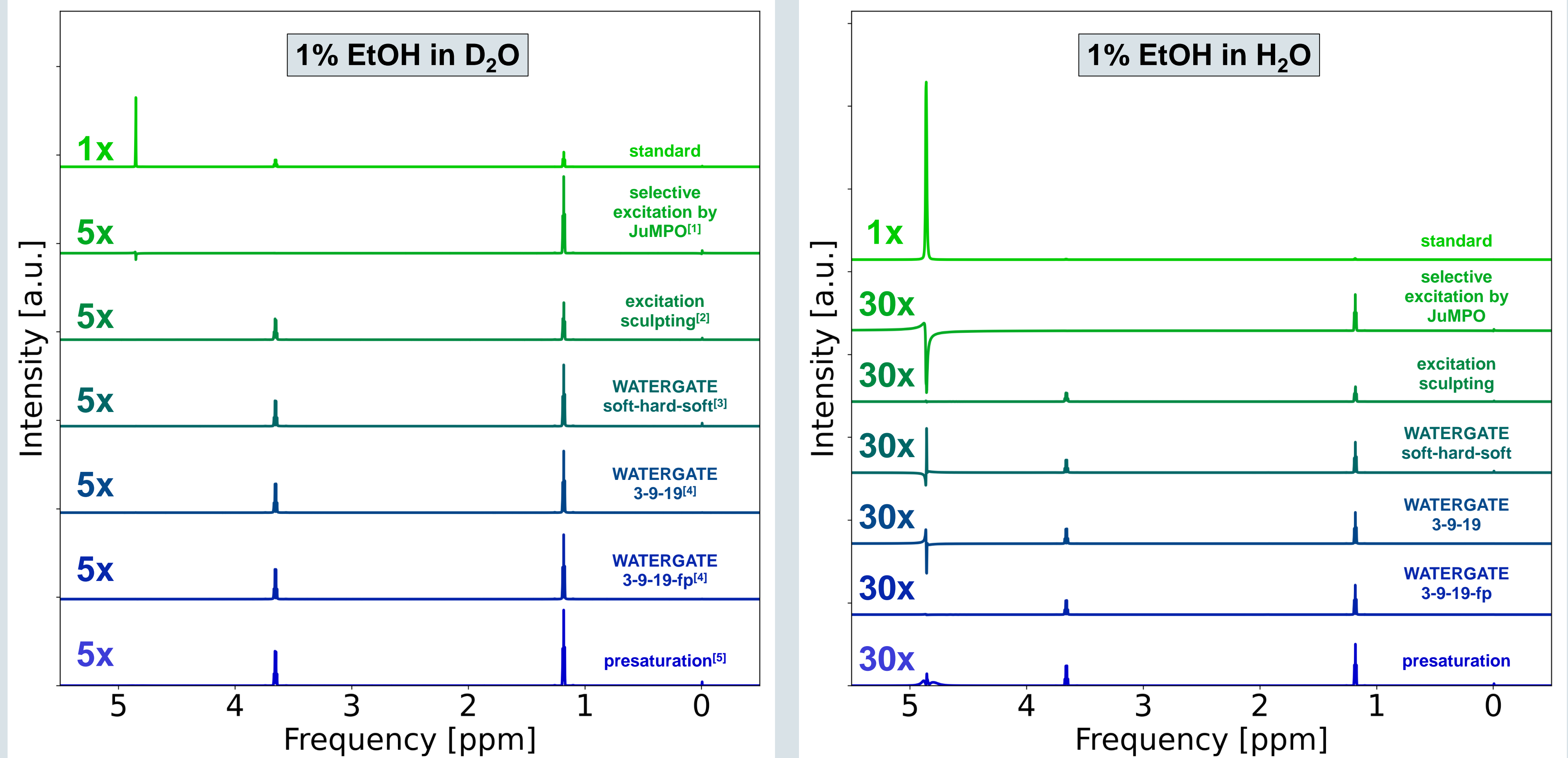
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## Current difficulties for *in operando* NMR investigations of electrochemical experiments

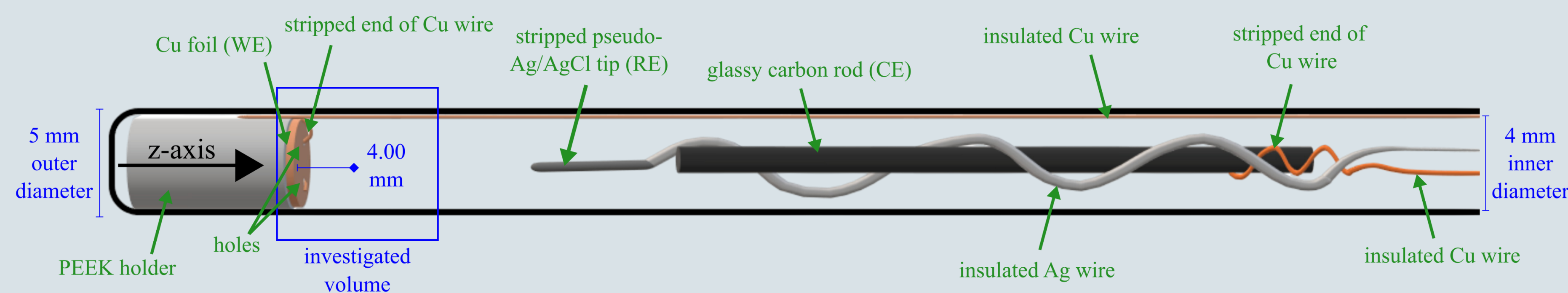
- Suppression of solvent signal during *in operando* NMR measurements of aqueous electrolysis experiments
- Quantitative analysis of signals close to the suppressed solvent signal
- Excitation of specific regions of an electrochemical cell setup i.e. Helmholtz- and diffusion-layer on the working electrode

## Conventional vs. OC-based pulses for low (D<sub>2</sub>O) as well as high (H<sub>2</sub>O) spin densities



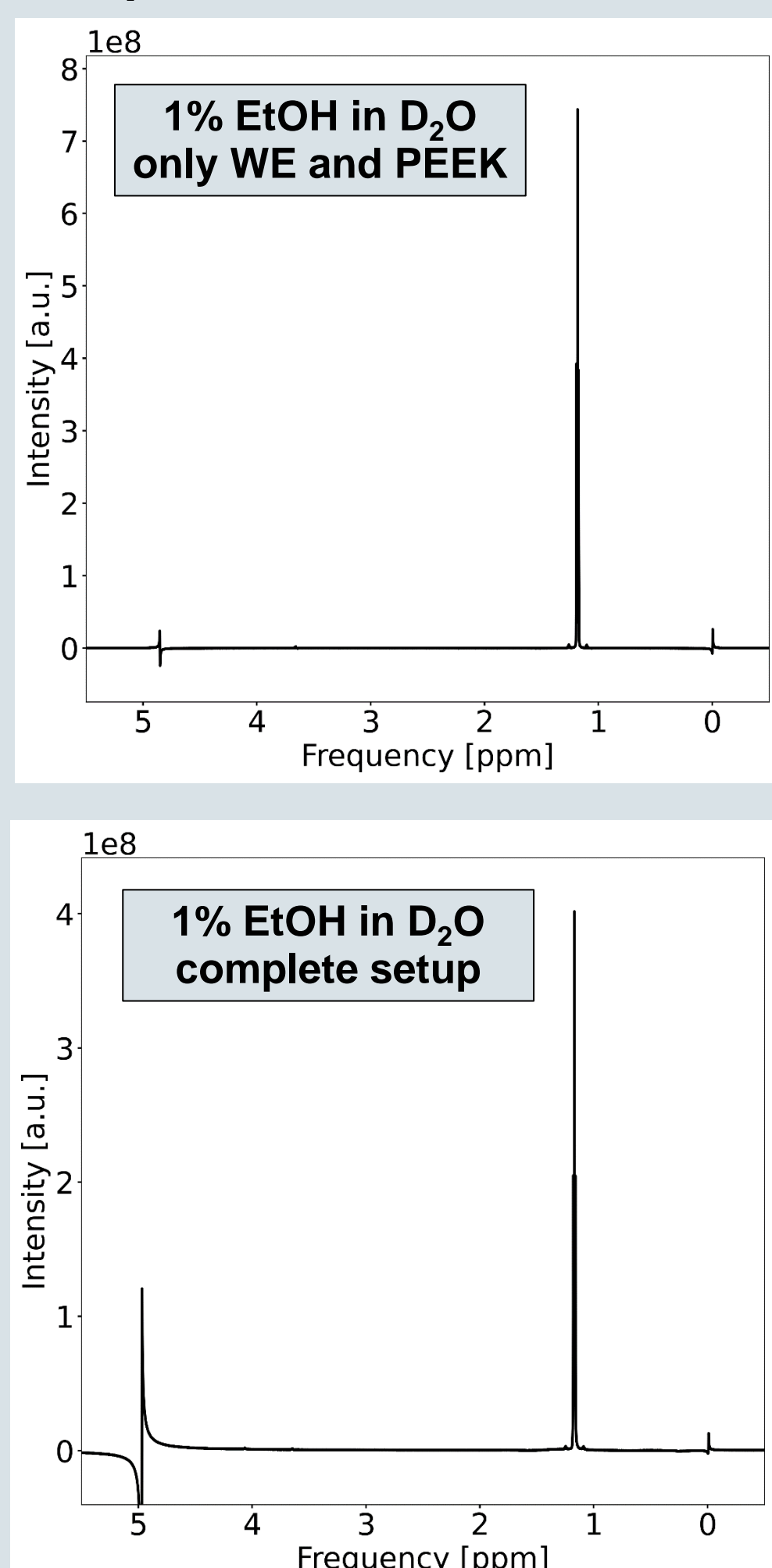
- Similar to some conventional pulses, suppression efficiency of OC pulses reduces with spin density

## Sketch of the *in operando* NMR setup for electrochemical measurements with working electrode (WE), reference electrode (RE) and counter electrode (CE)



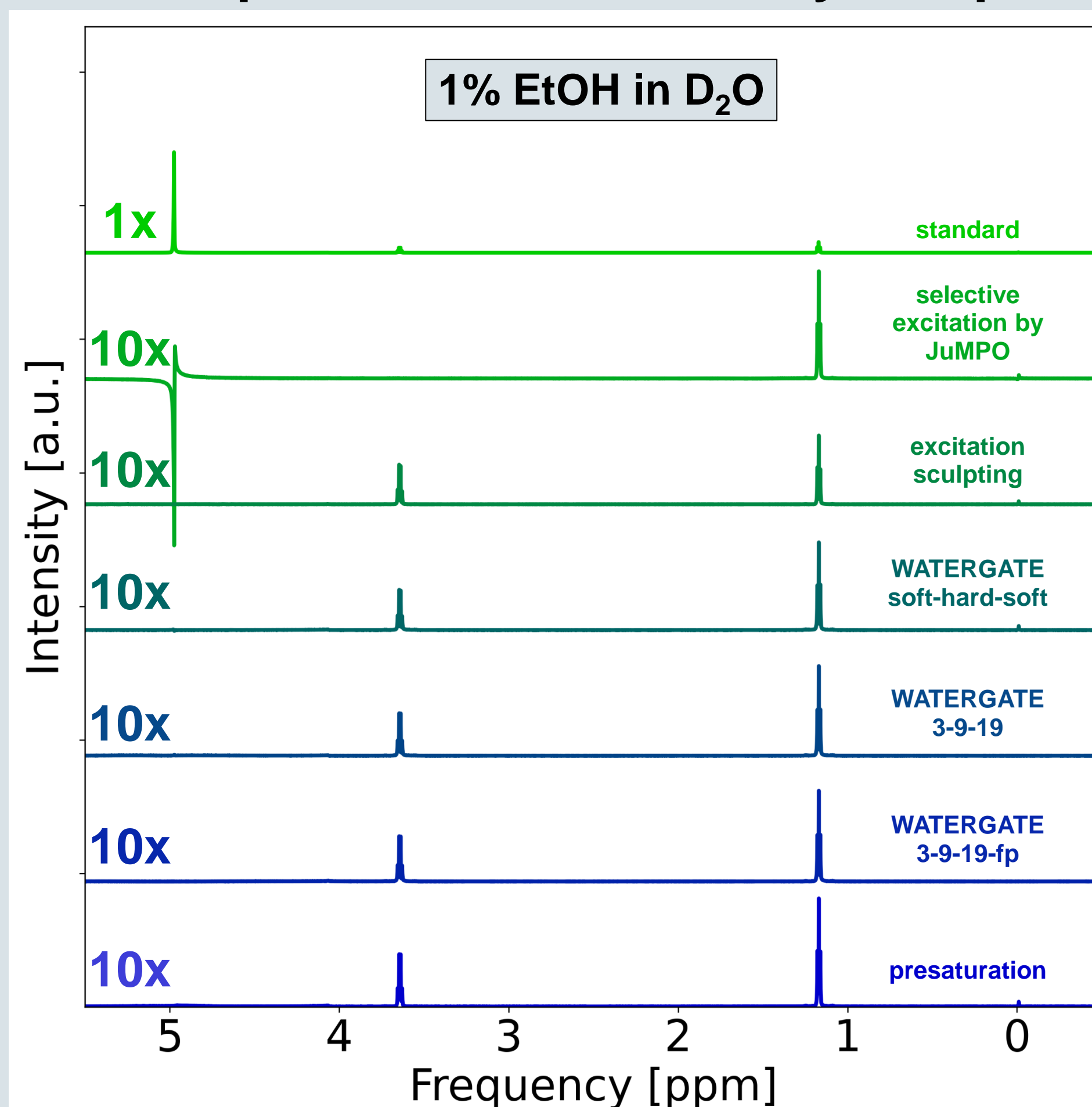
- conductive cell components cause B<sub>0</sub> and B<sub>1</sub> field distortions
- miniature electrochemical cell setup with optimized alignment of working electrode parallel to B<sub>1</sub> field<sup>[6]</sup>
- OC pulses based on JuMPO<sup>[1]</sup> package are applied to maximize suppression efficiency despite the induced magnetic field distortions

## OC pulses applied to samples with complete electrochemistry setup vs. WE with PEEK holder



- selective methylene excitation not impaired by components
- solvent suppression efficiency decreased with complete setup

## Application of OC pulses to Ethanol sample in electrochemistry setup



## Conclusion

- OC pulses effective for selective spin excitation in any setup
- solvent suppression by OC is less efficient but on the same scale as conventional pulses
- suppression efficiency of OC pulse decreased by electrochemical setup, specifically by placement of RE and CE

## Outlook

- OC pulses for online product distribution of electrochemical experiments in typical aqueous electrolytes
- incorporation of transfer functions to account for magnetic field distortions and thus increase suppression efficiency of OC
- adjustment of OC pulses for selective excitation of spins near electrode surface

## References

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## Acknowledgement

This research has been supported by the German Research Foundation (DFG) under Germany's Excellence Strategy Cluster of Excellence 2186 "The Fuel Science Center" (grant no. 390919832).