Control, Hyperpolarisation & Signal Processing for Quantum Sensing in the Life Sciences

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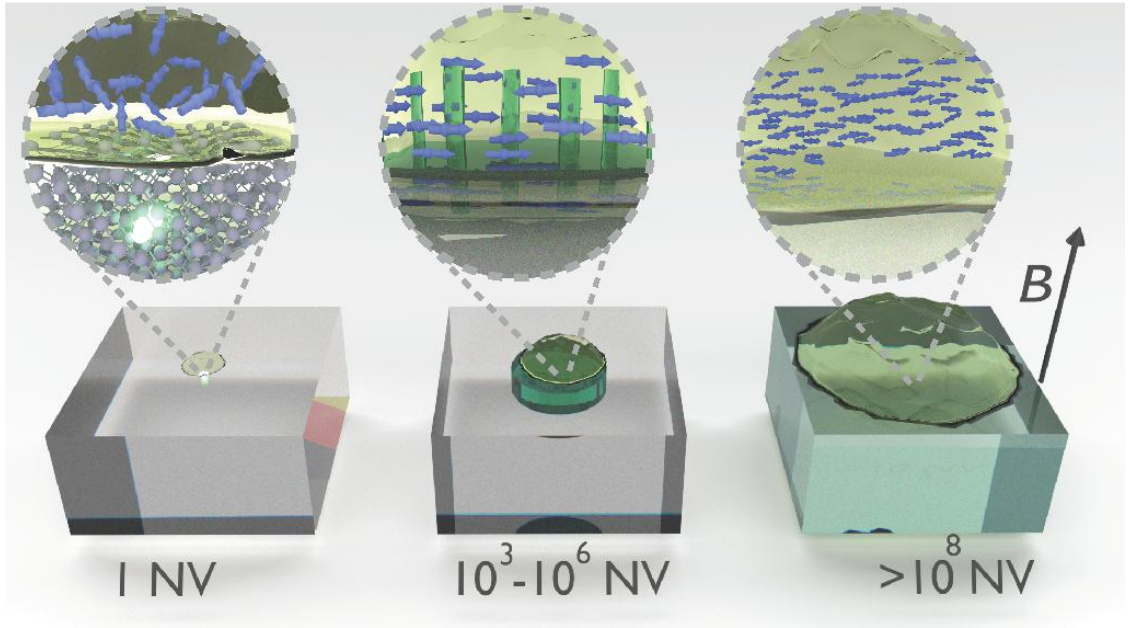
Our Goals for Quantum Sensing in the Life Sciences



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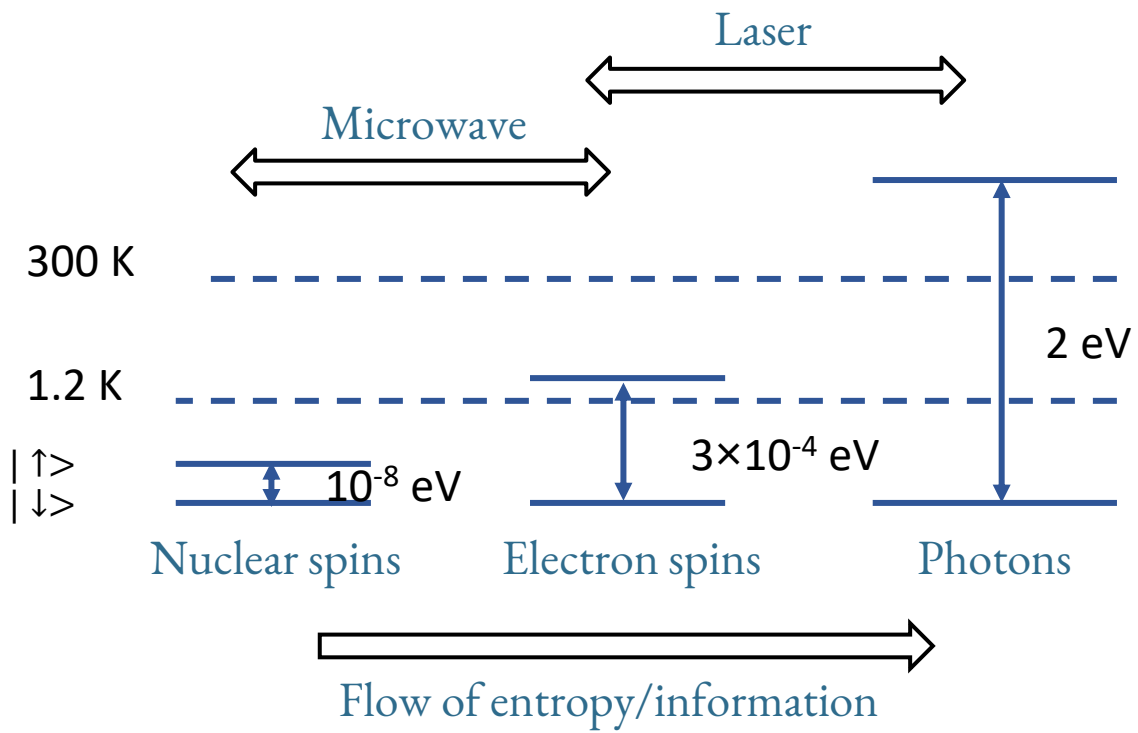
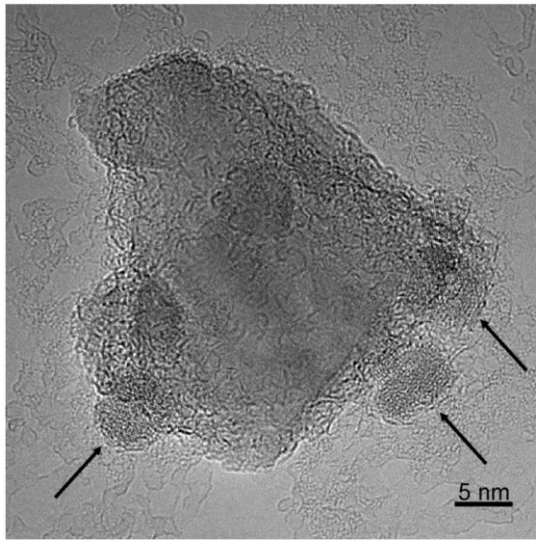
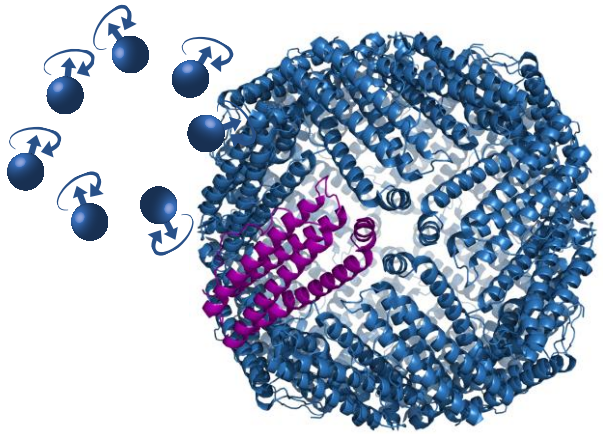
Enhancing ESR and NMR from the Nano- to the Macroscale to access metabolic information.

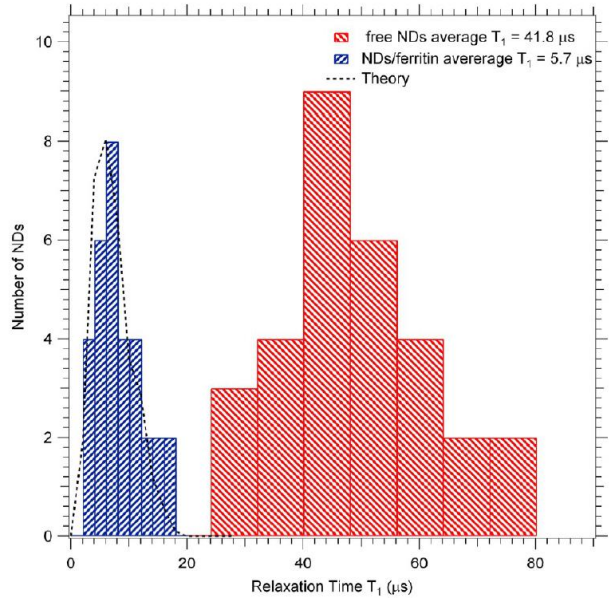
Optically Detected Magnetic Resonance

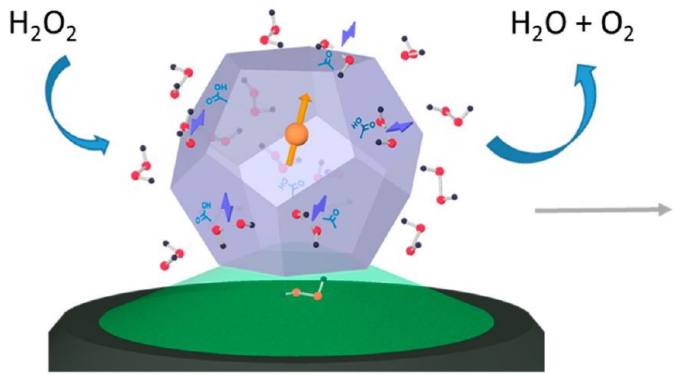


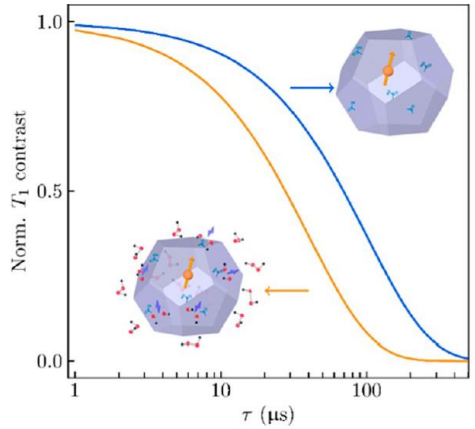
ESR at the Micron- and Nanoscale

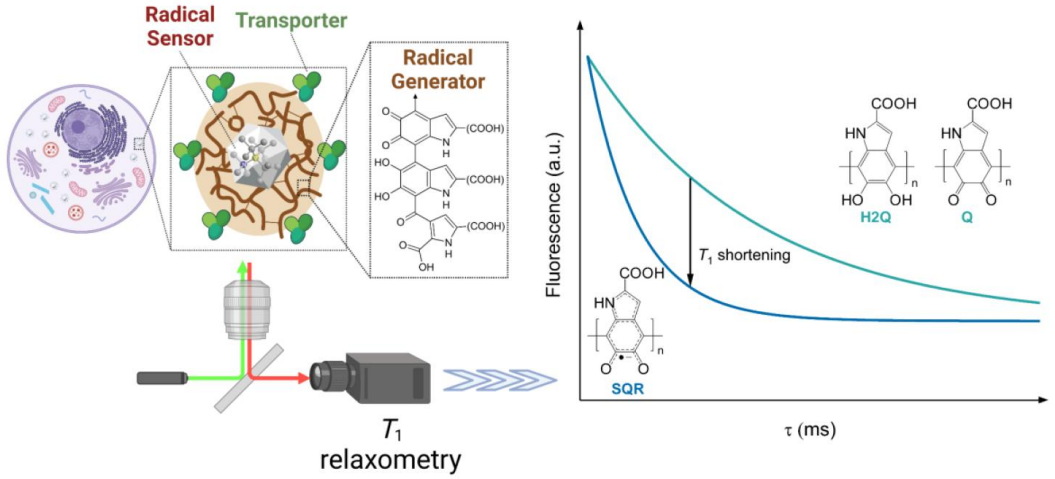




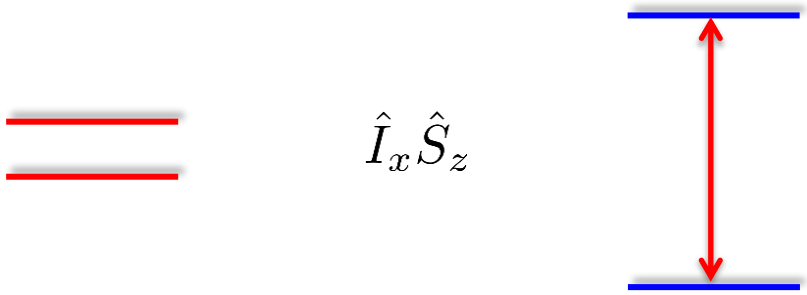




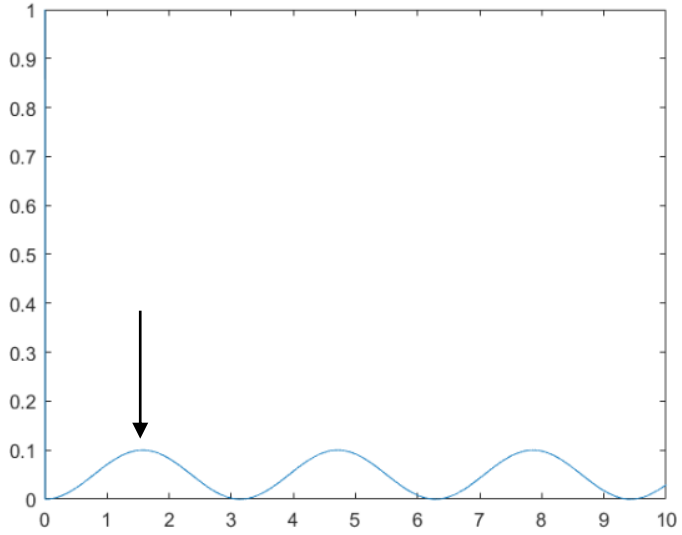




Elements of Quantum Control

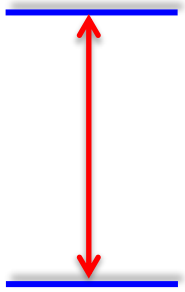


Use sharp pulses to flip sensing spin with period of target



Elements of Quantum Control

$$\hat{I}_x \hat{S}_z$$



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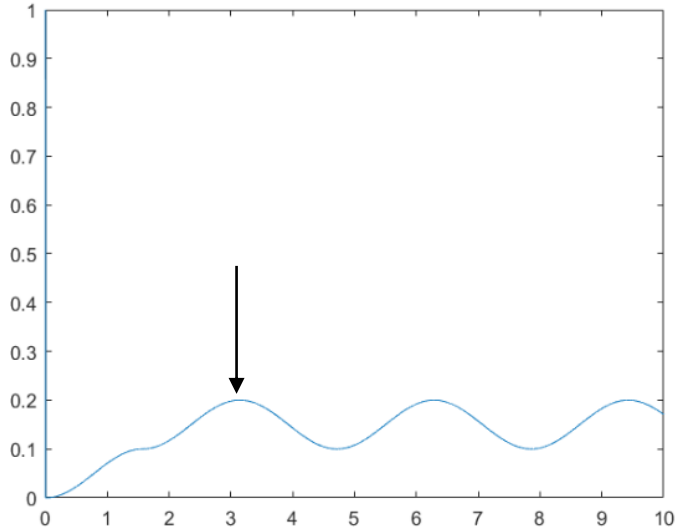

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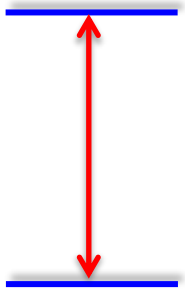

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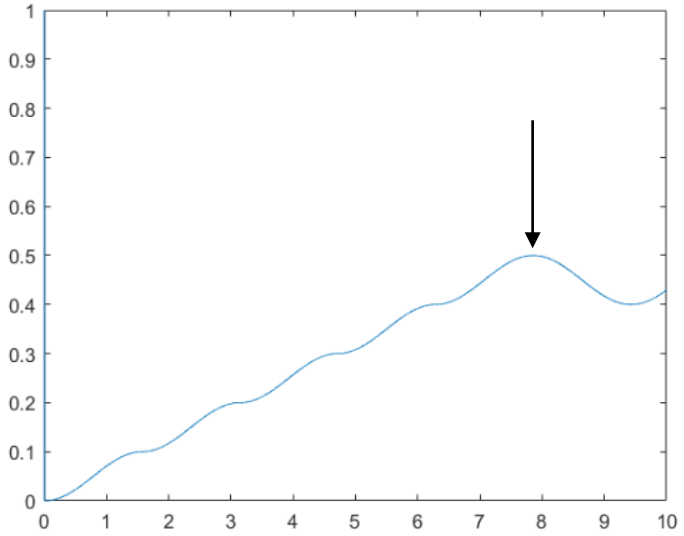

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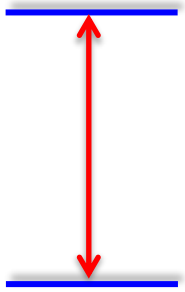
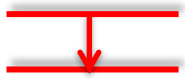
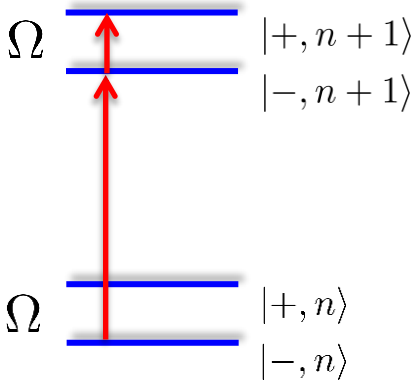


Use cw-field to create dressed states with energy splitting that matches target





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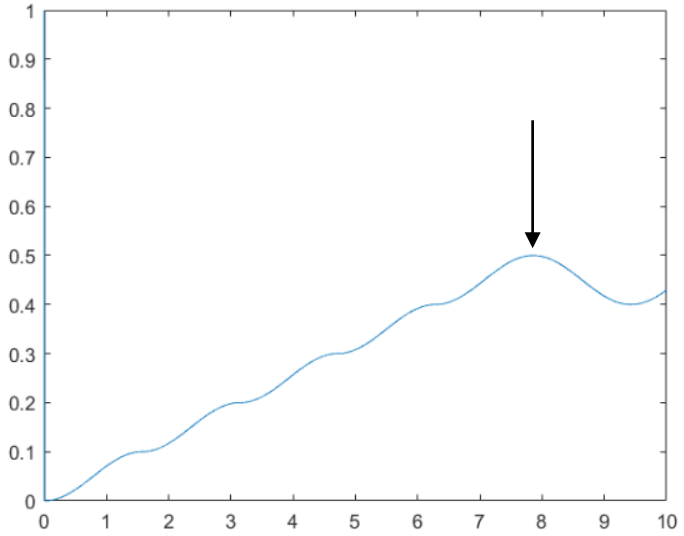

Elements of Quantum Control

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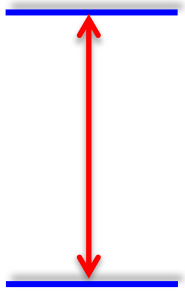

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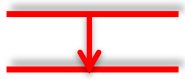
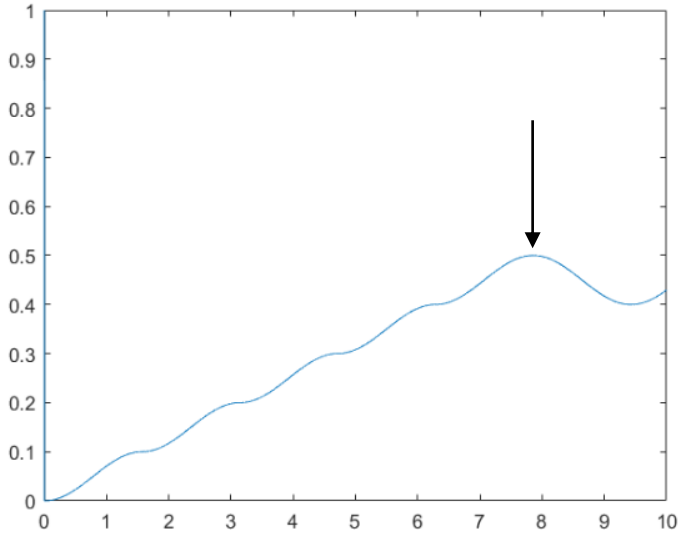


Ω

$|+\rangle$

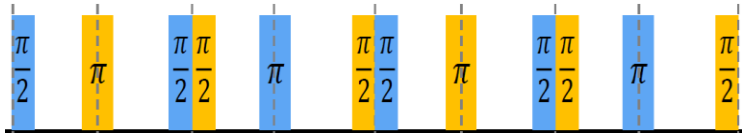
$|-\rangle$

Use sharp pulses to flip sensing spin with period of target



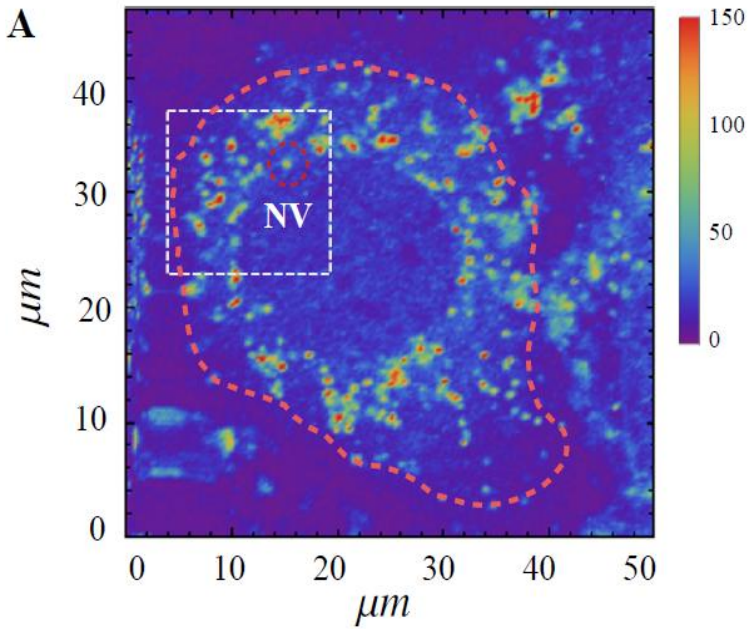
Elements of Quantum Control

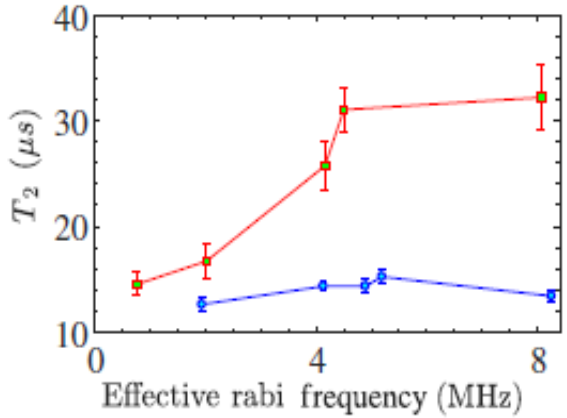
Generalities



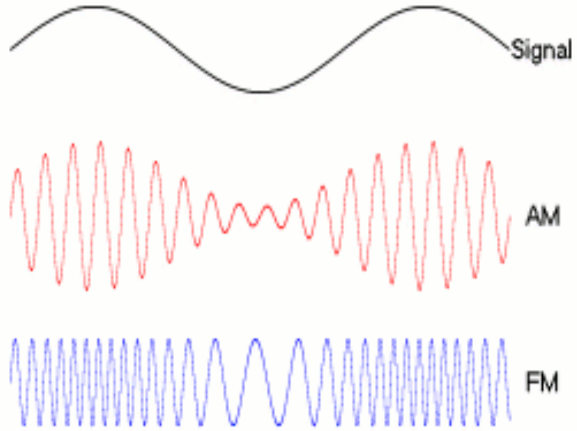
Continuous Wave Control	**Pulsed Control**
control intensity/phase	control timing/phase
Susceptible to energetic disorder	Robust to energetic disorder
Low energy consumption	High energy consumption
Interaction while pulse on	Interaction “in between” pulses

Continuous Wave vs Pulsed Control: Energy Efficiency

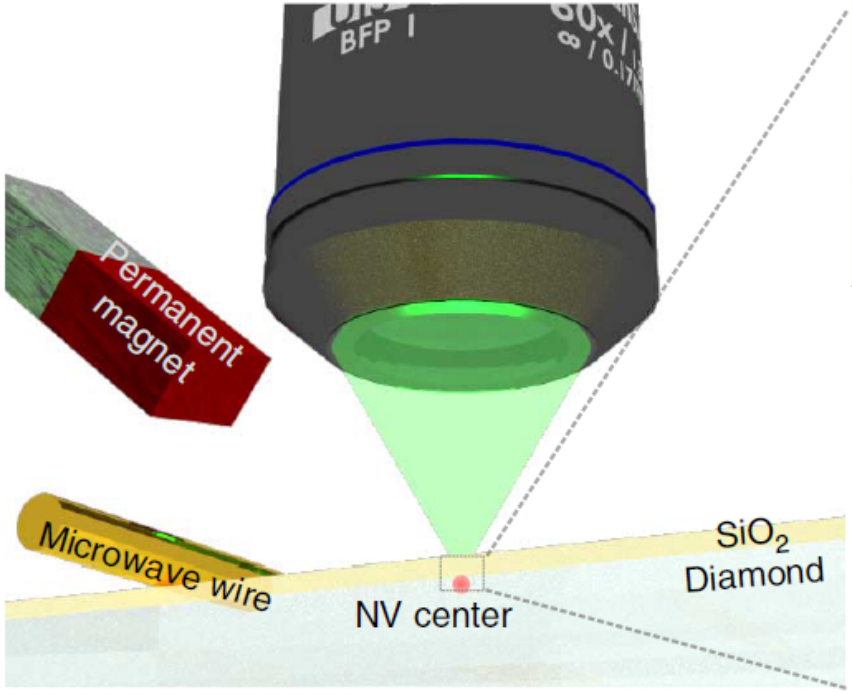


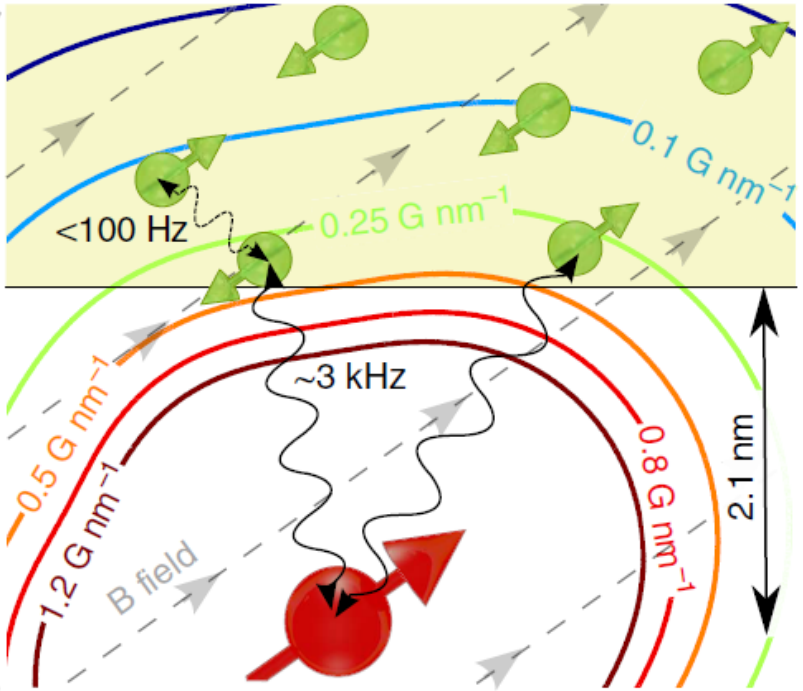


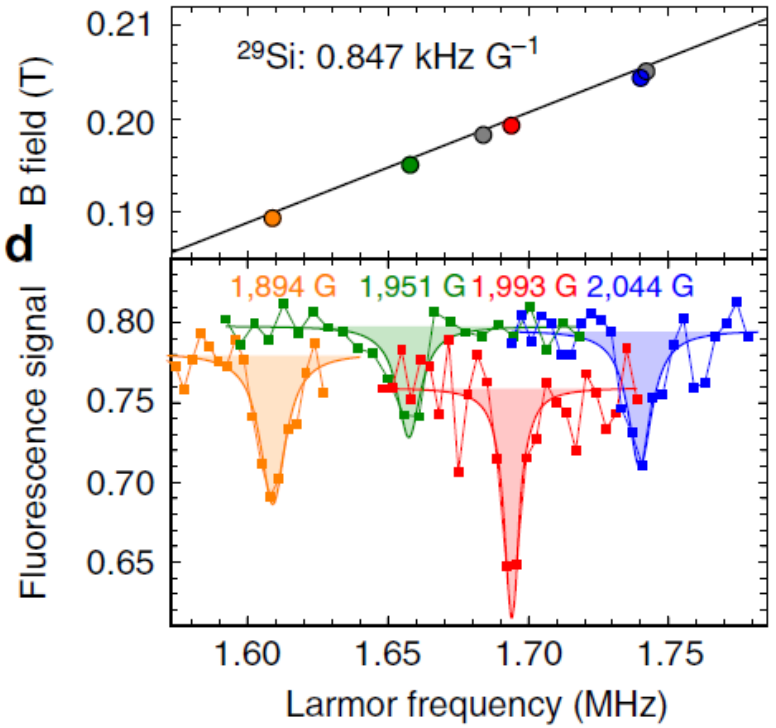
Comparison coherence time XY (blue) vs
Continuous concatenated drive (red)



The Sensitivity Challenge

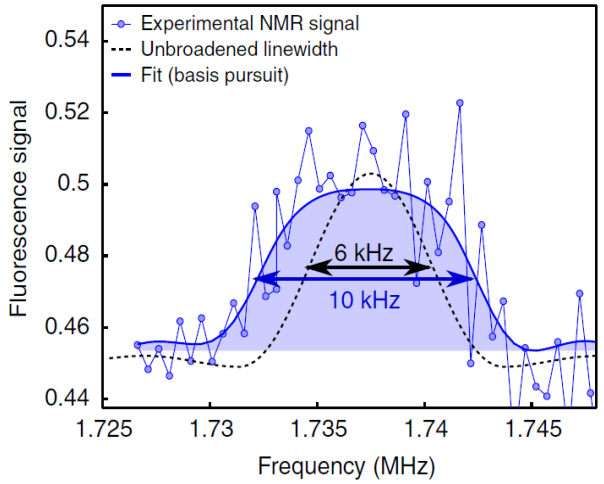






The Sensitivity Challenge

Signal Processing Methods Use Prior Knowledge to Enhance SNR



- Denoising Basis Pursuit

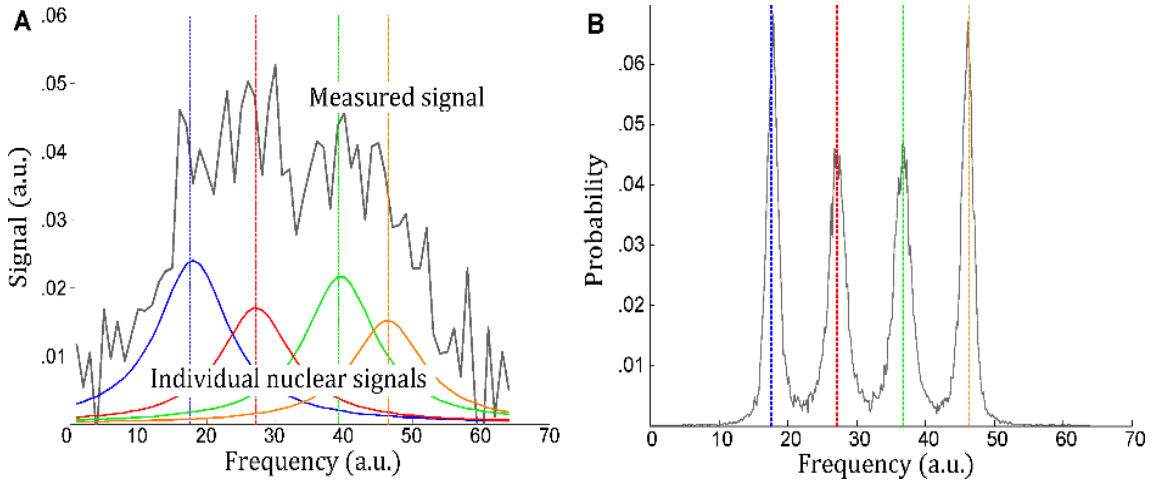
Add 1-norm penalty for number of nuclei

$$\min_{\alpha} \frac{1}{2}\|\mathbf{y} - \Phi\alpha\|_2^2 + \lambda\|\alpha\|_1$$

Encode lineshapes in matrix Φ

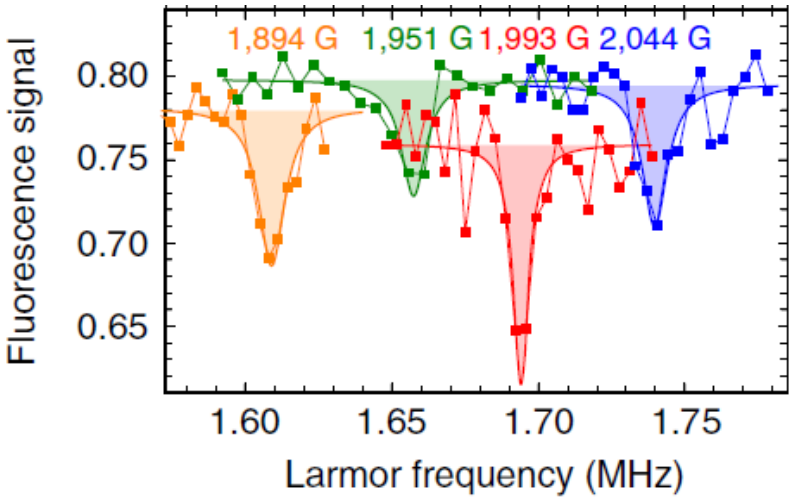
Reconstruct measured signal $\mathbf{y}$

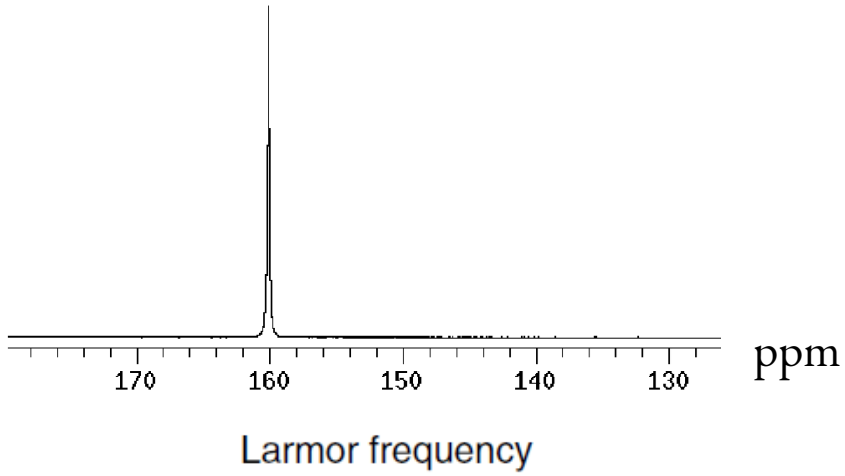
Numerical test:



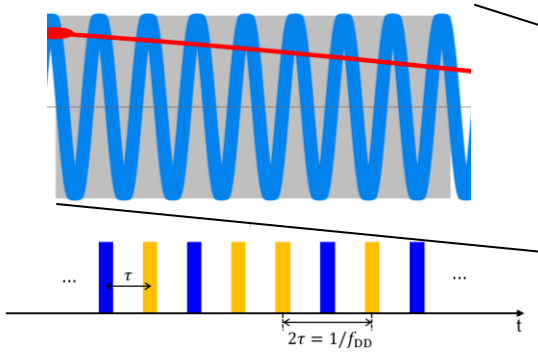
The Spectral Resolution Challenge

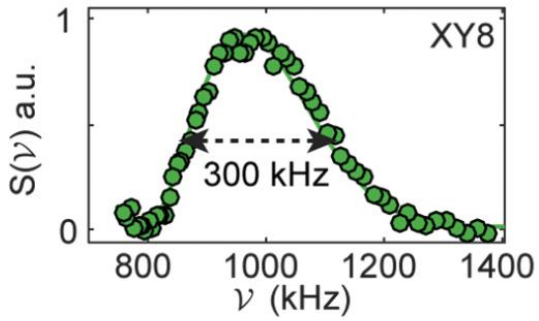
Great Sensitivity but Limited Resolution

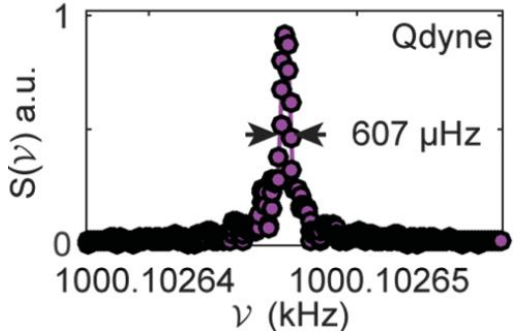




NMR at the Micron- and Nanoscale

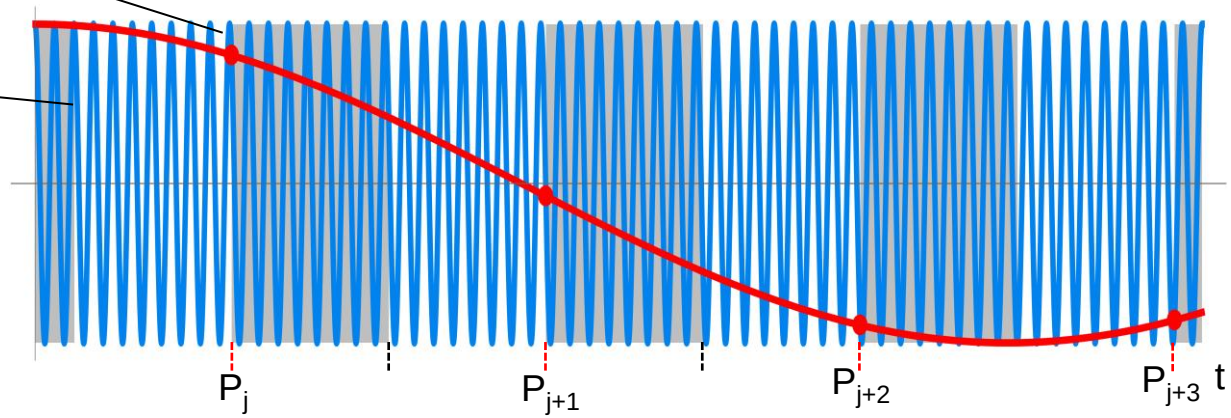






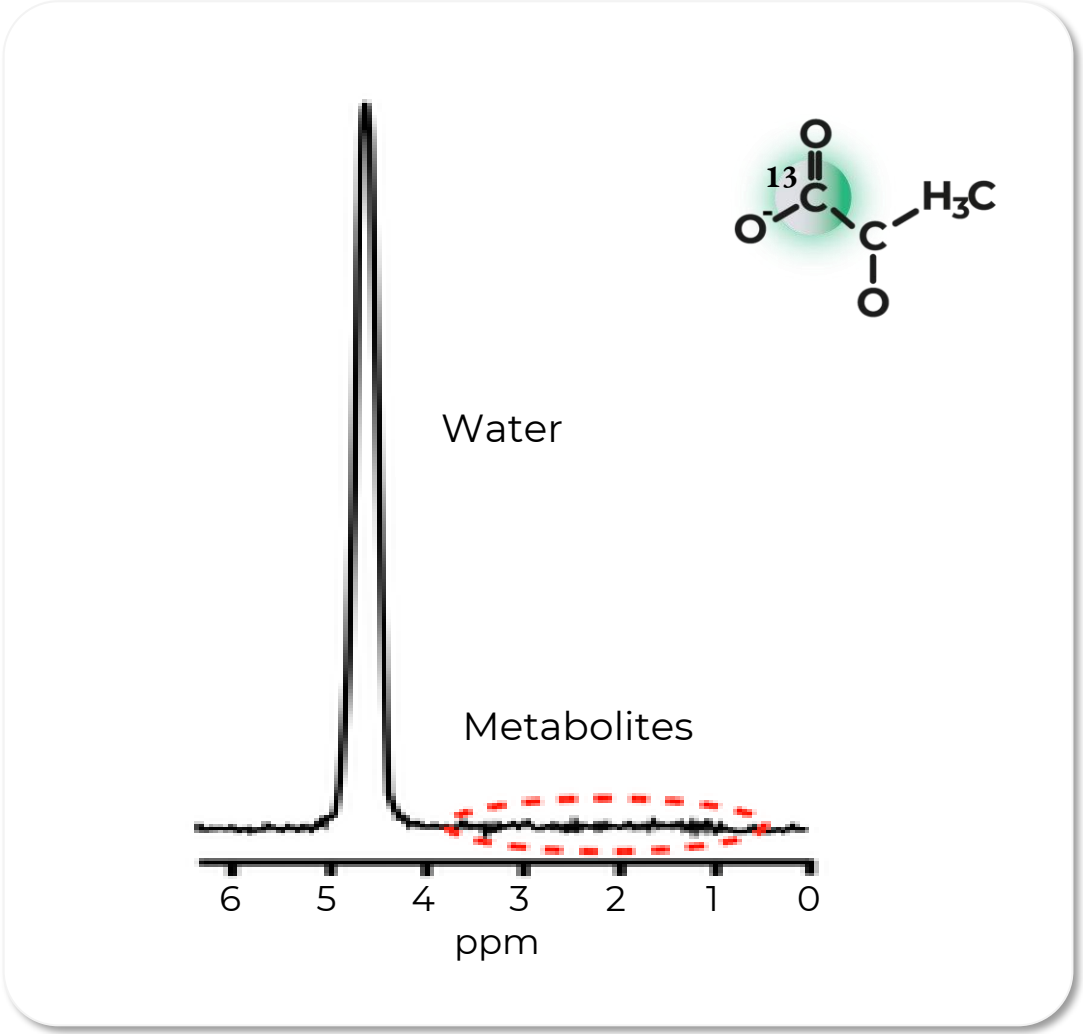
Quantum heterodyne protocol (QDyne)

$B(t) = \cos[2\pi f_L t]$ $P(t) = \cos[2\pi(f_L - f_{DD})t]$



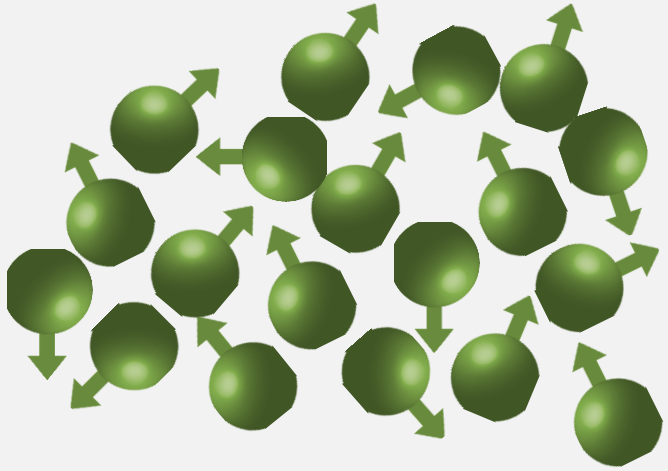
The Challenge of Metabolic Imaging by NMR

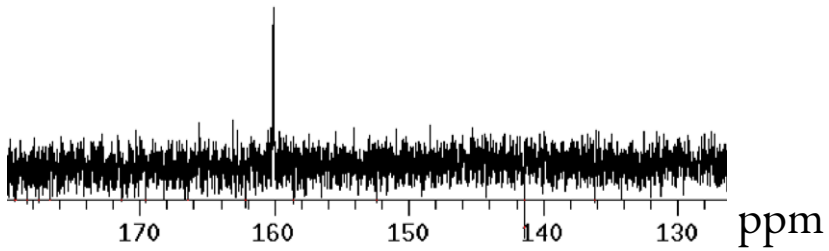
The road to Single Cell Metabolic NMR



Key Challenge in Magnetic Resonance

Thermal Nuclear Spins — Weak Signal

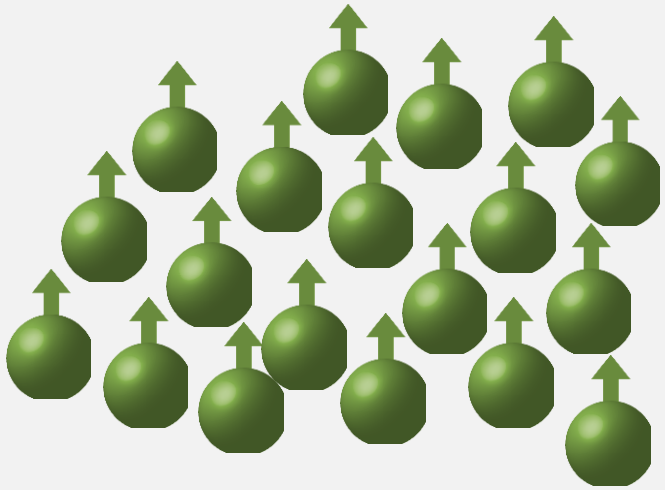


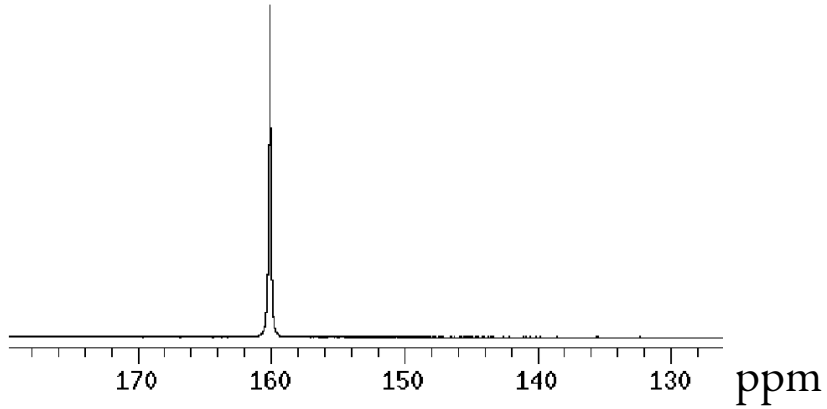


From molar concentration detection limit ...

Quantum technology allows for **spin control** (hyperpolarization)

Hyperpolarised Nuclear Spins — Strong Signal





... to micromolar concentration detection

Quantum Enabled Hyperpolarisation Requires Four Key Ingredients

1

Readily available low entropy SOURCE

Polarised electron spin

Singlet order in para-hydrogen

2

Ability to bring source in close CONTACT with polarisation target

Physical mixture

Chemical bonding

3

Coherent CONTROL methods for robust & efficient polarisation transfer

Microwave & rf-fields

Magnetic field control

4

VERSATILITY
Polarise a wide variety of targets by the same procedure

Polarisation Transfer

Generic Mechanism

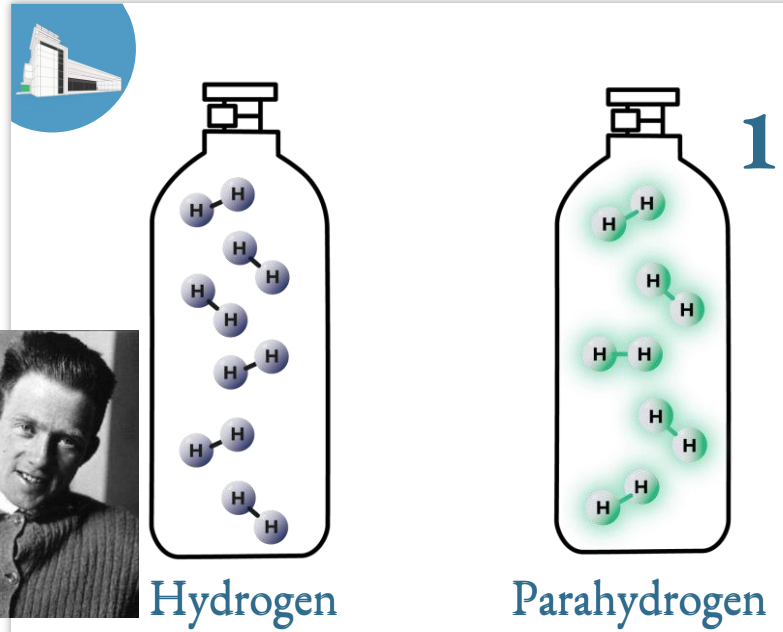
Quantum Enabled Rapid Room-temperature Hyperpolarisation

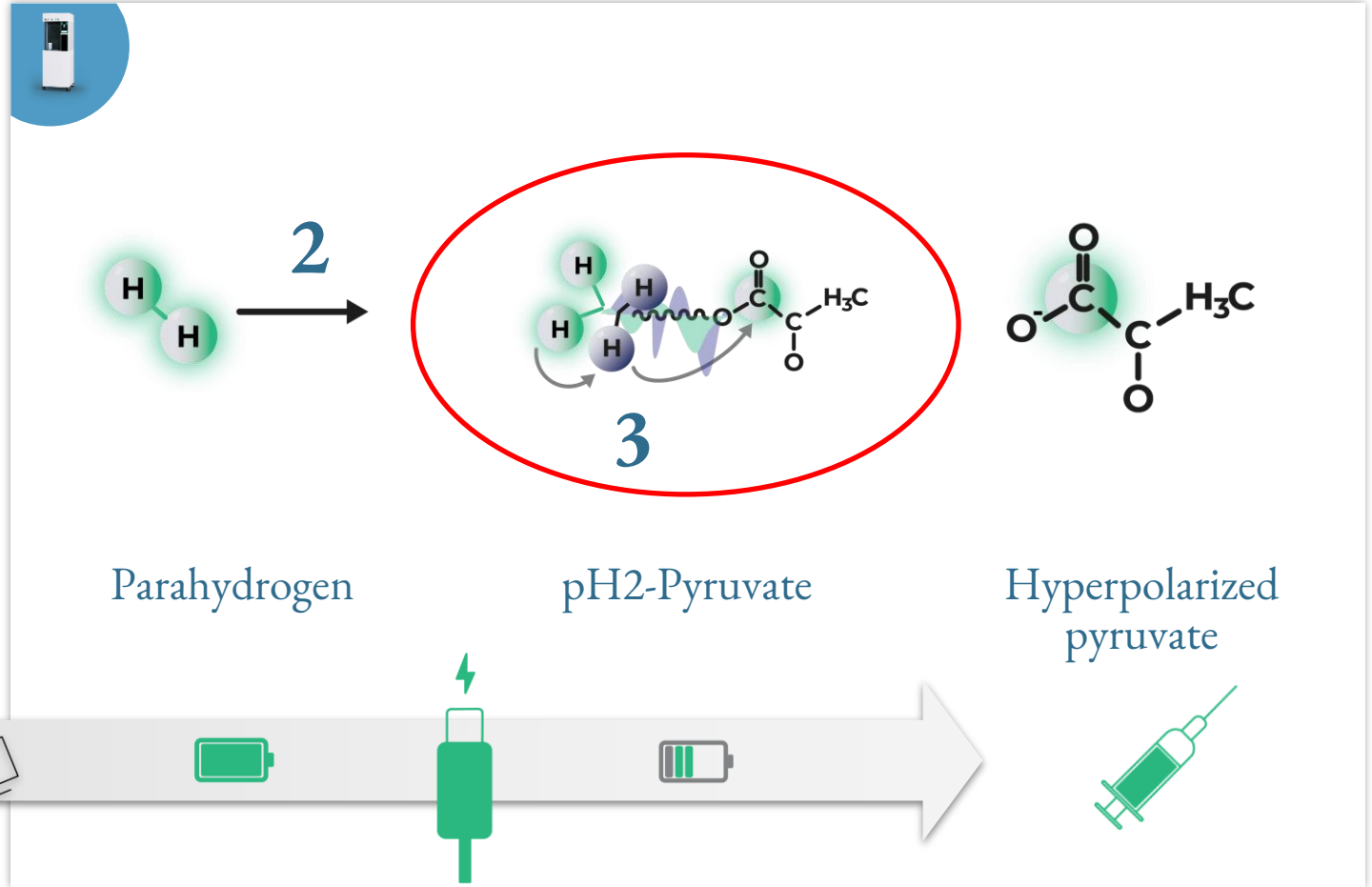
1 Polarisation source is parahydrogen gas (singlet quantum order), serves as "battery" that keeps its quantum order for months

2 Singlet order hydrogen is attached chemically to target

3 Quantum control converts singlet order to polarisation on ^{13}C target in 3 minutes

the award recognises his development of quantum mechanics, "the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen.





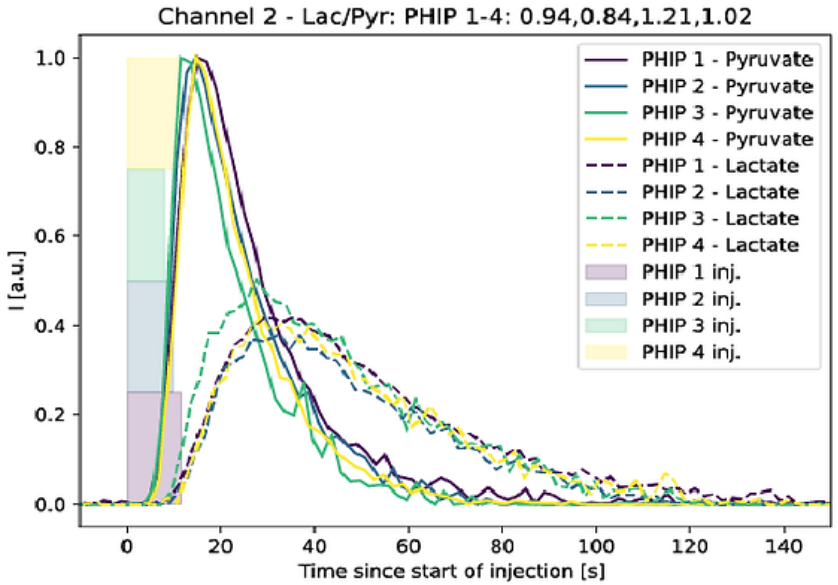
Patent US 11,940,510 Patent filed PCT/IB2023/059050

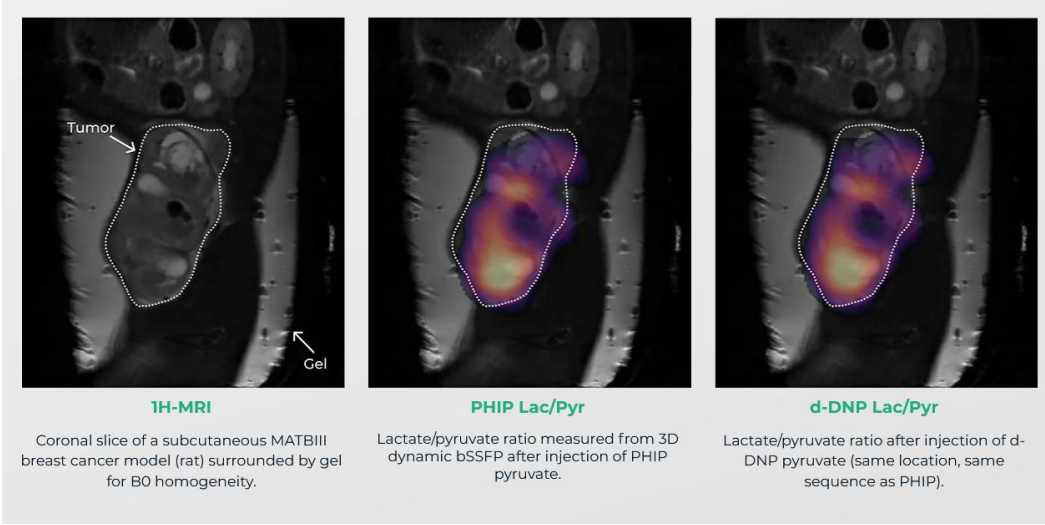
Bowen & Weitekamp, PRL 1986 ; JACS 1987
Reineri, Boi, Aime, Nat Comm. 2015

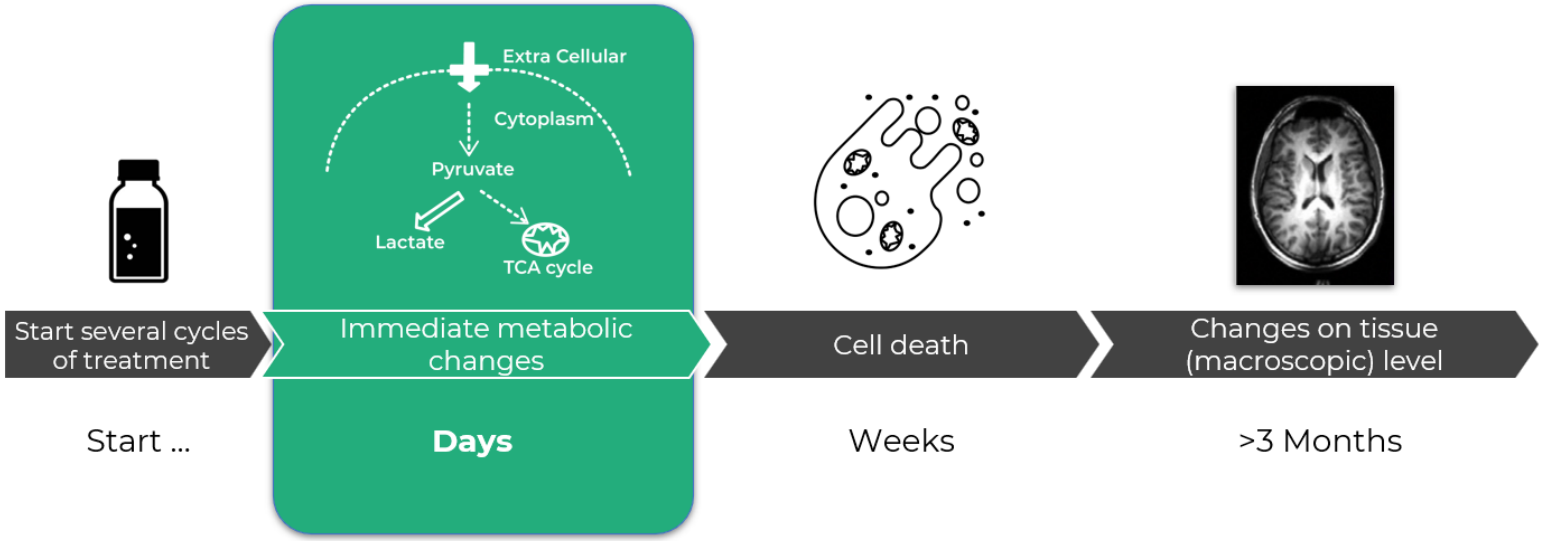
Quantum Technologies for the Life Sciences

Korzeczek, Dagys, Müller, Tratzmiller, Salhov, Eichhorn, Scheuer, Knecht, Plenio, Schwartz, JMR 2024
Dagys, Korzeczek, Parker, Eills, Blanchard, Bengs, Levitt, Knecht, Schwartz, Plenio. Sci. Adv. 2024
Korzeczek, Schwartz, Plenio, JMR 2026

Hyperpolarised MRI In Action







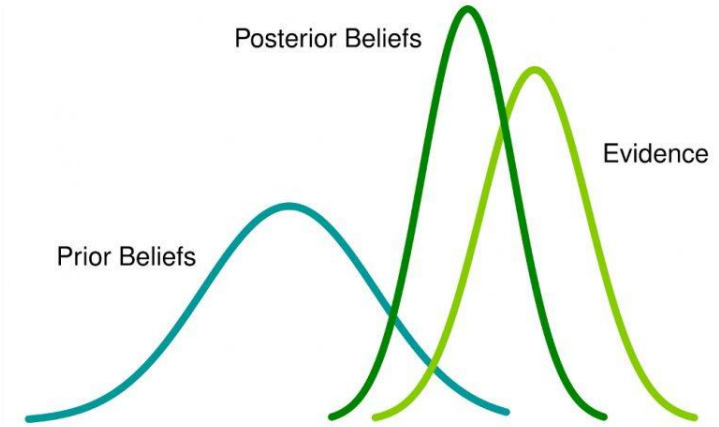
Polarisation
~50% in device
~30 % at point of injection

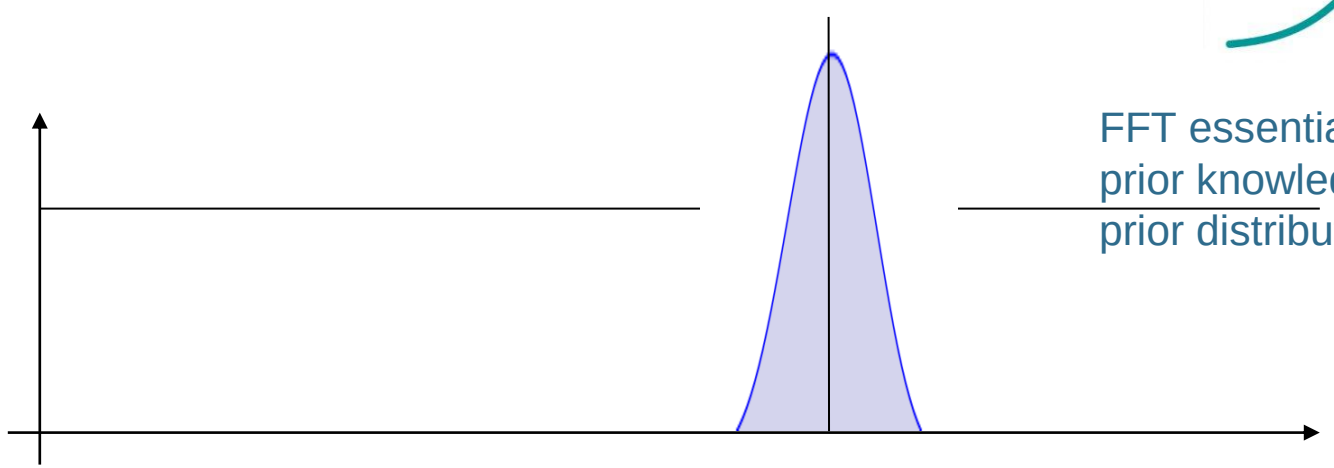
POLARIS by NVision

Extracting Signals from Very Noisy Data

Use all available knowledge

- You know the shape of the signal
- You know your nuclei & magnetic field





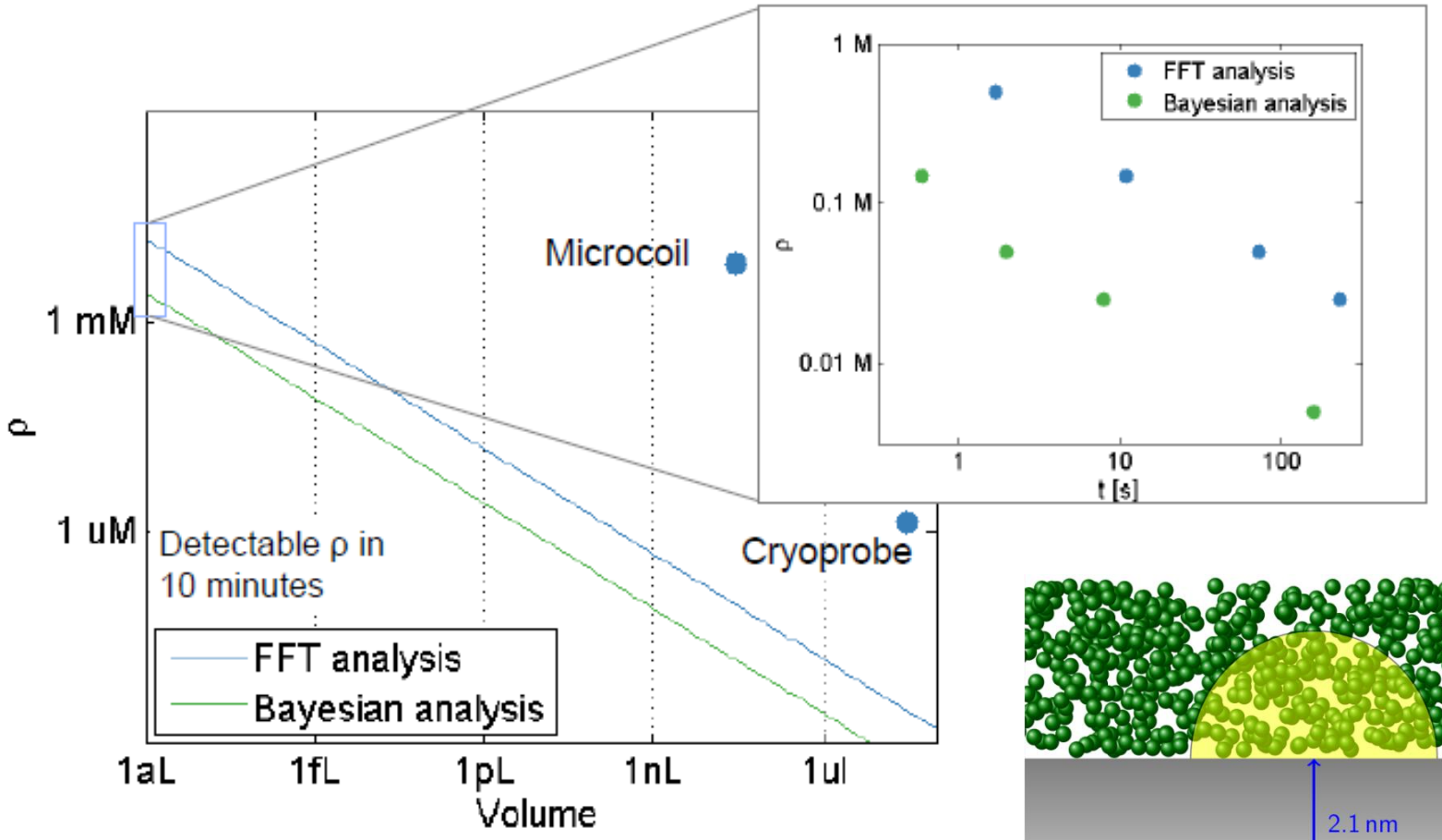
FFT essentially blind to prior knowledge hence prior distribution is flat

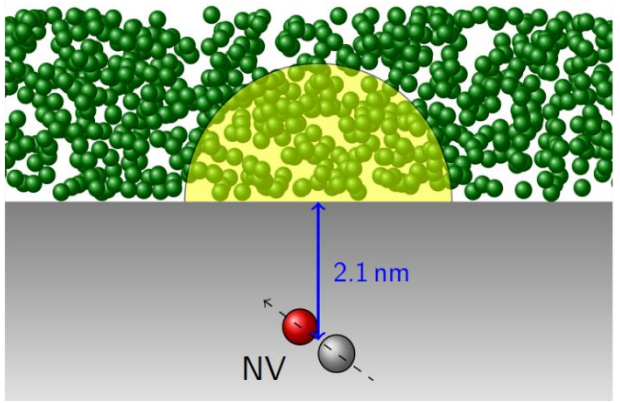
You look for small chemical shifts around known Larmor

- ….

Patent: US 11,181,494

Extracting Signals from Very Noisy Data

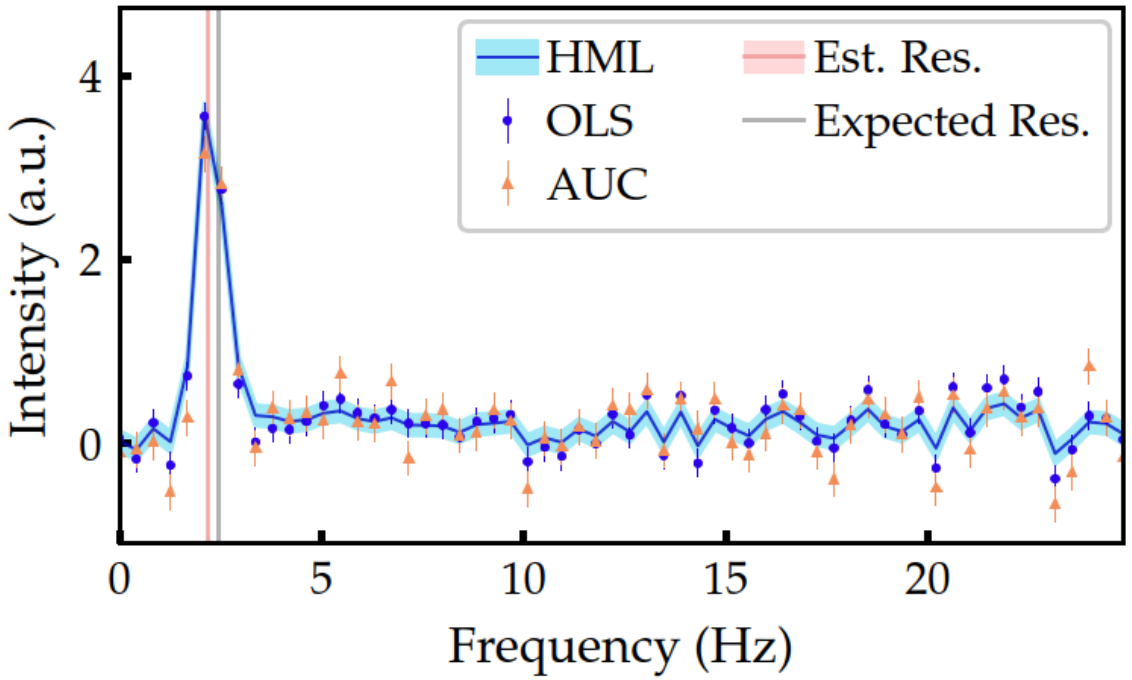


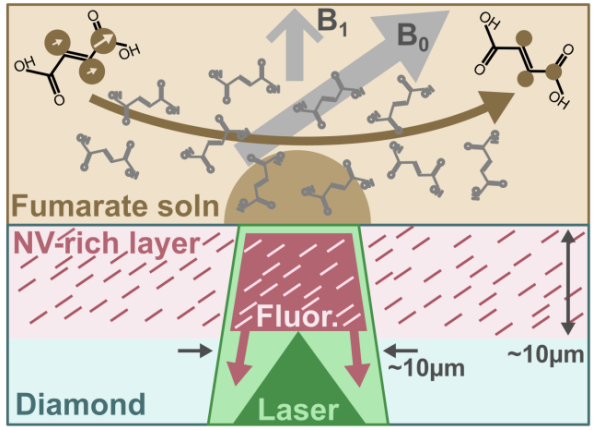


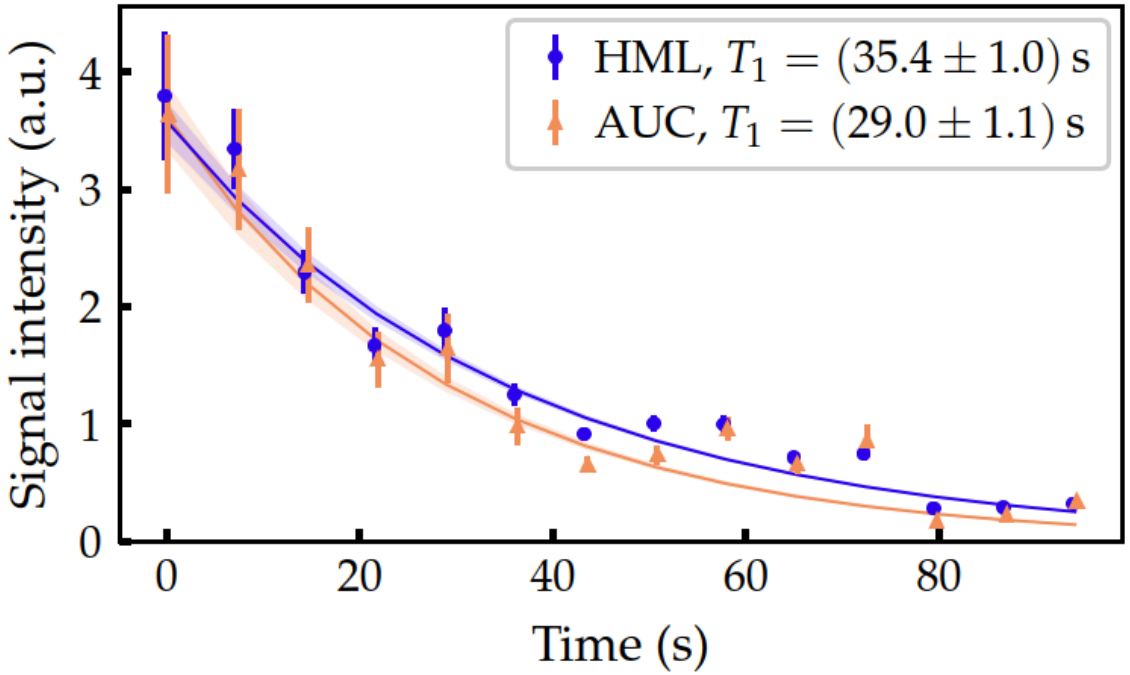
Patent: US 11,181,494

NMR at the Micron- and Nanoscale: J-coupling spectroscopy

The road to Nanoscale NMR



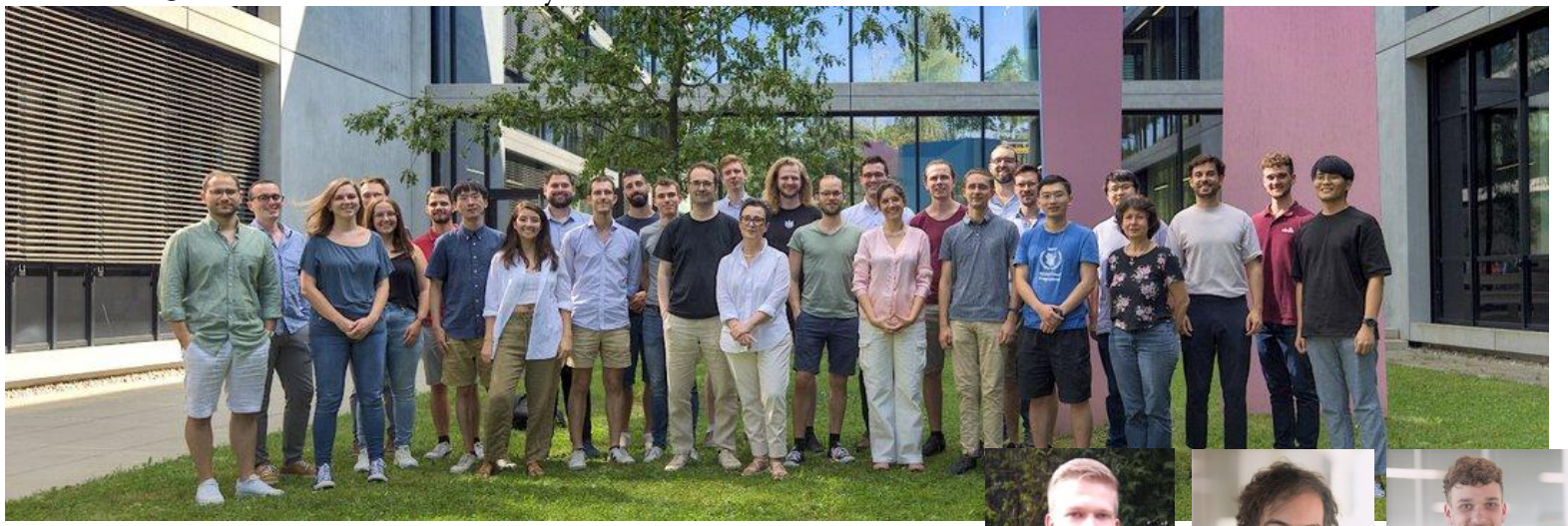




Hierarchical Bayesian analysis yields 2.6-fold SNR enhancement

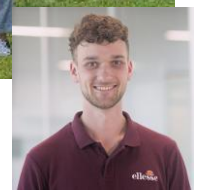
Team & Sponsors

The Team @ Institute of Theoretical Physics



Benedikt Tratzmiller

Martin Korzeczek



Lennart Bosch

The Team @ NVision Imaging Technologies

Ilai Schwartz
Co-founder & CTO

Humboldt Professorship

Henriette-Herz-Scouting Programme

Synergy Grants:
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