β-NMR in liquids

Opening new frontiers for biomolecular studies and nuclear physics

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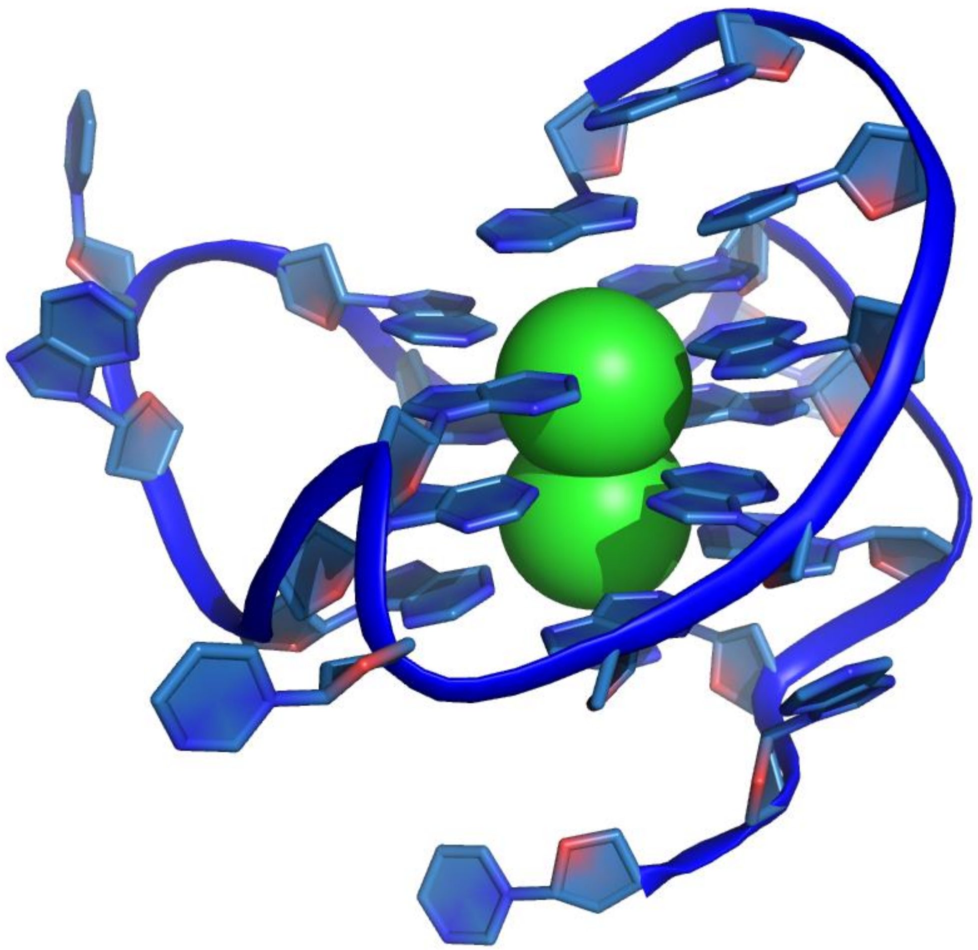
Outline

- β-NMR for biology
- Principles of β-NMR
- Experimental setup
- Measurements & results
- Conclusion and outlook

β-NMR for biology

Advantage over conventional NMR

- 10 billion times more sensitive
- Use probe nuclei with complementary properties
- Real-time observation of chemical reactions

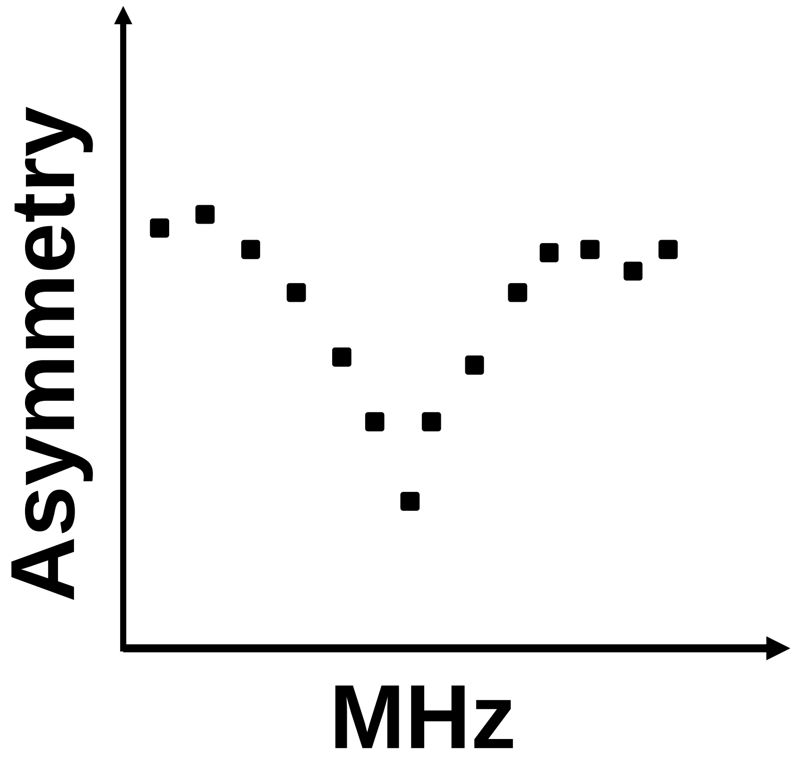


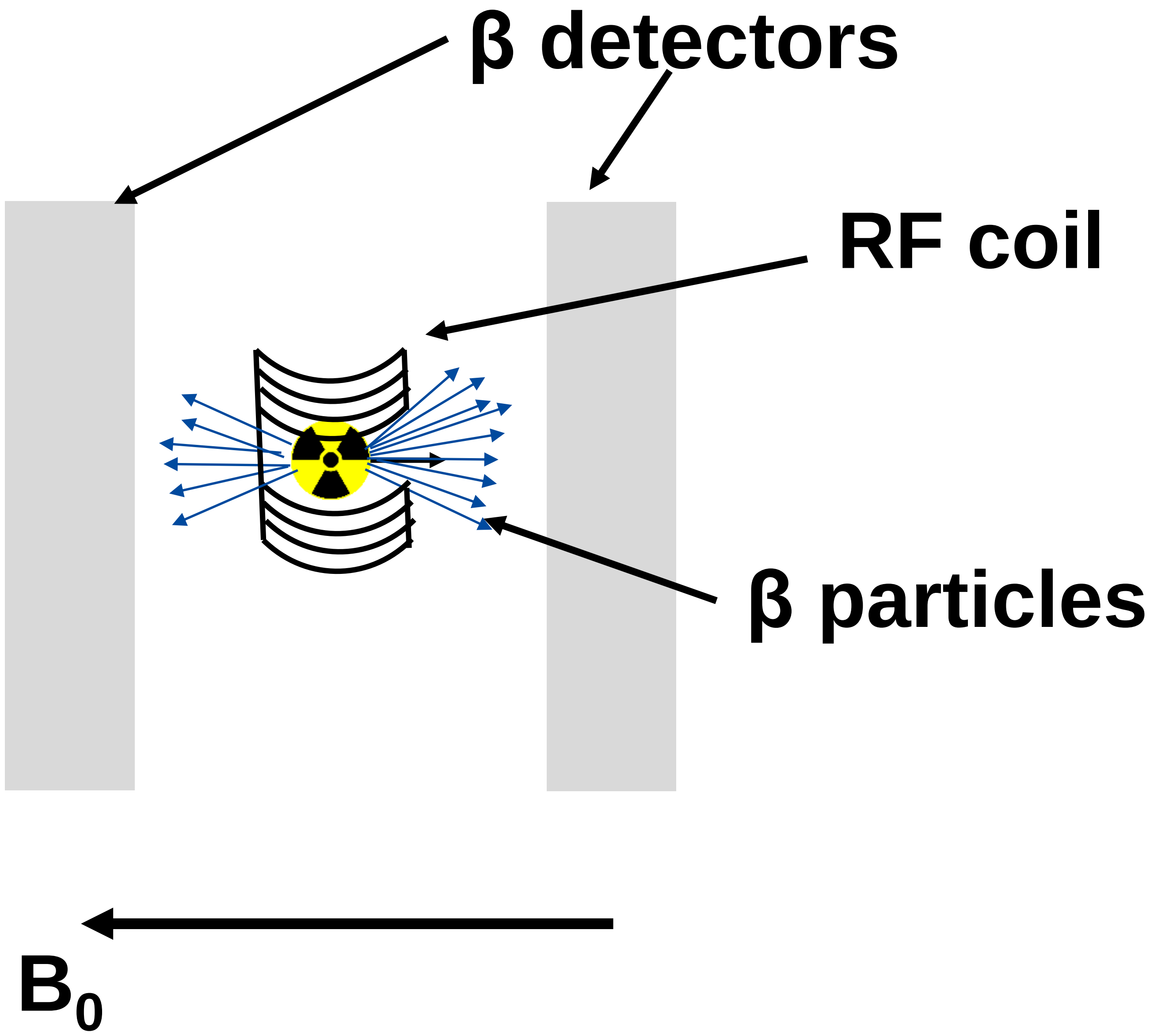
picture courtesy of B. Karg

Principles of β-NMR

β-NMR

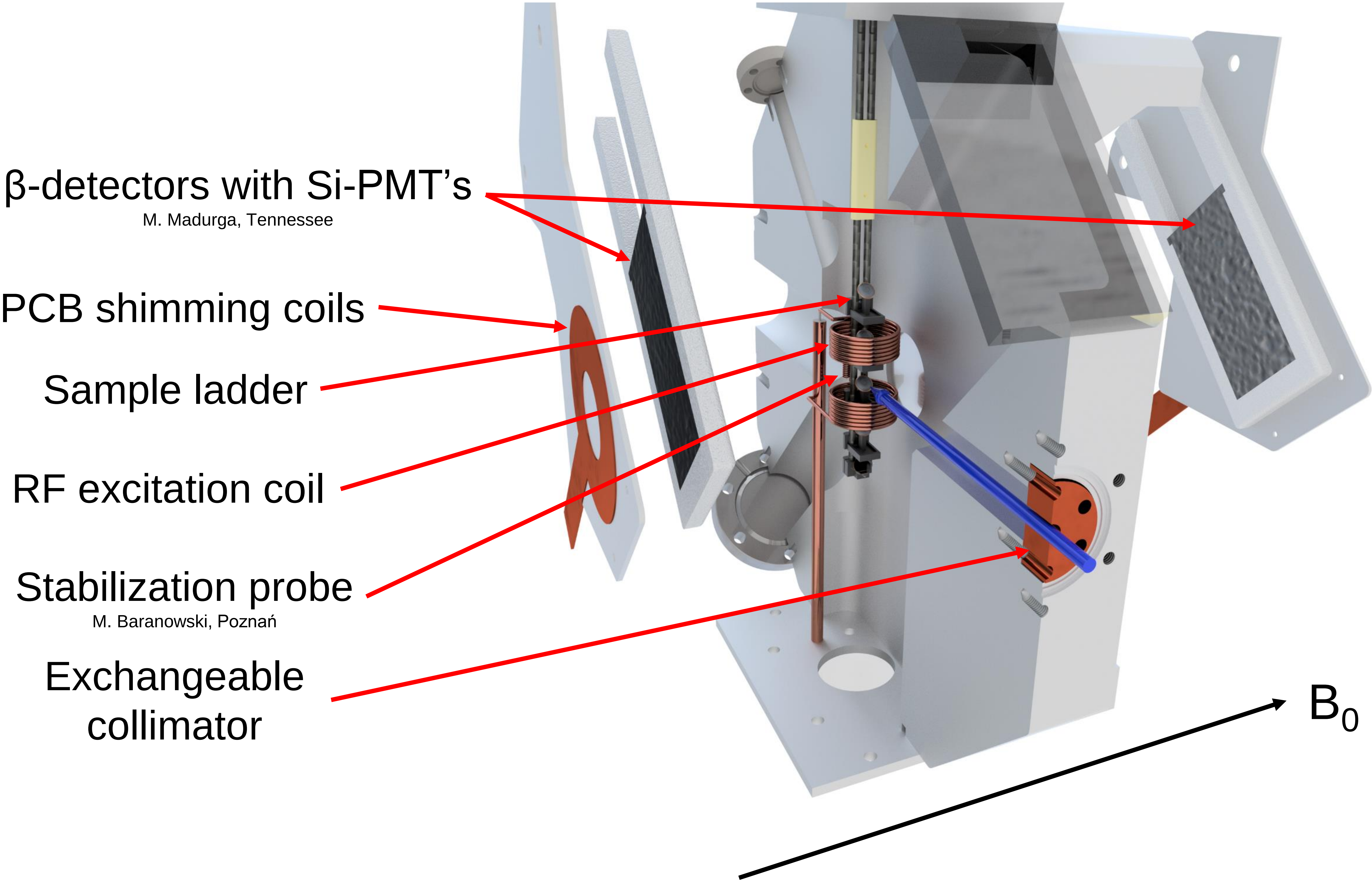
- Asymmetric β-decay from polarized nuclei
- Detection of the resonance by β-decay asymmetry





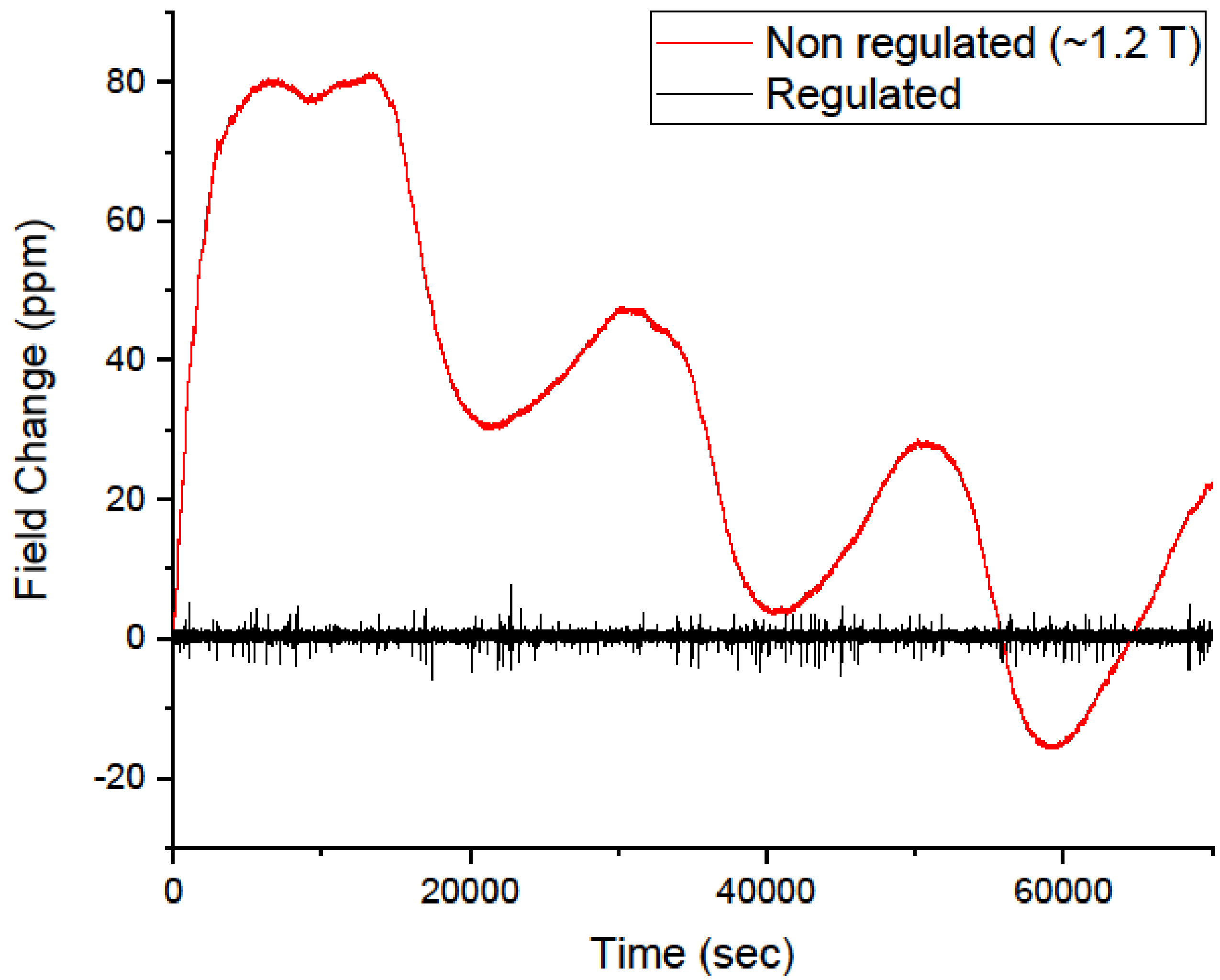
Experimental setup

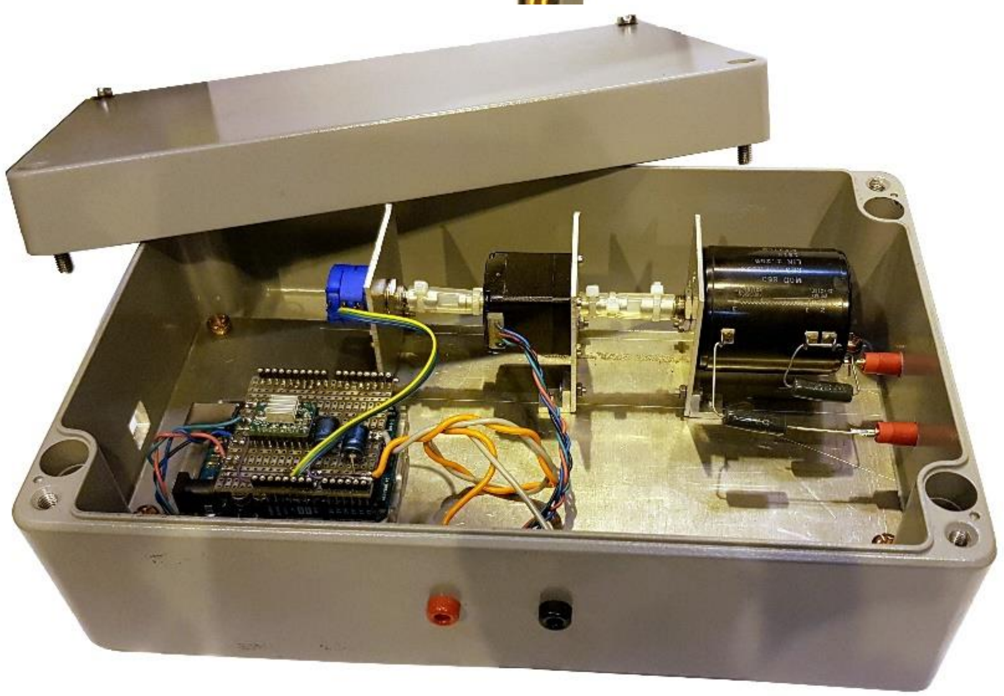
β-detectors & chamber



B_0-field stabilization

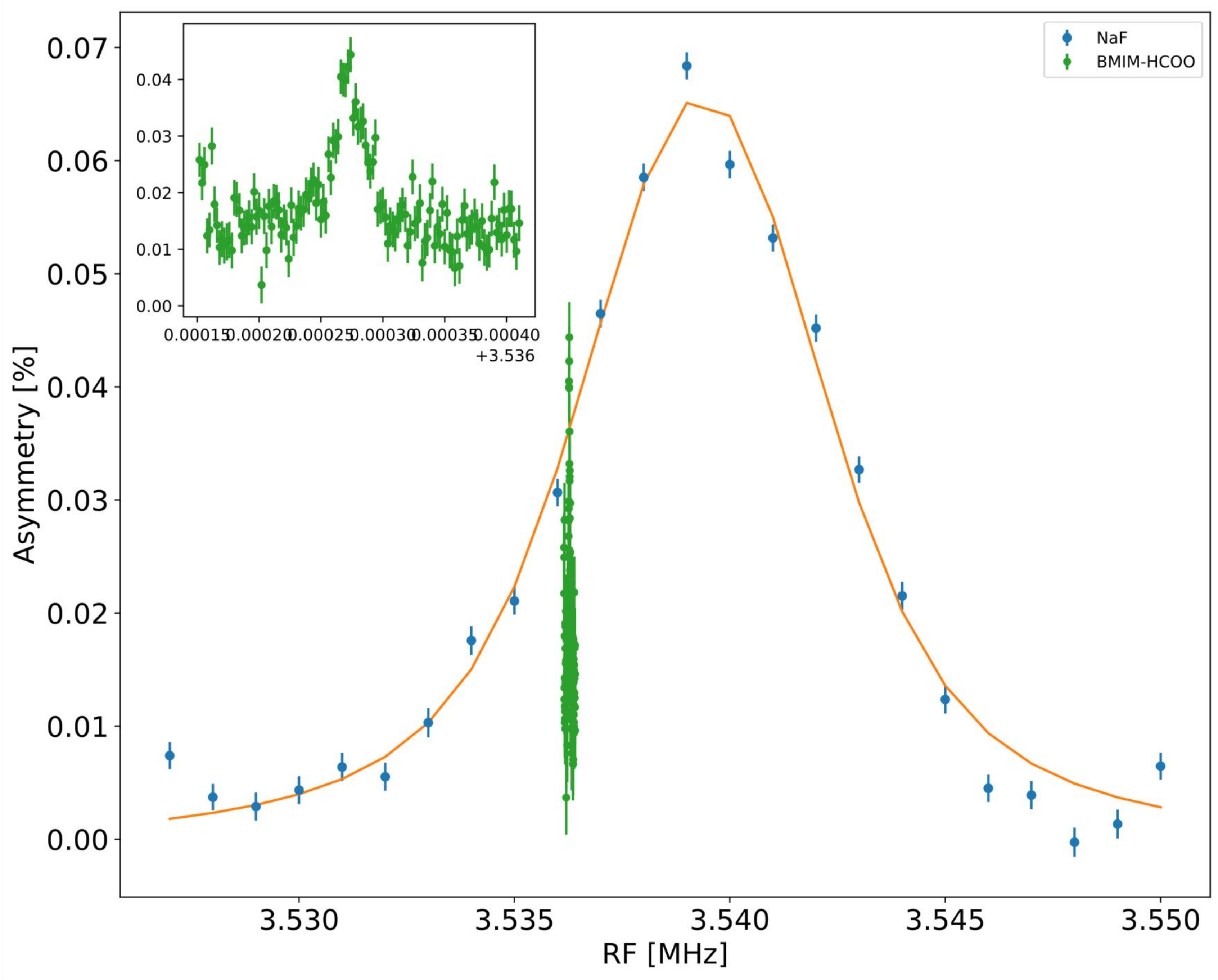
- Compact vacuum-compatible pulsed NMR probe
- PID driven variable resistor
- **From 100 ppm drift to ~1 ppm stability**





NMR in liquids

- Molecular tumbling leads to narrow peaks



Measurements & results

β-NMR reference

- Conventional NMR spectra always relative to a reference
  - (e.g 0.1 M ^{23}NaCl in D_2O)

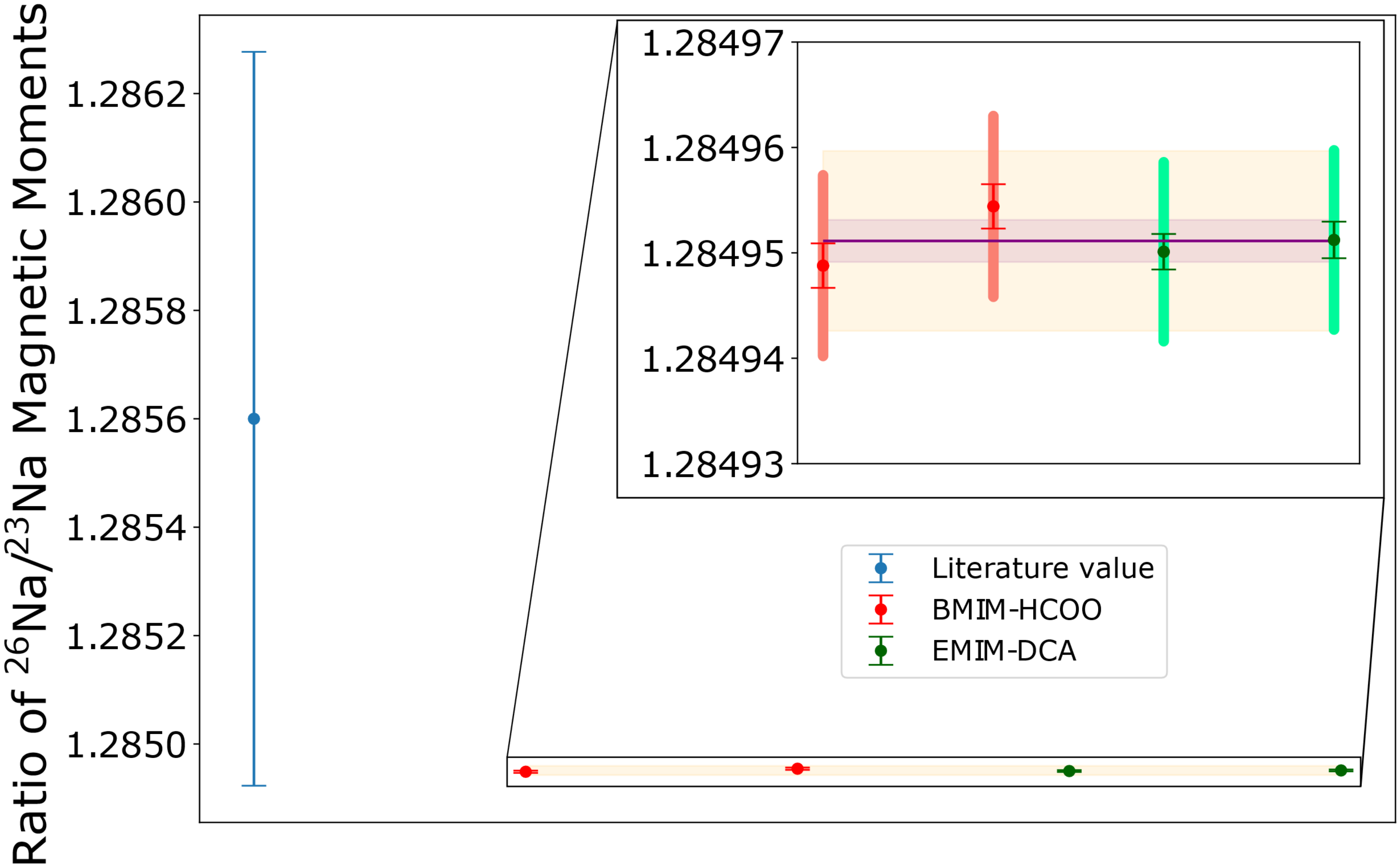
- References needed for β-NMR
  - Indirect use of conventional NMR reference

$$\frac{\nu_{^{26}\mathrm{Na}_{1.2T}}}{\nu_{^{1}\mathrm{H}_{1.2T}}} \sim \frac{\nu_{^{23}\mathrm{Na}_{7,05T}}}{\nu_{^{1}\mathrm{H}_{7.05T}}}$$

  - Use an absolute scale
    - (bare nucleus)

Indirect reference

- ppm precise $^{23}Na/^{26}Na$ magnetic moment ratio



Absolute scale: reference

- Accurate magnetic moments needed
  - Diamagnetic correction not accurate (up to 30% off)

Method	Literature ^{23}Na magnetic moment[1] (μ_n)
ABMR	+2.217522(2)
NMR	+2.2176556(6)

  - A difference of 134 ppm!

- New ab initio NMR shielding calculations save the day!

Method	New ^{23}Na magnetic moment[2] (μ_n)
ABMR	+2.217495(2)
NMR	+2.217500(7)

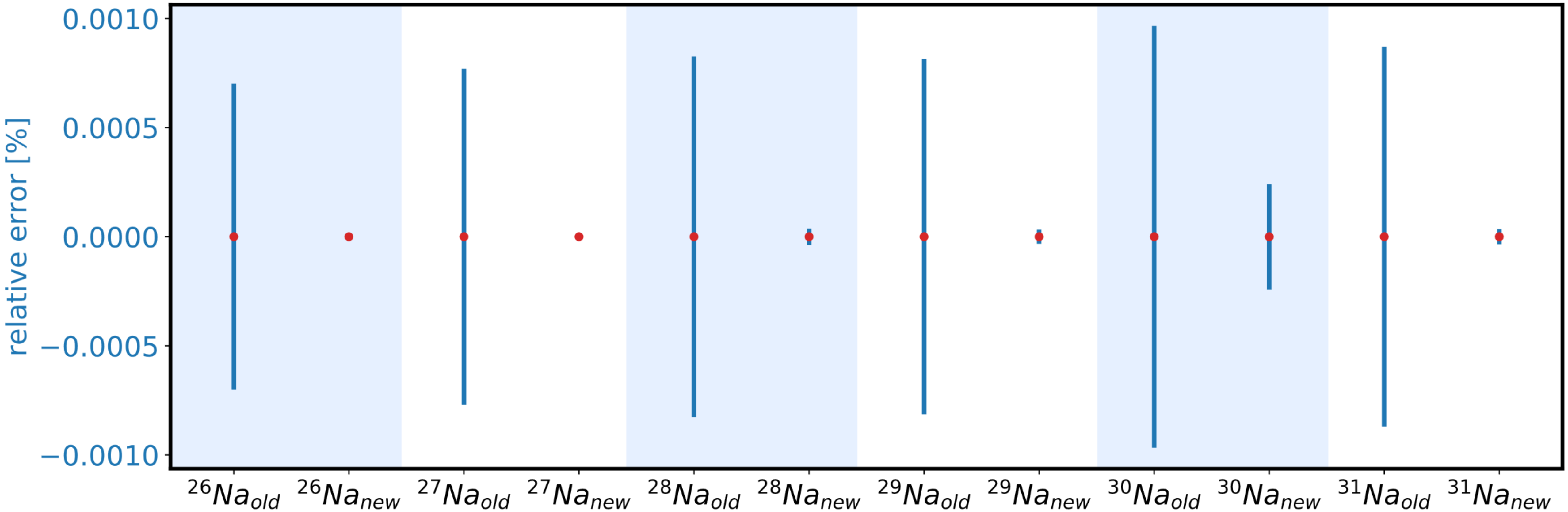
A. Antušek, Bratislava

  - This gives us an accurate reference
    - Combined with ratios leads to accurate moments

[1] N. J. Stone, Atomic Data and Nuclear Data Tables 90, 75 (2005)
[2] R.D. Harding et al. article in preparation

Absolute scale: accurate μ_I

- 100 times increase of precision of the magnetic moment of ^{26}Na
  - 10 times increase for $^{27-31}Na$ (from solid state β-NMR)[1]



ppm precise magnetic moments

- set of beta-NMR isotopes with ppm precise magnetic moments allow for probing different chemical effects

Nuclear properties of $^{23,26-31}$Na relevant for NMR and magnetic moments determined in this work compared to literature values.

Isotope	I	$T_{1/2}$(ms)	$Q(mb)$[1]	old μ_I (μ_N)[1]	new μ_I (μ_N)[2]
^{23}Na	3/2	stable	+105.6(12)	-	2.217500(7)^a
^{26}Na	3	1071	-5.3(2)	2.851(2)	2.849378(20)^b
^{27}Na	5/2	301	-7.2(3)	3.894(3)	3.89211(11)
^{28}Na	1	31	+39.5(12)	2.420(2)	2.41843(9)
^{29}Na	3/2	44	+86(3)	2.457(2)	2.45534(8)
^{30}Na	2	48		2.069(2)	2.0681(5)
^{31}Na	3/2	17		2.298(2)	2.29668(8)

^{a} Corrected $\mu(^{23}$Na) based on NMR experiment

^{b} Based on our improved ratio of the magnetic moments of ^{26}Na to ^{23}Na

- Applicable to:
  - Beta-NMR : Biomolecular studies, Material science & Nuclear Physics
  - Other fields

Summary

- β-NMR up to 10 billion times more sensitive
- Liquid state β-NMR 100 x increased resolution
  - referenced to conventional NMR
  - referenced to an absolute scale.
  - precise magnetic moments
- Interpretation of first biological measurements ongoing. **See poster 18 – Kasia**

Acknowledgements

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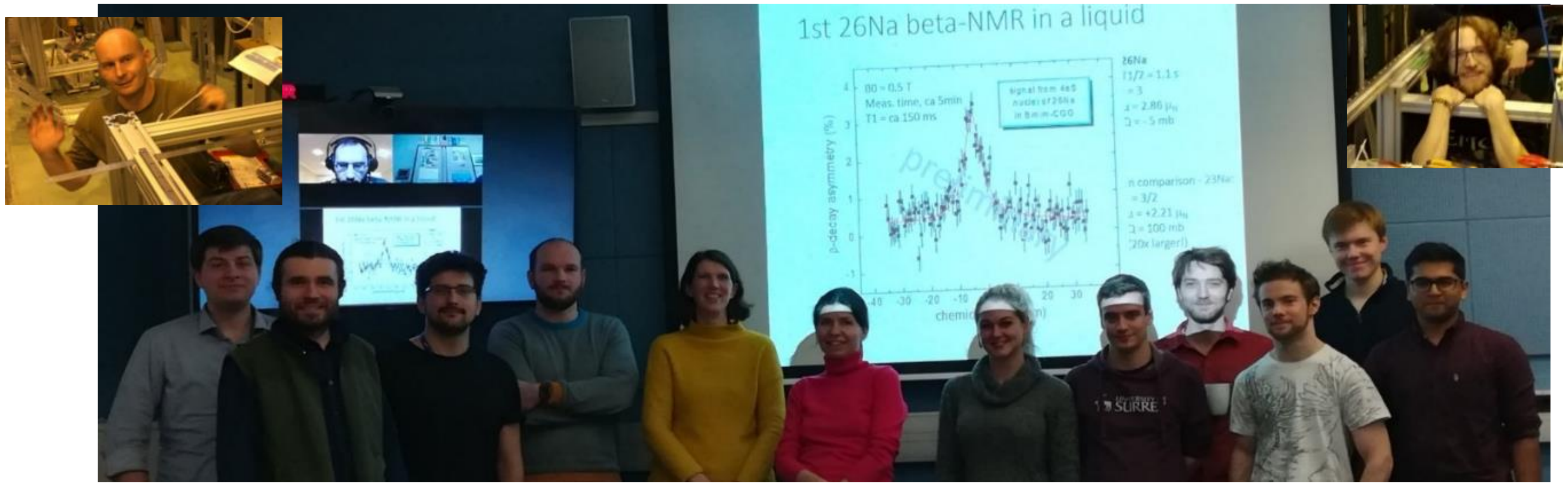
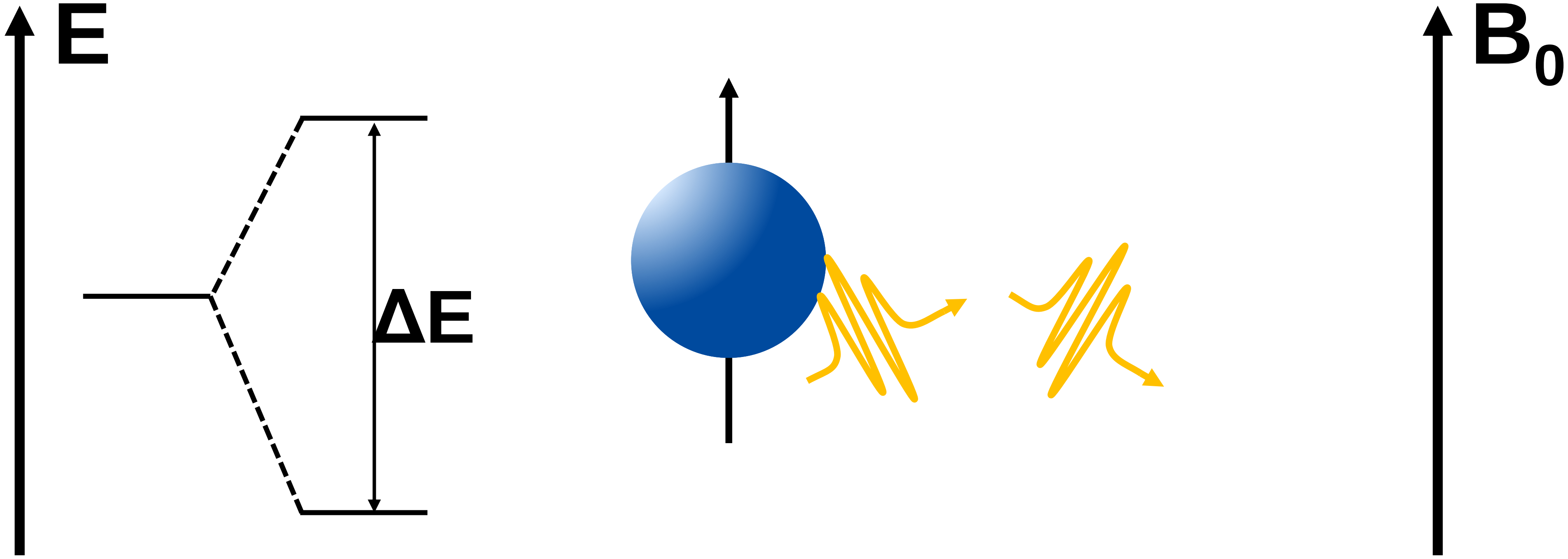


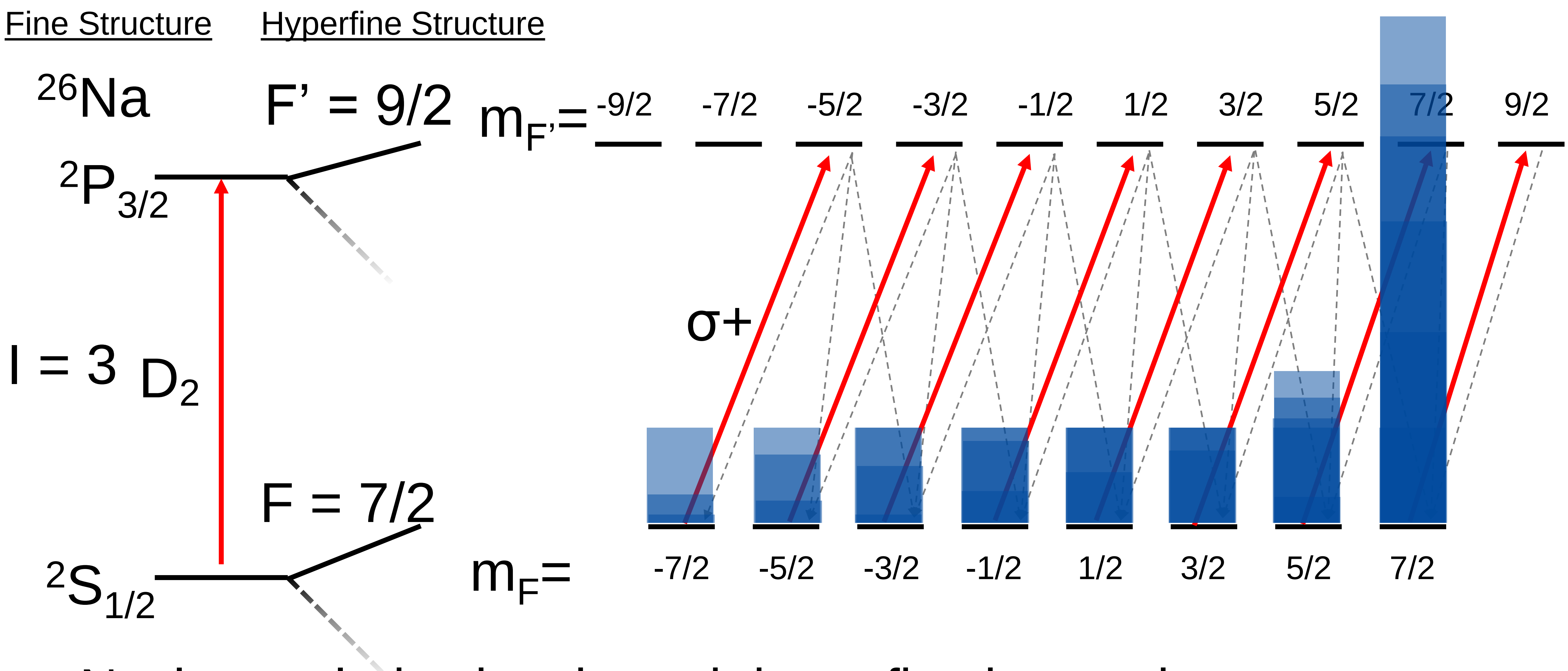
Nuclear Magnetic Resonance

- Nuclear spin ≠ 0
- B0 induces Zeeman effect
- Unequal distribution over magnetic substates (polarization)
- Spins flip due applied RF photons
- Detect emitted RF photon’s



Laser spin polarization

- Polarize atomic spins
- A laser accessible strong atomic transition (strong -> short T1/2)
- Circularly polarized light
- A closed "loop"



- Nuclear polarization through hyperfine interaction

VITO Beamline