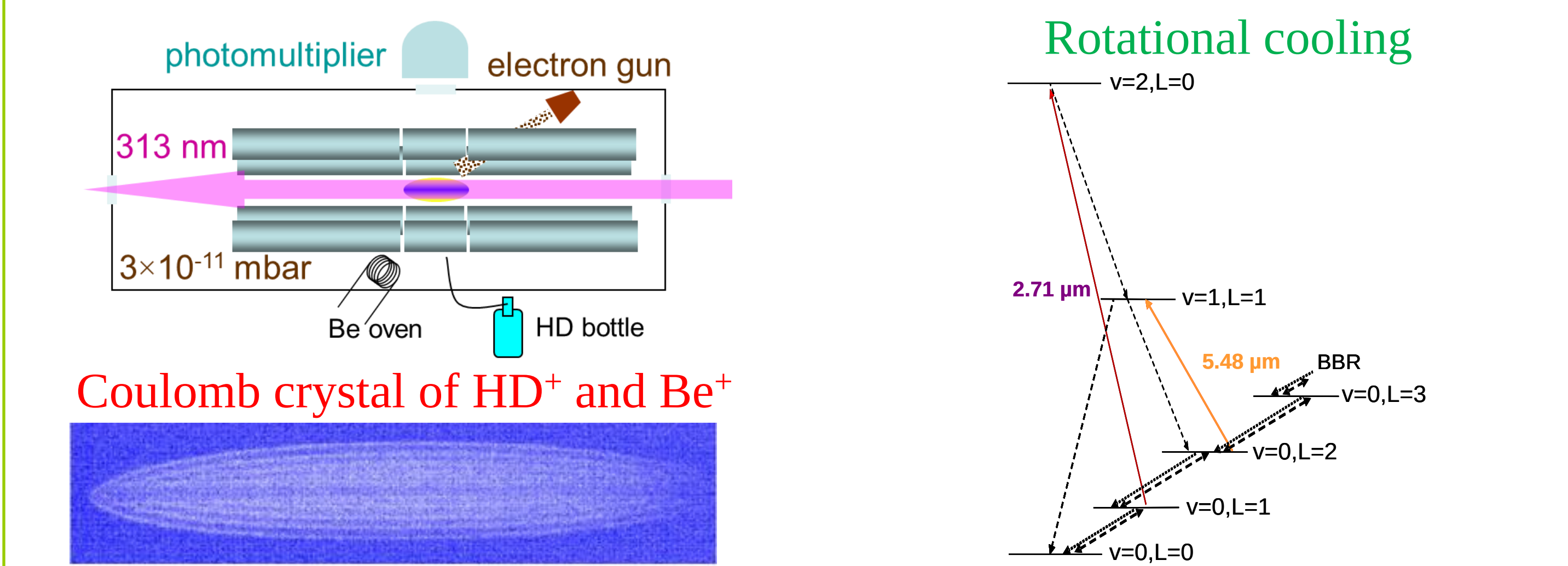


Motivation

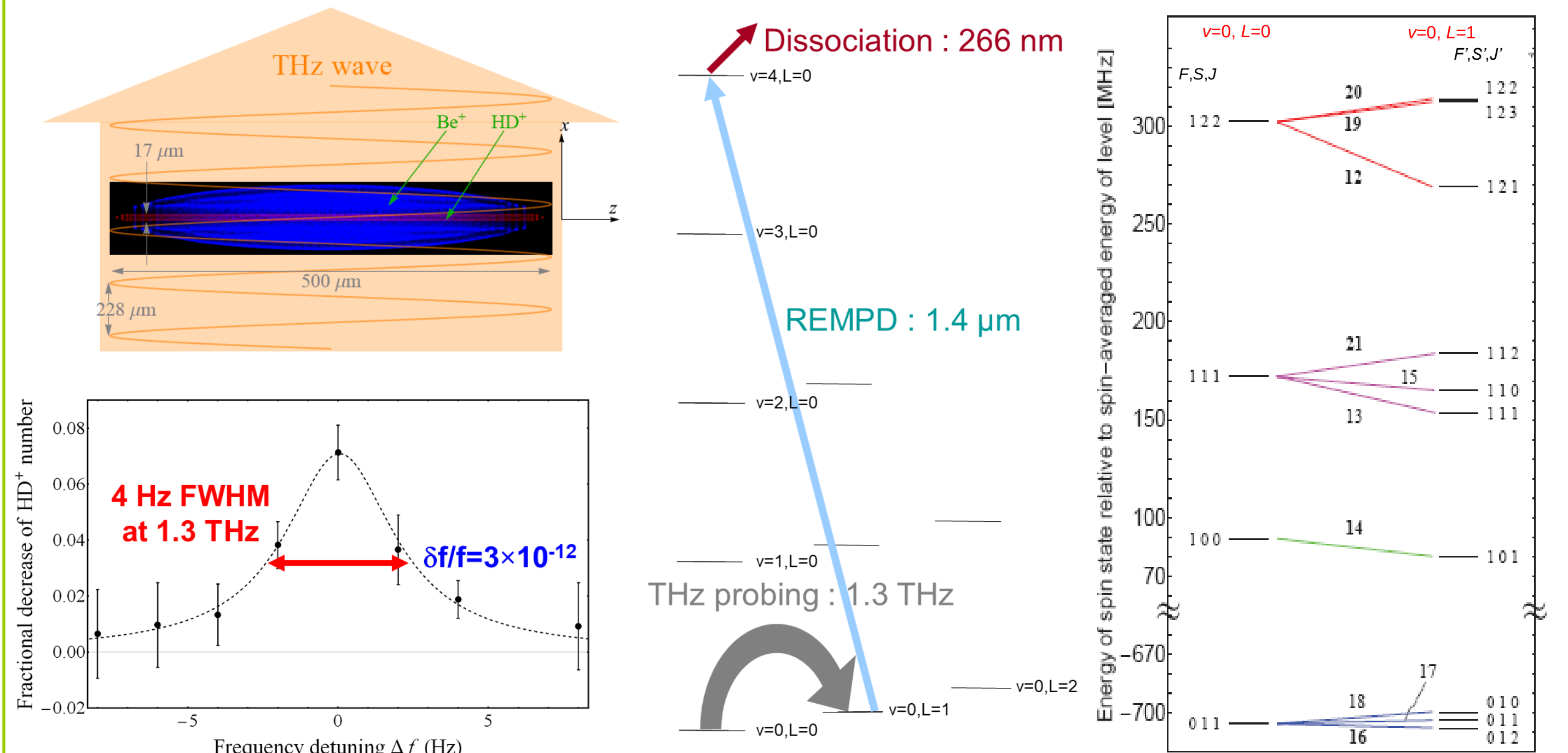
Matching accurate theory and precision measurements performed on single particles or simple quantum systems is exploited by CODATA for determination of fundamental physical constants.

The hydrogen molecular ions, one of the simplest three body quantum systems, are described with accurate molecular theory. They allow high spectroscopic resolution and are ready for quantum state control. Experiment-theory comparisons are exploited to address Rydberg constant, particle masses, proton and deuteron radii, testing quantum electrodynamics and searching effects of New Physics beyond the Standard Model. The physics of the hydrogen molecular ions links one-body physics of particle masses and two-body physics of hydrogen-like atomic systems.

Doppler-free spectroscopy of cold trapped HD⁺ ions



- Spectroscopy in the Lamb-Dicke regime with THz and IR-waves [5-8]



=> record-high resolution in the THz range, improved accuracy

- Two-photon IR spectroscopy of HD⁺ [9]

=> record-high fractional uncertainty

- Extension to spectroscopy of H₂⁺ [10]

=> access to extremely long radiative lifetimes

Determination of fundamental constants

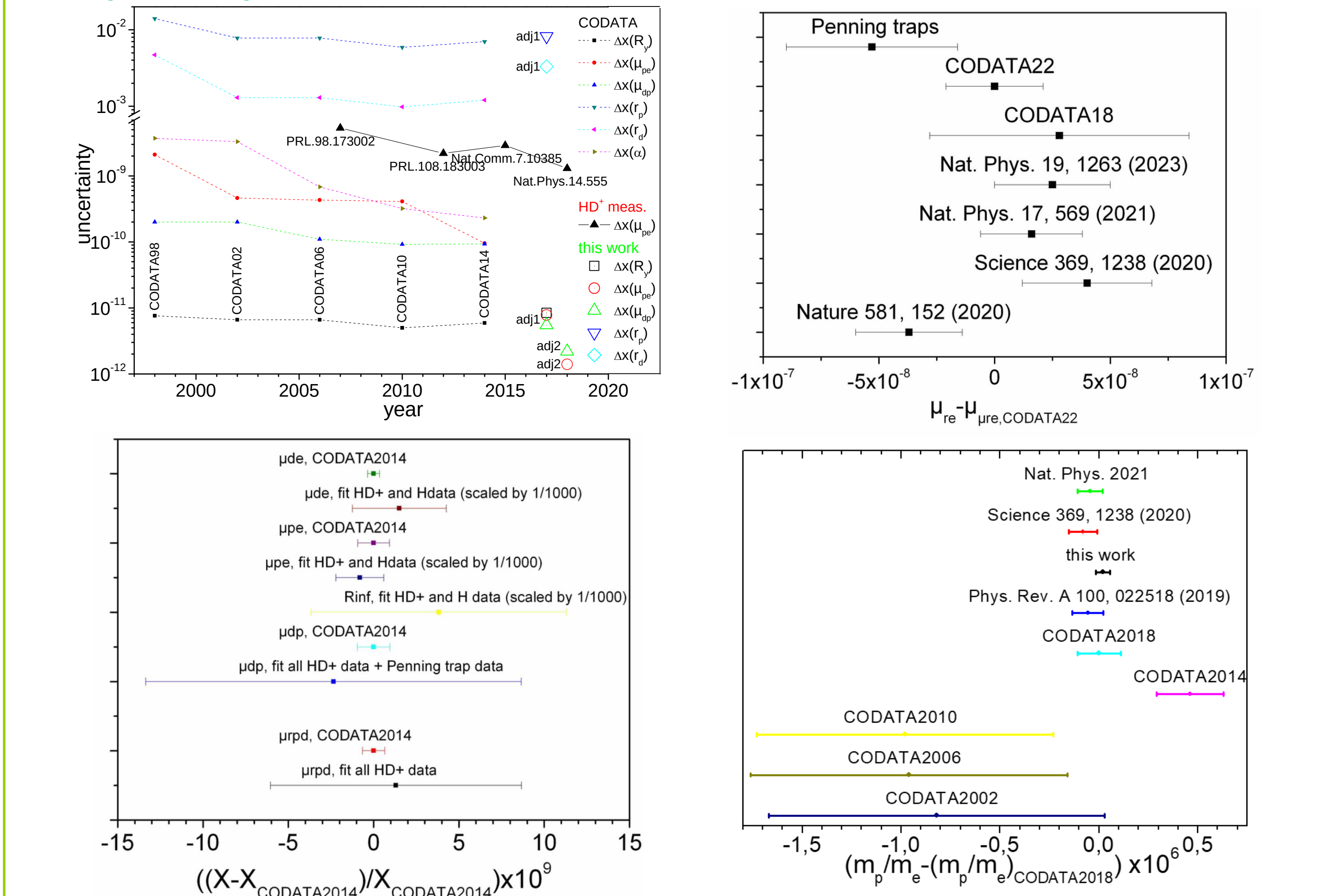
- Comparisons following CODATA approach between :

-experimental frequencies of HD⁺, H₂⁺, H

-QED ab-initio calculations of the energy levels

$$f_{spin-avg}^{(theor)} = f_{spin-avg}^{(exp)} + K_{R_\infty} \cdot (R_\infty - R_{\infty, CODATA}) + K_{m_p} \cdot \left(\frac{m_p}{m_e} - \left(\frac{m_p}{m_e} \right)_{CODATA} \right) + K_{m_d} \cdot \left(\frac{m_d}{m_p} - \left(\frac{m_d}{m_p} \right)_{CODATA} \right) + K_{r_p} \cdot (r_p - r_{p, CODATA}) + K_{r_d} \cdot (r_d - r_{d, CODATA}) + K_\alpha \cdot (\alpha - \alpha_{CODATA})$$

- Adj1 & Adj2 are from [11]



=> Uncertainties better than CODATA

=> New insights in the proton radius puzzle

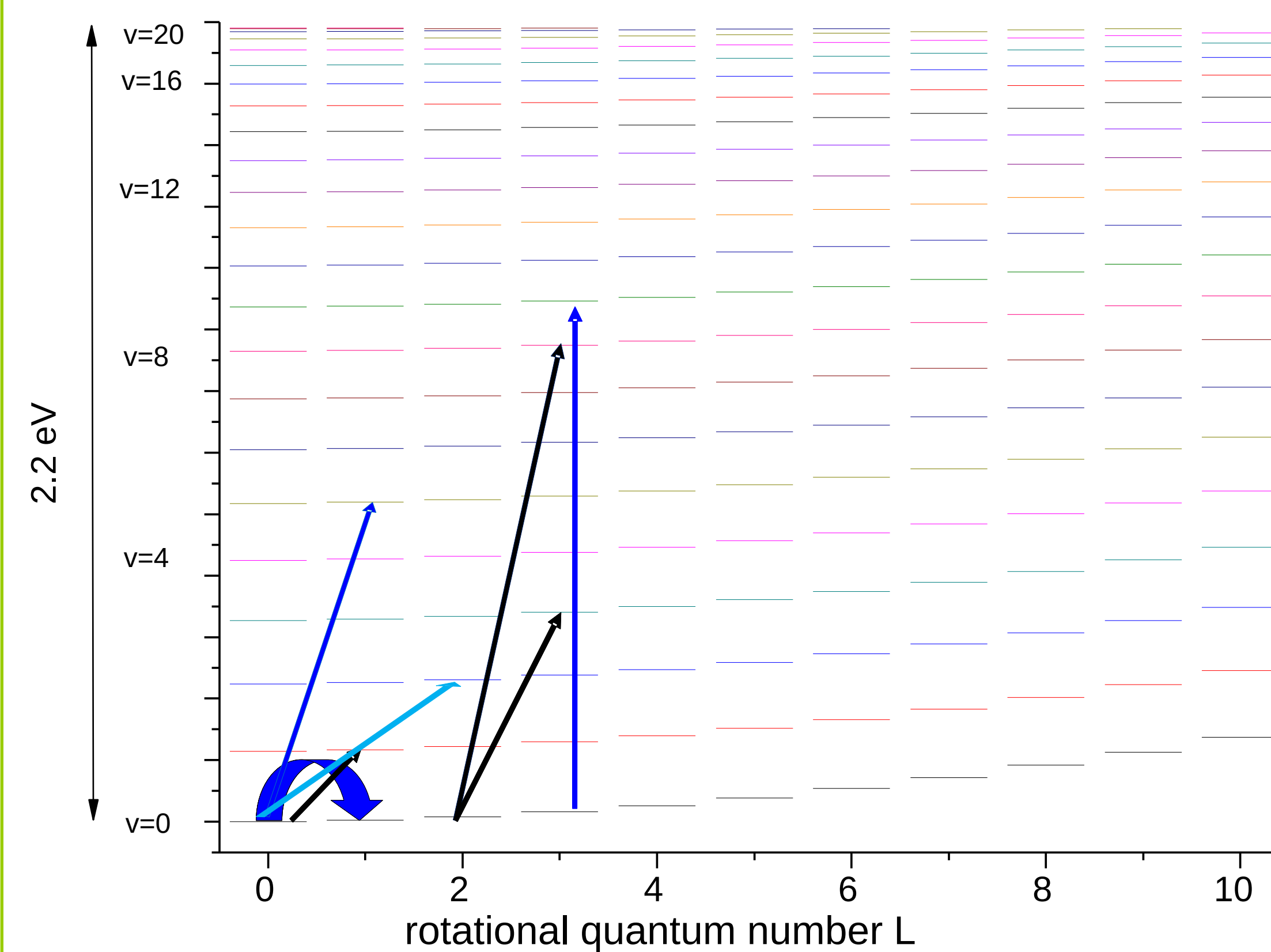
=> particle masses better than Penning trap measurements

=> Confirmation of consistency of two-body QED and three-body QED [12]

Fundamentals on hydrogen deuteride molecular ion theory

- 647 rovibrational energy levels with 10⁴- level E1, 2E1, E2 transitions

- radiative lifetimes at 10 ms level



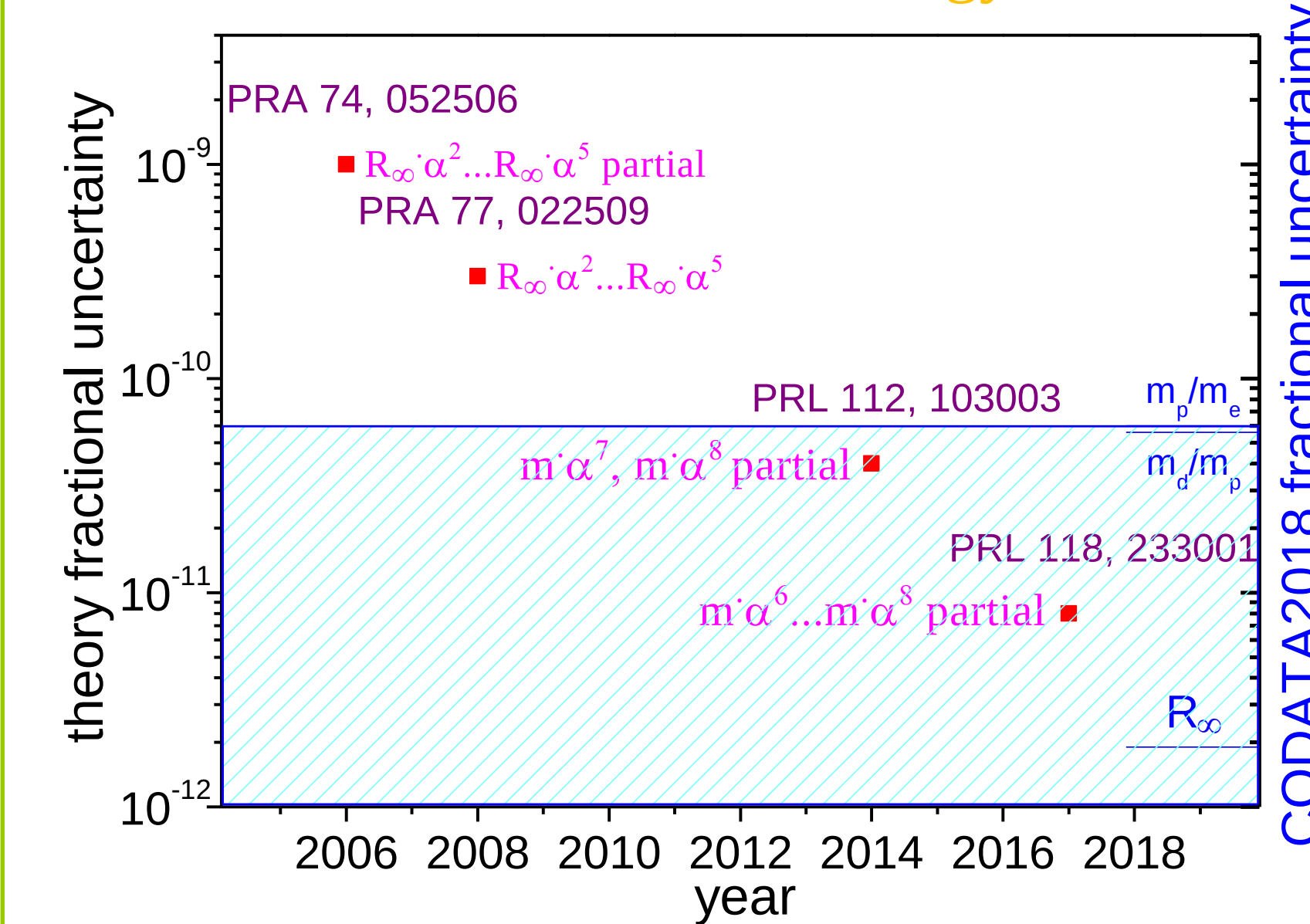
Rotational transitions

$$f_{rot} \approx R_\infty c m_e \left(\frac{1}{m_p} + \frac{1}{m_d} \right)$$

Vibrational transitions

$$f_{vib} \approx R_\infty c \sqrt{m_e} \left(\frac{1}{m_p} + \frac{1}{m_d} \right)$$

Rovibrational energy [1]



Spin structure [2]

$$\vec{F} = \vec{S}_e + \vec{I}_p$$

$$\vec{S} = \vec{F} + \vec{I}_d$$

$$\vec{J} = \vec{S} + \vec{L}$$

NRQED approach [3]: $E = E_{NR} + \alpha^2 (E_{rel} + E_{rel}^{FS}) + \alpha^3 E_{QED}^{(3)} \left(\frac{m_e}{m_p}, \frac{m_e}{m_d} \right) + \alpha^4 E_{QED}^{(4)} \left(\frac{m_e}{m_p}, \frac{m_e}{m_d} \right) + \dots$

+ $E_{spin} + E_{ext fields}$

=> *ab-initio* transition frequencies:

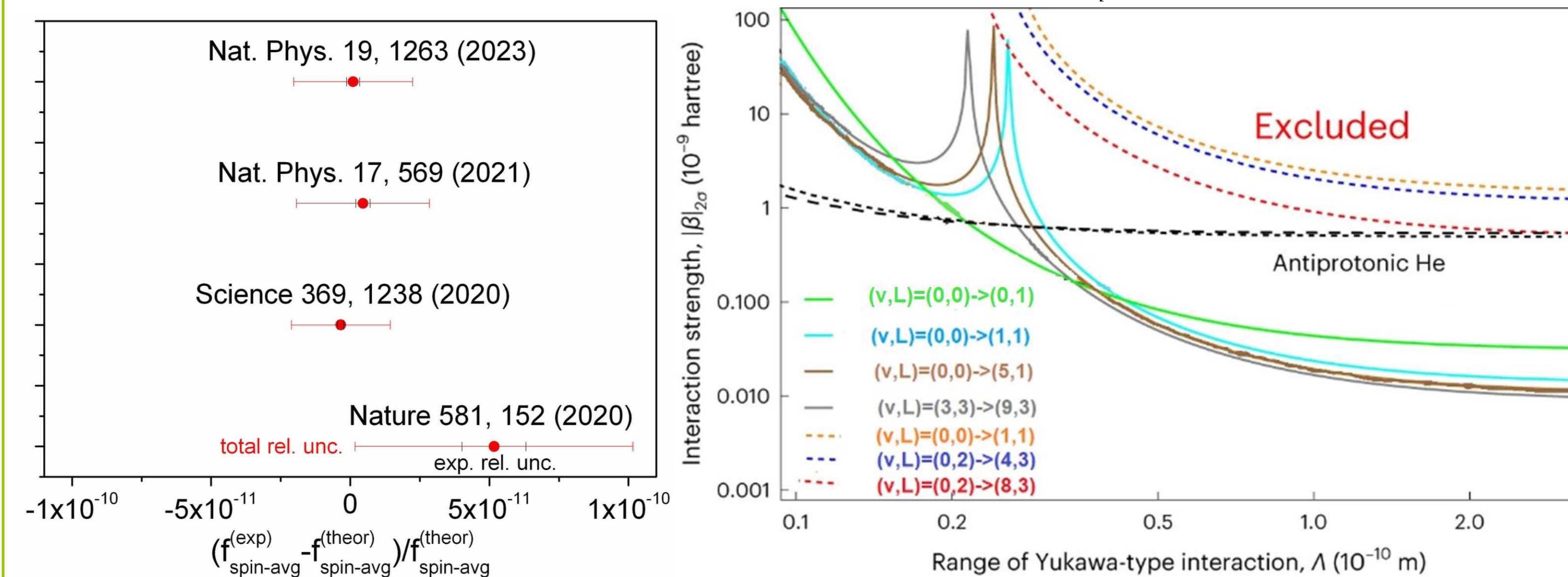
$$\begin{cases} f_{ab-initio,i} = f_{spin-avg}^{(theor)} + f_{spin,i}^{(theor)} \\ f_{spin-avg}^{(theor)} \approx R_\infty c \left[m_e \left(\frac{1}{m_p} + \frac{1}{m_d} \right) \right]^{-K_{\mu re}} \\ \mu_{re} = \frac{m_p m_d}{m_e (m_p + m_d)}; K_{\mu re} = \frac{\partial \ln f_{spin-avg}^{(theor)}}{\partial \ln \mu_{re}} \end{cases}$$

Comparison between theory and experiment

- Spin frequency uncertainty brings major contribution to the *ab-initio* frequency

- Comparison of spin-averaged frequencies $f_{spin-avg}^{(theor)} = f_i^{(exp)} - f_{spin,i}^{(theor)}$

- Error minimization with composite frequency $f_{spin-avg}^{(exp)} = \sum_i b_i (f_i^{(exp)} - f_{spin,i}^{(theor)})$



=> Test the validity of the QED at the order α^6

=> Constraints on effects of new nuclear forces [4]

Acknowledgements



References

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