1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: New quantum technologies for future optical primary SI standards of gas concentration, pressure and temperature

1.1. Project goals

- Development of optical methods for measuring light absorption that will be insensitive to systematic errors related to measurement of light intensity.
- Demonstration of new optical primary standards of gas concentration, pressure and temperature based on quantum properties of matter and its interaction with light.

1.2. Outline

The redefinition of SI units in 2019 was a consequence of the departure from artifacts, man-made metrology standards, which, due to their aging and temporal instability, prevented further improvement of measurement technologies and hampered progress in achieving high-accuracy results. It also initiated the ongoing trend of developing new, basic methods for measuring physical quantities, based on the quantum properties of matter and its invariance over time [1]. Because the interaction of light with matter gives us insight into this quantum world, high-resolution spectroscopy enabling selective measurements of gas components appears as a very promising tool for developing new optical standards for gas concentration, pressure and temperature.

Optical measurements of gas concentration and pressure use the frequencies and intensities of spectral lines. Accurate measurement requires integrating the absorption over the entire shape of the line. In case of non-isolated lines a thorough line shape analysis needs to be performed [2]. Knowing the line strengths from quantum-mechanical calculations consistent with the Standard Model and physical SI constants, one can demonstrate gas concentration and pressure standard with reasonably accurate absorption measurements for a given molecular line [1]. The gas temperature can be determined optically from the molecular Doppler line width [3] or from measuring the relative intensities of rovibrational lines resulting from the Boltzmann distribution of the population of quantum rotational states [4]. Therefore, an optical temperature standard and non-contact measuring systems can be developed based on accurate, high-resolution spectroscopy.

Achieving high accuracy in absorption measurements is, however, a difficult task. This requires a well-linear light intensity detection system, which is difficult to obtain in practice. As a result, although the relative precision of the measured spectral line intensities can be very high (0.001%), its relative accuracy is usually 1% or less [5,6]. The most probable cause is non-linearity in the measurement of light intensity [6]. The presented doctoral project addresses this current problem and focuses on developing new spectroscopic techniques that will be insensitive to the problems of measuring light intensity.

Our team has an extensive experience in developing molecular spectroscopy techniques that are insensitive to systematic errors in light-intensity detection. In our dispersion methods based on the optical cavity, implemented in various speed variants, the spectrum is obtained only by measuring the frequency of the optical cavity modes [6]. This approach enables SI traceability of the spectrum by connecting both its axes to an optical atomic clock using an optical frequency comb. Our methods show the most accurate line intensity uncertainties below the permille level [6], with spectroscopy alone contributing to an overall measurement uncertainty of less than 0.006%. We recently achieved the world's first compliance to sub-permille levels of line intensities measured in NCU and world-class metrology NIST and PTB laboratories and calculated *ab initio* at UCL [7].

New spectroscopy methods developed as part of this doctoral project will have wide applications in various fields of science, industry, and economy. They are particularly important when measuring in low-pressure gaseous media. They will contribute to supporting research on the state of the Earth's atmosphere by providing ultra-accurate reference spectroscopic data, meeting the accuracy requirements of less than 0.1% in satellite remote sensing. They will also enable non-contact measurement of gas temperature, which is currently disturbed by the presence of a temperature sensor.

1.3. Work plan

- Work on improving the accuracy of acquired molecular spectra in cavity-enhanced spectroscopy systems (measuring the transfer function of the light intensity detection system, construction of necessary optical and electrical systems to verify hypotheses, performing numerical calculations and simulations)
- Demonstration of gas concentration and pressure measurement based solely on a comparison of spectroscopically measured and determined from first principles (*ab initio*) spectral line intensity. Demonstration of gas temperature measurement based on the Doppler width of the line and/or measuring the relative intensities of ro-vibration lines. (controlling the measurement procedure, acquiring and analysis of molecular spectra, preparation of the uncertainty budget, comparison of results with the literature data).
- Presentation of results including publications and conference presentations
- PhD thesis preparation

1.4. **Literature** *(max. 7 listed, as a suggestion for a PhD candidate preliminary study)*

[1] K. Jousten, et al., Metrologia 54, S146-S161 (2017).
[2] R. Ciuryło, Phys. Rev. A 58, 1029 (1998).
[3] G.-W. Truong et al., Nature Commun. 6, 8345 (2015).
[4] L. S. Amato, et al., New J. Phys. 21, 113008 (2019).
[5] A. J. Fleisher et al., Phys. Rev. Lett. 123, 043001 (2019).
[6] A. Cygan et al., Science Advances 11, eadp8556 (2025).
[7] K. Bielska, et al., Phys. Rev. Lett. 129, 043002 (2022).

1.5. Required initial knowledge and skills of the PhD candidate

Knowledge of optics, spectroscopy, atomic and molecular physics. Good skills and experience in numerical methods and programming (preferred Labview, Mathematica, Fortran, Python). Mathematical skills in theoretical calculations. Experience in laboratory work is desirable, especially in building and using optical laser-based systems. Independence at work is welcome. High commitment to work and excellent problem-solving skills. Written and verbal communication and presentation skills (including English). Teamwork skills.

1.6. Expected development of the PhD candidate's knowledge and skills

Knowledge, skills, and experience in laboratory work: building electro-optical systems (especially cavity-enhanced spectrometers), techniques of phase and intensity modulation of light, techniques of laser frequency stabilization, experimental techniques of molecular spectroscopy. Good knowledge of molecular spectroscopy, theoretical skills in description of interactions of light with molecules and with optical cavity. Skills in programming and numerical methods. Experience in finding solutions, making hypotheses and formulating final conclusions. Presentation skills, including research papers and conference presentations.