# Precise and accurate spectroscopy of weak molecular transitions supported by ab initio calculations

Spectroscopy is a powerful tool to achieve a deep insight into the microscopic world physics. Precise studies of the internal structure of molecules and of fundamental molecular interactions play an important role in a variety of applications such as monitoring of the Earth's atmosphere to identify sources of pollution and model climate changes, detection of contaminants in semiconductor industry, non-invasive medical diagnostics, detection of trace amounts of explosives, understanding of the origin and evolution of galaxies, or search for extraterrestrial life. From a point of view of basic research the spectroscopy can be used to search of new physics beyond the Standard Model, to assess whether physical constants experience changes over cosmological times, or to validate assumptions about the dynamics of molecular collisions. Many of these applications have demanding requirements for the quality of spectroscopic data. The satellite-based monitoring of greenhouse gases concentration already needs sub-percent accuracy of reference data. In case of molecular hydrogen the validation of comprehensive sets of theoretical line-shape parameters and of the quantum electrodynamics (QED) predictions about the transitions frequencies requires experimental values determined with accuracy at the $10^{-3}$ and $10^{-10}$ levels, respectively. In modelling of exoplanets atmospheres the completeness of global theoretical fits of line-shape parameters (e.g. line intensities) for more complex molecules requires inclusion of – usually very weak – lines having higher transition energies.

In the project we plan to combine both experimental and theoretical efforts in order to address these problems. The targets will be molecular hydrogen and carbon monoxide, i.e. simple systems important in fundamental, environmental, and astrophysical studies.

Within the project a highly accurate and precise measurements of selected near-infrared transitions of these molecules will be performed for the first time. To reach this goal we will develop the state-of-the-art spectrometer to enable a high-resolution molecular line-shape study with the frequency axis referenced to the primary frequency standards. We aim to take advantage of the most recent advances in laser-based spectrometers, which have experienced a tremendous boost with respect to performance metrics such as sensitivity, spectral resolution, and frequency stability. We plan to use high-accuracy cavity-enhanced techniques: cavity ring-down spectroscopy (CRDS), cavity mode-width spectroscopy (CMWS) and cavity mode-dispersion spectroscopy (CMDS). The last technique is based solely on the measurement of the frequency, i.e. the physical quantity currently measured the most accurate, and has the potential to become the most accurate of all spectroscopic methods. The use of these three ultra-sensitive spectroscopic techniques will allow to eliminate the instrumental errors affecting determined line-shape parameters and increase the metrological capabilities of the spectrometer.

The proper data analysis will require a model including a number of physical effects affecting line shapes. Nowadays the spectroscopic databases are switching to the description of the spectral lines going beyond a simple Voigt profile. Recently a new standard profile, which was shown to be able to reproduce molecular spectra in a wide range of pressures with the desired accuracy below 0.1%, was adopted. The line-shape analysis with the use of such sophisticated model will be supported by the calculations based on the first principles of quantum mechanics. We plan to collaborate with the world leading theoretical molecular spectroscopy groups to calculate the line-shape parameters such as the line intensities or collisional widths and shifts.

The project results will allow to compare theory and experiment at a new ultimate level. The determined line positions of molecular hydrogen, one of the most important systems in basic research, will allow the tests of quantum electrodynamics for molecules at an unprecedented level of accuracy. Since the targeted molecular species play a key role in atmospheric, environmental as well as astrophysical studies, the project can have impact on these fields. The list of line-shape parameters generated within the project will be incorporated into the most popular spectroscopic databases thus making the results of the project accessible to a broad scientific community.