LABORATORY FOR LIGHTWAVE METROLOGY

RPTU Rheinland-Pfälzische Technische Universität Kaiserslautern Landau

MSc Thesis at the Laboratory of Lightwave Metrology, Prof. Ioachim Pupeza

Digital Twin of Field-Resolved Mid-Infrared Spectroscopy for Biomedical Diagnostics

Biological gases, such as exhaled breath or the headspace of microorganism cultures, contain a rich set of volatile organic compounds that reflect metabolic and inflammatory processes in real time. Yet, the molecular complexity in such samples render their quantitative, multivariate analysis an ongoing challenge.

Vibrational spectroscopy in the molecular fingerprint region provides specific, quantitative access to biological samples – from exhaled breath to single cells in flow – and holds strong promise for medical diagnostics. Yet, predicting which spectroscopic architecture will deliver the best performance on real samples remains a challenge: such samples usually contain thousands of molecular species with concentrations spanning the range from parts per trillion to thousands of ppm – dominated by a strong water and, for breath, CO_2 background.

At our lab, a small team is developing a digital twin of field-resolved mid-infrared spectroscopy [1,2] and of other promising fingerprint-region technologies, such as Fourier-transform infrared spectroscopy, Fourier-transform coherent anti-Stokes Raman scattering and cavity-enhanced spectroscopy. The twin represents each spectroscopic setup as a circuit of optical and electronic building blocks connected by data streams – such as optical pulse trains, analog and digital electronic signals. This enables physically meaningful modeling of the measurement noise sources, which are decisive for the real-world performance. Combined with quantitative models of complex samples, the twin yields realistic performance predictions for medical applications, which we validate against measurements from our experimental systems – among them field-resolved spectrometers operating at 1-µm and 2-µm gate-pulse wavelengths and a self-built fast-scanning Fourier-transform spectrometer for the overtone region with single- or multi-color delay calibration.

As an MSc student, you will contribute to the twin's codebase: you will implement and refine optical and electronic components, benchmark simulations against measured data, and analyze the performance of spectroscopic architectures for breath analysis. We aim to tailor the thesis – e.g., toward hardware-level modeling, sample modeling, or data analysis – to your interests and strengths. The project offers hands-on experience with the numerical modeling of state-of-the-art spectroscopy, exposure to ultrafast laser experiments, and work at the interface of simulation and experiment in an international research environment.

[1] I. Pupeza et al., “Field-resolved infrared spectroscopy of biological systems,” Nature 577, 52 (2020) [2] C. Hofer et al., “Linear field-resolved spectroscopy approaching ultimate detection sensitivity,” Optics Express 33, 1 (2025)

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