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## Motivation

Quality control of drinking water has been and will be an important technology. Current methods of evaluation of ionic indicators are, for example, ion chromatography and ion selective membranes. However an alternative method which uses NIR light seems promising.

Near-infrared (NIR) spectroscopy can be used to record part of the complex spectral absorption of water.<sup>[1]</sup> Insight on the perturbations of ions on water can be gained by measuring the change in absorbance.

We wish to investigate the possible use of near IR-light to identify and quantify solutions of inorganic salts by near-IR spectroscopy, using optofluidical chips.

## Technological challenge

The changes due to ionic interaction are small and hardly observable by direct comparison of the absorbance spectra (Fig. 1). To observe these effects, absorbance spectra are taken for both water with (sample) and without (reference) certain concentration of an electrolyte. Distinguishable features can be observed for 18 different electrolytes after subtracting the spectra of the solution from reference spectra of demi water (Fig. 2). This could potentially be used for identification of electrolytes. The limit of quantification is roughly 30 mM.

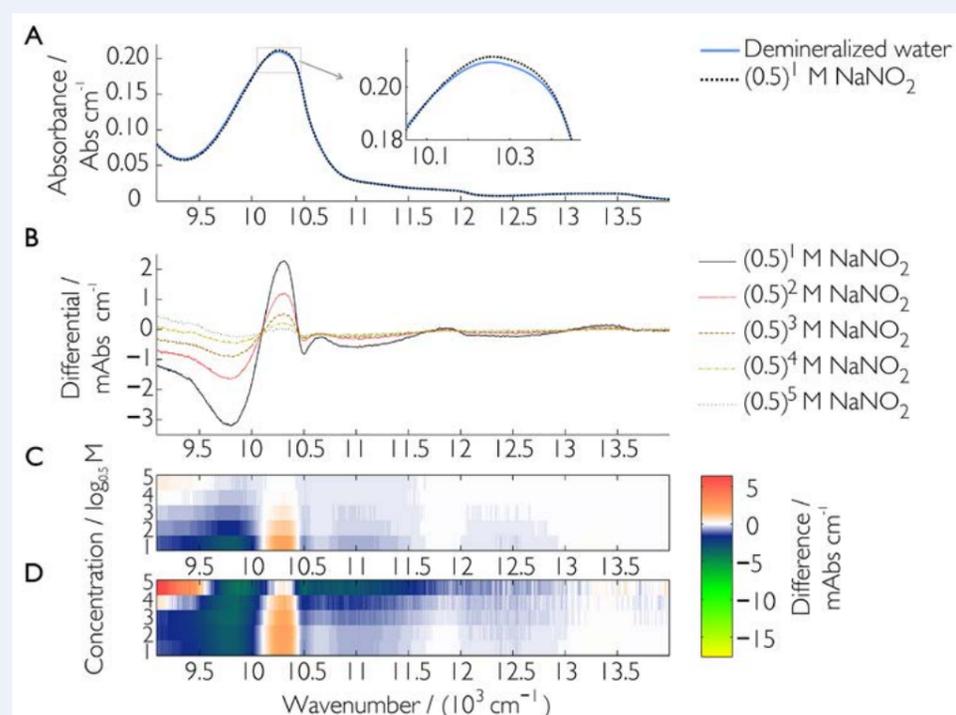


Fig 1. (A) Absorbance spectrum of demineralized water (blue-line) and (0.5)<sup>1</sup> M NaNO<sub>2</sub> dissolved in demineralized water (black-dots). (B) Difference absorbance spectra of demineralized water and aqueous NaNO<sub>2</sub>, showing the effect of the dissolved salt at different concentration. (C) A different representation of the effect of (0.5)<sup>1</sup> M, (0.5)<sup>2</sup> M, (0.5)<sup>3</sup> M, (0.5)<sup>4</sup> M and (0.5)<sup>5</sup> M dissolved salt: Five 2D plots are stacked on top of each other with color coded absorbance difference. (D) Multiplication of the difference absorbance spectra shown in (C) with the dilution factor of the electrolyte shows a deviation from the expected Beer-Lambert law, concentrations given in powers of (0.5).<sup>[2]</sup>

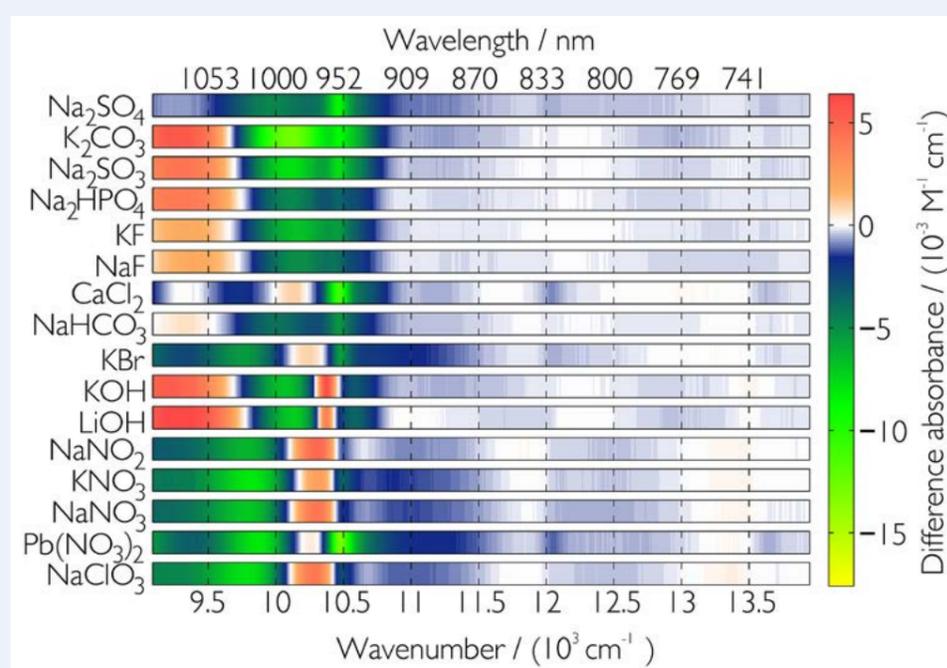
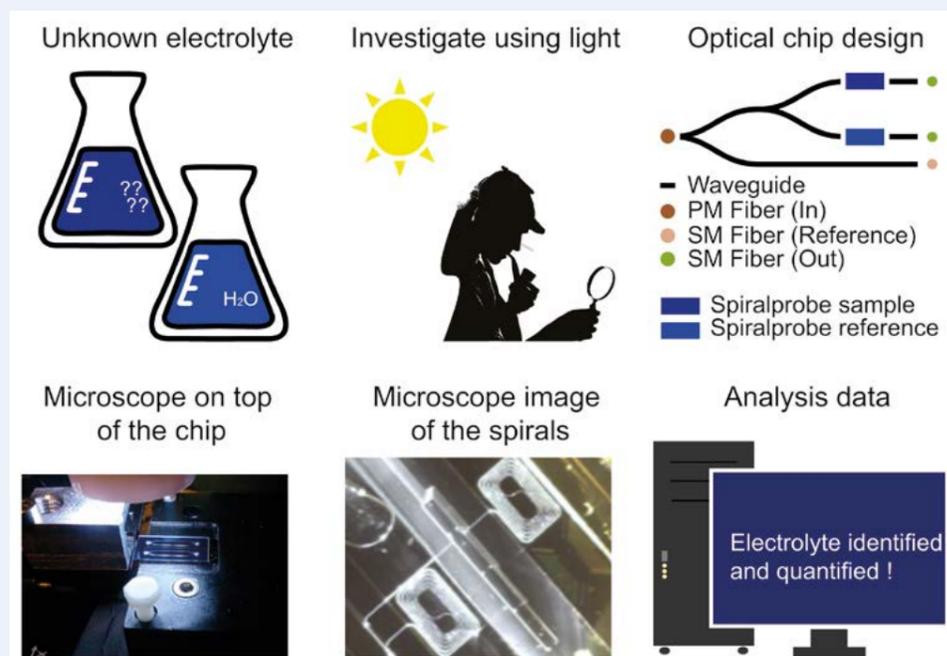


Fig 2. Stacked 2D plots of the differential absorbance spectra per Mol electrolyte using the FWLR Beer-Lambert method.<sup>[2]</sup>

The technology has to be integrated into high-tech but low-cost optofluidic chips which will enable direct and fast concentration measurement of relevant ions in drinking water.

## Research goals

- To investigate the influence of temperature
- To understand underlying physics of the differential absorbance spectra due to different ions.
- To design and characterize the optofluidical chip

[1] J. Lin et al., *Applied Spectroscopy*, vol. 50, no. 4, pp. 444–448, 1996.

[2] G. Steen, E. C. Fuchs, A. D. Wexler, H.L. Offerhaus. "Identification and quantification of 16 inorganic ions in water by Gaussian fitting of Near-Infrared (10754 – 9618 cm<sup>-1</sup>) difference absorbance spectra". *Applied Optics*. 2015. 5937-5942.