PROCEEDINGS OF SPIE

SPIEDigitalLibrary.org/conference-proceedings-of-spie

Optical tastebuds for water quality testing

Justin Sperling, Laurie Savage, Liam Wilson, Calum Cuthill, Katie McGuire, et al.

Justin R. Sperling, Laurie Savage, Liam T. Wilson, Calum Cuthill, Katie McGuire, Jill Robbie, William D. Sloan, Caroline Gauchotte-Lindsay, William J. Peveler, Alasdair W. Clark, "Optical tastebuds for water quality testing," Proc. SPIE 12372, Optical Fibers and Sensors for Medical Diagnostics, Treatment and Environmental Applications XXIII, 123720M (6 March 2023); doi: 10.1117/12.2647396

SPIE.

Event: SPIE BiOS, 2023, San Francisco, California, United States

Optical tastebuds for water quality testing

Justin R. Sperling*[, a], Laurie Savage[a], Liam T. Wilson[b], Calum Cuthill[a], Katie McGuire[b], Jill Robbie[c], William Sloan[a], Caroline Gauchotte-Lindsay[a], William J. Peveler[b], Alasdair W. Clark[+, a]
[a] James Watt School of Engineering, University of Glasgow, Glasgow, United Kingdom
[b] School of Chemistry, University of Glasgow, Glasgow, United Kingdom
[c] School of Law, University of Glasgow, Glasgow, United Kingdom

ABSTRACT

To achieve the UN Sustainable Development Goal of universal access to clean water and sanitation, we need to rethink centralized water systems with global net-zero carbon and sustainability in mind. One approach is to develop scalable off-grid systems that are reliable and easy to use and maintain. A major challenge for such systems is translating the standard laboratory-based monitoring of centralized systems to a more sustainable and scalable model for regularly and routinely monitoring system outputs, which consist of complex mixtures with varying concentrations of molecules and ions in water. Here, we demonstrate a preliminary sensor that, once fully developed, could allow for point-of-use measurements with a single output to monitor. Rather than developing multiple sensors to monitor the levels of each individual component in the water, our label-free, array-based design mimics the biological system of taste. The sensor is comprised of an array of nano-tastebuds made of tailored plasmonic metasurfaces. The combination of different signals from each nano-tastebud to the same sample yields a unique fingerprint for that sample. Through training, these fingerprints build an identification model. By integrating a fully developed sensor into decentralized water systems, we seek to provide non-expert end-users with an easy-to-read output capable of warning of imminent system failures.

Keywords: plasmonics, water, environment, sensor, nanophotonics, array-based sensing, cross-reactive sensing, metasurface

1. INTRODUCTION

According to the UN Sustainable Development Goals Report 2022, eight out of ten people who lack basic drinking water services live in rural areas[1], where providing access to centralized systems is either too costly or not existent. While research is being done to come up with alternative solutions to this problem[2], most feasible solutions would be unable to implement the same monitoring methods for the health of the water treatment system as is done for centralized systems. Centralized systems in Scotland, for example, use regular and routine sampling and laboratory analysis to monitor system outputs[3], which consist of complex mixtures with varying concentrations of molecules and ions in water. Finding alternative methods to this standard monitoring practice is essential to ensure any new technological advances in the water sector are scalable and sustainable.

Here, we demonstrate a preliminary sensor that allows for point-of-use measurements with a single output to monitor. Rather than developing multiple sensors to monitor each individual component of interest in the water, our label-free, array-based design uses combinatorial sensing[4-6]—a sensing mechanism that mimics the biological system of taste. The sensor consists of an array of tailored plasmonic metasurfaces that serve as nano-'tastebuds.' When exposed to a sample, the metasurface of each nano-tastebud acts in a partially selective way by only allowing certain components of the mixture to come within the local environment, and thus plasmonic sensing region, of the nanostructures of that particular element (see Figure 1). Since nanostructures are highly sensitive to changes in their local environment[7], this elicits a resonance shift that can be linked to that local environment change. The signal combination from all the nano-tastebuds yields a unique fingerprint for that sample that, through training using statistical analysis techniques like principal component analysis (PCA)[8] and linear discriminant analysis (LDA)[9], can be used to build an identification model[4,10,11].

* justin.sperling@glasgow.ac.uk
+ alasdair.clark@glasgow.ac.uk

Optical Fibers and Sensors for Medical Diagnostics, Treatment and Environmental Applications XXIII,
edited by Israel Gannot, Katy Roodenko, Proc. of SPIE Vol. 12372,
123720M · © 2023 SPIE · 1605-7422 · doi: 10.1117/12.2647396

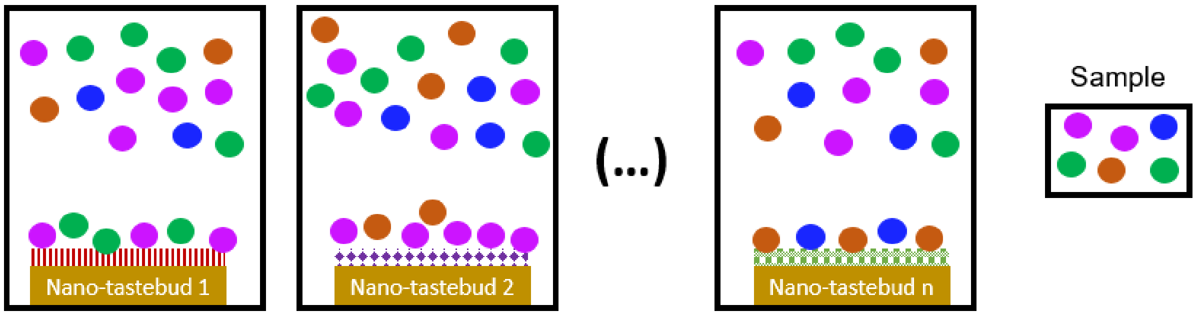

Figure 1. Rendered drawing of nano-'tastebuds'. Each nano-tastebud has a unique plasmonic metasurface that serves as a means of partial selectivity for the components in the sample (a complex mixture). The signal from each nano-tastebud creates a unique fingerprint that can be used to build an identification model.

2. METHODS

2.1 Sensor fabrication

Devices were fabricated on borosilicate glass using a standard electron-beam lithography (Raith EBPG 5200) patterning into a poly(methyl methacrylate) (PMMA) bilayer followed by titanium/gold metal evaporation (Plassys MEB 550S) and PMMA/metal lift-off. The nanopatterned surfaces were then chemically modified with self-assembled monolayers of functional thiol molecules to create an array of cross-reactive elements.

2.2 Transmission spectroscopy

Devices were submerged in a sample of interest. A custom-built microspectrophotometer was used to measure five transmission spectra across each element of the device (0.5 nm resolution). Light from a visible to near-infrared light source (broadband LED with 10dB wavelength range from 470 nm to 850 nm,) was used to probe the sensor. A 10x objective was used to couple the transmitted light into an optical-fiber attached to a StellarNet Microspectrophotometer (StellarNet Blue Wave). Transmission minima (peaks) were calculated using the second derivative of a high order polynomial fit of the data.

2.3 Sample collection

Influent (2), effluent (2), and tap (3) water samples from various water treatment sites and randomly selected consumer taps across Scotland were provided by Scottish Water. Samples were frozen upon collection. Prior to experimentation, samples were defrosted and filtered using a 0.45 µm filter.

2.4 Statistical classification methods

Principal component analysis (PCA) and linear discriminant analysis (LDA) of the shift of transmission minima from deionized (DI) water were used as classification strategy techniques using Systat 13 software.

3. RESULTS AND DISCUSSION

A sensor comprising 8 tailored plasmonic metasurfaces was used to measure DI water and seven samples from various water treatment sites and randomly selected consumer taps across Scotland. Figure 2 shows the PCA scatterplot of the first two principal components of these samples (that explain 51.6% of the total variance). The PCA analysis was calculated by finding the transmission spectra minima for each nano-tastebud and subtracting it from the averaged transmission spectra minima value of that same nano-tastebud for DI Water. As can be seen by the PCA, DI water (black), tap waters (TAP, 3 samples, shades of green), effluent waters (EFF, 2 samples, shades of blue), and influent waters (INF, 2 samples, shades of red) all cluster by the aforementioned 'type' of sample. The inset to Figure 2 shows the Eigenvectors for each of the nano-tastebuds, numbered 1-8 for the first two principal components. As can be seen by the Eigenvectors, nano-tastebud 4 had the least amount of variability sample to sample and nano-tastebud 0 mostly affected the first principal component.

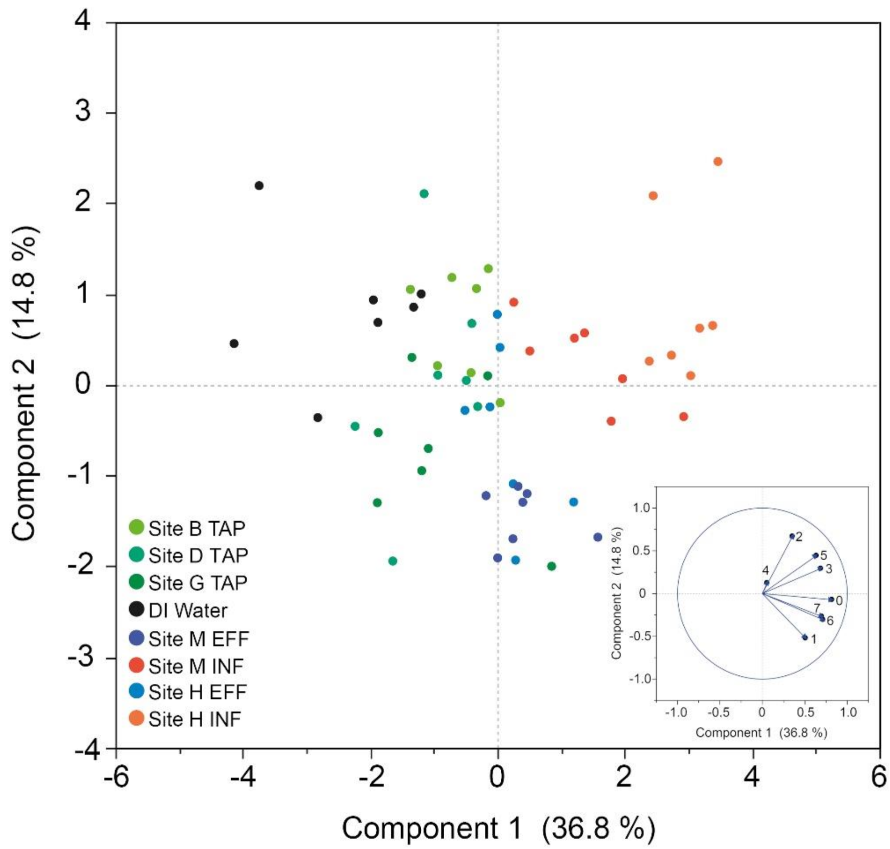

Figure 2. PCA of transmission peak (average shift from DI Water) of water samples from various sites across Scotland. (Inset) Eigenvectors of the 8 nano-tastebuds.

To determine classification capabilities of this device, a supervised analysis technique is required[9]. LDA was chosen for its strength in being able to maximize separation between known clusters whilst minimizing variance within each cluster. Figure 3a shows the resulting LDA scatterplot of the first two canonicals when classifying by 'DI water', 'tap water', 'effluent water', and 'influent water'. Figure 3b shows the comparison between all 3 possible pairings of canonicals, which is useful to demonstrate, for example, how DI water is fully separable from the other samples when all three canonical dimensions are taken into account. Table 1a shows the classification matrix for this LDA, using leave-one-out cross validation. The sensor was able to successfully classify DI water in all instances (100%), with 93% accuracy for effluent water, 90.5% accuracy for tap water, and 93% accuracy for influent water. There were two counts of misclassification of tap water for effluent water, one count of effluent for tap, and one count of influent for effluent.

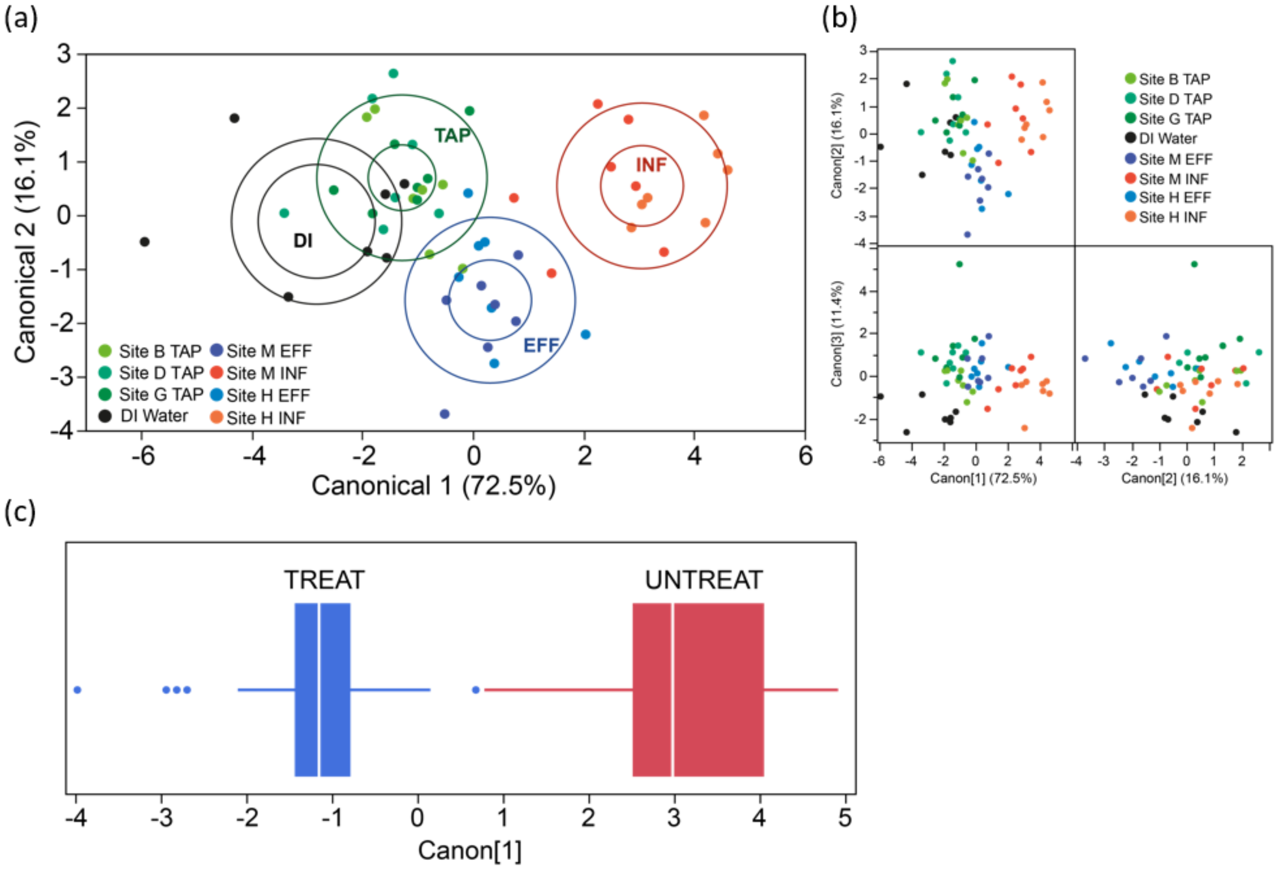

Figure 3. Linear discriminant analysis of transmission peak (average shift from DI Water) of water samples from various sites across Scotland. (a) LDA of first two canonicals using groups DI Water, tap, influent, and effluent. (b) LDA plots comparing all 3 iteration of pairs of canonicals to demonstrate separation in all LDA dimensions. (c) Focused LDA combining tap and effluent samples as 'treated' and influent as 'untreated'.

The few misclassifications between effluent and tap water is not too surprising as both are considered 'treated' water. For any water treatment application, the more important result is seeing how well the sensor is able to distinguish treated and untreated water. To determine this, a second LDA was done, grouping tap water and effluent water as 'treated' and influent water as 'untreated'. Figure 3c and Table 1b shows the resulting LDA and classification table, respectively. For this analysis, the sensor was able to identify with an overall accuracy of 98%: 1 misclassification for untreated water (93% accurate) and 0 misclassifications for treated water (100% accurate). These results demonstrate a good starting point for the development of an optical nano-tastebud sensor for water systems.

Table 1. Classification matrices for LDA shown in (a) Figure 3a and (b) Figure 3c.

(a)		Predicted			
	Label	DI	EFF	INF	TAP
Actual	DI	7	0	0	0
	EFF	0	13	0	1
	INF	0	1	13	0
	TAP	0	2	0	19

(b)		Predicted	
	Label	Treated	Untreated
Actual	Treated	35	0
	Untreated	1	13

4. CONCLUSIONS AND FUTURE WORK

In this manuscript, we successfully demonstrated the use of a nano-tastebud sensor to discriminate between 0.45 micrometer filtered influent and effluent water from various sites across Scotland. Further testing is required to determine the best array of tailored plasmonic metasurfaces for this particular application. Once fully developed, this technology could be fully integrated into water treatment facilities and provide non-expert, end-users with an easy-to-read output capable of warning of imminent system failures.

REFERENCES

[1] "The Sustainable Development Goals Report 2022." Department of Economic and Social Affairs, The United Nations. ISBN: 978-92-1-101448-8 (2022). https://www.un.org/sustainabledevelopment/water-and-sanitation/

[2] "Decentralised Water Technologies Annual Report 2022: Year 1." Decentralised Water Technologies Project. https://www.offgridwater.org.uk/updates/ (accessed: Dec 2022)

[3] "Drinking water quality in Scotland 2021 public water supply." Drinking Water Quality Regulators for Scotland. (2021) https://dwqr.scot/media/jj0l5oof/annual-report-public-supplies-2021.pdf (accessed Dec 2022)

[4] Macias, G., Sperling, J. R., Peveler, W. J., Burley, G. A., Neale, S. L. and Clark, A. W. "Whisky tasting using a bimetallic nanoplasmonic tongue," *Nanoscale*, 11(32), pp. 15216-15223 (2019).

[5] Rodriguez-Mendez, M. L.; De Saja, J. A.; Gonzalez-Anton, R.; Garcia-Hernandez, C.; Medina-Plaza, C.; Garcia-Cabezon, C.; Martin-Pedrosa, F. "Electronic Noses and Tongues in Wine Industry." *Frontiers in Bioengineering and Biotechnology*, 4 (2016).

[6] Guerrini, L.; Garcia-Rico, E. ; Pazos-Perez, N. ; Alvarez-Puebla, R. A. "Smelling, Seeing, Tasting-Old Senses for New Sensing." *ACS Nano*, 11 (6), 5217-5222 (2017).

[7] Minopli, A., Acunzo, A., Della Ventura, B., Velotta, R. "Nanostructured Surfaces as Plasmonic Biosensors: A Review". *Advanced Materials Interfaces*, 9(2), 2101133 (2022).

[8] Wold, S.; Esbensen, K.; Geladi, P. "Principal Component Analysis." *Chemometrics and Intelligent Laboratory Systems*, 2 (1-3), 37-52, (1987).

[9] Stewart, S.; Ivy, M. A.; Anslyn, E. V. "The Use of Principal Component Analysis and Discriminant Analysis in Differential Sensing Routines." *Chem. Soc. Rev.*, 43 (1), pp. 70-84 (2014).

[10] Tomita, S; Ishihara, S.; Kurita, R. "A polymer-based chemical tongue for the non-invasive monitoring of osteogenic stem-cell differentiation by pattern recognition of serum-supplemented spent media." *J. Mater. Chem. B*, 10, 7581-7590 (2022).

[11] Rodriguez-Quijada, C.; Gomez-Marquez, J.; Kimberly Hamad-Schifferli, K."Repurposing old antibodies for new diseases by exploiting cross-reactivity and multicolored nanoparticles." *ACS Nano*, 14, 6, 6626–6635 (2020).