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Smelling chemicals with a photonic nose

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A new sensing platform that uses photonic crystals and simple imagery techniques has applications in security, food monitoring, and water quality analysis.

The area of chemical sensors has grown over the years driven by the development of a wide variety of sophisticated sensing platforms. In the past decade, the preference has been for simplicity, that is, for low-cost, portable, and versatile sensing systems. The general class of multiplexed sensors known as artificial noses are among the best candidates to realize these characteristics. Using mechanisms based on the modulation of electric, gravimetric and optical signals, artificial noses combine the response from a number of different sensors when the array in which they are located is exposed to one or more chemicals. Despite the existence of a few commercially available, portable electronic noses,[1,2] the development of cost-effective and versatile platforms remains a significant challenge.

The photonic nose (P-Nose) is a sensing system that provides a viable alternative to existing devices. Created at the University of Toronto in Canada and currently under commercial development by Opalux Inc.,[3] the technology combines inexpensive methods for large-scale production of materials known as photonic crystals, and a simple analysis routine based on colors in digital photographs.

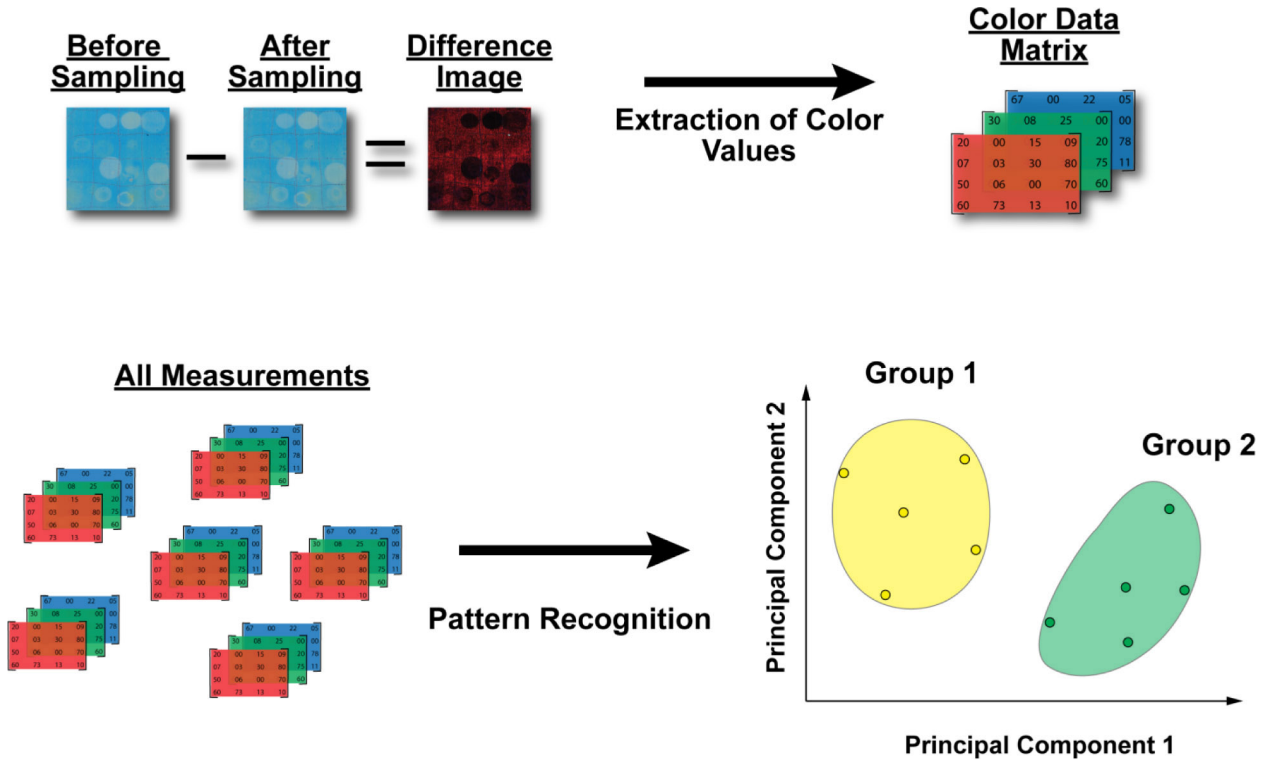

Figure 1. Diagram of the data analysis' process for the photonic nose. The principal components in the final panel are the variables resulting from a mathematical procedure known as principal component analysis.

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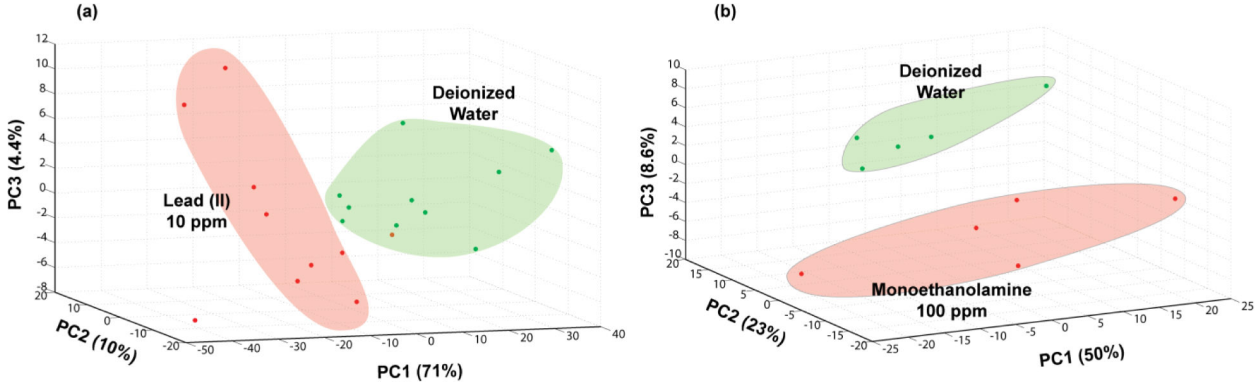

Figure 2. *(a) Discrimination between groups composed of pure water samples and a 10 parts per million (ppm) lead aqueous solutions. (b) Same study for monoethanolamine in water. PC1, 2 and 3: Principal components. In panel (a), for example, PC1 explains by itself the most variance in the dataset, 71% of the total, followed by PC2, which accounts for 23%, and PC3, responsible for 10%.*

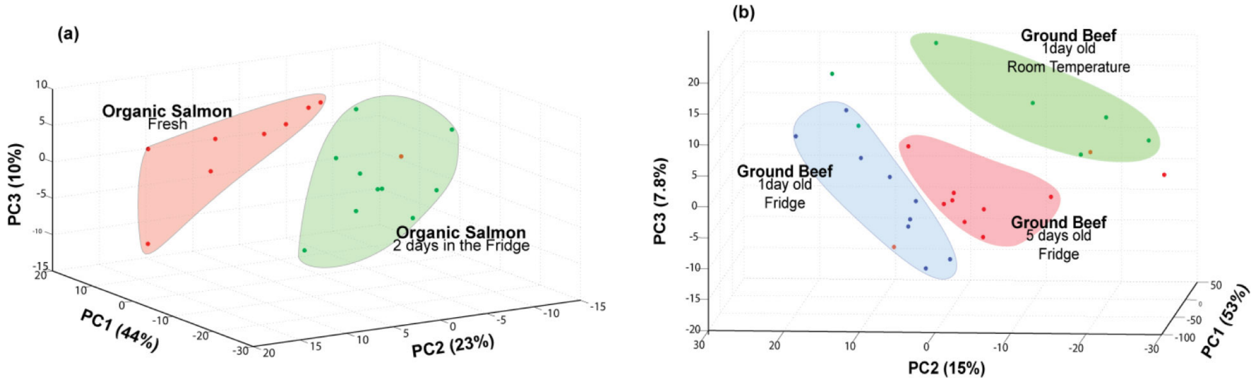

Figure 3. *(a) Discrimination based on the headspace composition between samples of fresh organic salmon fillets and of fillets kept in a fridge (5°C) for two days. (b) Same study for ground beef stored as indicated.*

Photonic crystals are materials that exhibit a so-called photonic band-gap: a range of forbidden frequencies for electromagnetic wave propagation. These frequencies are reflected off the surface of the photonic crystal and, if the range happens to be located within visible light, the object displays brilliant colors. It is the periodic modulation of the crystal's refractive index that generates these colors, similarly to what is observed in butterfly wings, sea-mouse whiskers, and abalone shells.

If porous materials are used in the fabrication of photonic crystals, they exhibit an additional characteristic: tunability. When vapors or liquids infiltrate the voids, the effective refractive index is modified. This leads to a shift in the position of the photonic band-gap and a change in color. The extent of this color alteration can be modulated by employing nanochemistry and surface chemistry concepts. Examples include the use of nanoparticles of various types as components in the photonic crystals, and the modification of surface properties by including self-assembled mono- and multi-layers into the porous surfaces.

We obtain a photonic nose by using an array of several tunable photonic crystals with distinct adsorption properties. The color changes in the system are easily monitored and quantified by employing conventional and low-cost digital imagery methods. More specifically, we use a commercially available digital camera to photograph a test piece before and after the sampling step and then calculate the absolute difference between the images (see Figure 1). With this simple approach, the P-Nose can be used in various problems of technological relevance. Complex mixtures of interest can be analyzed without individual components needing to be identified.

In its first demonstration,[4] the platform discriminated different bacteria strains from each other and from a control culture based on the headspace volatiles generated as by-products of bacterial growth. P-Nose's ability to 'smell' and differentiate the strains can be illustrated by principal component

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analysis. This mathematical procedure combines the response from all sensing units in the array into linear combinations of sensor outputs known as principal components. These are hierarchically ordered so that the first (PC1) accounts for as much of the variability in the dataset as possible, PC2 has the second highest variance, and so forth. The data points from this examination cluster into separate groups, providing a clear picture of the platform's discrimination capabilities (see Figure 1).

Besides detecting chemicals in the vapor phase, the P-Nose can also be used to analyze solutions. In this case, the sensing array is immersed into the liquid for a specific time, as opposed to sensing only the volatiles that emerge from the sample. We have shown that the platform can detect heavy metals in water, including lead, being potentially useful to evaluate the quality of drinking water. The system recognized concentrations of heavy elements as low as 10 parts per million: see Figure 2 (a). We are currently exploring the potential for detection at even lower concentrations. Organic contaminants can also be recognized as exemplified by the identification of an organic amine in water when compared to a control solution: see Figure 2 (b).

The platform is also capable of monitoring food quality. By using multivariate statistical analysis, it is possible to monitor food spoilage processes associated with prolonged storage by comparing the sensor responses when the device is exposed to either fresh or stored samples. We executed successful tests on the analysis of raw meat and fish (see Figure 3).

These proof-of-concept demonstrations show the potential of the P-Nose as the next generation cost-effective sensing platform. Large-scale printing methods for the production of photonic crystals, and a simple analysis scheme that uses low-cost digital cameras, are features that we hope will pave the way for applications in a number of relevant areas. We are currently developing a working prototype that can serve as a portable sensing platform based on the P-Nose technology and exploring its possible applications.

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Leonardo Bonifacio received his BSc, BEd, and MSc from the University of Sao Paulo in Brazil. He moved to Canada in 2006 to pursue a PhD at the University of Toronto. After obtaining his degree in 2010, he joined Opalux Inc. as a research scientist.

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Geoffrey Ozin studied at King's College London and at Oriel College, University of Oxford, before completing a postdoctoral fellowship at the University of Southampton in the UK. Currently he is the tier-1 Canada research chair in materials chemistry, a distinguished university professor at the University of Toronto, a distinguished research scientist at Karlsruhe Institute of Technology, and a founding fellow of the nanoscience team at the Canadian Institute for Advanced Research.

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