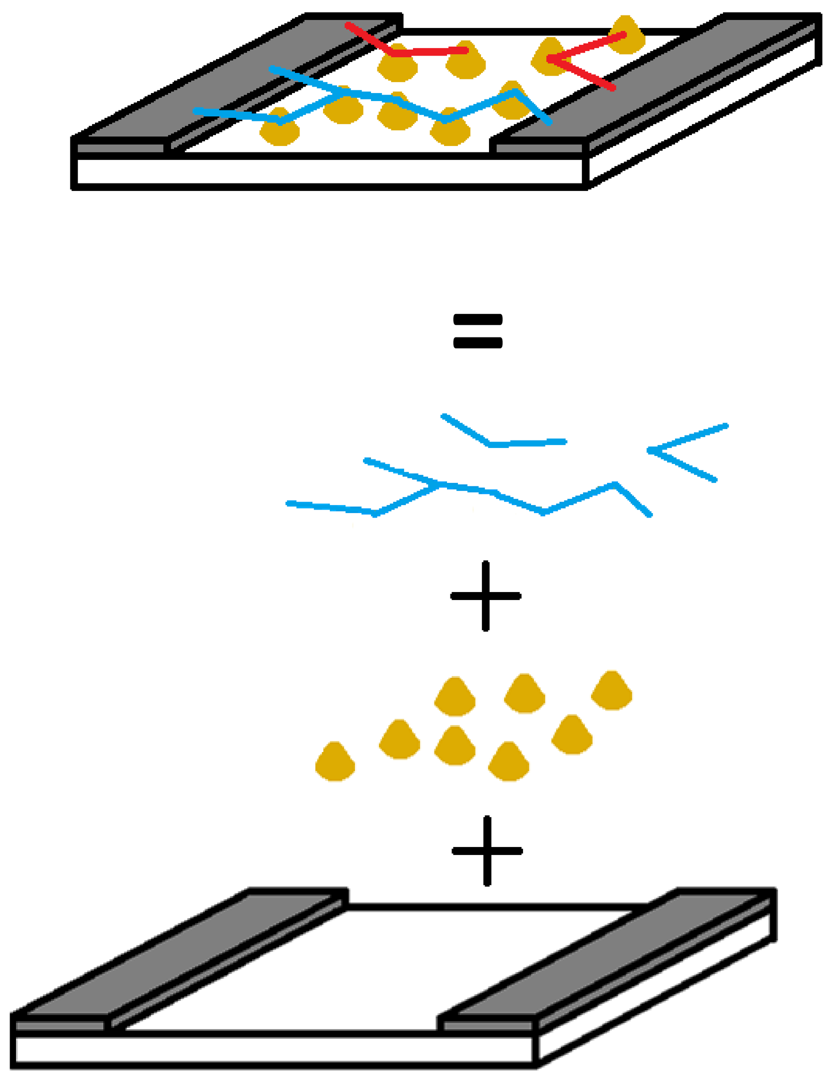
Ultra-Sensitive Molecular Detection of Explosives

Merel Lefferts, Krishnan Murugappan, Ben Armitage, Tabitha Jones, and Martin Castell
Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK

Introduction

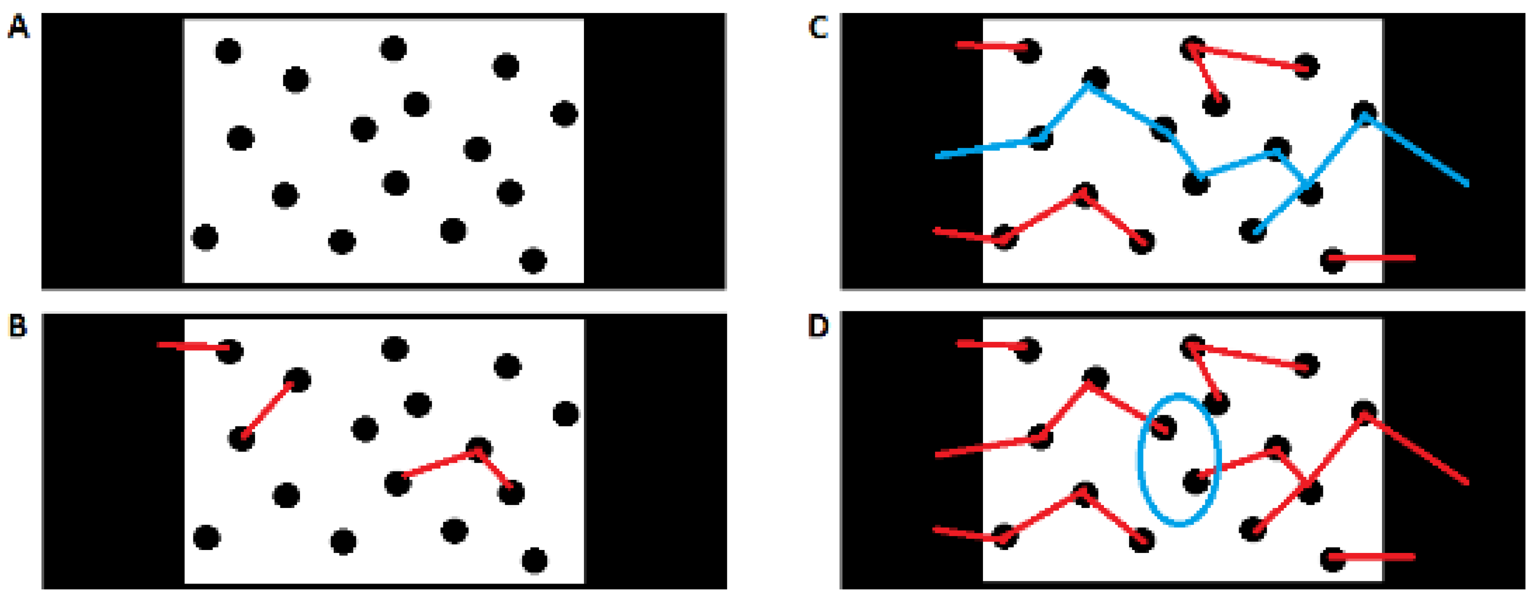
Explosives vapour sensing is especially challenging because of the low vapour pressures of explosive materials. Most existing explosives vapour sensing methods require a pre-concentration step to be able to detect the low vapour pressures. Furthermore, many require bulky pieces of equipment.[1-3]

The aim of this project is to develop a chemiresistive sensor based on a percolation network of conductive polymers on a metal nanoparticle scaffold, as shown in the diagram.



Percolation network based sensor

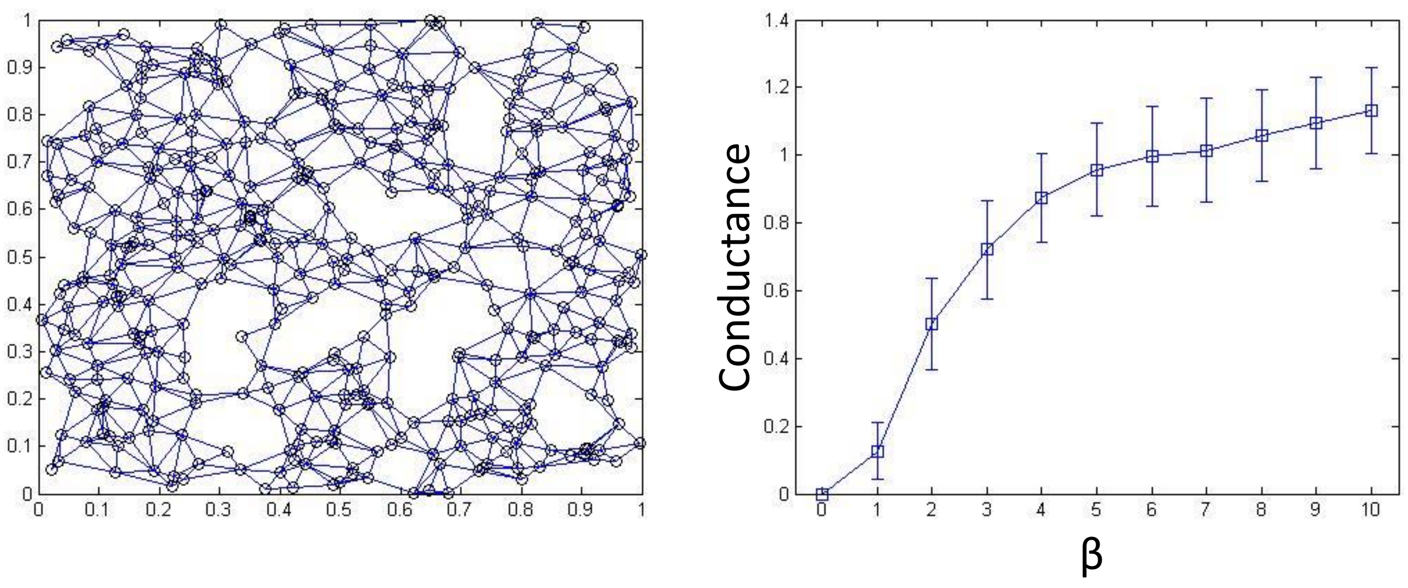
When operating the sensor at the percolation threshold a small, local change due to an interaction with an analyte molecule has a large effect on the resistance through the network, resulting in a sensitive sensor.



Schematic representation of a sensor based on a percolation network. A) Substrate with electrodes and nanoparticles, B) polymer connections (red) have been added but not enough to form a connection between the electrodes, C) more polymer connections have been added (red and blue) connecting the two electrodes (blue), D) breaking one of the connections can interrupt the entire network.

Simulations

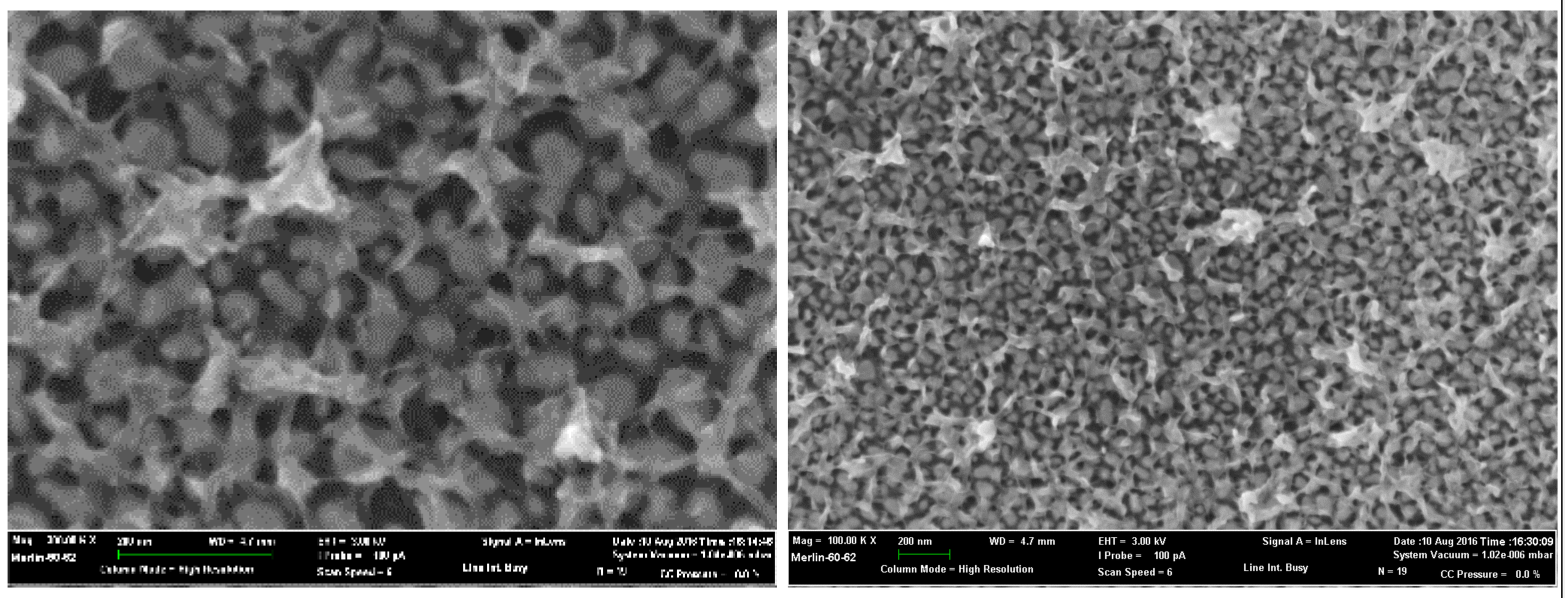
A percolation network based sensor was simulated and the conductance through the network is calculated for different β, or different levels of 'connectedness' of the network. As expected, initially there are very few connections and the conductance is zero, then there is a sharp increase as more connections are added, and finally it levels off again. Simulations have been run for various different networks and the influence of various parameters has been studied.



Simulated network based on a random node distribution, 400 nodes per unit area and a maximum connection length of 0.1 (left). The conductance calculated through that network, for various values of β (right).

Conductive polymer networks

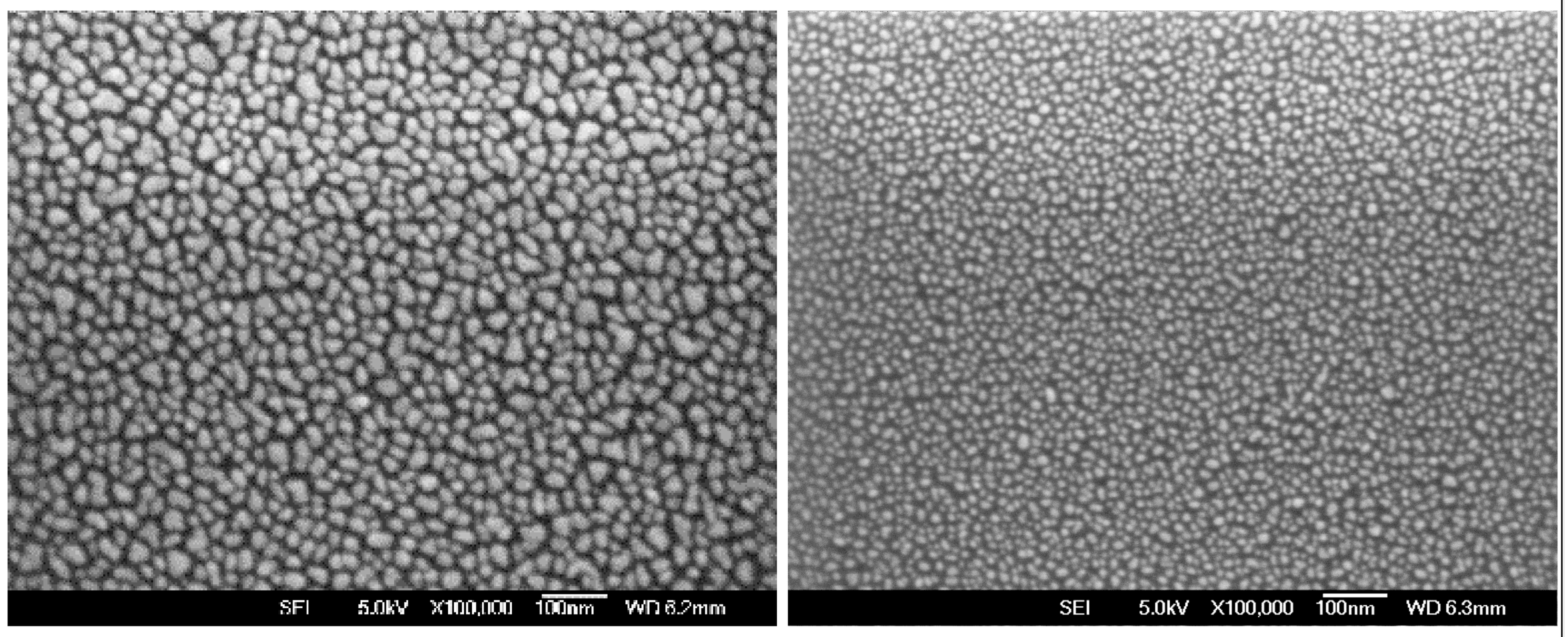
Conductive polymer networks have been created on the gold nanoparticles by electrochemical polymerisation.



SEM images of PEDOT networks on a gold nanoparticle scaffold on a glass substrate.

Gold nanoparticle scaffolds

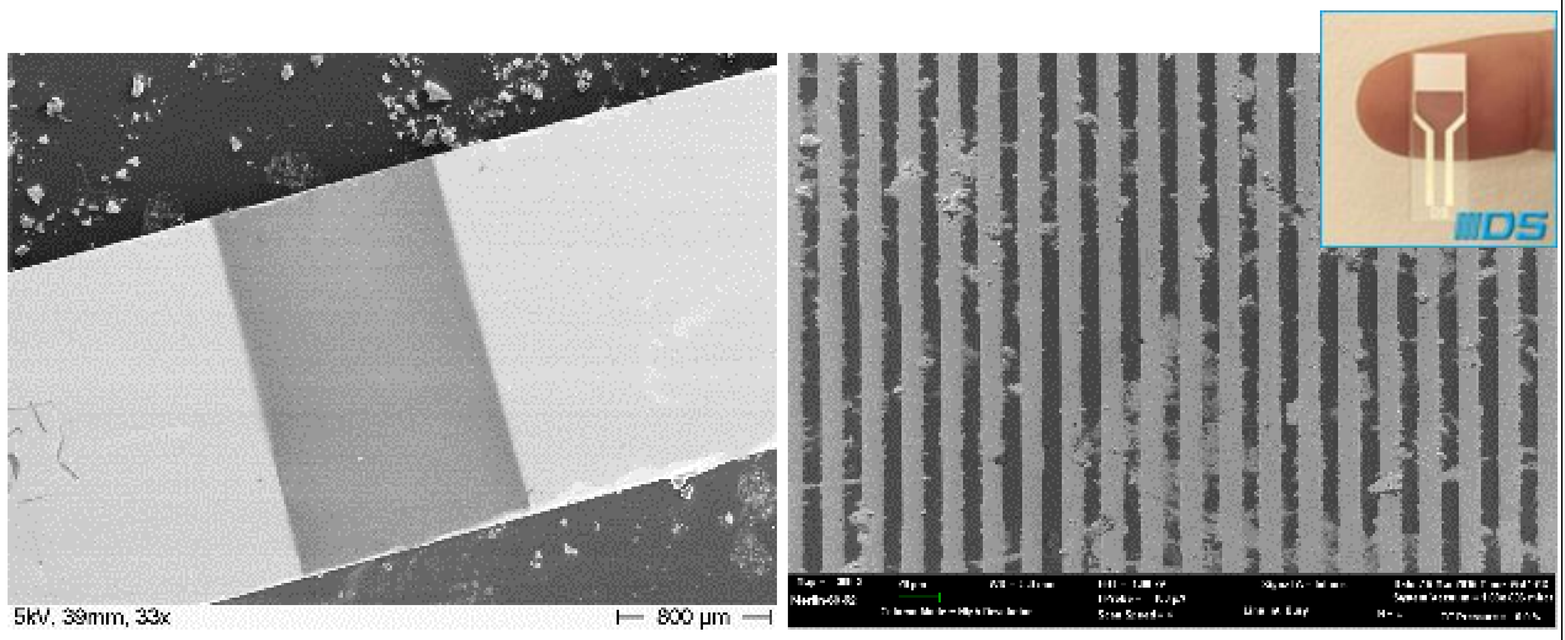
Gold was thermally evaporated onto the substrates in UHV. Next, the sample was annealed, which causes the gold film to dewet into individual particles. The particle size and separation can be controlled by controlling the thickness of the initial gold thin film and the annealing time and temperature.



SEM images of gold nanoparticles on a SiO_2 substrate.

Substrates and electrodes

Insulating substrates such as SiO_2, MgO and glass have been used, with an electrode separation between 5 µm and 1 mm.



SEM images of a SiO_2 substrate with Pt electrodes (bright) with a 1 mm separation (dark) (left), and Pt interdigitated electrodes (bright) with a 10 µm separation on glass (dark) (right).

Summary

A sensor based on a percolation network of conductive polymers on a gold nanoparticle scaffold has been created. Future work includes testing the sensor, and exploring a range of polymers and flexible substrates.

References

1. Lefferts, M. J.; Castell, M. R., Vapour sensing of explosive materials. *Analytical Methods* **2015**, 7 (21), 9005-9017.
2. Parmeter, J. E. In The challenge of standoff explosives detection, *Security Technology*, **2004**. 38th Annual 2004 International Carnahan Conference on, IEEE: 2004; pp 355-358.
3. Steinfeld, J. I.; Wormhoudt, J., Explosives detection: a challenge for physical chemistry. *Annual review of physical chemistry* **1998**, 49 (1), 203-232.

Wearable and Flexible Technologies (WAFT)

This work was funded under Dstl contract 10000810