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Nano-scale reservoir computing

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ABSTRACT

This work describes preliminary steps towards nano-scale reservoir computing using quantum dots. Our research has focused on the development of an accumulator-based sensing system that reacts to changes in the environment, as well as the development of a software simulation. The investigated systems generate nonlinear responses to inputs that make them suitable for a physical implementation of a neural network. This development will enable miniaturisation of the neurons to the molecular level, leading to a range of applications including monitoring of changes in materials or structures. The system is based around the optical properties of quantum dots. The paper will report on experimental work on systems using Cadmium Selenide (CdSe) quantum dots and on the various methods to render the systems sensitive to pH, redox potential or specific ion concentration. Once the quantum dot-based systems are rendered sensitive to these triggers they can provide a distributed array that can monitor and transmit information on changes within the material.

1. Introduction

In our work we investigate a combination of recent advances in materials science and information processing (see [1] for a discussion on the role of inter-disciplinary research in nano-scale communication). The goal of this research is to enable new classes of devices through the development of smart molecular systems incorporating nanoparticles serving in accumulator-based sensor applications. The sensing system that is being developed aims to mimic that of a neural network, in terms of its sensing and signal propagation. In this system, active particles with simple capabilities per device serve a triple function. First, as input units in a physical realisation of an artificial neural network, they can collect and transfer information from external stimuli. Second, in internal layers, they accumulate information from neighbouring regions. Third, and perhaps most critically, they are able to respond when the input exceeds a certain threshold.

From the information processing point of view, Reservoir Computing (RC) appears to be a suitable approach to achieve this goal (for a recent overview of this field, see [8]). RC computing approaches have been employed as mathematical models for generic neural microcircuits, as well as to investigate and to explain computations in neocortical columns (see, e.g., [9]). A key element of RC approaches is the randomly constructed, fixed hidden layer—typically, only connections to output units are trained.

The vision for the work described in this paper is to create a network of particle-sized units that collectively process information coming from the surface of a material. Such a technology would have a variety of applications,

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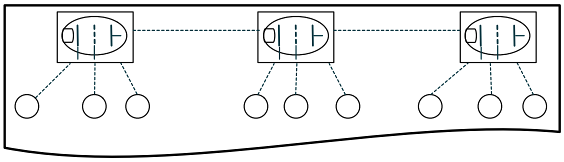

Fig. 1. For a first working prototype, a network of sensors will be created using QDs as sensors, with help of nano-scale triodes.

from monitoring the conditions of a structure (e.g., corrosion or stress), to responding to changes in the environment. Potentially, with many simple and low-power units connected to a large network, this technology could also perform generic computations similar to a processor, but instead of single operations executed at a high frequency make use of massive parallelism at lower frequencies.

We focus on quantum dots (QDs) as the devices to be used for sensing changing properties of a material. It may also be possible to get QDs to communicate signals in order to form a network. We describe the steps we have taken so far in creating an information-processing network of QDs in the subsequent sections. These steps include the materials science aspects of manufacturing the actual QDs, and also a simulation of processes in a material, as a testbed for further developments. Using this simulation, we can evaluate effects of changes in the material on the QDs attached to it. Using another software implementation, we simulate a nano-scale RC network to investigate the potential of recurrent neural networks with the topological constraints of an implementation in hardware. The physical implementation of this connectivity in hardware can be realised in various ways and is subject of our ongoing research. A first, pragmatic approach is to aggregate groups of QDs, to treat these groups as a single sensors, and to pick their signals up using nano-scale triodes for further communication (see the schematic in Fig. 1). We are currently working on such an approach, but are also planning to investigate optical or chemical signalling at a later stage.

Section 2 contains some details of the chemical processes involved in our quantum dot system. In essence, the idea is to use quantum dots to sense, to accumulate and transmit information from the surrounding environment. The sensory stage will be located physically close to external stimuli which may be in the solid, liquid or gaseous state. As a result of this interaction, a signal that may be chemical, electrochemical, thermal or optical in nature is propagated through the medium until it reaches the accumulating stage. These accumulating particles are affected by the signal in a characteristic way such that the accumulator is influenced by each signal, but does not undergo a change in the physical quantity being measured until a critical number of signals have reached it. Once this critical number of signals has been reached, the accumulator changes one of its properties and in doing so sends an intense signal to the responding particle; the latter either changes the properties of the structure or sends an amplified signal from the structure. Advantages over software-based RC implementations would be speed, parallelism, as well as energy efficiency.

In Section 3 we describe some aspects of our software simulation and some of the processes involved: the system that we use to experiment with possible configurations and network architectures, an abstract simulation of some of the chemical processes above in software.

Alternative physical implementations of RC have been proposed before. The work of Vandoorne et al. [14], for example, proposes the use of coupled semi-conductor optical amplifiers. These devices can be placed on a small chip and implement a number of units. A different approach, using electronic circuits, nano-wires and self-assembly, is presented in the paper of Stieg et al. [13]. Our approach uses essentially nanoparticle-sized units, so that it may allow an embedding of the entire reservoir network into, for example, the coating of a material.

2. Experimental work using quantum dots

QDs are spherical submicron particles (typically 1–10 nm), normally of a semi-conducting material, and often have a surrounding shell of a second semi-conducting phase. The optical properties of the QDs may be tailored by doping them with other elements or by particle size control. The most notable characteristic of QDs is their ability to absorb energy over a wide range whilst fluorescing with a relatively narrow bandwidth at a longer wavelength. One of the most widely investigated QD systems is Cadmium Selenide (CdSe) with a Zinc sulphide (ZnS) shell. These QDs absorb strongly through the mid- and near-UV and into the visible, yet emit a strong fluorescence signal in a relatively narrow band in the red region of the visible spectrum, with a high quantum efficiency.

The focus of our experimental work thus far has been on the development of the accumulator-based sensing system, which utilises CdSe/ZnS QDs coupled with a signal conversion molecule that reacts to changes in the environment. The signal conversion molecules selected have been either pH-sensitive dye materials (Section 2.1) or redox potential-sensitive dye materials (Section 2.2). The accumulator consists of the quantum dots surrounded by a medium containing either the pH or redox sensitive dye molecules. These surrounding dyes either block the incoming light that stimulates the quantum dot fluorescence, or serve to absorb and hence shut down the QDs outgoing fluorescence. The QDs used in this work has an emission peak centred at 646 nm (FWHM $\approx$25 nm).

2.1. pH system

The pH sensitive dye molecule selected for this demonstration was p-nitrophenol (4-hydroxynitrobenzene) as it possesses suitable optical properties for blocking the incoming optical stimulus to the quantum dots. p-nitrophenol is a weak acid with a pK_a of 7.08. In its neutral form, i.e., when the dye molecule is not an ion, at pH $<$ 4 the molecule is colourless, with transitions occurring in the UV near 300 nm. At pH $>$ 4, the molecule progressively deprotonates at the phenolic group, and transitions near 400 nm emerge, resulting in a yellow colour. This anionic form of the molecule has several resonance-stabilised forms, causing lower-energy transitions appear, compared to those of the neutral form. Above pH 7, the process is essentially complete. Thus progressive accumulation (or