Accelerating Molecular Electronics with Open Source Instrumentation

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Abstract—Molecular electronics offers a promising route towards high-performance, efficient electronic devices in the future, with myriad potential applications including sensing, computing, cooling and energy harvesting. High throughput electrical characterisation of molecular devices is essential in order to explore the vast design possibilities provided by modern synthetic chemistry in the search for viable molecules for the next generation of devices. This work presents a concept for an inexpensive open-source mechanically controlled break-junction (MCBJ) integrated into a printed circuit board (PCB), which may facilitate rapid parallel studies of single-molecule junctions.

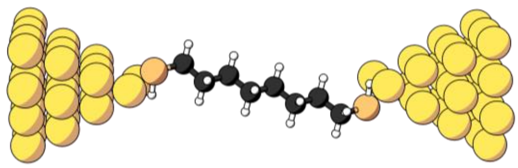
I. Introduction

Molecular electronics is a rapidly growing interdisciplinary field concerned with the development of electronic devices built from individual molecules, rather than from bulk materials. The motivations for pursuing molecular electronics research are twofold:

From a perspective of scientific curiosity, molecular devices provide a fascinating platform for the study of quantum transport in a highly customisable nanostructure. The freedom in molecular design afforded by synthetic chemistry provides greater control over the properties of the device than is available in other devices of comparable dimensions. This flexibility has facilitated access to a rich assortment of quantum phenomena, and molecular electronics experiments continue to provide valuable insight into quantum transport regimes which are not yet well understood theoretically.

There is also a strong technological motivation for molecular electronics research. Conventional devices are created from bulk materials via subtractive manufacturing. This 'top down' approach is limited by the properties of the available materials and the precision of the manufacturing process. In contrast, molecular electronics devices could use a 'bottom up' approach to fabrication, where components consist of individual bespoke molecules which may form larger devices via self-assembly. Molecular devices can also leverage phase-coherent quantum transport effects, such as quantum interference, which are not available to conventional electronics. This could lead to the realisation of highly efficient devices with unparalleled performance, such as chemical sensors with single-molecule detection thresholds and enhanced thermoelectric materials for waste heat harvesting.

The most basic implementation of a molecular device is a single-molecule junction (SMJ) formed by connecting a molecule between two metallic leads:



This configuration, despite its apparent simplicity, can exhibit a vast range of phenomena, and much of the progress in molecular electronics to-date has been achieved via the study of SMJs.

Due to their nanoscale dimensions, the controlled formation of SMJs presents a significant experimental challenge, and a number of different techniques have emerged in the last few decades. Perhaps the most versatile and widely adopted approach for SMJ formation is the break-junction technique, in which nanoscale metallic junctions are repeatedly formed and broken in the presence of the target molecule; each time the metallic junction breaks, a single-molecule may enter the gap and bind to each side of the junction, resulting in a molecular junction with two metallic leads.

The most common variant of the break-junction technique is the mechanically controlled break junction (MCBJ), in which the junction consists of a thin metallic wire affixed to a `bending beam'. A motorised `coarse' motion system applies pressure to the centre of the beam, and the wire is stretched by the resulting deflection. Once the wire reaches its breaking point, a piezoelectric `fine' actuator then modulates the deflection of the bending beam with sub-nanometre precision to form and break metallic junctions.

II. Related Work

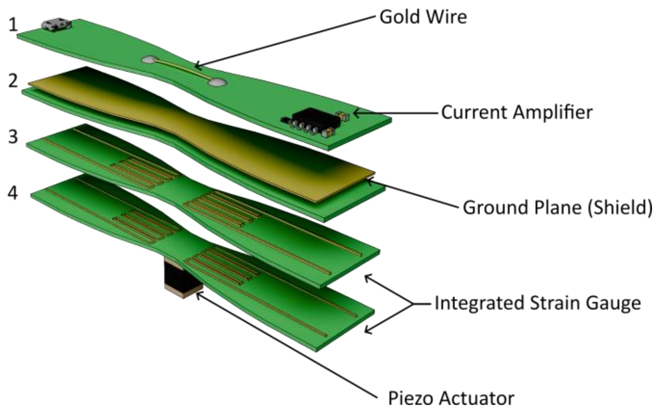
The MCBJ is among the most important experimental methods in molecular electronics, and many important phenomena have been observed in break-junction experiments[1]. Despite the ubiquity of the technique within the field, off-the-shelf commercial MCBJ instruments are not available; instead, individual labs typically implement `home-made' systems[2].

An open-source platform which can be more readily reproduced and modified allow more groups to utilise MCBJ techniques. Additionally, a lower cost solution opens the possibility to operate many instruments in parallel, with the potential to vastly accelerate the search for high-performance molecular device candidates. A standardised platform may also improve the reproducibility of results between different labs.

The most demanding technical aspect of the MCBJ is the measurement of the conductance of the junction. Over the course of a typical measurement the conductance of the junction can vary over 9 orders of magnitude as the metallic junction breaks and a single-molecule junction is formed in its place. A low-cost amplifier design for MCBJ based on a bridge configuration, which offers sufficient dynamic range while retaining a high bandwidth (>20KHz), has been demonstrated in the literature[3]. This may form the basis of the instrument developed in this work.

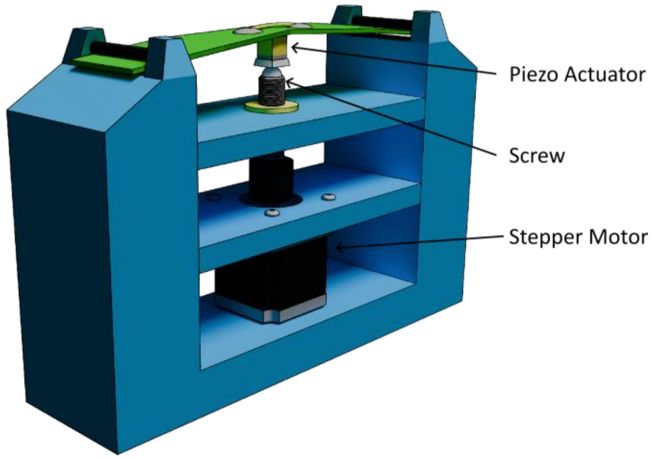
III. PROTOTYPE CONCEPT

In the interest of ensuring that the MCBJ instrument can be reproduced and modified at minimal cost and without specialised tools or expertise, the `bending beam' will consist of a 0.4mm thick FR4 PCB. This enables the use of inexpensive small-batch PCB production services in the fabrication of the MCBJ, and also facilitates the integration of electronic systems (such as the amplifier) onto the bending beam itself. Additionally, the use of a multi-layer PCB allows additional functionality to be incorporated into the inner layers, for example an integrated strain-gauge could be included for closed-loop deflection control, as illustrated in the exploded view below:

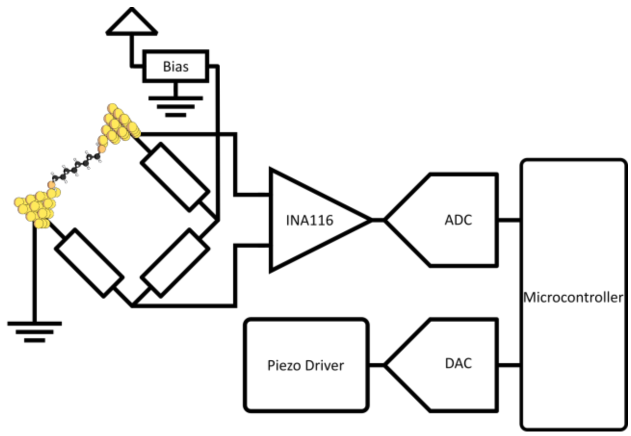


The fine positioning system will consist of a multilayer piezoelectric stack actuator (Thorlabs PA4DGW) with a sensitivity of 15.3nm/V. Since a piezo actuator is a capacitive element, current is required to change the drive voltage (and therefore displacement). The capacitance of the PA4DGW piezo stack is 50nF. If the piezo is driven with a triangle wave of amplitude 45V (corresponding to a displacement of 690nm) at 1kHz, the required drive current will be 2.3mA. This could be achieved using audio amplifier ICs as a low-cost alternative to the off-the-shelf piezo drivers typically used in MCBJ instruments.

The coarse motion system will consist of a NEMA 17 stepper motor and off-the-shelf driver module, connected via a flexible coupling to a fine pitch screw with a spherical tip. This system will be housed in a 3D printed frame which holds the bending beam in place over the screw with two push-fit steel rods, such that driving the screw and/or piezo stack will result in a deflection of the bending beam. For mechanical stability the frame will be printed from carbon-fiber reinforced nylon.



The control and data acquisition system will be based on a low-cost general purpose microcontroller interfaced with ADC and DAC ICs over SPI to measure the junction conductance and generate the piezo drive signal. A minimum resolution and bandwidth of 16-bit and 20KHz should be targeted for both converters. The low-cost amplifier configuration introduced in [3] will be implemented to measure the junction conductance.



IV. RESPONSIBLE INNOVATION

The purpose of the prototype device is to help accelerate the search for viable molecular-scale devices for a number of applications which could have a significant positive impact, for example:

- High figure-of-merit organic thermoelectric devices could enable the wide scale recovery of energy from low-temperature waste heat, which is estimated to account for over 60% of industrial waste heat[4]
- Molecular memristors could assist in overcoming the Von-Neumann bottleneck in computing, and may be a path towards efficient machine-learning inference "on the edge", helping the minimise the environmental impact of a growing sector of computing

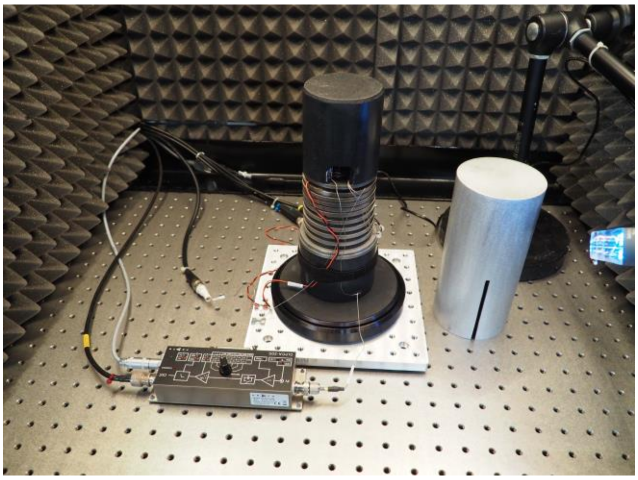
- The realisation of low-cost ultra-sensitive chemical sensing elements will have a wide range of applications including drug discovery and medical diagnostics[5]

The environmental cost of the construction and operation of the MCBJ must be considered and minimised. For example, the system should be designed to be easily cleaned and reused, and the cleaning process should be carefully optimised to minimise the quantity of solvents used.

V. Author bio

I am a postdoctoral researcher in the Lancaster University department of Physics, specialising in the characterisation of molecular scale devices using scanning probe microscopy and break-junction techniques. I have a keen interest in developing novel instrumentation in order to study molecular junctions with enhanced precision and detail.

During the course of my research I have developed a number of bespoke instrumentation systems, including a scanning tunnelling microscope (STM), pictured below, optimised for advanced multivariate break-junction modes which access additional information beyond electrical conductance. I also have experience in designing sophisticated data analysis approaches, leveraging deep networks and variational inference to extract additional information from the large datasets generated by break-junction experiments.



In my spare time I enjoy electronic prototyping and DIY, and I have worked on a wide range of hobbyist hardware projects, from guitar effects pedals to smartwatches.

VI. References

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