

University  
of Victoria

# Electronic Transport in Gold Nanoparticle-Molecular Networks

Tristan Zaborniak<sup>1</sup>, Anusha Venkatamaran<sup>2</sup>, Eberechukwu Victoria Amadi<sup>2</sup>, Chris Papadopoulos<sup>2</sup>

<sup>1</sup>Department of Physics and Astronomy, <sup>2</sup>Department Electrical and Computer Engineering



ENGINEERING

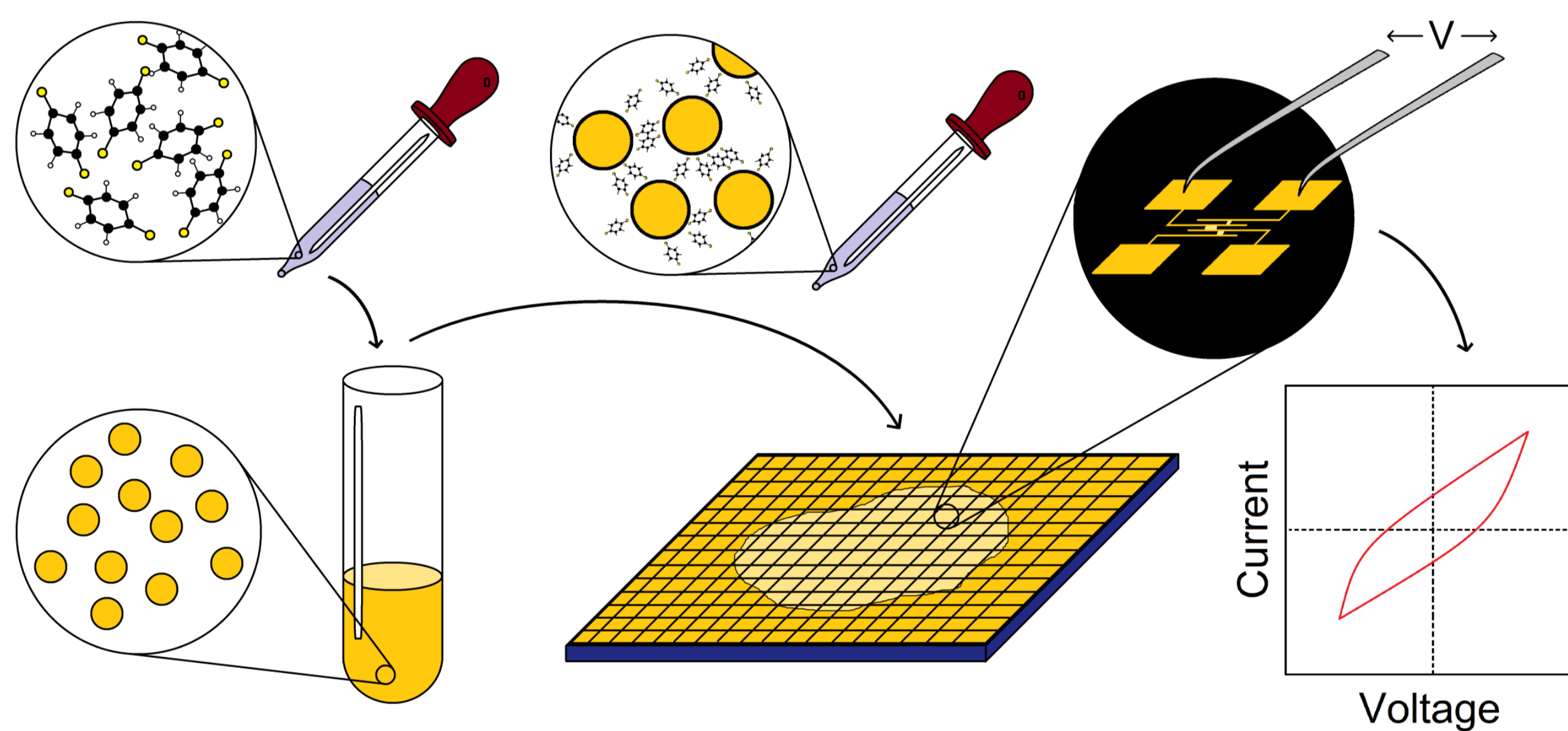
## Abstract

Electronic transport is investigated in self-assembled gold nanoparticle-benzenedithiol networks with tunable molecule:nanoparticle ratios (1:5-50:1) deposited between planar electrodes. Two-terminal current-voltage measurements reveal linearity at low bias (to  $\pm 0.3$  V), and negative differential resistance and hysteresis at high bias (to  $\pm 5.0$  V) in these networks. This suggests their application in molecular integrated circuits as memory and switching elements. Additionally, density functional theory is used to explore the electronic transport properties of gold-benzenedithiol junctions from first principles.

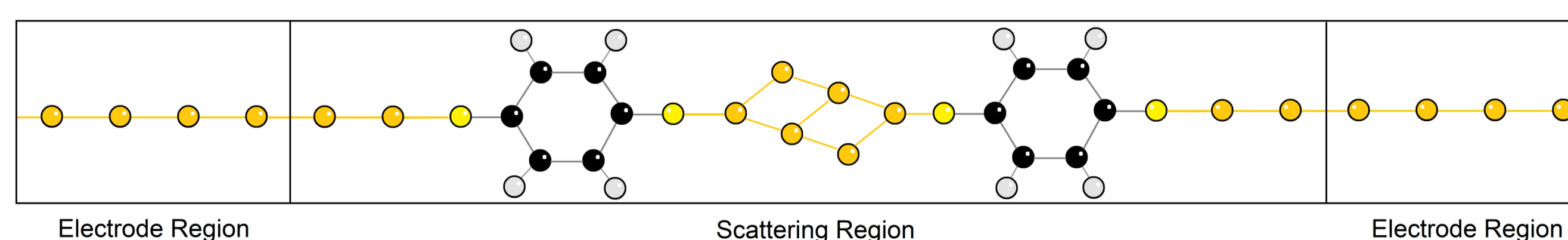
## Motivation

- Replacing electronic components with molecule-sized analogs or hybrids promises to further miniaturize electronics [1].
- Studying electronic transport through molecules is a necessary step in engineering their application as electronic components [2].
- Measuring the electronic properties of self-assembled metal nanoparticle-molecular thin-films offer a way to achieve this [3].

## Methods

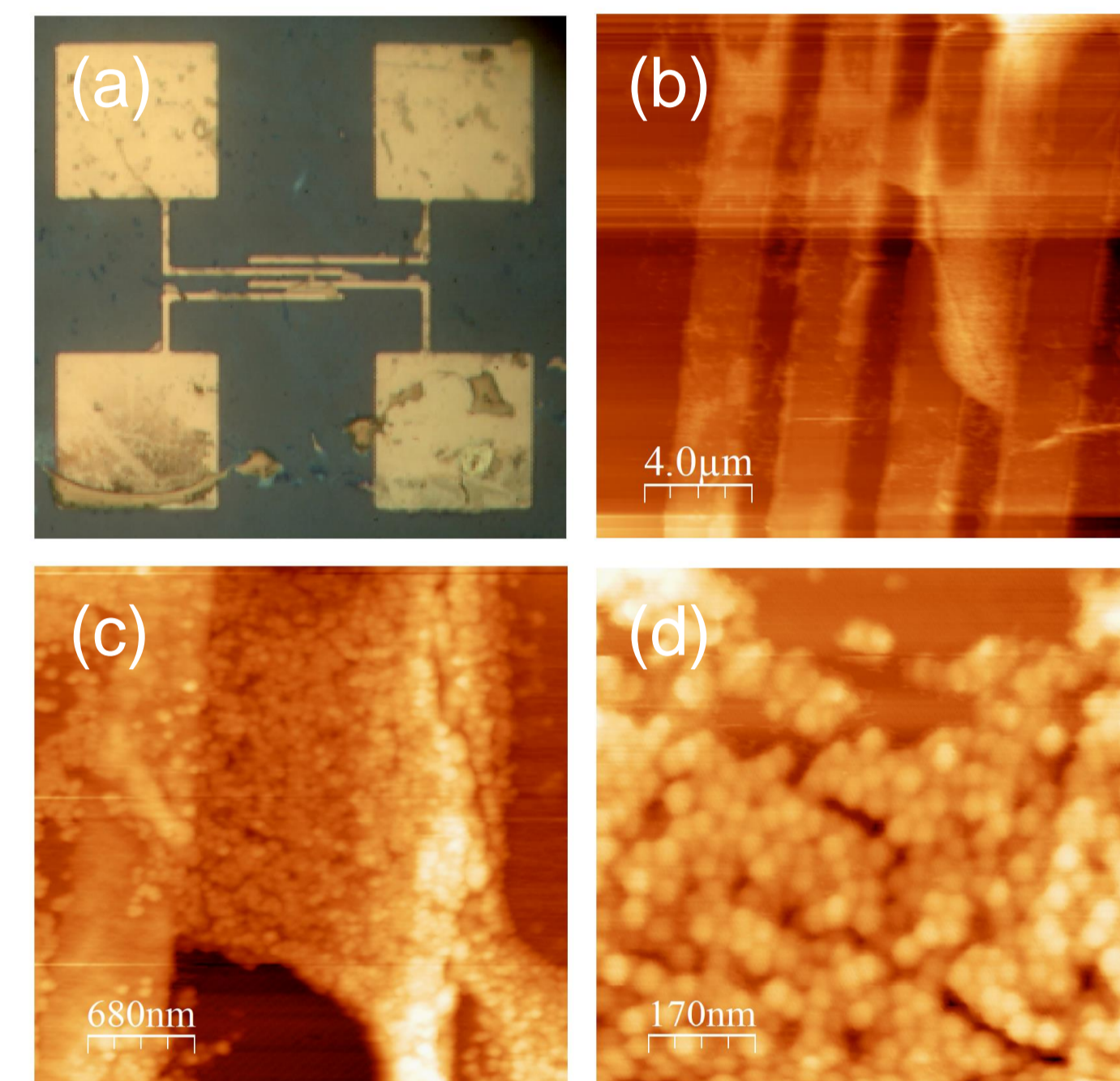


1. Mix benzenedithiol and gold nanoparticles in solution [4]
2. Drop solution onto patterned gold electrodes, allowing to dry
3. Measure current as a function of voltage between electrodes



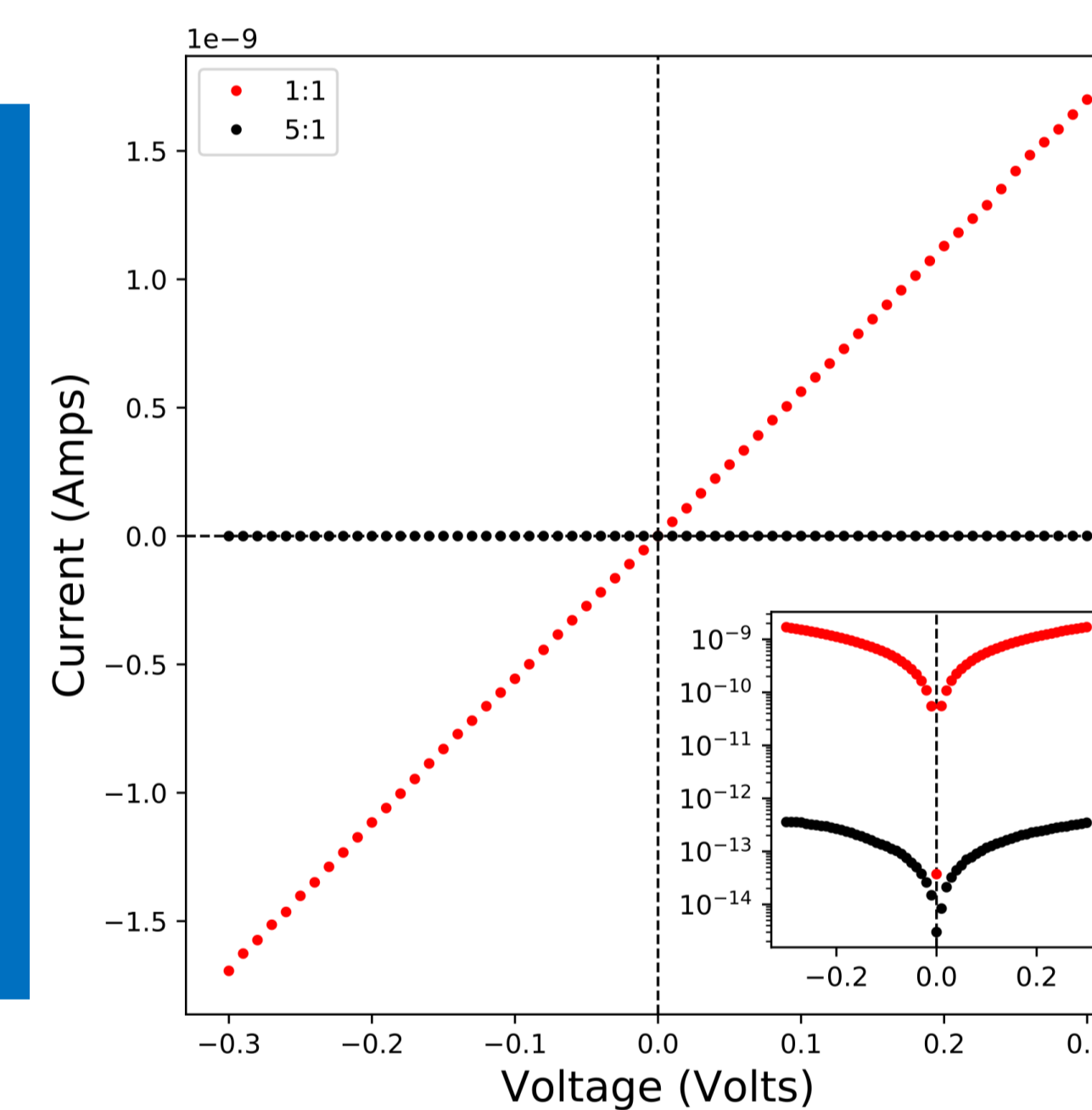
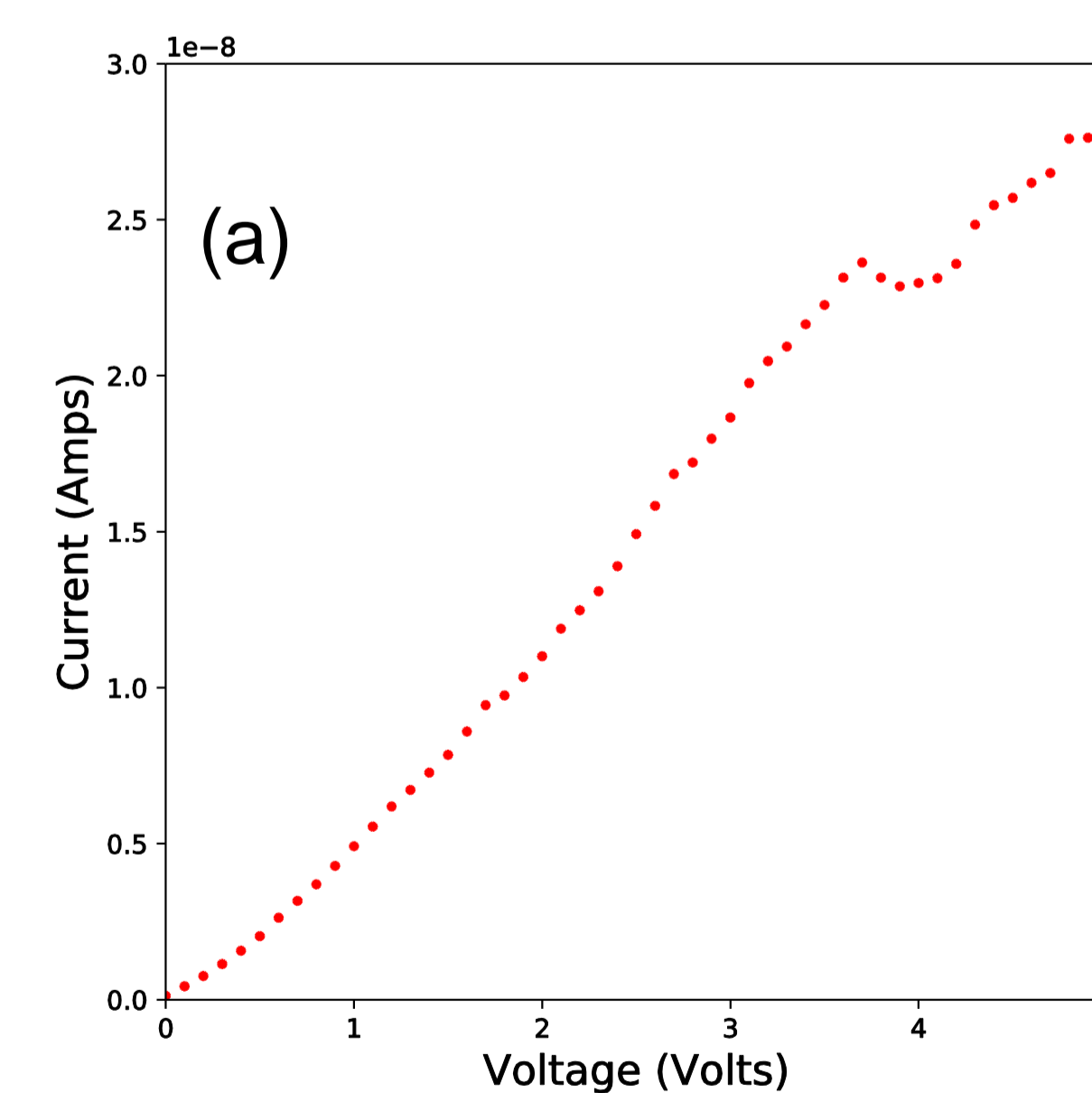
1. Build electrode-molecule-electrode structures in software
2. Calculate electronic transport and properties via Transiesta [5]

## Results



**Figure 1:** Self-assembled 1:1 30 nm colloidal gold nanoparticle-benzenedithiol networks bridging electrodes on  $\text{SiO}_2/\text{Si}$  substrate, as seen (a) optically, and (b-d) by atomic force microscopy. (c-d) show networks as having a thin-film nature, as well as particle clustering and defects in some regions.

**Figure 2:** Linear current response of 1:1 and 5:1 30 nm colloidal gold nanoparticle-benzenedithiol networks as a function of voltage at low bias showing decrease in current magnitude with increasing molecule: nanoparticle ratio.



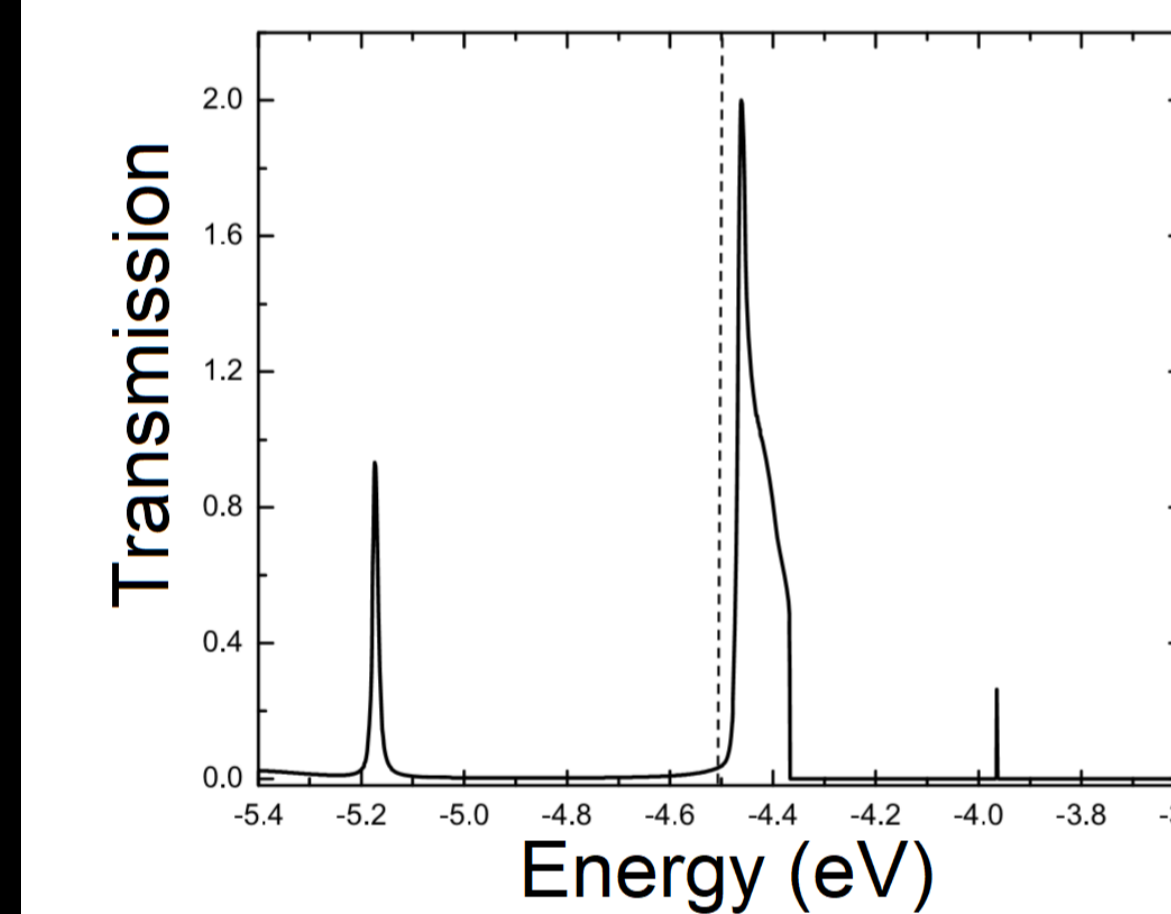
**Figure 3:** (a) Current response of 50:1 30 nm colloidal gold nanoparticle-benzenedithiol network to voltage exhibiting negative differential resistance (NDR), and (b) 1:5 and 50:1 samples displaying hysteric behaviour at high bias (semi-log inset showing current magnitude). Continuous voltage sweep of (b) from  $0 \rightarrow 5 \rightarrow -5 \rightarrow 0$  volts. NDR was only observed in 50:1 samples, with peaking typically between 3-4 Volts.

## Conclusions

- Electrical properties of gold nanoparticle-benzenedithiol networks are a function of molecule:nanoparticle ratio (M:N). At low biases, network resistance increases with M:N. At high biases, negative differential resistance (NDR) and hysteric behaviours become evident, their markedness increasing with M:N.
- These effects suggest that gold nanoparticle-benzenedithiol networks might be employed in nanoscale switching and memory applications.

## Future Work

- Experiments with other molecules and nanoparticles with the goal of designing specific components for molecular integrated circuits.



- Using first principles density functional theory to predict current response to applied voltage through networked molecule-nanoparticle structures, building on previous work [6]. Example transmission corresponding to structure shown in methods section previously calculated shown at left.

## References

- [1] J. R. Heath, *Annual Review of Materials Research*, **vol. 39**, no. 1, pp. 1–23, Aug. 2009.
- [2] D. K. James and J. M. Tour, *Chemistry of Materials*, **vol. 16**, no. 23, pp. 4423–4435, Nov. 2004.
- [3] H. B. Akkerman, P. W. M. Blom, D. M. de Leeuw, and B. de Boer, *Nature*, **vol. 441**, no. 7089, pp. 69–72, May 2006.
- [4] P. Zhang, A. Venkataraman, and C. Papadopoulos, *Physica Status Solidi B*, **vol. 254**, no. 9, p. 1700061, May 2017.
- [5] M. Brandbyge, J. L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, *Physical Review B*, **vol. 65**, no. 16, p. 165401, Mar. 2002.
- [6] A. Venkataraman, P. Zhang, and C. Papadopoulos, *AIP Advances*, **vol. 9**, no. 3, p. 035122, Mar. 2019.

## Acknowledgements

This work was carried out under the supervision of Dr. Chris Papadopoulos. Funding provided by the Jamie Cassels Undergraduate Research Award and the Natural Sciences and Engineering Research Council of Canada. We acknowledge the computational support of Compute Canada.