Solvent effects in molecular junctions

Iain Grace* and Colin Lambert
Department of Physics, Lancaster University, Lancaster, UK
*e-mail: i.grace@lancaster.ac.uk

Molecular electronics is a rapidly growing field, which offers the possibility of using molecules to build nano-electronic devices. Current experimental approaches, including STM and break junction techniques rely on a statistical approach to measure the conductance through individual molecules. Therefore, theoretical models of these junctions can help to analyse and understand experimental measurements. Recent work [1] has shown the importance of the environment surrounding the molecule, and has shown that the conductance of molecular wires can change significantly in the presence of water as compared to vacuum. This also opens up the possibility of using these devices as sensors.

Therefore, theoretical models should include the environment, and here we show that by combining molecular dynamic simulations with a DFT based transport approach, using the newly developed GOLLUM code, we can gain better agreement with experimental measurements.

[1] Phys. Rev. Lett. **102**, 086801 (2009).