

[subject category: Information technology]

TOWARDS SINGLE-MOLECULE COMPUTERS

Computers are forever shrinking and becoming more powerful. But the days of the computer based on the silicon chip are numbered. The transistors – the essential electronic ‘units’ of a computer – that are etched into a silicon wafer can be made only so small and that limit is likely to be reached in the next few years.

So scientists are looking to the next generation of transistor – based upon single molecules. Professor Colin Lambert, of the Lancaster University, says, “We are aiming to develop this new research field of single molecule electronics, and if we are successful we will deliver transistors that are 100 times smaller than those we have at present, so that computers can be 100 times more powerful or have a memory that is 100 times greater – that is the long-term goal.”

However, the field is in its infancy and there are huge theoretical and experimental challenges ahead. A transistor is sandwiched between two electrodes, and one of the big unknowns is how a single molecule will interact with its electrodes. To predict how such a system will behave, powerful supercomputers are necessary to carry out the relevant calculations.

“At the scale of individual molecules the rules of quantum mechanics apply and it is extremely complicated to describe how the molecular transistor will interact with the electrodes, how electrons will float from one electrode, through the molecule and to the other electrode,” says Professor Lambert. “We need to know what happens if the molecule is twisted, or has an external electric field applied to it – how would that influence the passage of the electrons? We need to consider every possible aspect of how these things sit together at the atomic and quantum scale, where everything is sensitive to everything else. This all requires fantastically complicated computations.”

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IMAGE CAPTION: Twist and stretch...computer-generated representation of how a single molecule transistor sits between two electrodes



