Coupling charge transport to internal degrees freedom at the single molecule level (acronym: **SINGLE)**

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Molecular electronics is a wide field of research, which consists of such diverging topics as *Organic Light Emitting Diodes (OLEDs)*, *Organic Field Effect Transistors (OFETs)* and *Single Molecule Devices*. Whereas OLEDs and OFETs exploit the properties of a large number of molecules, in the field of single-molecule electronics it is tried to condense the entire functionality of an electronic device into a single molecule. To obtain reliable devices, the composition of the devices has to be controlled to only a few atoms, a demand that seems to be infeasible for conventional lithographic methods. However, during the last few years it has been demonstrated, using different techniques, that it is possible to attach metallic contacts to individual organic molecules. This has opened up a new field of study for investigating transport of individual molecules, and of how this transport is influenced by parameters such as temperature, magnetic field and the interaction with phonons and photons. It is now largely understood how two independent properties define the gross features of the device: One is the strength of the contact between the molecule and electrode the other is the position of the electronic states. Time is ripe to go beyond this "State-of-the-art" and exploit the special responsive properties of organic molecules.

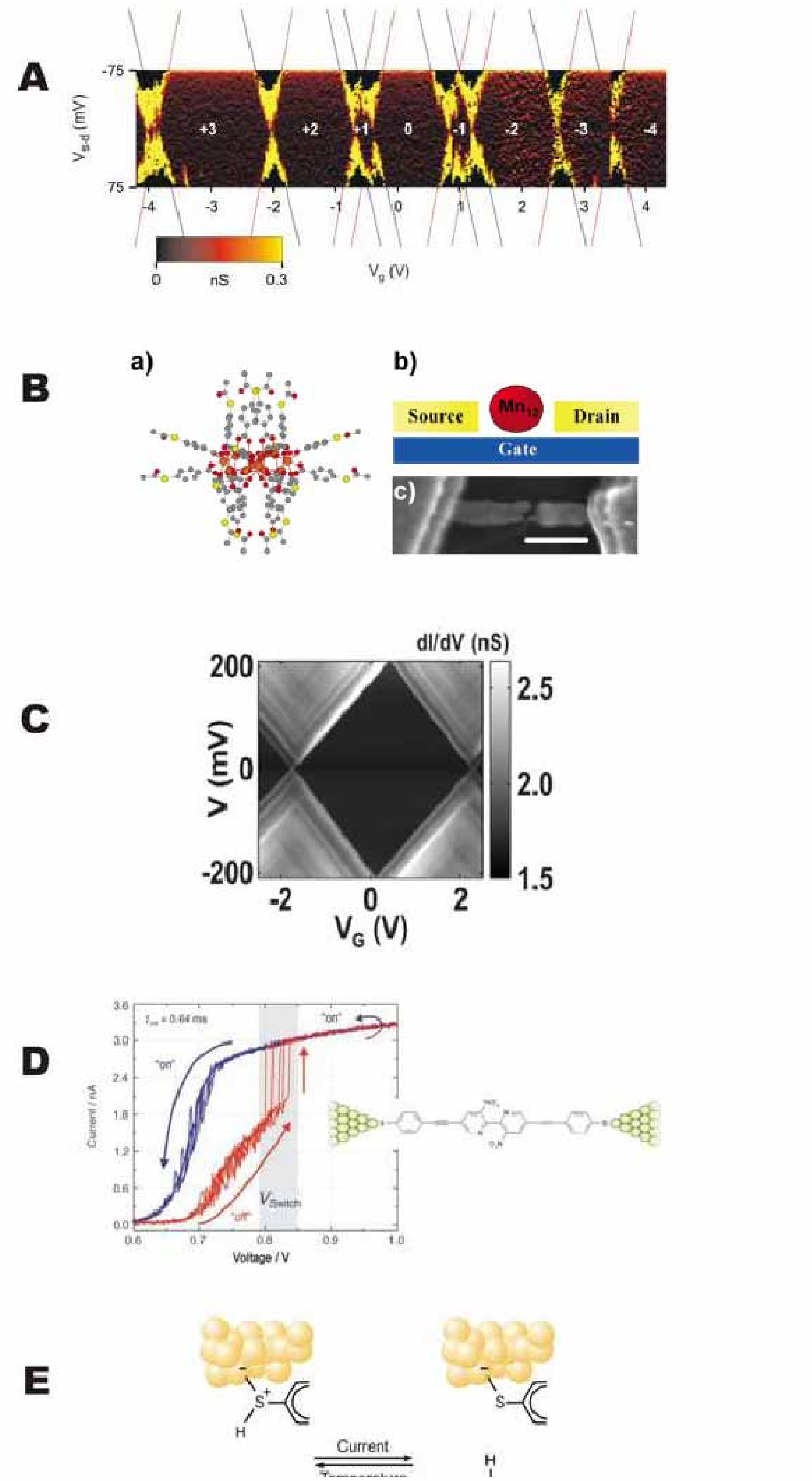
In this STREP project, coordinated by Prof. Thomas Bjørnholm from the University of Copenhagen- we will synthesize molecules, measure transport on the single molecule level and provide theoretical modeling (both DFT and toy-models) for the interpretation of the data. The scientific **objective** of the proposal is to

- understand transmolecular conductance of single organic molecules connected to electrodes and to
- exploit its relation to **internal degrees of freedom** in the molecules. These include: vibrations, conformational changes (nanomechanics), electronic levels, electron correlations and spin.

The final goal is to demonstrate new types of single molecule **switches**, **memory devices**, **diodes** and **transistors** that are radically different from classical semi conducting devices where crystallinety dominates the functionality of the material in the device. The concept underlying the proposal is hence to exchange the rigid "hard" crystalline semiconductors with the "soft" and structurally diverse organic molecules that respond much more vigorously and diversely to external stimuli.

Project participants

	Organization	*Principal investigators*
1	University of Copenhagen	Thomas Bjørnholm; Mogens Brønsted Nielsen; Kristine Kilså; Karsten Flensberg
2	Chalmers Technical University	Sergey Kubatkin; Göran Wendin
3	Delft University	Herre van der Zant; Jos Thijssen
4	IBM, Zürich	Heike Riel; Emanuel Lörtscher
5	Univ. of Mons Hinault	Victor Guestine; Jérôme Cornil; Roberto Lazzaroni



Recent examples taken from our own work demonstrating coupling of electron transport through individual molecules to ***A) charge*** *(Nature* ***425*** *(2003) 698),* ***B) spin*** *(Phys. Rev. Lett.* ***96*** *(2006) 206801,* ***C) vibrations*** *(Adv. Mater.* ***19*** *(2007) 281,* ***D) conformational changes*** *(Small* ***1*** *(2006) 973) and* ***E) proton transfer*** *(Nano Letters* ***6*** *(2006) 2184.*