# SELF-ASSEMBLED MOLECULAR DIODES ON SILICON

S. Lenfant, C. Merckling, D. Guerin and D. Vuillaume
*Institut d'Electronique, Micro-électronique et Nanotechnologie-CNRS*
*BP69, avenue Poincaré, F-59652cedex, Villeneuve d'Ascq (France)*
*Phone: +33 320 19 79 07, Fax: +33 320 19 78 84,*
*E-mail: stephane.lenfant@iemn.univ-lille1.fr*

We have recently demonstrated simple molecular rectifying diodes made of a π-group attached to silicon through an alkyl chain of a various length.[1] Another group has also demonstrated a negative differential resistance diode using a similar concept.[2] Current rectification was observed for the electronic transport though these Si($n^+$-type)/σ-π/metal junctions (with π=phenyl or thiophene), with rectification ratio up to about 37 and threshold voltages of in the range -0.3 to -0.9 V.[1]

***Here, we report on similar effect for a large number of π-groups of quite different chemical nature*** (pyrene, naphthalene, anthracene, terthiophene, quaterthiophene, anthraquinone, ethylene dioxyphenyl, ethylene dioxythiophene) ***with the aim of understanding how the π orbitals govern the rectification effect of the current-voltage curves***. We also demonstrate that changing from $n^+$-type silicon to $p^+$-type silicon (for a same given π-group) allow us to build complementary diodes, i.e. rectifying at negative or positive voltage, respectively.

The position of the π-orbital (with respect to the Fermi energies of the electrode) involved in the rectification phenomena is determined experimentally from the fit of a simple analytical model[3] of the current-voltage curve and from photocurrent experiments. A good agreement is found with our theoretical calculations for the different π-groups. Self-consistent tight binding calculations of the density of states for these Si/σ-π systems show that the rectification occurs due to a resonant tunnelling transport through the HOMO level of the conjugated group.[1] A recent attempt using acceptor groups (e.g. $C_{60}$ molecules) to get a resonant tunnelling transport through the LUMO, and thus a rectification effect for the opposite voltage (without changing the silicon doping), is in progress and will be reported at the conference.

This approach allows us to fabricate molecular rectifying diodes compatible with silicon nanotechnologies for future hybrid circuitries.

**References:**

[1] S. Lenfant, C. Krzeminski, C. Delerue, G. Allan, and D. Vuillaume, Nano Lett. **3,** 741-746 (2003).
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[3] I. R. Peterson, D. Vuillaume, and R. M. Metzger, J. Phys. Chem. A **105,** 4702-4707 (2001).