3D2.6 : Construction of QHC surface atomic circuit NOR and NAND gate on H:Si(100)

Unit 3-WP2: On-surface Atomic Scale Construction	**3D2.6:** Construction of QHC surface atomic circuit NOR and NAND gate on H:Si(100)
Lead participant: P10 (JUK Krakow); P9(Nottingham)	**Other participants:** P11 (IMRE Singapore)
Person Months (P10 Krakow)**:** 6; (P9 Nottingham): 24	**Person Months (other participant):** 1
Start date: 01/01/2011	
Planned End date: 31/12/2012	**Projected actual end date:** 31/12/2013

Description of the results:

The surface atomic structures of QHC Boolean logic gate were determined and optimized in Unit 2 (see the corresponding part of AtMol 3rd annual report). The practical construction of the selected QHC surface atomic circuits has been done following the appropriate STM tip-induced desorption protocols obtained in the previous reporting period as delivery 3-D2.3 of the Task 3-T2.2 (see 2nd AtMol annual report). STM-based extraction of H atoms to fabricate NAND gate has been performed by Krakow group (P10) on slightly doped H:Si(100) sample (p-type B doping) kept at liquid nitrogen (77K) temperature using Krakow's UHV LT STM system.

In the process of surface atomic circuit creation we used the following convention for encoding different Boolean logic operations depending on well determined surface network of dangling bonds: - the addition of two H atoms to the surface dimer encodes a logic "1" input, whereas two missing H atoms resulting in a dangling bond dimer encode a logic "0" input [H. Kawai et al., J. Phys.: Condens. Matter 24 (2012) 095911.].

The optimisation performed in Unit 2 consists of the determination of the proper H:Si(100) surface dangling bonds to be created for the corresponding quantum states to be manipulated while extracting one H dimer more per input. Without being interconnect to a drive and output metallic nano-pads in a full planar configuration, the gate truth table can be tested by dI/dV spectroscopy characterising how the surface states of this quantum circuit are shifted according to the binary input status. This spectroscopy testing is described in the report for deliverable 3D2.7.

In the first step of atomic circuit fabrication a simple follower design (H. Kawai et al., J. Phys.: Condens. Matter 24 (2012) 095911) has been constructed and is shown in Fig. 1. It is

seen that in going from left to right panel the circuit is open("OFF") when the logic input is "0" and closed ("ON")when the logic input is "1".

The Krakow group constructed a NAND gate and the resulting DB structures are shown in Fig. 2. It is striking that a change of the input from "00" to "11" causes a dramatic modification of the dangling bond structure appearance for both filled and empty states. Note that DB dimers are buckled in "00" gate structure for -2V at 77K. Such a buckling was not observed for the structures constructed in our previous work even at LHe temperature [1].

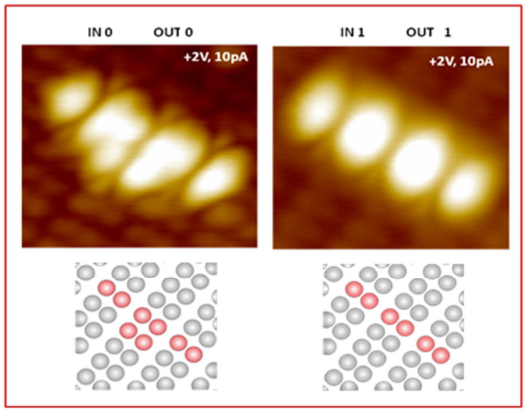

Fig. 1. *Construction of a dangling bond follower on a Si(100)-(2x1)-H surface. In going from left to right panel the circuit isOFF when the logic input is "0" and ON when the input is "1".*

P-11 has constructed the logic gates with other Boolean functions; namely, XOR and OR. The n-type phosphorus doped SiH was used as a substrate. The SiH was prepared in situ by conventional annealing followed by flashing. Hydrogen extraction was performed (Fig. 3) using the same protocol as described in the AtMol annual report for the year 2012 for Task 3.T2-2. The experiments were done using an Omicron LT-STM system at 4 K.

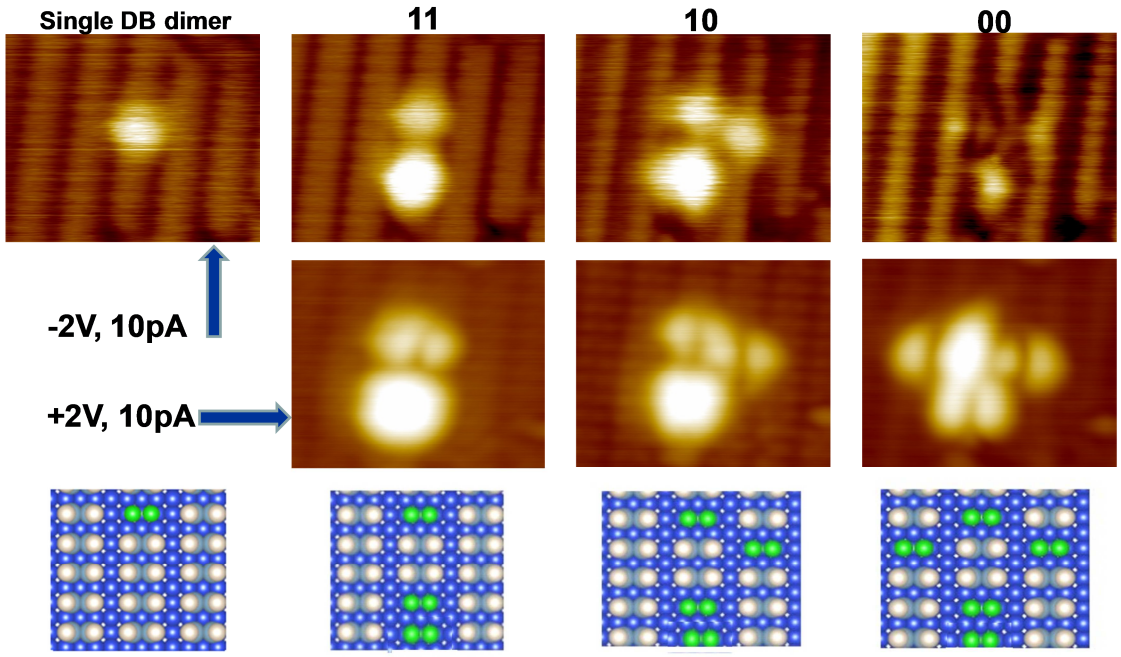

Fig. 2. *Construction of a dangling bond NAND logic gate on a Si(100)-(2x1)-H surface. The logic input values for different structures of the gate are given above the STM images. STM imaging parameters are -2V, 10 pA (upper row) and +2V, 10 pA (lower row) . The atomic structures of the DB dimer lines are shown below the corresponding STM images.*

Both single dangling bonds and dangling bond dimers can be created depending on the design of the logic gate. However, for the presented logic gates only single hydrogens were removed. Similar to Krakow's interpretation, the input function is "0" when there is a dangling bond and "1" when the bond is saturated. The dI/ dV spectroscopy of the created logic gates revealing the Boolean function is shown in the 3D 2.7 deliverable report. A schematic view of step by step construction of the gates is shown in Figs. 3 and 4.

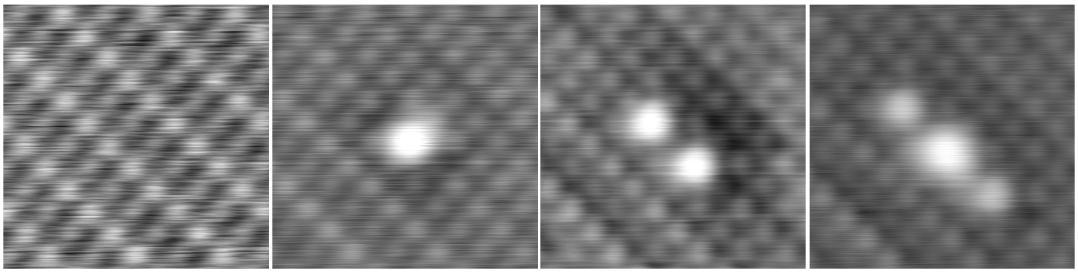

Fig. 3. *STM images of step by step construction of the XOR/OR logic gate at positive (+1.5 V; 20 pA) bias voltage*

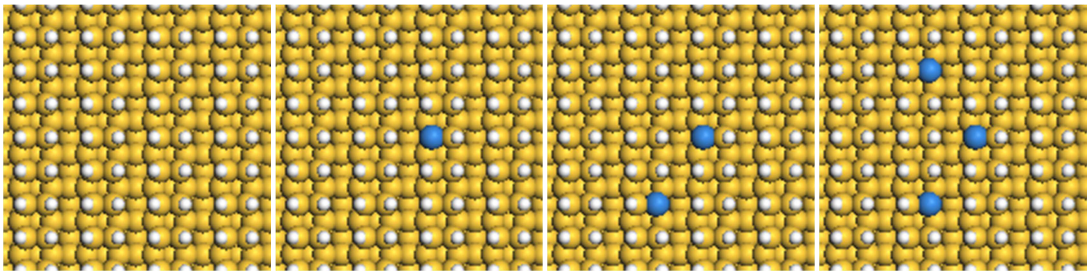

Fig.4. *Schematic view of the atomic structure of the XOR/OR logic gate*

Exploration of qPlus dynamic force microscopy for logic gate generation

A key objective of P9 (Nottingham) within work-package 3-2, as described in the AtMol proposal, is: "*Nottingham will use both qPlus- and STM-based extraction of H atoms from H:Si(100) to construct surface atomic circuits and thus encode different Boolean logic operations"*

From the start of the AtMol project, Nottingham has dedicated significant effort to exploring the efficacy of qPlus dynamic force microscopy for both imaging of hydrogen-passivated Si(100) and the generation of dangling bond patterns on H:Si(100) using a combination of experimental work and state-of-the-art density functional theory (DFT) calculations (carried out on a 1024 node high performance computing facility at the University of Nottingham). This work has produced three papers to date [3-5] and has been presented at five different international conferences thus far, including being part of keynote and plenary lectures.

Before briefly describing some of the key results associated with deliverable 3D2.6, it is important that we explain two points: P9's focus on atomic force microscopy (AFM), and, of course, the question of why deliverable 3D2.6 has yet to be delivered.

P9 has focussed on qPlus AFM as the manipulation tool for three key reasons: (i) AFM in principle should enable much more precise control over hydrogen extraction because it exploits single chemical bond formation, rather than a flow of tunnelling electrons, for imaging and manipulation; (ii) qPlus AFM also in principle will enable hydrogen *repassivation*, i.e. the transfer of a hydrogen atom from

the tip to a dangling bond (this is important for resetting an atomic logic gate); and (iii) to ensure complementarity of research objectives across the AtMol network.

Although, as part of progress towards deliverable 3D2.6, P9 published the first qPlus AFM study of the H:Si(100) surface [3], and a significant amount of time and effort has been dedicated to attempts to extract/restore hydrogen using qPlus AFM, our theoretical studies [4,5] have shown that the precise chemical nature of the tip, down to the single orbital level, plays an exceptionally important role in determining the efficacy of atomic manipulation attempts with AFM. A comprehensive series of imaging and force 'spectroscopy' experiments in parallel with this theoretical work clearly indicate that the apex of the scanning probe rapidly becomes hydrogen-terminated. This precludes hydrogen extraction. Indeed, even for a clean (i.e. silicon-terminated) tip, only certain classes of apex can yield reproducible hydrogen extraction [4].

Moreover, the commercial qPlus system (Createc) on which P9 carried out the H:Si(100) experiments is very far from being ideally suited for qPlus imaging and spectroscopy of semiconductor samples, exacerbating delays in sample throughput and analysis. (Partner P8 (Dresden) has experienced similar difficulties with this system). In late 2013, P9 therefore transferred its H:Si(100) activity to a separate UHV system equipped with an Omicron STM (but with no qPlus AFM facility). This also entailed transfer of the hydrogen passivation facility from the Createc to Omicron systems with consequent delays in the experimental programme.

A third frustrating delay has recently arisen because the postdoc employed on the AtMol project, Dr. Richard Woolley, left P9 in Dec. 2013 to take up a permanent position elsewhere at the University of Nottingham (in Engineering). Securing a postdoc for a year-long contract is always a challenge but a replacement for Dr. Woolley will start in Feb. 2014.

Fig.5 below shows a subset of qPlus AFM images of H:Si(100) which P9 has acquired in a series of experiments spanning almost a year. In each case, the atoms are resolved as depressions, rather than as protrusions. Indeed, we find that in 90% of our qPlus AFM data the atoms of the H:Si(100) surface appear as minima, rather than maxima, in constant frequency shift images. As we discuss in [3], and as was determined on the basis of a combination of experimental 'force spectroscopy' and theoretical calculations, this effect arises from hydrogen passivation of the tip apex.

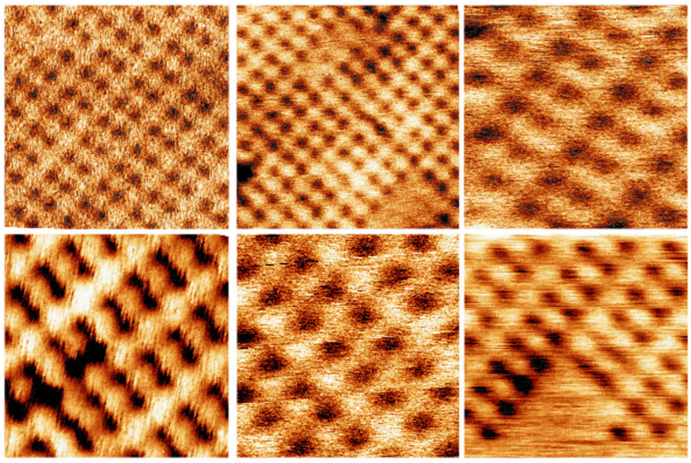

Fig. 5. Selection of constant frequency shift qPlus AFM images of the H:Si(100) surface. Note that in each case the atoms are imaged as depressions, rather than maxima.

Although it is possible to depassivate the tip via, for example, operation in STM mode (i.e. using the same types of vibrational heating desorption strategy exploited to remove hydrogen atoms from the surface), we find that there is a very strong propensity for the tip to become hydrogen terminated due qPlus AFM scanning. This becomes even more likely during force spectroscopy when the tip is pushed closer to the 'turn-around' in the interatomic potential such that high forces and force gradients are present.

Figs. 6(a) and (b) show two (of a number) of tip apices (and their associated orbital density) we have considered in theoretical studies of dynamic force microscopy imaging of the clean and H-passivated Si(100) surfaces. The remainder of the data in Fig. 6 provide an "at a glance" insight into the issue underpinning hydrogen depassivation with dynamic force microscopy: the orbital density/chemical reactivity of the tip plays a pivotal role in determining the possibility of extracting hydrogen from the surface. Despite the fact that both of the tip apices shown in Fig. 2(a) and (b) will produce very high resolution images in both STM and AFM modes, only the latter is capable of extracting hydrogen. Distinguishing between a variety of different tip types, each of which yields atomic resolution, remains a significant experimental challenge.

The upshot of our work on H:Si(100) to date is that it is significantly more difficult to exploit qPlus AFM for hydrogen extraction as compared to the tunnel current-derived vibrational heating process used for STM-derived depassivation. This is because the latter is not particularly sensitive to the precise orbital structure of the apex of the probe (the tip effectively acts as an 'electron source') whereas the fundamental chemical physics underpinning the acquisition of atomic resolution AFM images of semiconductors all relates to the chemical reactivity of the tip.

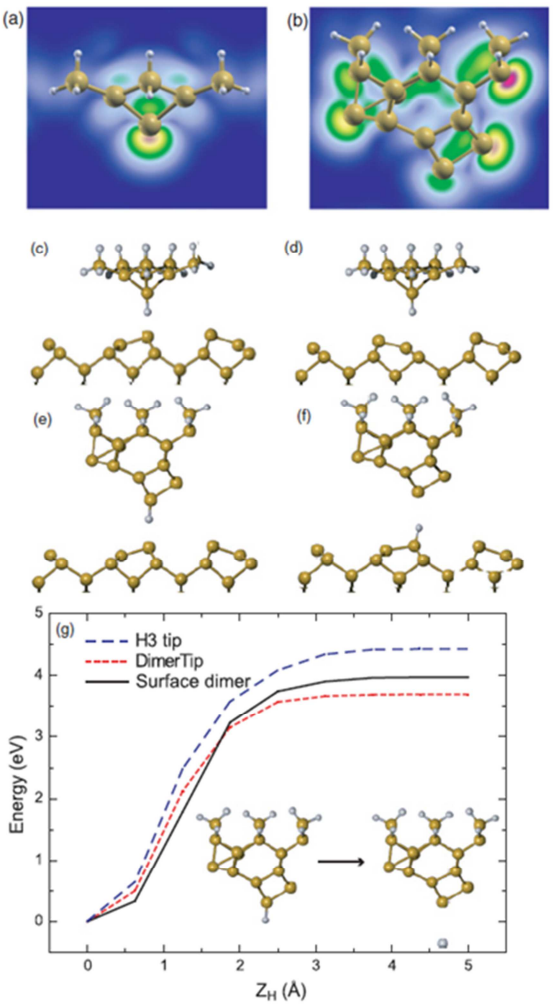

Fig. 6(a) Structurally rigid Si(111)-type tip apex; **(b)** dimer-like tip apex ; **(c)-(f)** Response of tip types shown in (a) and (b) to H-depassivation attempts ; **(g)** minimum energy pathway for removing a hydrogen atom from the surface upper dimer atom and from each tip type

Publications

[1] *Atomic scale fabrication of dangling bond structures on hydrogen passivated Si(001) wafers processed and nanopackaged in a clean room environment*, Marek Kolmer, Szymon Godlewski, Rafal Zuzak, Mateusz Wojtaszek, Caroline Rauer, Aurélie Thuaire, Jean-Michel Hartmann, Hubert Moriceau, Christian Joachim, Marek Szymonski, Applied Surface Science **288** (2014) 83-89.

[2] *Construction of atomic-scale logic gates on a surface of hydrogen passivated germanium*, Marek Kolmer, Szymon Godlewski, Jakub Lis, Bartosz Such, Lev Kantorovich, Marek Szymonski, Microelectronic Engineering 109 (2013) 262-265.

[3] *Identifying passivated dynamic force microscopy tips on H:Si(100),* P. Sharp, S. Jarvis, R. Woolley, A. Sweetman, L. Kantorovich, C. Pakes, and P. Moriarty Appl. Phys. Lett. **100**, 233120 (2012)

[4] *Role of orbital overlap in atomic manipulation*, S. Jarvis, A. Sweetman, J. Bamidele, L. Kantorovich, and P. Moriarty, Phys. Rev. B **85**, 235305 (2012)

[5] *Structural development and energy dissipation in simulated silicon apices*, S. P. Jarvis, L. Kantorovich and P. Moriarty, Beilstein J. Nanotechnol. **4**, 941 (2013)

Conference presentations

[invited] 4th European Nanomanipulation Workshop, Kraków, Poland, June 12-14, 2013, Szymon Godlewski: "Manipulation of single atoms and molecules on semiconductors - toward integration of prototypical switches"

[invited] 1st International Workshop on Nanopackaging, Grenoble, France, June 27-28, 2013, Marek Szymonski: “High resolution STM characterisation of dangling bond nanostructures fabricated on UHV de-bonded Si(001):Hx wafers” – invited oral presentation

18th Int. Conference on "Insulating Films on Semiconductors", INFOS 2013, Krakow, Poland, June 25-28, 2013, Marek Kolmer: “Atomic-scale logic gates on surfaces of hydrogen passivated germanium” – oral presentation

[poster] Int. Workshop on “Global Challenges - Opportunities for Nanotechnology”, Venice, Italy, April 15-18, 2013, Marek Kolmer: “Hydrogen passivated semiconductors as platforms for atomic-scale logic gates” – poster presentation

[Invited] “*Measuring manipulation and intermolecular forces using qPlus NC-AFM*”, A. Sweetman, NIST, Tsukuba, Japan. June 2012.

[Invited] “*Measuring manipulation and intermolecular forces using qPlus NC-AFM*”, A. Sweetman, OIST, Okinawa, Japan. June 2012

[Invited] “*Mechanical atom manipulation (and the Trouble with Tips)”*, P. Moriarty, 2013 Foresight Technical Conference: Illuminating Atomic Precision, Palo Alto, California, Jan. 11 – 13 2013

[Invited - Plenary] *“Mechanical Atom Manipulation”*, P. Moriarty, 6th Vacuum and Surface Sciences Conference of Asia and Australia, Islamabad, Oct. 9 – 13 (2012) [Declined due to family commitments]

[Invited] “*Mapping and Manipulating the Quantum World”*, P. Moriarty, Images and Visualisation, Norrköping, Sweden, 17 – 21 Sept. 2013

[Invited – Plenary] ""*Mechanical atom manipulation (and the Trouble with Tips)"*,P.Moriarty, Royal Society of Chemistry symposium on "Nanostructured Surfaces", Birmingham, Dec. 9 2012

[Invited – AtMol] "*NC-AFM 101*" and "*Manipulation of Matter at the Single Bond Limit*", P. Moriarty, Quantum Resources and Single Molecule Machines, AtMol Winter School, Les Houches, Jan. 28 2013

Probing chemical interactions at the Si(100):H surface, Sam Jarvis**,** Atomic Structure of Nanosystems from First-Principles Simulations and Microscopy Experiments, Helsinki, Finland - Stockholm, Sweden, May 15 - 17 2012

Measuring chemical interactions with dynamic force microscopy on H:Si(100), Sam Jarvis, ECOSS-29, Edinburgh, Sept. 3-7 2012

In addition to the presentations listed above, the Primary Scientist for P9 (Moriarty) will present aspects of the work associated with this deliverable during an invited talk at the upcoming American Physical Society meeting in Denver (March 5 2014)) and during a keynote lecture at the international MANA symposium at NIMS, Tsukuba on March 7 2014.