Preface

Driving the ultimate miniaturization of electronic circuits down to the atomic scale motivates the investigations of novel calculator and memory architectures and concepts, which involve a supported atomic structure or even a single molecule, to act as an independent calculating unit. This was the motivation of the third volume of the Springer Series "Advances in Atom and Single Molecule Machines" entitled "Architecture and Design of Molecule Logic Gates and Atom Circuits", to bring together the different theoretical architectures for a molecular or atomic systems to perform an elementary Boolean logic function at the quantum realm. For this new "On-Surface Atomic Wires and Logic Gates" Volume 10 of the series, we go a step further in this burgeoning field of atomic scale wires and circuits. To be more practical, this volume 10 is focussing on the hydrogenated (001) surfaces of silicon and germanium at a supporting surface to construct those calculating circuits atom by atom. On hydrogenated (001) surfaces, atom-by-atom extraction of single hydrogen can construct unique pre-designed and atomically perfect dangling bonds (DBs) structures with well identifiable states in the electronic band gap of those surfaces.

Starting from the description of two experimental processes to fabricate Si(100)H and Ge(0001)H surfaces, Chapters "Surface Hydrogenation of the Si(100)-2x1 and Electronic Properties of Silicon Dangling Bonds on the Si(100):H Surfaces"–"Si(100):H and Ge(100):H Dimer Rows Contrast Inversion in Low-Temperature Scanning Tunnelling Microscope Images" present the basic and measured electronic properties of DBs. This includes the standard laboratory ultrahigh vacuum (UHV) preparation protocols of passivated surfaces (Chapters "Surface Hydrogenation of the Si(100)-2x1 and Electronic Properties of Silicon Dangling Bonds on the Si(100):H Surfaces" and "Atomic Wires on Ge(001):H Surface"). In Chapter "Nanopackaging of Si(100)H Wafer for Atomic Scale Investigations", a more microelectronic industry like fabrication process is described with its nanopacking possibilities. Those chapters show also experimental strategies for atomic scale DB structures construction with the use of the scanning tunnelling microscopy (STM) vertical manipulation protocol. These results come together with a detailed analysis of DB electronic properties, which are determined experimentally by scanning tunnelling spectroscopy (STS) supported by advanced theoretical modelling methods. The combination of experimental and theoretical methodologies allows the identification of some interesting phenomena such as the formation of dispersive band structures during the DB wire atom-by-atom construction (Chapter "Atomic Wires on Ge(001):H Surface") or the counter intuitive half-row shift of STM constant current contrast observed for both Si(001H) and Ge(001)H substrates along the SiH dimer rows (Chapter "Si(100):H and Ge(100):H Dimer Rows Contrast Inversion in Low-Temperature Scanning Tunnelling Microscope Images").

In Chapters "Band Engineering of Dangling-Bond Wires on the Si(100)H Surface" and "Band Engineering of the Si(001):H Surface by Doping with P and B Atoms", the quantum engineering of the electronic structure of single and long DB wires is described. Chapter "Band Engineering of Dangling-Bond Wires on the Si(100)H Surface" details the geometrical arrangements of the DBs along single DB wires with the prospect to minimize the electronic energy band gap of those wires and increase the dispersion of their valence and conduction bands. This can also be obtained by a very specific surface doping with boron or phosphorus atoms well positioned along those long DB wires as described in Chapter "Band Engineering of the Si(001):H Surface by Doping with P and B Atoms".

Finally, different designs of simple Boolean logic circuits using DBs complemented by molecular latches are shown in next four Chapters. Starting from the experimental and theoretical analysis of atom-by-atom single DB wire construction and its corresponding STS characterization (Chapter "Electronic Properties of a Single Dangling Bond and of Dangling Bond Wires on a Si(001):H Surface"), Boolean logic circuits are described including purely atomic DB structures (Chapter "Quantum Hamiltonian Computing (QHC) Logic Gates") or with when necessary and for more realistic logical input, molecular latches adsorbed on hydrogenated surfaces (Chapters "The Design of a Surface Atomic Scale Logic Gate with Molecular Latch Inputs" and "Molecule Latches in Atomic Scale Surface Logic Gates Constructed on Si(100)H"). First experimental implantations of quantum Hamiltonian logic gates are also described. Volume 10 ends with Chapter "Complex Atomic-Scale Surface Electronic Circuit's Simulator Including the Pads and the Supporting Surface" describing what will be in the future an atomic scale circuit simulator expected to guide the construction of very complex DB logic circuits on hydrogenated surfaces.

Similar to the others volumes of the series, contributions included in this volume mainly result from a workshop organized by the AtMol and PAMS Integrated European projects. For this volume, it was the "International Workshop on Atomic Wires" held in Krakow from 10 September 2014 to 12 September 2014. Selected contributions were then completed by new results obtained in 2015 up to mid-2016 to finalize a volume in a comprehensive form.

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