Quantum Effects in Clusters and Nanowires

Project acronym: QCN

Coordinator: Prof. Dr. François Peeters

Report 2007-2009

April 2010
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<th>Description</th>
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<tbody>
<tr>
<td>AFD</td>
<td>Antiferrodistortive</td>
</tr>
<tr>
<td>AES</td>
<td>Auger Electron Spectroscopy</td>
</tr>
<tr>
<td>AFM</td>
<td>Atomic Force Microscopy</td>
</tr>
<tr>
<td>AMR</td>
<td>Anisotropic magnetoresistance</td>
</tr>
<tr>
<td>APW+lo</td>
<td>Augmented Plane Wave Method + local orbitals</td>
</tr>
<tr>
<td>BSE</td>
<td>Bethe-Salpeter Equation</td>
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<tr>
<td>B1</td>
<td>Hybrid Exchange-Correlation Functional</td>
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<td>CEMS</td>
<td>Conversion electron Mössbauer spectroscopy</td>
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<td>CMT</td>
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<td>CNM</td>
<td>Carbon NanoWall</td>
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<td>CNT</td>
<td>Carbon NanoTubes</td>
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<td>COK</td>
<td>Center for Surface Catalysis</td>
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<tr>
<td>CPM</td>
<td>Constant Photocurrent Method</td>
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<tr>
<td>CS planes</td>
<td>Crystallographic shear planes</td>
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<td>CVD</td>
<td>Chemical Vapour Deposition</td>
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<tr>
<td>DFT</td>
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<td>DFT-LSDA</td>
<td>DFT in Localized Spin Density Approximation</td>
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<td>DWNT</td>
<td>Double Walled carbon NanoTube</td>
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<tr>
<td>DWR</td>
<td>Domain wall resistance</td>
</tr>
<tr>
<td>d</td>
<td>Diameter</td>
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<tr>
<td>dc</td>
<td>Direct current</td>
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<tr>
<td>dV/dI</td>
<td>Differential resistance</td>
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<td>EBSD</td>
<td>Electron-BackScattered Diffraction</td>
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<td>EDX</td>
<td>Energy Dispersive X-rays</td>
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<td>EFTEM</td>
<td>Energy Filtered TEM</td>
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<td>ELISA</td>
<td>Enzyme-linked immunosorbent assay</td>
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<td>ELNES</td>
<td>Energy Loss Near Edge Structure</td>
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<td>EMAT</td>
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<td>EXAFS</td>
<td>Extended x-ray absorption fine structure</td>
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<td>Face Centered Cubic</td>
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<td>FD</td>
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<td>Field Effect Transistor</td>
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<td>FIB</td>
<td>Focused Ion Beam</td>
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<td>FLG</td>
<td>Few Layer Graphene</td>
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<td>FM</td>
<td>Ferromagnetic</td>
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<td>Ferromagnetic resonance</td>
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<td>FRAMs</td>
<td>Ferroelectric Random Access Memories</td>
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<td>FTIR</td>
<td>Fourier Transform Infrared Reflectivity</td>
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<td>FTPS</td>
<td>Fourier-Transform Photocurrent Spectroscopy</td>
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<td>FWO</td>
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<tr>
<td>LDOS</td>
<td>Local Density of States</td>
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<td>LECBD</td>
<td>Low Energy Cluster Beam Deposition</td>
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<td>LEED</td>
<td>Low Energy Electron Diffraction</td>
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<tr>
<td>LEID</td>
<td>Low Energy Ion Beam Deposition</td>
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<td>MBE</td>
<td>Molecular Beam Epitaxy</td>
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<td>MBPT</td>
<td>Many-Body Perturbation Theory</td>
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<tr>
<td>MC</td>
<td>Monte Carlo</td>
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<td>MD</td>
<td>Molecular Dynamics</td>
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<td>Magnetolectric</td>
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<td>MFM</td>
<td>Magnetic Force Microscopy</td>
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<td>MNM</td>
<td>Magnetization – magnetic field</td>
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<td>MRFM</td>
<td>Division of Molecular and Nanomaterials</td>
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<tr>
<td>MOKE</td>
<td>Magnet - Optical Kerr Effect</td>
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<tr>
<td>MS</td>
<td>Mössbauer spectroscopy</td>
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<td>MT</td>
<td>Magneto Transport measurements</td>
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<td>m</td>
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</tr>
<tr>
<td>NP</td>
<td>Nanoparticle</td>
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<tr>
<td>NRA</td>
<td>Nuclear Reaction Analysis</td>
</tr>
<tr>
<td>NW</td>
<td>Nanowire</td>
</tr>
<tr>
<td>PAC</td>
<td>Perturbed Angle Correlation Spectroscopy</td>
</tr>
<tr>
<td>PAW</td>
<td>Projector augmented wave</td>
</tr>
<tr>
<td>PC</td>
<td>Polycarbonate</td>
</tr>
<tr>
<td>PDA</td>
<td>Pyredocanoic Acid</td>
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<tr>
<td>PDS</td>
<td>Photothermal Deflection Spectroscopy</td>
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<tr>
<td>PECVD</td>
<td>Plasma Enhanced CVD</td>
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<tr>
<td>PIXE</td>
<td>Particle Induced X-ray Emission</td>
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<tr>
<td>PL</td>
<td>Photoluminescence</td>
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<tr>
<td>PNR</td>
<td>Polarized neutron reflectometry</td>
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<td>PS</td>
<td>Polystyrene nanospheres</td>
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<tr>
<td>pseudo-</td>
<td>Pseudo potential - self interaction</td>
</tr>
<tr>
<td>SIC</td>
<td>corrected approach</td>
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<td>PTIS</td>
<td>PhotoThermal Ionisation Spectroscopy</td>
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<tr>
<td>QDs</td>
<td>Quantum Dots</td>
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<tr>
<td>RBS</td>
<td>Rutherford Backscattering Spectrometry</td>
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<tr>
<td>RHEED</td>
<td>Reflection High Energy Electron Diffraction</td>
</tr>
<tr>
<td>RT</td>
<td>Room temperature</td>
</tr>
<tr>
<td>r1</td>
<td>Aspect ratio</td>
</tr>
<tr>
<td>S</td>
<td>Spectrometry</td>
</tr>
<tr>
<td>SAM</td>
<td>Scanning Auger electron Microscopy</td>
</tr>
<tr>
<td>SAM</td>
<td>Self-assembled monolayer</td>
</tr>
<tr>
<td>SBO</td>
<td>Strategisch basis onderzoek (Strategic basic research)</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning Electron Microscopy</td>
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<tr>
<td>SGM</td>
<td>Scanning Gate Microscopy</td>
</tr>
<tr>
<td>SHPM</td>
<td>Scanning Hall Probe Microscopy</td>
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<tr>
<td>SIESTA</td>
<td>Spanish Initiative for Electronic Simulations with Thousands of Atoms</td>
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<tr>
<td>SMEA</td>
<td>Spin and Molecular Electronics in Atomically-Generated Orbital Landscapes</td>
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<tr>
<td>SWNT</td>
<td>Single Walled NanoTube</td>
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<tr>
<td>SNOM</td>
<td>Scanning Near-field Optical Microscopy</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
<tr>
<td>----------</td>
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<tr>
<td>$f_{\text{m}}(H=0)$</td>
<td>Zero field resonance frequency</td>
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<tr>
<td>GGA</td>
<td>Generalized gradient approximation</td>
</tr>
<tr>
<td>GHz</td>
<td>Gigahertz</td>
</tr>
<tr>
<td>GL</td>
<td>Ginzburg-Landau</td>
</tr>
<tr>
<td>GMR</td>
<td>Giant magnetoresistance</td>
</tr>
<tr>
<td>GPLS</td>
<td>Gas Phase Laser Spectroscopy</td>
</tr>
<tr>
<td>GW</td>
<td>GW quasi particle method</td>
</tr>
<tr>
<td>H</td>
<td>Magnetic field</td>
</tr>
<tr>
<td>HAADF-STEM</td>
<td>High angle annular dark field scanning transmission electron microscopy</td>
</tr>
<tr>
<td>HMOD</td>
<td>Model Hamiltonian</td>
</tr>
<tr>
<td>HOPG</td>
<td>Highly Ordered Pyrolytic Graphite</td>
</tr>
<tr>
<td>HRTEM</td>
<td>High Resolution Transmission Electron Microscopy</td>
</tr>
<tr>
<td>Heff</td>
<td>Effective field</td>
</tr>
<tr>
<td>Hme</td>
<td>Magneto elastic field</td>
</tr>
<tr>
<td>$H_r$</td>
<td>Reverse field</td>
</tr>
<tr>
<td>$H_r$</td>
<td>Resonance field</td>
</tr>
<tr>
<td>II</td>
<td>Ion Implantation</td>
</tr>
<tr>
<td>IMO</td>
<td>Instituut voor Materiaalonderzoek (Institute for Material Research)</td>
</tr>
<tr>
<td>IR-MPD</td>
<td>Infrared multiple photon dissociation</td>
</tr>
<tr>
<td>IS</td>
<td>Impedance Spectroscopy</td>
</tr>
<tr>
<td>K</td>
<td>Kelvin</td>
</tr>
<tr>
<td>KFM</td>
<td>Kelvin Force Microscopy</td>
</tr>
<tr>
<td>keV</td>
<td>Kiloelectronvolt</td>
</tr>
<tr>
<td>kOe</td>
<td>Kilo-oersted</td>
</tr>
<tr>
<td>LDA</td>
<td>Local density approximation</td>
</tr>
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</table>

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I. Introduction

I.1 General information on the network

I.1.1 The project: Quantum effects in clusters and nanowires

The study of clusters and nanowires is a very important subfield in the area of nanoscience where the nanosize control of materials structures is realized in at least two dimensions. Nanoscience involves the understanding of physical and chemical phenomena at the atomic and molecular level. Nanotechnology provides the ability to precisely manipulate matter and energy at molecular scales. Based on unique electrical, magnetic, optical and structural properties of nanomaterials it will revolutionize existing architectures of computers or optical devices and lead to fundamentally new applications in, e.g., biomedicine and catalysis. Just as antibiotics, silicon transistors and plastics affected nearly every aspect of the society in the 20th century, nanotechnology will have profound influences in the 21st century.

The central objective is to design and control the structural, optical, magnetic, electrical and reactive properties through nano-engineering of the size, shape, structure, and composition of clusters and nanowires. Through the confinement of charges and spins a coherent control of the quantum mechanical states of the nano-device will be realized to achieve the desired physical properties for different applications.

Some key questions which are addressed in this project are:

- What is the influence of size and composition on structure and stability?
- How can the fundamentals of magnetism be understood (in particular ferromagnetism and superparamagnetism) through the investigation of very small magnets?
- What is the relation between structure (including the confinement geometry) and the functional properties (in particular optics, magnetism, electrical transport including superconductivity)?
- How can hybrid systems, where clusters and wires with different properties are combined at nanometer scale, be used in order to (i) understand these properties through their confrontation and (ii) create extra functionalities (e.g., magnetism and semiconducting behavior, superconductivity and magnetism)?
- To which extent does the chemical/physical environment of a cluster/nanowire modify its properties?

Our main effort is centered on clusters and nanowires consisting of metal (e.g., magnetic and superconducting or metals with different chemical properties), semiconductor, carbon and combinations of these materials (these are the so-called hybrid systems). We focus on the bottom-up approaches such as laser vaporization, ion implantation, electrochemical and vapor deposition (both physical vapor deposition, in particular molecular beam epitaxy and chemical vapor deposition) and self-assembly driven by chemical interactions to produce nanostructures, although the top-down (electron beam lithography) approach will not be discarded.

I. Introduction
Structural, chemical and electronic (including optical, magnetic and transport) characterization on different length scales (from nanometer to atomic size) are essential parts in the study. We use high-resolution electron microscopy, nuclear techniques with atomic probes and different types of local probe microscopy along with local chemical probing, SQUID based magnetometry, laser spectroscopy, X-ray reflectometry and others.

Computational studies are an important part of the research and are used for the interpretation of the experimental observations on the one hand and to provide feedback for an improved design and control of the physical properties of the systems on the other hand. Different modeling techniques, available in the proposed consortium (see details in Sec. I.3), ranging from Monte Carlo and molecular dynamics simulations, finite element and finite difference techniques to \textit{ab initio} approaches with different levels of sophistication. Genetic and other global optimization algorithms as well as multiscale approaches are also important techniques which are employed.

The contribution of the different partners is based on the available expertise and know-how of the partners (for more details, see Sec. I.3).

A single laboratory is not able to realize this program and an integrated effort was obviously necessary. In the previous IUAP/PAI V program on “Quantum size effects in nanostructured materials” the nanosize control of materials structures was realized in at least \textit{one} dimension. In the new network we go one fundamental step further and aim at realizing this control in at least \textit{two} and, finally, \textit{three} dimensions.

### I.1.2 Partners

<table>
<thead>
<tr>
<th>Partner</th>
<th>Name</th>
<th>Institution</th>
<th>Institution's abbreviation</th>
</tr>
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<tbody>
<tr>
<td>P1</td>
<td>PEETERS François</td>
<td>Departement Fysica, Condensed Matter Theory</td>
<td>UA-NANO</td>
</tr>
<tr>
<td></td>
<td>(Network Coordinator)</td>
<td>Universiteit Antwerpen</td>
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<tr>
<td>P2</td>
<td>VAN HAESENDONCK Chris</td>
<td>Departement Natuurkunde enSterrenkunde, Katholieke Universiteit Leuven</td>
<td>KULeuven (KUL)</td>
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<td>P3</td>
<td>PIRAUX Luc</td>
<td>Laboratoire PCPM, Université Catholique de Louvain</td>
<td>UCL</td>
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<td>P4</td>
<td>BOGAERTS Annemie</td>
<td>Departement Chemie, PLASMANT, Universiteit Antwerpen</td>
<td>UA-Plasmant</td>
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<td>P5</td>
<td>GHOSEZ Philippe</td>
<td>Institut de Physique, Université de Liège</td>
<td>ULg</td>
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<tr>
<td>P6</td>
<td>WAGNER Patrick</td>
<td>Instituut voor Materiaalonderzoek, Universiteit Hasselt</td>
<td>UHasselt-IMO</td>
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<tr>
<td>EU</td>
<td>PILENI Marie-Paule</td>
<td>Laboratoire des Matériaux, Mésoscopiques et Nanométriques, Université Pierre et Marie Curie</td>
<td>Paris LM2N</td>
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\textit{I. Introduction}
I.1.3 Budget

<table>
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<th>Name Partner</th>
<th>Institution</th>
<th>Budget (Euros)</th>
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<tr>
<td>P1 PEETERS François</td>
<td>UA-NANO</td>
<td>800 000</td>
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<tr>
<td>P2 VAN HAENSENDONCK Chris</td>
<td>KULeuven</td>
<td>1 250 000</td>
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<td>P3 PIRAUX Luc</td>
<td>UCL</td>
<td>1 200 000</td>
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<td>P4 BOGAERTS Annemie</td>
<td>UA-Plasmant</td>
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<td>P5 GHOSEZ Philippe</td>
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<td>P6 WAGNER Patrick</td>
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<td>EU PILENI Marie-Paule</td>
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<td>TOTAL BUDGET</td>
<td>4 547 250</td>
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</table>

I.1.4 Work Packages (WP)

WP1: Metallic and oxide clusters – leader: Dr. F. Remacle (P5)

WP2: Magnetic dots and wires – leader: Prof. K. Temst (P2)

WP3: Semiconductor quantum dots and wires – leader: Prof. S. Melinte (P3)

WP4: Superconducting nanosystems – leader: Dr. A. Silhanek (P2)

WP5: Carbon nanotubes and related materials – leader: Dr. E. Neyts (P4)
## I.2 History of the IAP Network

### Previous IAP-Phases

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<thead>
<tr>
<th>Phase I - IAP 1/12 (1987-1991)</th>
<th>Interphase Sciences</th>
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<td>KULeuven (Y. Bruynseraede)</td>
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<td>UCL (J.-P. Issi)</td>
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<td>UIA (F. Adams)</td>
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<td>UCL (P. Bertrand)</td>
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<td>UIA (F. Adams)</td>
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<td>UIA (R. Gijbels)</td>
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<td>UA-RUCA (G. Van Tendeloo)</td>
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<td>RUG (C. Dauwe)</td>
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<td>VUB (J. Vereecken)</td>
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<td>UA-UIA (F. Peeters)</td>
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<td>KULeuven (A. Vantomme)</td>
<td></td>
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<tr>
<td>Chalmers University of Technology – Sweden (B. Kasemo, T. Claeson)</td>
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<tr>
<td>Rheinisch-Westfälische Technische Hochschule (RWTH) – Germany (G. Güntherodt)</td>
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</tr>
</tbody>
</table>

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*I. Introduction*
The subsequent IAPs were characterised by an increased reduction of the scale and dimensionality of the materials and phenomena that were investigated. The first two IAPs concentrated on surfaces and interphases were the focus was on two dimensional physics and characterization was on the micrometer scale. In 'reduced dimensionality systems' the main accent was still on films and heterojunctions but inroads were made in lower dimensional systems as nanotubes, nanoparticles and quantum dots. In the previous IAP the effect of charge, spin and photon confinement on the electrical, magnetic and optical properties of nanostructured materials was investigated. The nanostructuring was mostly top-down and the nanosize control was in at least one dimension. The present IAP includes the bottom-up approach and focuses on quantum confinement in two and three dimensions.

In the last two IAPs there has been an increased participation of different theory groups contributing to theoretical modelling ranging from mean field to \textit{ab initio} approaches.

From the initial 4 groups participating in the IAP-phase-I only two groups (KUL and UCL) are still a part of the current IAP. Over the years new groups have emerged and (temporarily) incorporated in the IAP network if their expertise would bring added value to the consortium.

As an example of the evolution of the participation of research groups within the different IAP-phases, the involvement of the team UA-CMT of F. Peeters (P1) is discussed. In phase IV-IAP 4/10 the team UA-UIA (F. Peeters) was a young emerging research group that participated for the first time as a partner. In phase V-IAP 5/01 the team UA-CMT joined EMAT and participated as the coordinator group UA (G. Van Tendeloo). In the current phase VI-IAP 6/P42 the team UA-CMT and UA-EMAT are joined as the coordinating group UA-NANO.

Over the last 20 years the participating groups have been able to build up state-of-the-art characterization infrastructures and experimentation facilities.

\section*{I. 3 General Objectives of the Research Project and Partnership}

Except in the life sciences, there are only a few examples of materials that are naturally structured on scales of the order of a few to a hundred nanometers. Most nanostructured materials are synthetic. Important technological efforts have been made, driven by the increasing needs of the electronics industry, to understand and control the growth of semiconductors at the atomic level. In parallel to these developments, nanostructured materials have been developed by materials scientists and chemists. The science and technology of nanostructured materials is a broad and interdisciplinary field of research (from biology to physics and chemistry) and is currently at the forefront of science [1-3].

A comprehensive research program is proposed in the important subfield of clusters and nanowires. Because of the small dimensions, these systems enable direct observation of many quantum phenomena that would not otherwise be possible. The aim is to develop new nanoscale structures with an emphasis to control at different length scales with atomic precision the morphology, size, structure, composition and doping since these will define and enable control over physical properties. Understanding the fundamental physical properties of nanostructures is central to the rational development of functional devices, enables an efficient mechanism through coupling to synthetic studies for rapid variation and optimization of properties, and is central to discovery of potentially new device concepts.
The IAP-network combines nano-fabrication, characterization, measurement of physical properties, and theoretical modeling. Focus will be on bottom-up approaches, hybrid systems and new measuring, characterization and modeling approaches. Expertise in each area is present in the network (expertise of different partners is described in detail below).

The realization of new materials and more specifically nanomaterials can enable revolutionary versus evolutionary advances in science and technology. This motivated several industrial countries (USA, Japan, Germany, The Netherlands, …) to set up national programmes and initiatives (e.g., nanocenters) to advance the knowledge in nanoscience. In the 2005 ITRS (International Technology Roadmap for Semiconductors) [4] the growing importance of new nanoscale devices was stressed relying very heavily on new materials and new material properties. The IAP network joins the efforts of 6 research groups from 5 Belgian universities in the area of nanomaterials with one research group of France. It intends to give Belgium a leading position in the very promising subfield of clusters and nanowires.

The present proposal builds upon the base of activities and support by previous IAP’s. When compared to the previous IAP V programme on “Quantum size effects in nanostructured materials” where the nanosize control of materials structures was realized in at least one dimension, in the new network we go one fundamental step further and aim at realizing this control in at least two and, finally, three dimensions with a focus on the “bottom-up” paradigm.

**Specific objectives and research goals**

The research program is built around the central objectives to design and control the structural, optical, magnetic, electrical and reactive properties through nano-engineering of the size, shape and composition of clusters and nanowires. Through the confinement of charges and spins a coherent control of the quantum mechanical states of nano-size systems will be realized to achieve the desired functional properties for different applications.

*Fabrication* will be focused on the “bottom-up” paradigm. Different synthesis routes will be followed: gas phase, chemical, electro-chemical, electro-deposition, implantation…

*Characterization* is a critical part of any nanotechnology process. Highly specialized tools are required to measure physical and chemical properties at the nanoscale. The partnership houses a variety of advanced characterization techniques that are listed below in Table 1.

A combination of analytical and numerical tools, as well as computer simulations will be used in the *modeling* efforts which can be grouped into three main classes of approaches:

1) Model-type approaches based on, e.g., tight-binding, effective mass approximations, mean-field theory… where the resulting equations are solved using, e.g., finite difference and finite element techniques,

2) Ab initio approaches using established software like, e.g., ABINIT, SIESTA, GAUSSIAN, Wien2k…

3) Simulations: Monte Carlo, Molecular Dynamics…

To avoid a split up between theory and experiment, the theoretical groups are integrated into the different WPs in order to optimize the feedback and cross-fertilization between the modeling and the experimental activities.

Below we specify the objectives and research goals with reference to the different systems which we plan to study.

I. Introduction
METALLIC AND OXIDE CLUSTERS

Many years before nanoscience has been established as a new field of interdisciplinary research, both chemists and physicists were studying clusters as intermediates between atoms/molecules and bulk solids. Clusters, generally conceived as agglomerates of atoms or molecules in a size range where properties depend on their size in a non-scalable way, contain between a few and several thousands of atoms. Early cluster investigations led to the discovery of numerous emerging phenomena, e.g., the discovery of electronic shell structure in alkali and simple metal clusters, enhanced stabilities for densely-packed closed-shell structures, the discovery of buckminsterfullerenes, enhanced magnetic moments for small sizes, size-dependent catalytic activity for small noble metal clusters, and size-dependent optical properties of ligand stabilized nanoparticles [5]. Currently, fundamental research of nanoclusters continues building on ongoing developments of cluster synthesis and experimental methodologies, in close synergy with advanced theoretical studies. This is, for example, the case for mixed cluster systems, where adjusting composition may lead to new and improved nanomagnets, catalysts, and optical materials. Because of the richness and diversity of the properties of clusters and nanoparticles, and the ample possibilities of stabilizing them as individual units, they are considered as promising candidates for building blocks of tailored nanostructured materials [6]. The following objectives are defined where the synergistic interplay between experiment and theory will be crucial:

1) Determination of **design principles** for tailor-made cluster synthesis based on profound theoretical understanding through multi-scale modeling. Different complementary synthesis methods for metallic and oxide clusters and nanoparticles will be optimized for this purpose.

2) To understand the transition from **small clusters towards the bulk crystal structure**, in particular for binary and ternary systems. High-resolution transmission electron microscopy will be employed to determine the atomic arrangements and structure in combination with theoretical modeling. Classical modeling (molecular dynamics, Monte-Carlo) and first principles (density functional, quantum chemistry) approaches will be used.

3) To determine and describe the **physical, chemical, and optical properties** of (mixed) metallic and oxide clusters which, e.g., will be used as key input for the investigation of their magnetic and superconducting properties.

4) Insight into the influence of the **chemical environment** (organic ligands, embedding matrices, interfaces) of individual nanoclusters and assemblies of clusters (e.g., cluster-assembled films and arrays of ligand-stabilized nanoparticles).

MAGNETIC CLUSTERS AND NANOWIRES

The magnetic properties of materials with nanometer dimensions are substantially different from those of their bulk counterparts [7]. The spins at the surface of a nano-precipitate have a reduced coordination number, making the magnetic interaction highly anisotropic. Furthermore, interfacial interactions may result in interlayer coupling, magnetic frustration, or various kinds of magnetic anisotropy. Finally, as the total spin of a nanoparticle is very small, its magnetic properties may be dominated by single-domain behaviour, spin excitations, spin-fluctuations and quantum spin tunneling. To further advance the field, it is essential to fundamentally understand:

1) the **onset of magnetism** in nanoscale materials,

2) the origin of **magnetic anisotropy**,

3) **spin-dynamical effects** on the nanoscale,

4) **spin transfer** in nanowires.
The onset of magnetism in hybrid nanoscale materials is optimally studied in ultrasmall binary clusters. We will investigate whether the Slater-Pauling curve, describing the average value of the magnetic moment per atom as a function of alloy composition, continues to hold at the nanometer scale. Besides the 3d alloy clusters, magnetic clusters consisting of a 3d metal and a 4d or 5d metal and magnetic oxide clusters will be studied as well.

Exchange bias [8] results in a unidirectional anisotropy along the magnetic field when a hybrid ferromagnetic-antiferromagnetic system is cooled below the Néel temperature. The exchange interaction at the interface is strongly affected by the domain size of both the ferromagnet and the antiferromagnet. It is therefore interesting to investigate the anisotropy in single-domain particles. The focus will be on the prototype Co/CoO system. We will investigate oxidized Co dots that are obtained via MBE-growth followed by an in-situ oxidation process. We will also attempt to achieve oxidation via implantation of Co films. Finally, multilayers of electrodeposited oxidized Co pillars may yield new artificial domain structures as a result of the combination of shape anisotropy of the Co pillars and exchange anisotropy at the Co-CoO interface. Experimental results will be compared to theoretical models, taking into account the confinement of the systems.

For the study of the dynamic properties of ultrasmall magnetic clusters, the techniques of conversion electron Mössbauer spectroscopy and of nuclear resonant scattering of synchrotron radiation will be further developed, as they also could yield information on the spontaneous dynamics in the GHz regime [9]. The experimental results about the transition between the superparamagnetic and ferromagnetic behaviour will be combined with numerical modelling and theoretical studies. The high-frequency and dynamical properties of magnetic nanowires will be studied up to 50 GHz using ferromagnetic resonance. These wires are synthesized with accurate control of the composition, size and aspect ratio. This will allow investigating the various contributions to magnetic anisotropy in the nanowires. The Co nanowires can also be used as the source of a very large magnetic field gradient in magnetic resonance force microscopy (MRFM). In this respect, we will further develop MRFM detection with high spatial resolution. Finally, the GHz to THz superradiance from molecular magnets [10] in fast-sweeping magnetic fields will be investigated both experimentally – by using bolometers, network analyzers and time domain spectroscopy – and theoretically.

It was recently discovered that a large spin-polarized electrical current injected into a thin ferromagnetic layer can result in a switching of its magnetization or, under certain conditions, in a steady precession of the magnetization at GHz frequencies [11]. Such phenomena will be investigated in nanowired magnetic spin valves fabricated by electrodeposition in nanoporous alumina templates. This approach is very flexible and it was recently demonstrated that current densities as high as ~ 10^9 A/cm² can be achieved without degradation of the nanowire.

SEMICONDUCTOR QUANTUM DOTS AND WIRES

Semiconductor (SC) materials properties are especially sensitive to size reduction, and consequently their inclusion into modern opto-electronic devices requires an extreme control of their properties at nanoscale. For instance, the integration of silicon-based chips with III-V - based optoelectronic components that are at the heart of modern telecommunications networks is still unachieved. The ability to squeeze light out of nanometric silicon objects and create silicon optoelectronics would not only revolutionize telecommunications but would provide a means to remove electrical interconnects from integrated circuits. Semiconductor nanowires are particularly interesting as they are required to
interconnect functional units in nanoelectronics. Recently, using nanowires, novel semiconductor devices have been fabricated, including memories and biosensors. Clearly, the new quantum effects appearing at the nanometer scale might lead to unexpected high-tech applications [12]. We intend to synthesize, characterize and understand from a fundamental point of view the properties of semiconductor quantum dots (QD) and nanowires both free standing and in the presence of a substrate or embedded in a matrix.

The following main objectives can be defined:

1) To gain detailed understanding of the behavior of individual free standing SC nanodots and nanowires. The effect of the large fraction of surface atoms and of the geometric confinement on the nano-object properties has to be clarified and various techniques available will provide the required knowledge (EELS, TEM, PL, XRD, pulsed magnetic field, ab initio and \( k.p \) calculations...). Semiconductors dots, rings and wires (group IV, III-V, II-VI...) will be investigated, with a focus on the effect of composition, surface passivation, shape, ligands, and electro-magnetic field on the structural, optical (luminescence), dielectric (effective Coulomb interaction), and electrical properties (e.g., ferroelectricity).

2) Spin is the only internal degree of freedom for the electron. Employing it for creating new electrical or optoelectronic devices is the ambitious goal of spintronics. Abandoning magnetic elements and relying on spin-orbit coupling is the dominant concept of modern semiconductor spintronics [13]. To fully exploit the potential of nanostructured semiconductor materials for spintronics and quantum computation, it is necessary to better understand the dynamics of elementary excitations and, in particular, the dynamics of spin carriers. The spin dependent transport in 0D and 1D semiconductor nanostructures will be studied experimentally by local probes: scanning gate microscopy and electron force microscopy, both at very low temperature and high magnetic fields.

3) Determination and understanding of the optical properties of self-assembled quantum dots and rings, and molecular structures and networks made of them [14]. Investigation of the influence of a strong magnetic field (e.g., diamagnetic shift, Aharonov-Bohm oscillations) as a tool to obtain microscopic information on excitons and exciton complexes.

SUPERCONDUCTING NANOSYSTEMS

When a particle’s size is strongly reduced, quantum size effects of the superconducting properties will arise. In this project, we will study the size dependence of the superconducting properties and the critical parameters and we will investigate the electron pairing correlations at the nanometer scale. Experiments designed to gain insight in the size dependence of superconductivity are limited and leave many fundamental questions unanswered. Recent experiments deal on the one hand with measurements of the thermodynamic macroscopic properties of ensembles of small grains [15, 16]. On the other hand, pioneering tunneling experiments on individual nanoparticles could resolve the discrete energy spectrum in individual nanosize Al grains and revealed a spectroscopic gap strongly dependent on the number of electrons being odd or even [17]. In even smaller grains, where both the average spacing \( d \) between the discrete energy levels and the variations of \( d \) from grain to grain can significantly exceed the bulk superconducting gap \( \Delta \), pairing correlations can hardly be detected through tunneling spectra. Alternative ways to detect and study pairing correlations in ultra-small grains are necessary in order to address the fundamental problem of pairing correlations at the nanometer scale.

The main objectives are to investigate:

1) nanoscale evolution of \( T_c \) and the gap in individual 3D structures (smaller than the coherence length, so in fact, in real space we shall deal with 3D nanograins, nanocrystals and nanoclusters, but the effective dimensionality of superconductivity in these objects is 0D).

I. Introduction
2) confined condensate and phase-slip phenomena in superconducting nanowires.
3) controlling vortex patterns and achieving vortex manipulation in superconductors and S/F hybrids with nanoscale pinning centers and magnetic field templates.
4) superconductivity in cluster-assembled diamond films and nanodiamonds.

CARBON NANOTUBES AND RELATED MATERIALS

Carbon is a light, versatile element that exists in a number of hybridization states. Since their discovery in 1991, carbon nanotubes (CNT) have become a major research subject. These nanostructures are nearly perfect and made of pure carbon and the fact that large-scale production methods have been rapidly developed in the 90's are reasons for this fast and growing interest [18]. The physical (mechanical, electrical, thermal, optical...) and chemical properties of carbon-based materials can be tailored by tuning either the growth parameters and/or doping. The possibility to tailor their electronic and transport properties using defects, doping or functionalization is an open avenue for building nanoelectronic devices [19]. Nanostructures made of a few graphene layers have recently been discovered and display both gate controlled conductivity and massless fermionic behavior [20,21]. Nanodiamonds are promising clusters where on the one hand superconductivity can be observed at nanoscale [22] and on the other hand can be used to covalently immobilize biomolecules.

This project will focus on carbon nanotubes and, more generally, on carbon-based nanostructures (nanodiamonds, fullerenes, graphite containing only one or a few layers...). Within this rich field of research the following issues will be addressed:
1) Perfect carbon nanotubes exhibit ballistic transport that is strongly affected by doping and the presence of defects. Using transport and spectroscopic measurements, down to very low temperatures, and inelastic electron tunneling spectroscopy (IETS) in combination with semi-empirical and ab-initio simulations, we aim at a better understanding of the effect of both doping and defects.
2) Although growth of carbon-based nanomaterials is routinely performed on a large scale, the control of the atomic structure is rather limited (diameter, chirality and number of layers for CNTs; exact sp²/sp³ hybridization and doping composition for nanodiamond). To better understand the principles determining the growth, simulations of the growth mechanism will be performed at different scales: atomistic simulation, molecular dynamics and rate equations in a plasma CVD environment. In parallel the nucleation and growth characteristics will be studied in-situ at the atomic scale by Field Ion Microscopy combined with atom-probe Pulsed Field Desorption Mass Spectrometry. High resolution electron microscopy will complete the structural analysis of the produced carbon-based nanostructures.
3) Optical and electro-dynamical properties of carbon clusters (nanodiamonds, carbon multishell fullerenes) will be investigated. Several questions concerning the optical properties of nanodiamond remain unanswered: the role of nitrogen doping, the effect of the surface hydrogen passivation or the possible formation of diamond core surrounded by sp² shells. It is also believed that multishell spherical fullerenes have shielding properties for microwaves.

Education and Training

An important component of the proposed research is training and education of students in this highly interdisciplinary area, which includes theory, computational modeling, nano-fabrication, modern characterization techniques and advanced (local) measurements of physical properties. A vigorous
scientific investigation in a research university setting can only be effective if there is a synergistic blend of research and teaching activities. This is especially true for a young and dynamic interdisciplinary field such as nanoscience, for which there are no established textbooks, since the foundations of the field are being established in stride by active researchers working at the intersecting boundaries of several disciplines. Several partners are active in developing and implementing undergraduate and graduate educational modules in nanotechnology.

Providing hands-on research experience for advanced and highly motivated undergraduates is one of the most effective methods of training. In the new master program of the different universities laboratory work at a different university is required. The proposed IAP network is a perfect vehicle to streamline this exchange of students. These students will have the opportunity to experience the stimulating research environment at the different teams.

References

I.3.1 Main skills of the Partners

P1 - Name: PEETERS François

(including: D. Lamoen, W. Magnus, B. Partoens, M. Milosevic, D. Van Dyck, G. Van Tendeloo, S. Bals, and J. Verbeeck)

Institution: UA-NANO

Main Skills:

UA-NANO consists of the research groups CMT (Condensed Matter Theory, Prof. F. Peeters) and EMAT (Electron Microscopy for Materials Science, Prof. G. Van Tendeloo).

CMT has a long standing expertise in computational modeling of mesoscopic and nanostructured systems with emphasis on superconductors, semiconductors and hybrids. They have collaboration with several experimental groups over the world with joint publications. Finite difference and finite element techniques have been used to solve coupled nonlinear differential equations. First-principle calculations are pursued to model semiconductor clusters and nanowires.

EMAT has a long experience in advanced electron microscopy for characterizing materials on a nanoscale and even on an atomic scale. Particularly electron microscopy applied to nanosystems (layered materials, nanowires and nanoparticles) has been the main interest of the group in recent years. Advanced electron microscopy includes real space imaging on an atomic level, chemical information through EELS, on a (sub)nanometer scale, or on an atomic scale through HAADF-STEM and electronic information on a nanometer scale (through quantitative EELS). EMAT is an internationally renowned microscopy center, coordinating, e.g., the EU project ESTEEM (2006-2011), that groups the main European microscopy centers.

P2 - Name: VAN HAESENDONCK Chris

(including: P. Lievens, V. Moshchalkov, A. Vantomme, and K. Temst)

Institution: KULeuven

Main Skills:

The planned research activities involve the input of 5 professors of the Department of Physics and Astronomy who focus on solid-state physics at nanometer scale: Peter Lievens, Victor Moshchalkov, Chris Van Haesendonck, K. Temst and André Vantomme. Their present research activities are coordinated in the framework of a KULeuven “Concerted Research Action” program on “Magnetism and Superconductivity in Hybrid Nanosystems”. They are also members of the KULeuven “Institute for Nanoscale Physics and Chemistry” (INPAC), which provides a broader interdisciplinary nanoscience background involving 8 research teams of the Department of Physics and Astronomy and the Department of Chemistry.

In order to study the influence of nanostructuring and nanoscale confinement of charge, spin and photon on the physical properties, the KULeuven partner can rely on a unique collection of fabrication, characterization and physical measurement techniques. The available facilities include the “Ion- and Molecular Beam Laboratory” (IMBL), a facility in which *in situ* solid-state physical fabrication (MBE deposition, ion implantation and soft landing), characterization, and measurement technology is combined with nuclear solid-state physics techniques. Nanometer size mixed clusters
can be produced with laser vaporization sources and are studied in the gas phase with laser spectroscopy or after deposition on a substrate. Various scanning probe techniques can be applied down to low temperatures, while electrical transport, magnetic and optical properties can be measured in pulsed fields up to 70 T.

P3 - Name: PIRAUX Luc

*Including: V. Bayot, P. Bertrand, J.-C. Charlier, A. Delcorte, X. Gonze, S. Melinte, G.-M. Rignanese*

Institution: UCL

Main Skills:
The UCL partner has an outstanding experience in the fabrication, characterization and investigation of the physical properties (electrical, thermal, magnetic and high frequency properties) of nanostructured materials such as magnetic and superconducting nanowires, carbon nanotubes, quantum dots and various low-dimensional carrier systems.

The UCL partner has a recognized expertise in materials modeling and simulation from first-principles (ab initio) calculations and beyond (GW, TDDFT,...) to empirical techniques, including molecular dynamics, relying on high performance and parallel computing. It is synchronizing the development of the world-wide used ABINIT software.

The UCL partner has also a strong expertise and is fully equipped for the elemental, functional and structural characterization of surfaces and interfaces of inorganic and organic layers by the ionic spectrometries (TOF SIMS).

The UCL partner has micro-nanofabrication facilities ranging from e-beam lithography to electrochemical templating synthesis, ion implantation, thin film and submonolayer deposition techniques, high resolution electron microscopies (SEM-FEG; TEM), scanning tunneling spectroscopy, scanning gate microscopy, electron force microscopy...

P4 - Name: BOGAERTS Annemie

Institution: UA-Plasmant

Main Skills:
The research group PLASMANT has about 15 years experience with modeling of plasmas, by means of fluid dynamics, Monte Carlo or particle-in-cell / Monte Carlo simulations and hybrid models. In the last 4 years, research was focussed, among others, on the formation and behavior of nanoparticles in plasmas. This is an interesting and emerging new research field, with still many unresolved questions, which we hope to solve further in the coming years.

Equally in the last 4 years, research was started on molecular dynamics simulations for the deposition of thin amorphous carbon films. We now want to extend this study to the simulation of nanostructured carbon films (e.g., (ultra)nanocrystalline diamond) and carbon nanotubes.

Finally, in the last 3 years, research was started on the fluid dynamics modeling of processes occurring during and after laser-solid interaction (laser ablation), i.e., heating, melting and vaporization of the solid, vapor expansion and plasma formation.

I. Introduction
In the coming years, we want to use this model as a basis, for a description of nanoparticle formation occurring as a result of laser ablation, by various mechanisms.

P5  - Name: GHOSEZ Philippe  
(including: J.-Y. Raty, F. Remacle)  
Institution: ULg  
Main Skills:  
First-principles (DFT, TD-DFT, GW) and semi-empirical (tight-binding, model Hamiltonian fitted on ab initio results or experimental data) study of the properties of nanoparticles, nanoparticles arrays and nanowires. Specific expertise in the structural, electronic, dynamical, optical and transport properties as well as in the modeling of structural phase transitions controlled by external constraints (temperature, electric field, mechanical constraints). Active developer of the ABINIT software.

P6  - Name: WAGNER Patrick  
(including: H.-G. Boyen, K. Haenen, M. Nesládek)  
Institution: UHasselt-IMO  
Main Skills:  
UHasselt-IMO has more than 15 years experience in the deposition and characterisation of CVD diamond films and thin PVD AlN layers. The main studied topics are doped and undoped single crystal and microcrystalline diamond films. Since a couple of years, more focus is put on the novel ultra- (UNCD) and nanocrystalline (NCD) diamond films and thin layers of BN. Especially hexagonal BN has received a lot of renewed interest because of the peculiar opto-electronic properties of this material. Many structural, morphological as well as highly sensitive opto-electronic spectroscopic techniques are available within the research group such as x-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron-backscattered diffraction (EBSD), atomic force microscopy (AFM), Kelvin-probe force microscopy (KPFM), photothermal deflection spectroscopy (PDS), constant photocurrent method (CPM), Fourier-transform photocurrent spectroscopy (FTPS), photothermal ionization spectroscopy (PTIS), Fourier-transform infrared spectroscopy (FTIR), scanning near-field optical microscopy (SNOM), impedance spectroscopy and magnetotransport from cryogenic to elevated temperatures. The trend towards nanoscale science at Hasselt University is emphasised by the recent appointment of a professor of theoretical physics, who is specialized in nanoscale transport mechanisms. Also, a professor of experimental physics (specialized in nanostructures) will be appointed by the start of the academic year 2006/2007. Both colleagues will be actively involved in the current project proposal. Development of affinity biosensors based on the covalent binding of functional biomolecules (e.g., single-stranded DNA and proteins) to nanocrystalline diamond films.

I. Introduction
The “laboratoire des matériaux mésoscopiques et nanométriques”, LM2N is involved in the study of the collective physical properties (optical, electric, magnetic…) induced by the organization of inorganic nanocrystals. The LM2N has developed new routes of synthesis by soft chemistry, allowing the fabrication of nanocrystals differing by their size and/or their shapes. These nanocrystals can be assembled in 2D and 3D mesoscopic superlattices. Thus organization can be achieved with inorganic nanocrystals. The collective physical properties are mainly due to the dipolar interaction between the nanocrystals in the 2D or 3D organization. The structure of the mesoscopic assembly is one of the key parameters in the collective response. The LM2N is concerned by the fabrication of magnetic nanocrystals Cobalt, CoPt, ferrites and their organization in mesostructures and by the study of their magnetic properties at microscopic and macroscopic level.

The LM2N is concerned by the fabrication of metallic nanocrystals having optical properties like gold, silver, copper and by the study of their optical properties depending on the size, the shape and the level of organization (self-organized at 2D or 3D in ordered superlattices or disordered films).

The LM2N has also recently shown that the organization of silver nanocrystals in fcc supra crystals could induce intrinsic physical properties due to the organization. This opens a new way in the study of the physical properties of the organization of inorganic nanocrystals.
### I.3.2 Network instrumentation

**Table 1: Experimental tools and theoretical techniques of the partners**

<table>
<thead>
<tr>
<th>Fabrication</th>
<th>Characterization</th>
<th>Modeling</th>
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<tbody>
<tr>
<td><strong>P1</strong></td>
<td>SEM, TEM, STEM, XRD</td>
<td>EDX, EELS</td>
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<td><strong>P2</strong></td>
<td>MBE, LEID, II, sputtering, clusters, lithography, laser vaporization, LECBD</td>
<td>RBS/C, PIXE, NRA, XRD, RHEED, LEED, AES, AFM, STM, PAC, MS, CEMS, ToF-MS</td>
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<td><strong>P3</strong></td>
<td>ED, lithography, sputtering, II</td>
<td>SEM, HRTEM, XRD</td>
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<td><strong>P4</strong></td>
<td>MD, MC and fluid modeling</td>
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<tr>
<td><strong>P5</strong></td>
<td>ABINIT, SIESTA, GAUSSIAN, TB, HMOD</td>
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<tr>
<td><strong>P6</strong></td>
<td>sputtering, PEMWCVD</td>
<td>AFM, EBSD, FTIR, SEM, SNOM, TEM, XRD</td>
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<tr>
<td><strong>EU</strong></td>
<td>Chemical synthesis in solution</td>
<td>XRD, TEM, SEM, TED, AFM, VSM</td>
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</table>

*including transport, magnetic and optical

**Abbreviations:**

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AES</td>
<td>Auger Electron Spectroscopy</td>
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<tr>
<td>AFM</td>
<td>Atomic Force Microscopy</td>
</tr>
<tr>
<td>APW+lo</td>
<td>Augmented Plane Wave Method + local orbitals</td>
</tr>
<tr>
<td>CEMS</td>
<td>Conversion electron Mössbauer spectroscopy</td>
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<td>CPM</td>
<td>Constant Photocurrent Method</td>
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<tr>
<td>DFT</td>
<td>Density Functional Theory</td>
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<td>EBSD</td>
<td>Electron-BackScattered Diffraction</td>
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<td>Energy Dispersive X-rays</td>
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<td>Electron Energy Loss Spectroscopy</td>
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<td>EFM</td>
<td>Electrical Force Microscopy</td>
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<td>ELISA</td>
<td>Enzyme-linked immunosorbant assay</td>
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<tr>
<td>FD</td>
<td>Finite difference techniques</td>
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<td>FE</td>
<td>Finite element techniques</td>
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<tr>
<td>FTIR</td>
<td>Fourier Transform Infrared Reflectivity</td>
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<td>FTPS</td>
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<td>Gas Phase Laser Spectroscopy</td>
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<td>GW</td>
<td>GW quasi particle method</td>
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<td>HMOD</td>
<td>Model Hamiltonian</td>
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II. Research Results

WP1: Metallic and oxide clusters

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1. Aims and Objectives

At the molecular and nanoscale, the properties of bare and passivated clusters depend on their size and composition in a non scalable way and this non scalability is responsible for various emerging properties: e.g., electronic shell structure in alkali and simple metal clusters, enhanced stabilities for densely-packed closed-shell structures, buckminsterfullerenes structures for metallic clusters, enhanced magnetic moments for small sizes, size-dependent catalytic activity for small noble metal clusters, and size-dependent optical properties of ligand stabilized nanoparticles. In addition to providing an understanding and to characterizing the properties of nanostructures, essential objectives of WP1 are to predict and control the emergence of new properties in nanoscale structures in order to engineer tailored multi-functional nano-structured materials.

The detailed four main objectives of WP1 below rely upon the synergistic interplay between experiment and theory:

1. Provide understanding about the transition from small clusters towards the bulk crystal structure and the emergence of new properties, in particular for binary and ternary systems. High-resolution transmission electron microscopy will be employed to determine the atomic arrangements and structure, together with theoretical investigations. Classical modeling (molecular dynamics, Monte-Carlo) and first principles (density functional, quantum chemistry) approaches will be used.

2. Determination of design principles for tailor-made cluster synthesis based on theoretical understanding through multi-scale modeling. Different complementary synthesis methods for metallic and oxide clusters and nanoparticles will be optimized for this purpose.

3. To determine and characterize the physical, chemical, and optical properties of (mixed) metallic and oxide clusters which, e.g., will be used as key input for the investigation of their magnetic and superconducting properties.

4. Insight into the influence of the chemical environment (organic ligands, embedding matrices, interfaces) of individual nanoclusters and assemblies of clusters (e.g., cluster-assembled films and arrays of ligand-stabilized nanoparticles).

2. Scientific activities and results

2.1 Metallic and oxide clusters

Progress towards the first three objectives of WP1 requires the investigation of the physical properties of isolated clusters, as these are the building blocks for designing applications for catalysis. Various doped metallic and semi-conducting clusters were investigated experimentally by P2-KULeuven. The reactivity of doped nanometric size gold clusters was theoretically investigated by P5-ULg. Another theoretical study, undertaken by P4-Plasmant also aims at a better understanding of catalysis, this time in the context of the control of the synthesis of SW-CNT by size selected Ni NP.
2.1.1 Cluster synthesis and structure

P2-KULeuven investigated the following clusters, semi-conducting and metallic, with emphasis on doped coin metal ones. The self-organization properties of these clusters were also characterized. The work carried out belongs to objectives 1, 2 and 3.

Structure of pure and doped Si clusters. The structure of pure Si ($n = 6 – 21$) and doped Si$_n$X ($n = 6 – 20; X = Cu, V, Mn$) clusters, prepared in a laser vaporization source, was investigated by infrared spectroscopy (P2, i.c.w. the Chemistry Department at K.U.Leuven and FHI Berlin, G. Meijer). This has led to the identification of the structure of pure Si and several doped Si clusters by means of IR multiple photon dissociation (IR-MPD) combined with the atom messenger technique at the FELIX facility (Nieuwegein, the Netherlands). Adding a dopant atom to a Si backbone structure facilitates the formation of cage-like structures. Both, for Ar physisorption and IR-MPD experiments a transition between exo- and endohedral structures is observed depending on the dopant atom. Vibrational information on neutral Si clusters was obtained via tunable IR-UV two-color ionization.

Stability of doped Ge, Si and Li clusters. An experimental and theoretical study of Li-doped Ge clusters focused on the periodic appearance of abundance peaks in the mass spectrum, corresponding to Ge$_n$Li$_m$ ($n=6–20, m=5–12$). This clearly suggests the existence of the Ge$_n$ building block, which is a well-known feature for the group-14 elements. Theory supports the fact that doping with Li atoms enhances the stability of the Ge cluster, in which the Li atom mainly acts as a charge balancer. In smaller Li doped Ge and Si clusters (5-11 atoms) the Li atom can also take a substitutional position, resulting in more stable structures. The stability of small Ge-doped Li clusters ($Li_nGe^{n+}$ ($n=1–7$) shows odd−even alternation for both neutral and cationic clusters. Because of electronic shell closure, the 8- and 10-electron systems have enhanced stability, with the 8-electron species ($Li_nGe, Li_nGe^+$) more favored than the 10-electron ones ($Li_nGe, Li_{n-1}Ge^+$). Ge- and C-doped Li clusters behave differently due to the difference in atomic radii.

Structure of doped noble metal clusters. Neutral Y-doped Au clusters were investigated by IR-MPD. Besides the structure assignment of these clusters, also the fluxional behavior of Au$_6$Y was calculated. The corresponding Au$_6$Y anion has a planar cyclic D$_{6h}$ form and can be regarded as a σ-aromatic six-member ring. Fragmentation studies on doped Au and Cu clusters (Au$_n$X$:X= Y, Er, Nb and Cu,X$:X= Sc, V, Fe, Co) show the most stable structures as well as the fragmentation channels for both pure and doped clusters. For doped clusters, monomer evaporation is the most likely fragmentation channel with the exception of Au$_{18}$Y$^+$ and Au$_{20}$Y$^+$ for which gold dimer evaporation is also observed. The dissociation energies show an odd−even staggering and enhanced stabilities for certain cluster sizes, in agreement with electronic shell model predictions.

2.1.2 Doping of Au$_{20}$ cage conformers

When their size is large enough, metallic clusters can take cage structures, with the ability to trap atoms or small molecules in a similar way to C$_{60}$. It is expected that it should be possible to manipulate reactivity of the surface atom through the chemical nature of the dopant atom and thereby control the catalytic activity of the gold cluster. Several low-energy nanosize Au$_{20}$ hollow cage clusters in three charge states $Z=0, ±1$ were identified by P5-ULg(TPC) using ab initio quantum chemistry computations at the DFT level and their properties compared with the ground-state cluster Au$_{20}$($T_d$). Their energies lie within a 2 eV interval above the Au$_{20}$ ($T_d$) which suggests that some of the identified hollow cages may be experimentally observable. Hollow cages are characterized by the existence of a void inside the cage. Special attention was devoted to understanding which structural transformations the void undergoes as the cluster charge state alternates from 0 to ±1, under, for example, ionization and electron attachment. General trends of the void reactivity in

![Fig. WP1.1: MEP mapped from -0.016 (red) to +0.016 (blue) $\epsilon/(4\pi\epsilon_0a_0)$ onto the 0.001 $e^2/\AA^3$ isosurface of the one-electron density $\rho(r)$ for cages I, II, and III respectively. $\rho(r)$ is computed at the B3LYP computational level. In the color coding, green corresponds to a neutral MEP.](image-url)
hollow gold cages in relation with the confinement of a guest atom or molecule into the void region were identified, based on the analysis of the molecular orbital patterns and of the molecular electrostatic potential (MEP) (figure WP1.1).

We show computationally that rare gas atom He, Ne and their dimer He2 and Ne2 can be trapped in these voids and analyze how their trapping modifies the MEP. Both endohedral and exohedral doping by CO is computed to be stable while the trapping of the polar LiF molecule is exclusively endohedral (see figure WP1.2). These studies show that doping can be used to manipulate the reactivity of the cluster and that the analysis of the MEP characteristics is a good prediction tool. This work contributes to objectives 2 and 4.

2.1.3 Numerical study of the size dependent melting mechanisms of nickel nanoclusters

The unique electronic, mechanical and optical properties of carbon nanotubes (CNTs) render these materials excellent candidates for application in numerous fields, including microelectronics, medical applications and materials science. CNTs can be produced by catalytically decomposing hydrocarbons on metal catalyst NP. Depending on the phase state of the NP, the formed C-atoms may or may not diffuse in the particle, affecting the possible growth mechanism. P4-UA Plamant studied the size dependent melting mechanisms of Ni NP with size applicable for Single Walled CNTs (SWNTs).

Molecular dynamics simulations using a recently developed interatomic many-body potential were carried out to investigate the melting mechanism of nickel nanoclusters with sizes between 1 and 2 nm diameter, which are typically used for the catalytic growth of single walled carbon nanotubes. The melting process was followed by monitoring the cluster Lindemann index (see figure WP1.3), the caloric curve, and the atomic Lindemann indices of each investigated cluster. In agreement with literature, a linear decrease in melting temperature is found with increasing inverse diameter. A gradual transition from a dynamic coexistence melting mechanism for the smallest clusters (diameter ~ 1 nm) to a surface melting mechanism for the larger clusters (diameter ~ 2 nm) is observed. These results may be of importance for understanding the catalytic nucleation process of SWNT’s from nickel clusters with sizes between 1 and 2 nm. This work belongs to objectives 1 and 2.

2.2 Interaction with organic molecules and environment: hybrid complexes

Changing the environment of nanoparticles often offer a very good handle on controlling their properties in view of applications to catalysis, sensing, storage medium and logic applications. The WP1 partners have undertaken several efforts in this direction both experimental and theoretical. The progress made relates on the long term to objective 4 and also to objectives 1 and 2. Joint work of P2-KULeuven and P1-UA-NANO shows that hydrogenation can be used to modify the size distribution of the Pd-Au NP. These two groups also used insulin fibrils as a template to form helical patterns using Ag NP. Finally, P5-ULg investigated theoretically the effect of ligation and solvation on the electronic properties of Au55 NP and on the redox process occurring when Au55 is functionalized by a redox active ligand.

Fig. WP1.2: The endohedral LiF@Au20 complex. Li forms 8 bonds with the neighboring Au atoms which bond lengths in the interval 2.65 – 2.92 Å. F forms a single bond with Au (2.504 Å).

Fig. WP1.3: Calculated melting points for the investigated clusters of different sizes, based on the cluster Lindemann index (+, lower line) and the total energy (x, upper line).
2.2.1 Pd-Au bimetallic nanoclusters upon hydrogenation

In collaboration with P2-KU Leuven, P1-UA-NANO has investigated the effect of hydrogen on Pd-Au bimetallic nanoclusters using Z-contrast STEM. The nanoclusters were deposited by P2 on TEM grids by dual-target dual-laser vaporization and half of the identical samples were exposed to hydrogen at 1 bar for 2 hours. The intensity in Z-contrast images can be interpreted in terms of sample thickness and composition and in this manner, particle size and average intensity are obtained for many particles from a large number of Z-contrast images. An example of such an image is shown in Figure WP1.4. A change in size distribution is found for the nanoclusters before and after hydrogen treatment. This is interpreted as being the result of hydrogen induced Ostwald ripening. The palladium and gold atoms must have moved freely over the amorphous carbon layer. Furthermore, this study indicates that after hydrogenation the smaller nanoclusters have a higher gold content (from 24% Au to 38 ± 2%). This work mainly fits within objectives 1 and 2.

2.2.2. Ag nanoparticles deposited on insulin fibers

Silver-coated insulin derived amyloid fibrils, prepared by P2 were characterized by TEM by P1-UA-NANO. The challenge here is to simultaneously image a hard (Ag particles) and a soft (insulin fibrils) compound. For this purpose Z-contrast TEM was found to be very useful. This study demonstrates that the Ag particles are clearly deposited along the amyloid fibrils and are found to form a nanochain of particles. Interestingly, a helical pattern of the nanoparticles was often found, which is in agreement with previous AFM data carried out by P2. Unfortunately, TEM images are only 2D projections of 3D nanochains. To visualize the 3D arrangement of the Ag particles along amyloid fibrils, 3D reconstruction was done by electron tomography.

The result of this procedure is shown in Figure WP1.5 and confirms that the particles indeed form a helical pattern, in agreement with the helical structure of the amyloid fibrils. This study is complemented by optical measurements carried out by P2, which show the presence of a circular dichroism band, in agreement with a helical arrangement of the Ag particles. Besides the helical arrangement of the particles, no specific periodicity was found, indicating that the interaction between the particles and the insulin is probably electrostatic. This knowledge has been used as an input for theoretical modeling of these systems. This work was carried out by Prof. M. Milosevic (P1-CMT). This work mainly fits within objective 2.

2.2.3 Theoretical investigation of ligation and solvation effects on Au55

P5-ULg (TPC in collaboration of CMT) has undertaken detailed quantum chemistry ab initio studies, at the DFT level, of the structural, electronic and redox properties of the Au55 cluster, bare, ligated by a non redox active ligand shells, Au55(PH3)12, Au55(PH3)2Cl6, Au55(SCH3)32 and Au55(SCH3)42. Au55(PH3)2Cl6 is a good model for the well characterized Au55(PPh3)12Cl6, as the H atoms induce about the same strain as the phenyl group on the Au55 core. We then studied the redox activity of the functionalized...
The Au$_{55}$($\text{SCH}_3$)$_{41}$($\text{S(CH}_2)_2\text{CO}_2$(CH)$_2$)$_{10}$bp$y^{2+}\cdot2\text{Cl}^-$ cluster (bp$y$ is bipyridine) in three charge states, positive, negative and neutral. It was shown experimentally\textsuperscript{10} that applying a negative potential to the surface triggers a mechanical motion of the ligand towards the latter which when the potential is sufficiently negative, allows for an electron transfer to the bp$y^{2+}$ unit which is reduced in bp$y^+$. In addition, the effect of a water layer of 54 molecules was also studied for Au$_{55}$, Au$_{55}$(PH$_3$)$_{12}$Cl$_6$, Au$_{55}$($\text{SCH}_3$)$_{42}$ and for Au$_{55}$($\text{SCH}_3$)$_{41}$S($\text{CH}_2$)$_2\text{CO}_2$(CH)$_2$)$_{10}$bp$y^{2+}\cdot2\text{Cl}^-$, 21 H$_2$O were added around the bp$y$ unit. Our computations were carried out at the DFT, B3LYP/6-31G+(d) level with the LANL2MB RECP pseudo potentials and a simple dzeta basis set on the gold atoms, as implemented in the Gaussian03 suite of programs. All the structures were fully relaxed and geometrically optimized. The initial geometries of the ligated and solvated complexes were first optimized using the VASP solid-state plane wave implementation of the DFT in collaboration with P5-CMT.

We found\textsuperscript{11} that taking explicitly the effect of a water layer is essential for describing the electronic properties, such as the charging energy and the metal or insulator character. The reason is that the water molecules engage in a network of H-bonding with the ligand shell which reduces the charge transfer from the outer shell of gold atoms to the ligands and lowers the values of the charging energy, in agreement with experimental studies of P6-UHasselt for Au$_{55}$(PH$_3$)$_{12}$Cl$_6$.\textsuperscript{12}

In the case of the redox active bp$y$ ligand, three complexes were investigated, Au$_{55}$($\text{SCH}_3$)$_{41}$($\text{S(CH}_2)_2\text{CO}_2$(CH)$_2$)$_{10}$bp$y^{2+}\cdot2\text{Cl}^-$, the partially solvated Au$_{55}$ ($\text{S(CH}_2)_2\text{CO}_2$(CH)$_2$)$_{10}$bp$y^{2+}\cdot2\text{Cl}^-$. 21 H$_2$O complex and the thiol passivated Au$_{55}$($\text{SCH}_3$)$_{41}$($\text{S(CH}_2)_2\text{CO}_2$(CH)$_2$)$_{10}$bp$y^{2+}\cdot2\text{Cl}^-$. 21 H$_2$O one. The optimized geometries for the neutral complexes are shown in figure WP1.6. We chose the dense layer (SCH$_3$) passivation to mimic the short alkane thiol SAM that is used in the experiment to protect the gold surface. Au$_{55}$($\text{SCH}_3$)$_{42}$ has not been identified experimentally. The only thiolated Au$_{55}$ that has been experimentally identified is Au$_{55}$(SC$_{18}$)$_3$$_2$\textsuperscript{13} where the dilution of the ligand shell leads to the formation of Au-S-Au bridges. Our computations, not shown, also converged to a ligand shell with Au-S-Au bridges for the model cluster Au$_{55}$(SCH$_3$)$_{32}$ but it turned out that the dilute thiolated shell is not a good model for anchoring the bipyridine ligand. In figure WP1.6, we can see that the effect of the thiol layer is indeed to protect the Au$_{55}$ core and to prevent the formation of the cavity that is formed when a single thiolated bp$y$ ligand is anchored on the bare Au$_{55}$ (figure WP1.6a). In the relaxed geometries of the cationic, neutral and anionic overall charge states of the Au$_{55}$($\text{Slink-bpy}$)$_{21}$H$_2$O complex the shortest distance between the bp$y$ unit and the Au$_{55}$ core is observed for the negatively charged complex. It is equal to 5.23 Å. In the neutral the distance increases to 5.39 Å and to 5.57 Å in the positive one. Moreover, the analysis of the charge distribution of the negatively charge cluster shows that in the relaxed geometry, a significant part of the excess charge is localized on the bp$y$ unit while if the charge distribution of the negative ion is computed at the geometry of the neutral all the excess charge is localized on the Au$_{55}$ core. We interpret the charge transfer as a redox process between the negatively charge core and the positively charge bipyridinium ion, bp$y^{2+}$. The geometric reorganization leads to a shortest Au$_{55}$-bp$y$ unit distance, $l$ and is accompanied by a charge transfer that will be manifested by a molecular
hysteresis in the cyclic voltammetry (CV) for the redox process between the neutral and the negatively charge complex. Such a charge reorganization does not occur in the cationic state where the default of charge remains localized on the Au$_{55}$ both at the geometry at the neutral and after geometry relaxation. We have shown previously that hysteresis was a key aspect for implementing set-reset machines by cyclic voltammetry. The hysteresis can be either a current hysteresis induced by the finite rate of mass transfer to the electrode or a molecular one, due to a molecular change of geometry following the addition or removal of an electron. While our previous implementation on a copper rotaxane was realized in solution, the implementation that we have designed is for a self-assembled monolayer anchored on a surface.

These studies contribute to objectives 2, 3 and 4.

2.3 Monolayer and self-assembled nanoparticles

The studies reported in this section investigate how one can control the self-assembly of NP’s by controlling their individual properties, their environment and the template over which they self-assemble. P1-UA-NANO and P-EU have jointly studied the stability properties of 2D ordered and non-ordered assemblies of C-Co oxide core shell nanostructures. It is found that an ordered 2D structure is important for their stabilities. The arrangement of small size inclusions of Pb NP’s in a Si matrix was shown by P1-UA-NANO and P2-KULeuven to exhibit a special epitaxial relation with the Si matrix. The influence of the structure of the surface was also studied by P2-KULeuven for the self-organization of Fe-Silicide nanostructures. All these studies are very important for catalysis design. Finally, the composition fluctuation in FePt alloy NP’s as a source for supermagnetism in arrays of ferromagnetic NP’s was studied by P6-Hasselt in view of application to data storage. These studies belong to objective 4.

2.3.1 Self-assembly of Co-Co oxide core shell nanostructures

In collaboration with P-EU, cobalt–cobalt oxide core-shell nanostructures were investigated by P1-UA-NANO using different transmission electron microscopy (TEM) techniques. These NP are synthesized by P-EU from micelles in solution and they can self-assemble in 2D or 3D hexagonal arrays upon deposition on a grid. When exposed to air, cobalt–cobalt oxide core-shell NP form. The goal of this study was to prove a larger (chemical) stability (lower tendency to full oxidation and coalescence) of the particles arranged in 2D arrays, compared to the non-arranged and isolated particles.

Conventional TEM images and Z-contrast scanning TEM (STEM) images are taken to visualize the cobalt particles before oxidation and the core-shell particles after oxidation (see Figure WP1.7). The structure of the particles and core-shell structures is furthermore investigated by electron diffraction and high resolution images. To prove the chemical composition of the core and the shell, energy-filtered TEM and electron energy-loss spectroscopy are used. Using these techniques it has been shown that isolated or semi-isolated (at the edge of an array) particles form core-shell Co-CoO structures faster than hexagonally arranged particles, and that these structures have a larger tendency to coalesce and totally oxidize compared to...
2.3.2 Pb nanoclusters synthesized in Si by ion implantation

In collaboration with P2, P1-UA-NANO has investigated high dose ion implantation of Pb in a crystalline Si matrix. This implantation results in segregation of Pb and the formation of small size inclusions. High resolution images show that these inclusions show a specific epitaxial relation with respect to the Si matrix and it was found that the number of the smallest clusters increases for lower annealing temperatures of the sample. In addition the 3D size distribution of the samples was investigated. This was done using electron tomography using a full tilt range of 2D projections. This is remarkable since usually a so-called missing wedge of information is present in this type of experiments. An example of a 3D reconstruction is presented in Figure WP1.8. Our experiment on the other hand allows to quantify the size distribution and the size of the particles.

This work mainly fits within objectives 1 and 4.

The structural and thermal properties of Pb nanoparticles (NPs) embedded in a Si wafer, synthesized by high-fluence ion implantation and subsequent annealing, have been experimentally investigated by P2-KUL. A variety of techniques, such as X-ray diffraction (XRD), real-time XRD, small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM), have been used to study the formation, orientation, strain, size, size evolution, and melting/solidification behaviour of the NPs. Samples with different implantation fluences ranging from $0.5 \times 10^{16}/cm^2$ to $2 \times 10^{16}/cm^2$, which were accurately determined by Rutherford backscattering spectrometry (RBS), were annealed at $600^\circ$C in a N$_2$ atmosphere, using different annealing time intervals. After annealing, we observed the formation of fcc-structured Pb NPs by using a combination of XRD and TEM. With the exception of a fraction (~10 %) of Pb NPs that are rotated by $60^\circ$ in the (111) plane, the Pb NPs are well-aligned with the Si wafer, irrespective of substrate orientation (see figure WP1.9). Results of size evaluation obtained from SAXS and TEM measurements are in good agreement with each other, and the average size of the Pb NPs could be tuned from 8.7 nm to 12.1 nm. In addition, the scaling of the average radius of NPs with implantation fluence and duration thermal annealing can be explained by the kinetics of cluster growth.

Unlike the theoretical prediction and previous experiments for free standing metallic nanoclusters, the crystalline Pb NPs embedded in a Si matrix show a size-dependent dilatation of their lattice parameter. Quasi-pseudomorphism can be invoked to explain this result. The melting and solidification behavior of Pb NPs was investigated by real-time XRD measurements. The solid/liquid phase transition exhibits a hysteresis with a width of ~ 50 K during the heating up and cooling down process. The width of the hysteresis is due to a contribution from the low energy epitaxial interface between Pb and Si and a contribution from the Pb finite size effect. The shifting of melting/solidification points of Pb NPs can be explained by their size-dependent tensile strain.

2.3.3 Superstructure controlled self-assembly of Fe-silicide nanostructures

P2-KUL has studied the superstructure controlled self-organization of Fe-silicide nano-islands on Si(111) surfaces. In particular, the influence of noble metal (Cu, Au, Ag) induced surface reconstructions on the diffusion of deposited Fe–atoms and the subsequent growth kinetics of nanoscale islands was investigated. It is demonstrated that the presence of these buffer layers causes

![Fig. WP1.9: Real-time XRD measurements for the melting/solidification points' determination of Pb NPs. The integrated intensity of the Pb(200) diffraction peak clearly shows a hysteresis with a width ~ 50 K during the heating up and cooling down process. The shift of the melting/solidification points of Pb NPs correlates well with their average size.](image-url)
Section II. Research Results – WP1: Quantum effects in clusters and nanowires

2.3.4 Composition fluctuations in alloy nanoparticles as source for superparamagnetism in arrays of ferromagnetic nanoparticles

Further reduction of the volume of magnetic structures appears as a natural route towards the enhancement of information density stored by corresponding magnetic devices. Such a reduction, however, generally results in a superparamagnetic behavior for any material below a critical size (several 10 nm), the value of which is governed by its magnetocrystalline anisotropy energy. Among the materials with large anisotropy energy, P6-HUasselt investigates Fe<sub>50</sub>Pt<sub>50</sub> alloys in the face-centered tetragonal (L1<sub>0</sub>) phase which play a vital role since various techniques based on self-organization are available for the synthesis of nanoparticles and their organization into two-dimensional arrays. It turns out that, in the as-synthesized state, FePt particles exhibit a face-centered cubic structure, which has to be transformed by annealing into the desired L1<sub>0</sub> phase. Such phase transformation, however, can be achieved only within a limited range of compositions (X ≈ 40-60) raising the important question of whether or not statistical fluctuations during the formation of particles of equiatomic composition (Fe<sub>50</sub>Pt<sub>50</sub>) might result in significant variations of the magnetic properties as well.

In order to address this fundamental problem with a technique sensitive to fluctuations within macroscopic areas, XPS has been performed on FeₓPt<sub>100-x</sub> reference films (26 ≤ X ≤ 68) in order to study chemical shifts and changes in line shape of appropriate core levels (Fe-2p, Pt-4f) induced by
alloying. These reference data were used in a second step to decompose core level spectra measured on FePt nanoparticle arrays (size 6 nm, particles prepared by two different synthesis methods: micellar + standard colloidal). It turns out, that statistical fluctuations in alloy composition are present exceeding values of more than ±15 atomic percent independent of the synthesis strategy thus providing an explanation for the observation of superparamagnetic contributions to the hysteresis often found for such nanoparticle ensembles. Consequently, this leaves the potential of such alloy particles for magnetic data storage applications highly questionable, at least in the present state of particle preparation.

3. Main achievements in relation to the initial objectives

During the period 2007-2009, the partners of WP1 contributed to the four objectives listed above. They investigated experimentally and theoretically pure, binary and more complex metallic and oxide clusters and studied the influence of size, composition and electronic structure on the catalytic, chemical and physical properties and on their self-assembly in ordered layers. The interactions of metallic clusters with organic molecules, either as a support like in silver coated insulin derived amyloid fibrils complexes or as passivated and/or functionalized ligand shells in the case of gold nanoparticles were characterized. Possible applications to the design of magnetic particles for data storage (in collaboration with WP3), to hydrogen storage, for enhancing of catalytic activities and for the realization of logic operations were explored.

References

WP2: Magnetic dots and wires

The main contributors to work package 2 (WP2) are:

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The ULg focuses on theoretical research, while the other partners in this work package focus on experimental work.

1. Aims and Objectives

The four main objectives for this work package are:

1. The onset of magnetism in nanoscale materials,
2. The origin of magnetic anisotropy,
3. Spin-dynamical effects on the nanoscale, and
4. Spin transfer effects.

The research that has been carried out in the period 01/01/2007 – 30/04/2010 has adhered to these four main objectives, as will be shown in the following research summaries. One new item of common interest has emerged after the start of the network, namely the study of multiferroic materials, which is currently and worldwide a ‘hot’ research topic, not in the least because of its potential for future applications in memory devices. Furthermore, research on multiferroic materials fits into this work package because it addresses items (1) and (2) of the four main objectives that were stated above.

2. Scientific activities and results

2.1. Multiferroic materials

2.1.1 Magneto-electric multiferroics: theoretical study.

Magnetoelectric (ME) multiferroics, which combine ferromagnetic (or another kind of magnetic ordering) and ferroelectric orderings, are currently the subject of numerous investigations because they potentially open the way to totally new applications for multi-state memories or within the emerging field of spintronics.

It is worth to mention that a major drawback in the theoretical study of ME multiferroics is the difficulty to find a fully predictive and accurate DFT-based method to describe their properties. The ULg developed an alternative predictive tool for the study of multiferroics [1] and demonstrated that the recent B1-WC hybrid functional of Bilc et al. [2] provides very good overall agreement with experiments and can be considered as a valuable alternative to LDA, GGA and DFT+U. This opens interesting new perspectives for further and more predictive first-principles investigations of multiferroic materials.

In the search for alternative single-phase ME multiferroics, the ULg reinvestigated the physics of CaMnO$_3$, a magnetic insulator, which is considered as a prototypical example to reveal the antagonist role of partial d-shell occupancy in respectively yielding magnetism but penalizing ferroelectricity. In [3] the ULg partner pointed out that, contrary to common believe, CaMnO$_3$ does develop a weak ferroelectric (FE) instability at its equilibrium volume. However, like in CaTiO$_3$, the latter is hidden by a much deeper antiferrodistortive (AFD) instability, which is responsible for the orthorhombic ground-state. It was highlighted that CaMnO$_3$ can be made multiferroic under epitaxial strain in ultra-thin
films and/or when partially substituting Ca by Ba. All this suggests alternative strategies in the search of single-phase multiferroic ABO₃ compounds.

Ferroelectricity and multiferroism in oxides is commonly believed to be restricted to the family of ABO₃ compounds. Using first-principles density functional calculations, the ULg has shown recently [4] that ferroelectricity can be easily induced in simple alkaline earth binary oxides such as barium oxide (BaO) using appropriate epitaxial strains. It was also highlighted that magnetic binary oxides such as EuO, with the same rocksalt structure, behave similarly to the alkaline earth oxides, and can be made multiferroic under reasonable epitaxial strain. For EuO the epitaxial strain is expected to increase the ferromagnetic Curie temperature, so providing a route to higher temperature multiferroics in very simple compounds.

2.1.2 Magneto-electric multiferroics: experimental study

Recently, experimental work on the magnetoelectric material BiFeO₃ started, initiated by a new collaboration, with the group of Prof. Marlies Van Bael and Prof. An Hardy of the UH. The BiFeO₃ films are made at the UH by the sol-gel method. Characterization by x-ray diffraction and scanning electron microscopy was carried out at the UH, where via an external collaboration it was also established that these films are ferroelectric. Magnetization measurements carried out in a Squid magnetometer at KUL also proved the magnetic nature of the films. Finally, polarized neutron reflectometry experiments were carried out at the Helmholtz Zentrum Berlin, indicating a spin-glass like magnetic state.

2.1.3 New candidate multiferroic materials

Apart from the research into known multiferroic materials, there is also an initiative to develop new multiferroic materials within the network. The ULg partner highlighted the possibility to achieve improper ferroelectricity in short-period PbTiO₃/SrTiO₃ superlattices [5].

The UA partner works on the possibility to obtain multiferroicity in new perovskite based materials based with an A cation with a lone electron pair. A new family of perovskite based materials has been developed within this context, which has a general composition \(A_{4p+3q}Fe_{4(p+q)}O_{10p+9q}\) (up till now \(A = \text{Pb, Sr, Ba}\). [6-8] Also a new perovskite based homologous series was made that can be considered as part of this large family. These are made so far using solid state synthesis at UA, but within a new collaboration started in 2009 with University of Hasselt (Marlies Van Bael and An Hardy), optimization of the synthesis is also being attempted using the sol gel method. As the first attempts gave multiphased samples, all published structure studies were done using transmission electron microscopy. A characteristic high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) image and model of the relevant structure is shown in Figure WP2.1. The recently obtained samples are single phase and their structure will be refined using neutron and X-ray powder diffraction.

Future perspectives are to also make these materials with Mn instead of Fe, and with Bi instead of Pb, both with solid state synthesis (UA) and sol gel method (UH), to achieve multiferroic properties and/or Pb-free compounds. Preliminary results show that this leads to new variations within the family.
2.2. Magnetic anisotropy

The research work on magnetic anisotropy contains several subtopics, related to different relevant anisotropy contributions: research on FePt-based systems focuses on the intrinsic magnetocrystalline anisotropy, while the work on ion-sputtered epitaxial Fe films explores the consequences of competition between magnetocrystalline and induced surface anisotropy. The work on domain wall engineering is based on exploiting shape anisotropy effects. Finally, the contributions on exchange bias are based on the unidirectional anisotropy of ferromagnetic/antiferromagnetic interfaces.

2.2.1 Magnetocrystalline anisotropy in FePt-based systems

Due to its perpendicular magnetic anisotropy, FePt in the L_{10} phase is an attractive candidate for high-density magnetic recording media. Epitaxial FePt thin films, highly ordered in the L_{10} phase, can be obtained when grown directly onto MgO(100) substrates [9]. Furthermore, by depositing a thin Fe film onto such an L_{10} FePt layer, a new phenomenon emerges: while the hard FePt layer forces its magnetization perpendicular to the film plane, the soft Fe layer prefers its magnetic moments to orient in plane. Hence, a perpendicular exchange spring magnet is formed due to the interfacial exchange coupling between the soft and hard ferromagnetic layers.

The spin orientation in the soft Fe layer of Fe-FePt bilayers is investigated by the KUL partner by nuclear resonant scattering [10,11] for epitaxially grown 56Fe(x)/57Fe(0.7 nm)/56Fe(y)-56FePt(30 nm). For Fe layers close to the interface, the magnetically hard FePt pins the magnetization in the soft Fe layer to the out-of-plane direction. For Fe layers further away from the interface, the influence of the FePt diminishes and the magnetization cant to the in-plane Fe[001]-direction. It was deduced that the field required to cant the moments towards the external field decreases as the distance from the interface increases.

Using inelastic nuclear scattering of synchrotron radiation, the KUL partner also achieved to measure important dynamic properties, in particular the anisotropic phonon density of states in a 30 nm FePt film. Analysis of the phonon spectra provides understanding of the structural reorientation that is observed in such films at elevated temperatures.

2.2.2 STM and STS on Co nano-islands

Scanning tunnelling microscopy (STM) and scanning tunnelling spectroscopy (STS) at low temperatures and in ultra-high vacuum (UHV) have been used for investigating the structural and electronic properties of nanometer size Co islands (typically two monolayers high) that are obtained “in situ” in UHV by atom deposition and subsequent self-organization on Au(111) surfaces with “herringbone” surface reconstruction. Standing wave patterns, which appear on top of the atomically flat Co islands, can be quantitatively accounted for in terms of “particle-in-a-box” based calculations that take into account the polygonal island shape. Quantum confinement effects are present as well for higher lying image-potential states. Combined STM and STS measurements have also been performed for self-organized Cr and Au islands and wires [12,13] on Au(111) and for self-organized Co islands on “in situ” cleaved p-type InAs(110) semiconductor crystals [14].

Magnetic monolayer and bilayer Co islands on Au(111) films were successfully investigated with spin sensitive STM and STS [15]. This opens the way for detailed atomic-resolution magnetic measurements of magnetic nanoparticles.

2.2.3 Domain wall engineering

The KUL partner determined the intrinsic domain wall resistance (DWR) of 180° Néel walls in a polycrystalline Fe thin film by creating a periodic domain pattern. This was achieved by locally inducing the exchange bias effect by patterning with a template of antiferromagnetic CoO lines on top of a continuous ferromagnetic polycrystalline thin Fe film (21.5 nm thick). The exchange biased parts consist of 7.1 µm wide lines arranged in a period of 10 µm, by locally bombarding a fully exchange biased thin CoO/Fe film with Ar⁺ ions. By field cooling through the CoO blocking temperature (∼ 120
K), the coercivity of the Fe film is spatially modulated. Upon reversal of the magnetic field, the unbiased regions flip their magnetization first. This creates a periodic stripe domain pattern where uniformly magnetized regions are separated by 180° Néel domain walls. The resistance difference between the parallel and the antiparallel state can be attributed to the presence of domain walls. After correcting for the AMR contribution caused by the Néel walls themselves, as well as from a deviation from the perfect antiparallel state, the extracted DWR is positive and represents a local increase in resistivity of $9 \times 10^{-10} \Omega \text{m}$ [16]. This positive intrinsic DWR can be understood in terms of the giant magnetoresistance mechanism.

### 2.2.4 Exchange bias in Co-CoO systems formed by ion implantation

Opposed to archetypal exchange bias (EB) structures like bilayers or core-shell clusters, where the formation of the antiferromagnetic (AFM) oxide relies mainly on surface oxidation, the KUL-partner was able to induce EB in a novel way, i.e. by implanting O ions in thin Co films, forming cobalt oxide embedded in the Co film [17]. The interaction between the Co film and the formed CoO clusters causes EB. In a first stage of this research the determining parameters of the effect, like implantation energy, implantation fluence and post-implantation annealing were explored in a polycrystalline Co system. This constituted of Co films with a thickness in the range of 60-100 nm, grown on a (100)-oriented MgO-substrate. The implantations were performed at an energy of 30-60 keV and at fluences ranging from $3.3 \times 10^{16}$ to $2.3 \times 10^{17}$ ions/cm$^2$. The reversal mechanism was studied in detail with Polarized Neutron Reflectometry (PNR) and Anisotropic Magnetoresistance (AMR) measurements.

### 2.2.5 Anisotropy and exchange bias in glancing angle deposited Fe and Co films

Magnetic nanostructured thin films were fabricated on Si(100) substrates using the glancing angle deposition (GLAD) method. In GLAD the deposition flux arrives at the substrate surface at an oblique angle of incidence $\alpha$, with respect to the substrate normal. This leads to self-shadowing during film growth and a subsequent structuring of the film into nanocolumns whose direction of growth towards the incidence beam direction is at an angle $\beta$ from the substrate normal. For the Co films in-situ oxidation was carried out at an oxygen pressure of $\sim 4 \times 10^{-4}$ mbar for 90 seconds in a chamber attached to the deposition system. This resulted in the formation of a CoO shell of $\sim 3$ nm thickness around individual columns. Different Fe sample thicknesses were deposited, ranging from $\sim 7 - 180$ nm. These films were investigated for shape-induced magnetic anisotropy, and for the Co/CoO film exchange bias anisotropy and training effects were also investigated. The dependence of the easy magnetization axis as well as the direction with highest coercivity on thickness is related to changes in column morphology and shape during film growth.

### 2.2.6 Observation of exchange bias in Co/CoO ‘nanocaps’

The KUL partner worked on the magnetic properties of Co/CoO ‘magnetic nanocaps’, a term referring to the deposition of a magnetic thin film on a self-assembled lattice of polystyrene nanospheres. Since the thickness of the deposited film varies across the nanospheres boundaries and the exchange and dipolar interactions between the spheres are limited, the film on each nanosphere can be considered as an isolated ‘magnetic cap’. In this study, exchange bias results are reported on ultra-thin Co (10 nm) films deposited by MBE on polystyrene nanospheres (PS, 530 nm diameter).

![Fig. WP2.2: Panel (a) shows the SEM cross-sectional view of an Fe film deposited at oblique angle of 72°. Panel (b) shows the SEM topography image of the same Fe film.](image-url)

### Section II. Research Results – WP2: Magnetic dots and wires
For comparison, a reference film was simultaneously deposited on a plane Si(100) substrate. It is observed that the film deposited on PS shows higher coercivity than the film deposited on a plane substrate. The exchange bias measurements carried out on these thin film structures reveal a higher exchange bias field for Co on PS, than on Si substrate. It is also observed that this exchange bias field depends on the direction of external magnetic field and is higher for a perpendicular field rather than the parallel field. The observed results are attributed to the curved nature of the nanospheres surfaces, which significantly modifies the microstructure of the film and hence modifies the magnetic properties of the system.

2.3. Magnetic nanowires

2.3.1 Effects of layering on magnetostatic interactions in Co$_{x}$Cu$_{1-x}$/Cu nanowires

The UCL partner fabricated arrays of CoCu/Cu multilayered nanowires (NWs) by electrodeposition, which have been characterized by ferromagnetic resonance (FMR) in order to study dipolar interactions between layers as a function of the magnetic and nonmagnetic layer thicknesses [18, 19]. A model was developed, giving an accurate description of the behavior of the effective field $H_{\text{eff}}$, opening the possibility to determine the geometrical conditions needed to obtain multilayered NWs with $H_{\text{eff}}$ favouring an easy axis parallel or perpendicular to the NW axis, which can serve as a design guide in order to tailor specific magnetic properties.

2.3.2 Tunable zero field ferromagnetic resonance in arrays of bistable magnetic NW

Arrays of 30 nm diameter Co$_{35}$Fe$_{65}$ NWs with porosity ($P$) of 5%; have been grown by electrodeposition into the pores of polycarbonate (PC) membranes. Low density arrays of bi-stable NWs were considered, for which the magnetization $m$ along the wire axis has two equilibrium configurations, named positive $m^+$ and negative $m^-$. The rotation of the magnetization of the NW array corresponds to the successive reversal of individual wires. By decreasing the applied field the evolution of the FMR spectra shows how the two resonance peaks superpose by shifting in opposite sense their resonance frequencies, as indicated by the dotted lines, until zero-field is reached and the final absorption peak is the combination of the two FMR peaks corresponding to each $m_s$. Since the peak intensity is proportional to the number of wires magnetized in each direction, the absolute

![Fig. WP2.3: Field cooled magnetization measurements carried out on Co/PS and Co/Si thin films in perpendicular field direction. Insets show the orientation of the applied magnetic field for perpendicular geometry, showing the alignment of the field with respect to the Co/CoO layer following the nanospheres contours and Si substrate respectively.](image-url)

![Fig. WP2.4: FMR spectra for different non-saturated states obtained with $H_r$ of (a) -1.1 kOe and (b) -2.0 kOe and the spectra recorded at intermediate fields between $H_r$ and zero field. (c) Measured (symbols) and calculated (continuous lines) $f^{\text{meas}}(H=0)$ as a function of the reverse field $H_r$.](image-url)
minimum in the resulting spectra will be given by the peak that corresponds to the magnetization direction with the largest number of wires.

These results are interesting as a mechanism to develop new and more functional microwave devices.

2.4. Spin torque effects

The UCL partner developed a reliable and flexible method combining template synthesis and nanolithographic processes to fabricate current-perpendicular-to-plane giant magnetoresistance spin-valve nanowires very promising for the exploration of electrical spin transfer phenomena. Dense arrays of nanowires are synthesized by electrodeposition into the pores of anodic porous alumina supported on Si substrate. The nanolithography based contacting method allows to connect separately individual nanowires at different locations in a large assembly of wires (Fig. WP2.5(a)). Measurements were performed on single nanowires consisting either in a single trilayer spin valve or in a stack of several spin valves intrinsically electrically connected into series [20,21]. Both NiFe/Cu/NiFe and Co/Cu trilayers systems have been investigated and clear evidence for spin transfer torque effects were observed in these systems. The giant magnetoresistance curve was found to be typical of an almost uncoupled spin valve. In Fig. WP2.5(b), we show the variation of the differential resistance dV/dI versus injected dc current at small field for a selected nanowire sample. The experimental hysteretic curve is attributed to spin transfer induced magnetization reversal, usually observed at zero or low applied magnetic field. Under larger external magnetic field (typically larger than the coercive field of the thin ferromagnetic layer), the abrupt jumps in the variation of the differential resistance with the injected dc current are replaced by reversible peaks (see in Fig. WP2.5(c) the dV/dI curves recorded at selected H values). The shift from irreversible to reversible action of the spin transfer torque has been associated in standard nanopillars to the onset of sustained precession of magnetization.

![Fig. WP2.5: (left) schematic illustration of the single wire contacting process on an array of nanowires electrodeposited in supported nanoporous alumina template; (center) current-induced switching of magnetization for a Py(30nm)/Cu(10nm)/Py(6nm) spin-valve nanowire; (right) set of differential resistance curves obtained for various magnetic field GMR on the same sample. The peaks are associated to the onset of precession of magnetization in the 6nm thick Py free layer.](image)

The nanowire spin valves were designed with support from micromagnetic simulations to favor the nucleation of magnetization vortices. In such devices, narrow line microwave current emission associated with the spin transfer driven motion of magnetization vortices was measured, leading to high quality factor spectra under proper field and current conditions. These oscillations can be measured at zero magnetic field. This novel approach promises to be of strong interest for subsequent fabrication of phase-locked arrays of spin transfer nano-oscillators exhibiting high quality coherent emission by synchronization via their self emitted current and increased output power for microwave applications.

The KUL partner recently started work on spin torque effects in magnetic nanogranular materials, in particular the Co-Ag system. By selectively choosing the suitable Co concentration in Co-Ag system containing Co nanoparticles embedded in a Ag matrix, it is possible to optimize the giant magnetoresistance (GMR) which is a prerequisite for the observation of spin torque transfer effects.
3. Main achievements in relation to the initial objectives

During the period 2007-2009, the partners of WP2 contributed to the study of magnetic dots and wires. They investigated experimentally and theoretically the onset of magnetism in nanoscale materials, the origin of magnetic anisotropy, lattice and spin dynamics at the nanoscale, and spin transfer effects. Important progress was made in getting a deeper understanding of intrinsic (magnetocrystalline) anisotropy effects as well as of inducing new anisotropies by tuning the film morphology at the nanometer scale. In the field of exchange bias, an entirely new area was started by creating small clusters of antiferromagnetic oxide within a ferromagnetic film by using ion implantation. Scanning probe microscopy was used for the study of nanoscale magnetic islands and was also used to contact nanoparticles and nanowires to investigate spin torque effects. Apart from the four initial scientific objectives, several partners also started working on a new topic of common interest, namely multiferroic materials (in particular those multiferroics that display magneto-electric coupling). Since the start of the network, this has become worldwide a hot research topic with important implications for use in e.g. future magnetic data storage devices. Research on multiferroic materials fits into this work package because it also addresses the first two scientific objectives set forward at the start of the project (onset of magnetism and magnetic anisotropy).

References

WP3: Semiconductor quantum dots and wires

Four contributing partners have been actively involved in WP3 during the period of the report:

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<th>P3 UCL</th>
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1. Aims and Objectives

The initial objectives of the WP3 were:

1. Study of the optical properties of self-assembled quantum dots (QDs) by continuum elasticity and k.p theory;
2. Study of the electronic and optical properties of embedded semiconductor NWs (NWs) within the effective mass approximation;
3. Study of the electronic and optical properties of thick free-standing NWs, with a focus on the effects due to the dielectric mismatch;
4. Study of the electronic structure and optical properties of NWs and QDs using highly accurate first-principles simulation techniques, with application to Si and Ge NWs;
5. First-principles study of GeTe-based QDs and NWs, with a focus on the aspects related to the presence of ferroelectricity;
6. the development of a ultra-low temperature scanning gate microscopy setup (SGM)
7. imaging electron transport in semiconductor nanodevices, using the SGM, in various regimes (coherent, ballistic, quantum Hall transport regimes, ...).

2. Scientific activities and results

2.1 Self-assembled QDs, embedded NWs and thick free standing NWs

The CMT-UA group modelled QDs within the k.p theory. For example, magneto-optics of unstrained GaAs/AlGaAs QDs were investigated theoretically in the presence of an external magnetic field. An important aspect of this study focused on the effect of the substrate orientation and an external magnetic field on the exciton binding energy: this model was applied to (In,Ga)As capped InAs QDs grown on [11k] substrates. Next, the electronic structure of coupled QDs was studied. In collaboration with experimentalists from P2 and from the Instituto de Microelectrónica de Madrid, P1 investigated the charge confinement in InAs/InP self-assembled quantum NWs theoretically through the study of the exciton diamagnetic shift. The calculations were performed within the single-band effective mass approximation, including band nonparabolicity, strain effects, as well as the electron-hole Coulomb interaction energy. A detailed comparison was made between the theoretical and experimental data on the magnetic field dependence of the exciton diamagnetic shift. The theoretical analysis showed that excitons in the InAs/InP quantum well are trapped by local well width fluctuations. Together with experimentalists from the Universidad de Cádiz and the Instituto de Microelectrónica de Madrid this study was extended to the effect of the coupling between InAs/InP self-assembled NWs on the exciton energy [1].

Besides excitonic properties, P1 extended this study to charged excitons. The binding energy for charged excitons $X^-$ and $X^+$ was calculated within the single-band effective mass approximation, again including the effects due to strain for rectangular, triangular, and V-shaped quantum wires. Both $X^-$ and $X^+$ were found to be bound in rectangular InAs/InP quantum wires and V-shaped
GaAs/Al$_{0.32}$Ga$_{0.68}$As quantum wires. A remarkable dependence of the trion binding energy on the size and shape of the NWs was found and compared with available experimental data. Moreover, P1 studied free-standing NWs with a diameter of 5 nm and more within the effective mass and multiband approximation. (Thinner NWs were studied by first principles calculations.) An important aspect of free-standing NWs is the dielectric mismatch between the semiconductor NW and its surroundings. Taking advantage of previous investigations, the theoretical studies focused on the binding energy of trions in these free-standing NWs.

Furthermore, P1 looked at the effect of the dielectric mismatch on impurities. Shallow impurity states in a freestanding semiconductor NW and in a semiconductor NW surrounded by a metallic gate were studied. The total energy of the electron and the binding energy were calculated using (i) a variational approach, which provides an upper bound to the electron energy, and (ii) the finite element method which is “numerically” exact. The dependence of the binding energy and the extent of the shallow impurity wave function on the NW radius and the ionized impurity position in the NW were examined. Finally, P1 has investigated the effect of a metallic gate on the bound states of a shallow donor located near the gate and showed how a transverse electric field can tune the average position of the electron with respect to the metallic gate and the impurity.

Collaborations:
S.I. Molina - Universidad de Cadiz (Spain)
W. Magnus and V.V. Moshchalkov – P2
B. Li, B. Partoens, A.F. Slachmuyders, and F. Peeters – P1
D. Fuster, Y. Gonzalez, L. Gonzalez - Instituto de Microelectronica de Madrid (Spain)

2.2 Thin free standing NWs

Si and Ge NWs, Si/Ge, Ge/Si and Ge/SiGe core-shell NWs are expected to play an important role in future electronic devices as they could provide a robust integration in the mainstream Si technology. P1, P3 and P5 investigated the properties of these NWs grown in the [110] and [111] directions by means of ab initio calculations. All our calculations were performed using the ABINIT code.

Inspired by the importance of doping for future applications and the unexplained experimental result that B-doped Si NWs have higher conductivities than similarly P-doped NWs, P1 started in the past with an investigation of the electronic properties of doped H-passivated NWs on an atomic level. It was shown that the near edge position is the preferred position. As these NWs have a large surface to volume ratio, the number of a dangling bond defects can be larger than the number of dopants. Therefore the effect of such a defect on the preferred localization of dopants was also investigated. This defect increases the segregation energy substantially, especially in the case of P atoms. For B atoms this segregation energy is smaller. This work was published in Nano Letters [2]. Due to the small unit cells with a very high dopant concentration used in the calculations, the valid question can be raised if these NW structures are stable. Ground state calculations alone do not provide this information, therefore the ionic positions were addressed via first-principles perturbation theory. All previously used structures were found stable. Concerning core/shell NWs, P1 focused on Si/Ge and Ge/Si structures of various diameters. The effect of the NW diameter on the phonon spectra is twofold: the (longitudinal) acoustic mode is hardened, while the optical modes are softened. As the phonon density of states allows to identify different contributions to the spectra, it was used in core-shell NWs to distinguish between different core materials and shell sizes.

Furthermore, P5 used first-principles calculations to exhaustively address the structural and electronic properties of undoped bare and H-passivated Ge NWs and Ge/SiGe, Ge/Si and Si/Ge core/shell NWs. The diameters of the NWs considered are in the range of 0.6 to 2.9 nm and oriented along [110] and [111] directions (see Fig. WP3.1). The diameter, the surface passivation, and the substitutional effects on the binding energy, band structure, and effective mass were extensively investigated considering the relative contribution of quantum confinement and surface effects. This work as well as a complete study of the vibrational properties was published in Physical Review B [3].
Fig. WP3.1: Cross sectional views of HOMOs and LUMOs in Ge/Si and Si/Ge core-shell NWs with diameters of 2.9 nm along [110] direction.

Collaborations:
R. Shaltaf and X. Gonze – P3
H. Peelaers, B. Partoens, and F. Peeters – P1

2.2.1 Methodological developments

The methodological developments and associated implementation efforts within MBPT have been lead to the point that the GW approximation can be used now for the accurate study of NWs and QDs within ABINIT. With the available computing power, systems with characteristic size on the order of 2 nanometers have been studied. The developments involved: (i) the implementation of a finite-length cutoff for the Coulomb interaction, preventing the spurious interaction between neighbouring cells to appear; (ii) the use of the closure relation, allowing a drastic reduction of the number of unoccupied states to be used in the computation of the electronic susceptibility or the correlation part of the self-energy; (iii) the use of Wannier interpolation, in order to be able to predict the full electronic band structure, as well as derived quantities, such as the effective masses.

Work had also be done at the level of the Bethe-Salpeter equation, leading to optical spectra. In particular, the exciton-plasmon coupling has been shown to be quite large for nanostructures. The Tamm-Dancoff approximation, very often made for Bether-Salpeter studies, actually neglects such coupling to a large extent. It has been shown how to efficiently bypass this approximation thanks to a new numerical algorithm. The methodological aspects of these works have been published in Nano Letters [4].

Collaborations:
R. Shaltaf, M. Grüning, and X. Gonze – P3
H. Peelaers, B. Partoens, and F. Peeters – P1
A. Marini – Universita di Roma “Tor Vergata” (Italy)

2.2.2 Hybrid exchange correlation functional – hybrid B1

DFT within LDA is usually appropriate to describe the physics of most nanostructures with good accuracy. However, the well-known “DFT bandgap problem” reveals problematic for the investigation of experimentally relevant electronic and optical properties. To address this problem, we proposed an alternative hybrid B1 functional that mixes exact exchange with the recently proposed GGA of Wu
and Cohen which, for solids, improves over the treatment of exchange of the most usual GGAs. Our new B1 functional was shown to provide an accurate description of both the structural and electronic properties of typical ferroelectric oxides and might be an interesting alternative for the modelling of ferroelectric nanostructures involving metal/ferroelectric interfaces. This study was published in Physical Review B [5]. Well-studied systems were the hydrogen saturated SiNWs (Fig. WP3.2). Their accurate electronic and structural properties were obtained at the same time; the effect of the NW diameter on the bandspectra, where the lowering of the bands associated with the indirect bandgap in bulk Si could be observed. The formation of a B or P single impurity band, obtained by systematically reducing the concentration was observed and its localization with respect to the other bands was determined. Its width was also seen to converge towards a dispersionless band.

![Fig. WP3.2: Top views of optimized atomic structures of hydrogen saturated SiNW(N) for different sizes.](image)

Collaborations:
E. Durgun, D. Bilc, J.-Y. Raty, and Ph. Ghosez - P5
R. Shaltaf and X. Gonze - P3
H. Peelaers, B. Partoens, and F. Peeters - P1

2.2.3 Interaction of Si NWs with transition metals

We examined the interaction of hydrogen passivated Si NWs with TM atoms which are externally or internally adsorbed. We found that the adsorption of TM atoms generally resulted in magnetic ground states. We predicted that specific TM atoms adsorbed Si NWs have a half-metallic ground state. They are insulators for one spin-direction, but show metallic properties for the opposite spin-direction (Fig. WP3.3). This work was published in Physical Review Letters [6]. The obtained results were also verified using hybrid B1 functional which indicates that half-metallicity or high-spin polarization is not an artifact of DFT. These results are promising for spintronic applications of Si NWs.

![Fig. WP3.3: The structure and the energy band diagram of H-SiNW(45)+Cr. Bands described by dotted (blue) and continuous (orange) lines are for minority and majority spin-states, respectively.](image)
Collaborations:
E. Durgun, D. Bilec, J.-Y. Raty, and Ph. Ghosez – P5
R. Shaltaf and X. Gonze – P3
S. Ciraci - Bilkent University (Turkey)

2.2.4 GeTe nanoclusters and NWs

The study of GeTe-based bulk and nanosystem, performed in collaboration between P3 and P5, has been quite successful as well. In a first stage, the dynamical, dielectric, and ferroelectric properties of bulk GeTe have been carefully studied, leading to the publication of a series of articles in Physical Review B [7]. Then, nanoplatelets and NWs have been studied. A toroidal moment $G$ (with two different rotational orientations) has been found to develop in such nanosystems. The existence of such a toroidal moment was expected on the basis of previous studies based on a model Hamiltonian, but our study, in addition to being based on first principles, without adjustable parameters, uncovered the existence of a critical size for the appearance of the instability. At least one thousand atoms were needed to characterize correctly this effect. Also, the behaviour of the surface atoms was found intriguing. The two-state ordered behaviour, coupled with the possibility to have an amorphous state, opens the way to ternary logic in these nanosystems. This study was published in Physical Review Letters [8]. These GeTe nanostructures are possible candidates of building blocks of FRAMs where data can be stored as binary digits 1/0 (see Fig. WP3.4).

Similar formation of vortex pattern is also obtained for one dimensional NWs. The total polarization remains to be zero but $G$ is still significant. The switchable $G$ is calculated to be smaller than their counterpart cluster but also size dependent and increases with size. Interestingly, it is found that $G$ changes by strain and increases under compression. This part is still under investigation.

Collaborations:
R. Shaltaf and X. Gonze – P3
E. Durgun, J.-Y. Raty, and Ph. Ghosez – P5

2.2.5 Scanning gate microscopy

Low temperature experiments were performed by P3 on a quantum ring fabricated from an InGaAs/InAlAs substrate, in the low magnetic field range. The SGM conductance maps obtained at 90 mK exhibited a ten-fold enhancement of contrast with respect to data at 4.2 K (see Fig. WP3.5). This allowed to evidence a new range of details in the conductance images, and to clearly identify the phenomena at play. The smallest details that could be observed at low temperature have a typical dimension inferior to 10 nm, after optimization of the measurement parameters, which is exceptional for this technique. In parallel with the experimental side of the project, it was also crucial to develop simulation tools necessary to understand the mechanisms giving rise to the contrast of SGM images. At first, a specific simulation code was written by Dr. M. Pala (MINATEC, Grenoble), in collaboration with P3, to simulate the effect of a biased tip on the local density of states (LDOS) and on the transport properties of a mesoscopic device. This code was used to find the precise conditions that have to be met to obtain a map of the LDOS of a quantum ring using the SGM technique. The comparison of simulation results and experimental data led to a publication in Phys. Rev. Lett. [9]. Further work also demonstrated that the LDOS – conductance map correspondence still holds in the...
case of non-ideal mesoscopic systems, and when a weak magnetic field is applied (publications in Phys. Rev. B [10] and Nanotechnology [11]).

\[9.5 \text{T} , 100, 450 \text{ and } 960 \text{ mK on a quantum ring in the quantum Hall regime (around Landau filling factor 6). The contrast in region A originates from direct tunneling between counterpropagating edge states at the opening of the quantum ring. The other sets of concentric resistance fringes in (a-c) originates from tunneling between edge states and a specific Coulomb island, whose center corresponds to the center of the set of fringes. (d) Temperature dependence of the conductance fringe amplitude in region A and B in (c), and of the periodic magnetoresistance oscillations observed around B=9.5 T.]

Collaborations:
B. Hackens, S. Melinte, and V. Bayot - P3
F. Peeters - P1
X. Wallart - IEMN, Lille
M. Pala - MINATEC, Grenoble

3. Main achievements in relation to the initial objectives

Several theoretical developments are the core of the WP3 – in particular, first-principles simulations of nanoscale systems that are based directly on quantum mechanics and electromagnetism and do not involve adjustable parameters. In fact, the appropriate tool to study numerically the electronic and optical properties of NWs and QDs depends on the size of the structures. For systems with dimensions larger than 5 to 10 nm, the multiband $k_p$ method is a reliable approach. However, for smaller QDs and thinner NWs, the multiband approach breaks down and an atomistic approach is necessary. Accordingly, the major methodologies on which one is relying are DFT and the MBPT. While DFT is well established, it is, formally, only suited for studies of the system’s ground-state (e.g. ground state
energies and phonon spectrum). It is at best qualitative for the electronic structure or the optical spectrum. At variance, the more sophisticated schemes based on MBPT open the possibility of an accurate study of the excitations of the system, leading to accurate electronic structure (thanks to the GW approximation) and optical spectrum (thanks to the Bethe-Salpeter equation).

Experimental developments addressed electron systems confined within QDs and NWs that are, by nature, sensitive to minute changes of their environment. This is directly reflected in their transport properties, which can be influenced, for example, by the position or state of polarization of a single dopant, or the presence and the quantum state of a single electron. To take advantage of this sensitivity, it is necessary to develop experimental methods both to detect and to apply (under control) different kinds of nanoperturbations which will influence electron transport. The tip of an atomic force microscope (AFM) is a versatile tool, perfectly adapted for this task. In its SGM implementation, the AFM tip acts as a mobile electrostatic gate which alters the transmission of electrons through the device. Thus, SGM produces maps of electrical conductance variations measured while scanning the AFM tip above the device. These maps are directly related to transmission changes. Different experiments showed that SGM is a suitable technique to image electron flow in real space, inside QDs and NWs.

Concerning topics (1-3), P2 contributed to various experimental realizations. The multiband approach via increasing size \( k.p \) models (up to 8 X 8) was used by P1 to study the electronic properties of self–assembled QDs, embedded NWs and thick free-standing NWs within the effective mass approximation.

Concerning topic (4), the state-of-the-art implementation of MBPT for the study of NWs and QDs, addressed two key challenges: (i) the Coulomb potential is not screened in the vacuum region surrounding the NWs and QDs, and cause major numerical convergence problems, (ii) the number of electronic states is drastically increased with respect to simulations of the bulk, because the size of the supercell in which the nanosystem is embedded is typically one or two orders of magnitude bigger than the primitive cells for the bulk. Thus new developments had to be done in order to be able to deal efficiently with MBPT for nanosystems. The application of these methodological developments was done in collaboration between P1, P3 and P5. Also, the development and use of a hybrid functional to achieve good structural and electronic properties at much lower computational cost than the MBPT has been explored in collaboration between the 3 partners.

Concerning topic (5), the foreseen studies involved the use of DFT for the characterization of GeTe NWs and platelets. The properties that were targeted (geometric instabilities, Born effective charges, polarisation) were of the ground-state type, hence no direct methodological developments were needed in the first stage of the project. Yet, the number of atoms needed in the calculation to reveal the ferroelectric distorsions represented a major challenge. This study was lead in collaboration between P3 and P5.

The objective (6) consisted in building a new SGM system at P3, which could be operated at ultra-low temperature (mK regime) and high magnetic field (several Tesla), in order to investigate quantum electron transport phenomena at the local scale. The conception of such an instrument is challenging, mainly due to the limited space available inside a cryostat equipped with superconducting coils, and to the necessity to minimize the thermal link between, on one side, the sample and the scanning probe system, and, on the other side, the warmer parts of the cryostat.

Concerning topic (7), different QDs had to be designed and processed from semiconductor substrates, and, in particular, from semiconductor heterostructures (InGaAs/InAlAs substrates prepared by the group of X. Wallart, IEMN, Lille). The planned study included both an in-depth analysis of the working principle of SGM in the case of ballistic and coherent electron transport, and an exploration of other transport regimes, such as the quantum Hall effect, which had never been probed at the local scale in mesoscopic devices.
References

WP4: Superconducting Nanosystems

The main contributors to work package 4 (WP4) are:

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1. Aims and Objectives

The main objectives addressed within the WP4 are:

1. Nanoscale evolution of Tc and the gap in individual 3D structures
2. Confined condensate and phase-slip phenomena in superconducting nanowires.
3. Controlling vortex patterns and achieving vortex manipulation in superconductors and S/F hybrids with nanoscale pinning centers and magnetic field templates.
4. Superconductivity in cluster-assembled diamond films and nanodiamonds.

2. Scientific activities and results

2.1 Superconducting Nanograins and Cluster-Assembled Systems

The main motivation of this section is to investigate the confinement of the superconducting condensate in all spatial directions (zero dimensional limit) and its complementary limit of nanoinclusions in a superconducting matrix. Particular attention will be paid to the influence of these geometrical constraints on the maximum achievable critical field and critical temperature. In addition, we aim to study the electron pairing mechanism and the superconducting gap at these nanoscale dimensions. A selection of the most important achievements is highlighted below.

2.1.1 Cluster of magnetic particles embedded in a superconducting matrix

During the last years, the technical expertise of P1 has been upgraded to consider fully three-dimensional superconducting samples of arbitrary geometry. P1 started these studies with the simplest geometry possible, i.e. a superconducting sphere [1], where mainly the magnetic properties of different vortex states were analyzed and a possible distinction between giant- and multi-vortex states by magnetometry was proposed. Soon after, the research was expanded to the case of a superconducting cone [2], which is also of relevance to experiments, considering that recently superconducting tips of such shape are used for scanning tunneling microscopy of vortex structures in thin films. P1 also studied the critical behavior of spheres and cylinders with a cavity [3]. The main results comprise novel asymmetric vortex states, and the possibility of multi-quantum vortex entry in the sample. All these studies were conducted for samples in a homogeneous magnetic field. Additionally, P1 also studied S/F hybrids, where an

Fig. WP4.1: Complex system of vortex loops interconnecting magnetic particles inside a thick superconducting film (calculated by Ginzburg-Landau theory).
inhomogeneous magnetic field stemming from imbedded magnetic particles gives rise to very novel and rich physical phenomena inside the superconductor (see Fig.WP4.1). P1 first included a single magnetic dipole in the center of the sample, and studied the rise of vortex loops around the magnetic inclusion, which mimics the stray magnetic field lines of the dipole. The number and arrangement of these loops strongly depends on the shape and proximity of the boundary, as discussed in Ref. [4]. It was shown that loops nucleate in threes in a superconducting sphere, but their onset changes to doubles and quadruples in the case of cubic geometry. In addition, in the case of samples with multiple magnetic islands, vortex loops stemming from different sources may intertwine, and form a complex internal vortex phase [5].

2.1.2 Superconductivity in Boron doped diamond granular films with tuned diamond cluster density

Due to its outstanding electronic, mechanical, and thermal properties, diamond became a potential candidate for developing electronic devices which could meet the increasing demand for smallness, higher performance, less power consumption, and heat dissipation. Furthermore, the material rigidity and electrochemical robustness make it of interest for high-temperature electronic application such as diamond transistors that could operate at T=700 K. In 2004, the discovery of superconductivity in highly boron-doped diamond films has been reported, adding a new property to the already broad phenomena exhibited by these materials. Researchers from P2 and P6 have successfully prepared boron doped –nano-crystalline diamond films by chemical vapour deposition techniques, see Fig. WP4.2. Interestingly, it was found that the superconducting transition is determined by the Josephson coupling between neighbouring clusters. A positive magnetoresistance at high fields indicated orbital shrinking effects which start to decouple the overlapped boron orbitals [6]. In addition, low temperature scanning probe spectroscopy (in collaboration with the Universidad Autonoma de Madrid –Spain) showed that the superconducting gap D varies over a length scale much shorter than the structural grain size, revealing that the samples have an inherent (intrinsic) granularity. More importantly, it was shown in this report that the temperature dependence of the superconducting gap is consistent with early theoretical results describing the superconducting gap of a BCS superconductor in contact with a normal layer by solving the 1D Usadel equations on the superconducting side of the SN interface.

Fig. WP4.2: SEM picture of nanocrystalline diamond. Using different dilutions of seeds in solvent, the seeding density was tuned, giving rise from full covered layers to non-connected nano-diamond islands.

2.2 Superconducting Nanowires and Nanofilms

The 1-dimensional (nanowires) and 2-dimensional (nanofilms) confinement of the superconducting condensate and its impact on the superconducting properties is the goal of this Section. In these systems the primary dissipation mechanism corresponds to fluctuations of the order parameter, i.e. the non-equilibrium response, which leads to the development of phase-slip phenomena. This particular topic and the study of hot-spot formation, and non-equilibrium kinematic vortices in nanowires subjected to high currents, have been extensively investigated both, theoretically and experimentally, representing an important common point of interest for partners P1, P2, and P3. The most distinguished achievements within this Section, are listed below,
2.2.1 Quantum Size effects

When the characteristic size of a superconductor is of the order of the bulk Fermi wavelength, quantum confinement of electrons plays a major role. Solving numerically the Bogoliubov-de Gennes equations P1 found that [7] the band of single-electron states is split into a series of subbands moving in energy with changing film thickness. When the bottom of such a subband passes through the Fermi surface, a resonance appears leading to oscillations of the critical temperature as a function of film thickness [8]. This quantum confinement of the transverse electron motion is the major effect governing the superconducting properties of high-quality metallic nanofilms, leading to size-dependent oscillations of the superconducting properties with profound resonant enhancements. A nonuniform distribution of the pair condensate is typical for the resonant points (breakdown of the transverse translational symmetry). In this case, the order parameter exhibits significant local enhancements due to the quantum-size effects and, consequently, quasi-particles have lower energies when they avoid these local enhancements of the pair condensate in their spatial distribution. Such low-lying excitations can be considered as new Andreev-type quasiparticles but now induced by quantum confinement. By numerically solving the Bogoliubov-de Gennes equations and using Anderson's approximate solution to these equations, P1 (a) has formulated a criterion for such new Andreev-type states and (b) studied their effect on the superconducting characteristics in high-quality metallic superconducting nanofilms [9] and nanowires [10]. P1 has demonstrated that nanofilms made of low-carrier-density materials, e.g., of superconducting semiconductors, can be a more optimal choice for the observations of these new Andreev-type states and other quantum-size superconducting effects [9].

In high-quality nanowires [10], quantum confinement of the transverse electron motion splits the band of single-electron states in a series of subbands. This changes in a qualitative way the scenario of the magnetic-field induced superconductor-to-normal transition. P1 showed numerically, for a clean metallic cylindrical nanowire at zero temperature in a parallel magnetic field and diameters ~10–15 nm, that this transition occurs as a cascade of subsequent jumps in the order parameter (this is opposed to the smooth second-order phase transition in the mesoscopic regime). Each jump is associated with the depairing of electrons in one of the single-electron subbands. As a set of subbands contributes to the order parameter, the depairing process occurs as a cascade of jumps. Pronounced quantum-size oscillations of the critical magnetic field with giant resonant enhancements were found, where the paramagnetic breakdown of Cooper pairing also contributes but only for smaller diameters, i.e., D < 5 nm (see Fig. WP4.3).

2.2.2 Non-equilibrium phenomena in NbN microstrips

Heat dissipation is known to impact the electrical behavior of superconducting devices, especially for mesoscopic samples. The main challenge is to determine the real influence of Joule heating on the voltage-current characteristics. For the last years much attention has been devoted to both the experimental (P3) and theroretical (P1) comprehension of the non-equilibrium phenomena that compete in superconducting nanowires and microstrips. The distinction between phase-slippage phenomena (and to some extent to the motion of kinematic vortices) and the propagation of normal hotspot domains has been particularly studied. This led to a joined paper on the transport properties of superconducting NbN nanowires [11]. The main issue remains however to discriminate between the
latter competitive mechanisms because both result in voltage steps in the current-voltage characteristics. In this context new insights have been gained by performing transport measurements on NbN and Nb multicontacts microstrips. P1 and P3 have unambiguously demonstrated that the stabilization of normal domains properly is the ultimate cause for the stepwise current-voltage characteristics of superconducting microstrips. These dissipative states are stabilized both in the voltage- and current-biased regimes on a current interval limited by the retrapping current, i.e. by the normal-to-superconducting transition current. The heat-flow equations allow us to relate these features with the stabilization of localized normal hotspot domains [12] whose electronic temperature is above the critical one. The model of a normal hotspot maintained by Joule heating introduced two thermal characteristic currents, which quantitatively describe the boundaries of the stabilization current interval. As the heat transfer balance between the heat dissipated in the sample and the heat transferred through the substrate defines the characteristic current densities, the current spreading of the normal-to-superconducting transition is thought to result from nm-range modulations of the samples cross-section. Such localized non-uniformities prevent hotspot propagation by pinning the normal/superconductor interfaces. In addition P3 has shown that microwave irradiation induces an additional electron heating due to the generated rf currents. Insofar as the microwave power level is sufficiently high, some dissipative states are stabilized in a larger current interval. The smallest difference of resistance between two nearest states correspond to additional normal domains across the whole width and whose length amounts to around 40 nm and 200 nm for NbN and Nb, respectively.

The characteristic energy relaxation time of our samples being mainly determined by the electron-phonon interactions, and the thermal healing length of our samples appear to match the additional resistive length between two observed intermediate dissipative states.

2.3 Vortex manipulation in superconductors with nano-pinning centers and Superconductor/Ferromagnet hybrids

The main objective of this part of the research project is to develop new or alternative fluxonic devices which allow one to control the vortex statics and dynamics via nanostructuring. This goal can be achieved (i) by exploiting the interplay of two competing collective phenomena, namely Superconductivity (S) and Ferromagnetism (F), (ii) by geometrically confining vortices, or (iii) by using external “knobs” such as bias currents or fields. Some highlights, evidencing the success of these methods, are briefly presented below,

2.3.1 Manipulation of quantum states in mesoscopic superconductors by injected current

Current-driven phenomena at nanoscale are nowadays of great interest, as they can find direct application in electronic devices. At this moment, this topic is of highest priority in magnetic systems (for manipulation of domain walls in nanowires, and switching of magnetic vortices in disks), molecular electronics, and spintronics, but also in superconductivity. Namely, applied current exerts a lateral force on flux lines in superconductors (analogous to the Lorentz force), which forms the base of the modern field of fluxonics. Such very efficient local manipulation of vortices by strategically applied current directly leads to local tailoring of quantum properties of superconducting samples. Recently, P1 showed the first controlled manipulation of vortex states in a submicron superconductor. In both state-of-the-art experiment and simulation, P1 researchers were able to induce a splitting of a giant vortex, as well as manipulate its vorticity, by applied dc current. As a consequence, a current-driven ballistic quantum switch, analogous to the field-driven one proposed by Melnikov and Vinokur in Nature (2002), was realized. P1 also succeeded in manipulating the degenerate states, i.e. switching between states of same energy, which is relevant, for example, for the earlier concept of Fluxonic Cellular Automata (Milosevic et al. Appl. Phys. Lett. 2007). [13]

2.3.2 Kinematic vortices

Under an applied current drive vortex motion usually exhibits instabilities in the system. The latter effect results in shrinkage of the vortex core at temperatures close to the critical one. Using time-dependent GL calculations [14,15,16], we showed that with increasing applied current the moving vortex lattice changes its structure from a triangular one to a set of parallel vortex rows. This effect originates from the change of the shape of the vortex core due to nonequilibrium effects. The moving
vortex creates a deficit of quasiparticles in front of its motion and an excess of quasiparticles behind the core of the moving vortex. This results in the appearance of a wake (region with suppressed order parameter) behind the vortex, which attracts other vortices resulting in an effective direction-dependent interaction between vortices. When the vortex velocity reaches the critical value quasiphase slip lines (lines with fast moving vortices) appear, which may coexist with slowly moving vortices between such lines. These studies have been recently expanded to consider the tunability of phase slips by a magnetic dot [17]. More recently a joint research between P1 and P2 has lead to the first direct visualization of these very fast kinematic vortices [18].

2.3.3 Effect of sample geometry on the flux patterns of the intermediate state in mesoscopic type-I superconductors

Intermediate state (IS) of type-I superconductors usually exhibit complex flux structures – highly branched and intricate fingered patterns of flux domains (lamellae). Moreover, the temperature and magnetic field history of the sample strongly influence the IS flux structures. The reason for such complex IS flux structures is the competition between the magnetic field energy of the domains and the positive surface energy between the superconducting and normal regions. The 3D nature of the long-range magnetic interaction of the normal domains makes it difficult to model the IS and, therefore, approximate expressions are usually used for the magnetic energy. We studied for the first time the effect of sample geometry on the intermediate state flux structures in mesoscopic type-I superconductors using full 3D GL theory making no approximation for the magnetic energy of the domains [19]. In contrast to bulk type-I superconductors, where flux tubes represent the equilibrium topology of the IS [R. Prozorov, Phys. Rev. Lett. 98, 257001 (2007)] at intermediate field values, both tubular and laminar structures form the ground state of mesoscopic samples. In addition to these well-established patterns, we found at equilibrium (i) a phase of singly quantized vortices, which is typical for type-II superconductors and (ii) a ring of a normal domain. The stability region and the formation process of these IS flux structures are strongly influenced by the geometry of the sample.

3. Main achievements in relation to the initial objectives

A more critical analysis on the general performance of the WP4 can be obtained by contrasting the main achievements, obtained during the last three years, to the original goals. The evolution of the superconducting critical temperature in 2D and 3D nanostructures has been successfully and thoroughly investigated theoretically via the GL phenomenological approach and using the Bogoliubov-de Gennes formalism. This achievement was mainly developed by P1 in collaboration with non-Belgian Universities. In addition, highly relevant experimental investigations have been performed in nanocluster and nanofilms of Pb and Boron-doped diamond by partners P2 and P6. The phase slips phenomena, hot-spot formation, and non-equilibrium kinematic vortices in nanowires subjected to high currents have been extensively investigated both, theoretically and experimentally. These topics have represented an important common point of interest for partners P1, P2 and P3, which has led to several joint publications in top journals.

Arguably the most active area of research within WP4 has been that devoted to the control and manipulation of the vortex dynamics by using patterned superconductors and S/F hybrid systems. This success and productivity follows from the world-wide recognized experimental and theoretical expertise of partners P1 and P2, in this particular topic. To illustrate this point we should mention that the invigorated joint research between P1, P2 and P3 has resulted in 7 Physical Review Letters and 1 invited review devoted to S/F heterostructures.

References

WP5: Carbon nanotubes and related carbon materials

The main contributors to work package 5 (WP5) are:

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1. Aims and Objectives

Work package 5 (WP5) of the IAP network is concerned with the investigation of structural, electronic and transport properties of carbon nanostructured materials, as well as their formation processes, focussing on (ultra)nanocrystalline diamond ((U)NCD), graphene and carbon nanotubes. These studies are conducted both by experimental and simulation means. The main objectives of WP5 are:

2. The study of the structural, electronic and transport properties of graphene and graphene multilayers.
3. The study of the structural and electronic properties of ideal and defected carbon nanotubes.

2. Scientific activities and results

2.1 Nanocrystalline and ultrananocrystalline diamond

The main objectives regarding (U)NCD are (1) to accomplish and understand nucleation of NCD particles and subsequent film growth by a combination of experimental and simulation techniques, and (2) to experimentally accomplish biosensing by DNA functionalization of (U)NCD films. Compared to the initial work programme, the use of Ar-rich plasmas to grow UNCD has been replaced with the continuous bias technique that also leads to very small grained films.

2.1.1 Study of the nucleation step of diamond growth

The diamond nucleation step is critical for the CVD of diamond on non-diamond substrates, i.e., for heteroepitaxial as well as polycrystalline growth. In general, diamond CVD growth on such foreign substrates requires artificial formation of diamond nucleation sites on the substrate’s surface. Three different possible procedures to induce this nucleation are investigated in a collaborative effort by UHasselt (P6), UA-NANO/EMAT (P1) and UA-Plasmant (P4).

The first method is based on a monodispersed diamond nanoparticle aqueous based colloid. This solution yields reproducible nucleation densities higher than $10^{11}$ cm$^{-2}$ and is currently the state-of-the-art procedure used to produce closed films thinner than 100 nm making use of conventional hydrogen-rich methane-based plasmas for diamond deposition.

In collaboration with UA-NANO/EMAT (P1), a second technique was investigated based on a diffusion based transport of carbon atoms from nanodiamond particles of ~ 5 nm size through a thin (~ 10 nm) sol-gel based TiO$_2$ film [1]. When a TiO$_2$ interlayer is deposited on a pre-treated Si wafer that is covered with a monolayer of diamond seeds, successful diamond growth can be accomplished. UA-NANO/EMAT (P1) used EELS and EFTEM to obtain the elemental and chemical information of the films grown at UHasselt (P6) (see Fig. WP5.1). It was found that pure diamond crystals can be nucleated by dissolving carbon into the TiO$_2$ buffer layer which is transported through the layer with simultaneous growth of the clusters, reaching the TiO$_2$ surface as sp$^3$ bonded diamond nuclei clusters.
The role of the substrate temperature, the presence of atomic hydrogen in the plasma, and the solid state environment provided by the thin TiO$_2$ film, is currently further investigated by P6 and P1. In the 3rd and final method a continuous bias voltage is applied to control diamond grain size and sp$^2$/sp$^3$ ratio in NCD. By an increase of the negative bias voltage, an increase of the substrate current is obtained, i.e. the flux of overall ions arriving at the substrate surface. This flux increase clearly influences the surface morphology of the NCD films, while reducing the grain size below 30 nm and down to 10 nm.

\[\text{Fig. WP5.1: (a) EFTEM composite element map indicating carbon (red), titanium (blue) and oxygen (green). The image shows a silicon substrate (dark, bottom right) that was seeded with diamond grains which are shown as the red areas underneath the blue Ti-layer. The Ti-layer forms a barrier between the seeds and the growth interface of the NCD film (red area, top left). (b) SEM image after growth of a seeded sample with a pure Ti-layer on top. The right side was seeded twice, proving the importance of a high carbon concentration underneath the Ti or TiO$_2$ layer.}\]

To quantify the amount of crystalline diamond and amorphous carbon ratio, EELS spectra are modelled showing an increased sp$^2$/sp$^3$ ratio with decreasing grain size. The experimental data were supplemented by theoretical modelling based on hybrid MD/MC simulations, performed by UA-PLASMANT (P4) [2]. From these simulations, it is concluded that a higher substrate temperature promotes higher adatom coordination, which is required for the growth of diamond structures. This temperature-induced effect on the adatom coordination might explain why larger diamond crystals, as typical for NCD, can be grown at higher temperatures, and why UNCD, with its high percentage of disordered phases (up to 10%), can be grown at lower substrate temperatures than NCD. Finally, it was shown that highly reactive species such as C$_x$H$_y$ (x ≥ 2) contribute significantly to the growth of (U)NCD when attached to biradical sites.

2.1.2 Surface spectroscopy and biosensing with DNA-functionalized (U)NCD films

Biological functionalization of carbon-based materials with DNA strands in order to develop carbon-based biosensors was accomplished by UHasselt (P6) in collaboration with KUL (P2) [3]. P6 has further optimized their two-step linking method based on i) the photochemical attachment of ω-unsaturated fatty to hydrogen-terminated NCD and ii) the subsequent EDC-mediated coupling between the COOH groups of the fatty acids and amino-terminated DNA. A special achievement was the determination of the typical tilt angle of DNA fragments with respect to the diamond surfaces by spectroscopic ultraviolet ellipsometry, utilizing molecular-orbital transitions in DNA with preferential spatial orientations. P6 also determined the surface areal density of immobilized fragments by confocal fluorescence microscopy and integrated the diamond-based electrodes, functionalized with single-stranded probe DNA, into impedimetric sensor cells: this allowed monitoring label-free and in real-time the hybridization of DNA with complementary fragments and also the reverse experiment with chemically induced denaturation. The sensitivity is sufficient to distinguish clearly between complementary DNA and DNA with point mutations. All this could only be achieved due to the excellent thermal and chemically stability of the NCD platform materials.

2.2 Graphene and multilayered graphene

The recent synthesis of graphene and the experimental observation of Dirac charge carriers have awaken an enormous interest in these systems. In WP5, attention is focussed on the investigation of the Klein effect and the realization of quantum dot structures in graphene systems, as well as the study of the adsorption and absorption of small molecules on graphene. Another highlight is the first-time PECVD growth of carbon nanowalls that consist of only a few layers.
2.2.1 Klein tunneling and the theoretical demonstration of quantum dots in graphene systems

One of the most challenging tasks is to learn how to control the electron behavior using electric fields in this two-dimensional (2D) layer. This task is made complicated by the so-called Klein effect according to which Dirac electrons in graphene can tunnel through any electric barrier. As a consequence, in electrically created quantum dots there are no bound states but only quasi-bound states, or so called resonances which, however, under certain conditions can have a long life time.

UA-NANO/CMT (P1) investigated how the spectrum of single-layer graphene is modified due to an applied periodic potential resulting in a superlattice structure [4]. For a bilayer, Klein tunneling is not seen, however, the tunneling features of this material are remarkable and due to the possibility of generating a gap by applying a perpendicular electric field onto the sample, bilayer graphene can be tweaked easily. Bound states and tunneling were investigated for bilayer barrier structures with applied potential barriers with or without applied bias. Also bilayer superlattices were considered, and the spectrum, the density of states and the conductivity for such systems were investigated. To get more insight into the transport phenomena found for these structures in single and bilayer graphene, P1 also studied the Kronig-Penney alter egos of the barrier systems.

Alternatively, non homogeneous magnetic fields can be used to control the motion of electrons, e.g. by the deposition of nanostructured ferromagnets. First P1 looked at magnetic barrier structures with a nonhomogeneous magnetic field and showed that they are able to confine Dirac electrons in graphene and bilayer graphene [5]. Also finite size magnetic structures were considered where the magnetic field is nonzero only in a finite region of space: a homogeneous magnetic field that is non-zero in a circle is considered, i.e. a magnetic dot. Such a model system can be realized by having a magnetic vortex piercing through the graphene layer or by overlaying graphene with a type I superconductor with a circular hole in a perpendicular magnetic field. In order to reveal the peculiarities of the behavior of Dirac electrons in such a magnetic dot the results were compared with those for standard electrons with a parabolic dispersion law. It was found that in such a magnetic quantum dot no electrons can be confined. Nevertheless close to the Landau levels quasi-bound states can exist with a rather long life time. Given the importance of graphene, P1 studied this magnetic confinement more systematically by considering a magnetic Kronig-Penney model in graphene, i.e. a series of magnetic delta-function barriers that alternate in sign. Recently, also Fabry-Pérot resonances were studied in detail in the transmission through single and double, graphene-based barriers and wells as well as their dependence on an applied perpendicular magnetic field.

The Klein tunnelling prevents the electrostatic confinement of charged particles in graphene. However, P1 demonstrated theoretically that quantum dots in bilayers of graphene can be realized [6], by a position dependent doping in order to create nanometer-scale quantum structures and also proposed a new system where electron and hole states are electrostatically confined into a quantum ring in bilayer graphene. These structures can be created by tuning the gap of the graphene bilayer using nanostructured gates or by position-dependent doping. The energy levels have a magnetic field dependence that is strikingly distinct from that of the usual semiconductor quantum rings, i.e. there is no $B \rightarrow -B$ symmetry.

2.2.3 Adsorption and absorption of molecules on graphene

Soon after the experimental realization of graphene a lot of interesting properties of this material have been discovered. E.g. it was demonstrated that graphene has exceptionally good sensing characteristics. This motivated UA-NANO/CMT (P1) to perform a theoretical investigation of the adsorption of small molecules on this new material [7, 8]. Because the underlying mechanisms of the resistance changes are not immediately clear, the adsorption process of different small molecules on a graphene surface was simulated by DFT calculations. It was found that the main reason for the resistance changes is a small charge transfer between the molecules and graphene after adsorption.

The electronic properties of graphene with absorbed H atoms was investigated by UCL (P3). H atoms adsorbed on top of graphene sheets could provide confinement of carriers to a narrow strip centered on these lines. These adsorbed atoms are found to induce a band gap whose value depends on the spacing between the H lines. The adsorption of species other than H would provide a way of tailoring the conductivity of graphene, through the different chemical dopings that different atoms would entail. The effect of different chemical species acting as donors or acceptors on the electronic properties of the carbon sheet is therefore also investigated by P3. Results for lines and strips of H and K (donors),
and F (an acceptor) adsorbed on graphene, in the DFT-LSDA framework as implemented in the SIESTA code, have been obtained. P3 also calculated the quantum transport properties of graphene nanoribbons in presence of OH- and H+. The quantum conductance is predicted to be strongly modified by these chemical groups, which play the role of scattering centers. Indeed, some specific conduction drops can be observed either at the right or at the left of the Fermi energy, depending on the chemical nature of these impurities.

2.2.3 Plasma-enhanced CVD growth of few-layer graphene

PECVD has been used by P2 for the first-time growth of carbon nanowalls that consist of only a few atomic layers (down to 4 layers) [9, 10]. The vertically oriented few-layer graphene sheets can be conveniently used for field emission applications. The high-density networks of few-layer graphene sheets has a very high surface to volume ratio that offers unique possibilities for various other applications. In collaboration with P6 the networks were successfully used for the detection of the binding between complementary single-stranded DNA fragments.

2.3 Structural and electronic properties of carbon nanotubes

The main objectives in WP5 in the field of carbon nanotubes (CNTs) include

1) imaging of CNTs
2) electronic properties of CNTs and sensing properties of ideal and defected CNTs

Initially, also the simulated catalyzed growth of CNTs by classical MD was an objective. However, test simulations showed that the interatomic potentials described in the literature are not sufficiently accurate to model the growth process. Therefore, this objective was temporarily set on hold. Using a very recently developed interatomic potential (2009), much more realistic results were recently obtained by UA-PLASMANT (P4).

2.3.1 Imaging of carbon nanotubes

The growth of CNTs on silicon substrates is of great importance because of their potential applications in next-generation device technologies in semiconductor industry as interconnects. However, producing CNT-based devices starting from catalyst nano-particles on Si substrates still presents a major challenge. In order to understand and optimize in-situ CNT growth at predefined locations (“contact holes”) for interconnect applications, TEM is used by UA-NANO/EMAT (P1). A first step in this study is the investigation of different catalyst particles, including their composition analysis and size distribution. Next, growth of the CNT’s from the contact-holes in test arrays is studied by TEM as well (P1). This study required the preparation of samples from selected regions on a Si wafer, which was accomplished by FIB methods. The 3D structure of bamboo-like CNTs, grown from catalyst nanoclusters is studied by discrete electron tomography in combination with EFTEM by P1 (Fig. WP5.2a) 11, 12]. By using dark-field STEM tomography, it is possible to conclude that different compositions are present inside the catalyst clusters. By EFTEM maps, these different compositions have been identified as Cu and CuO2. Tomography furthermore reveals that cavities are present in the catalyst clusters. The volume fractions of the different compositions are determined quantitatively from the 3D reconstructions and it is found that 85% of the nanocluster consists of Cu2O, 6% of Cu and 9% of the cluster is expected to be hollow. Furthermore, the 3D structure and chemical composition of patterned samples containing CNTs grown inside contact holes was studied by 360-degrees on-axis rotation electron tomography by P1 in collaboration with IMEC and P2.

Fig. WP5.2: (a) 3D reconstruction of the carbon nanotube. The catalyst material fills up hollow compartments in the tube. (b) 3D visualisation of a contact hole (yellow) containing a 3D network of carbon nanotubes (red)
A tomography sample for this purpose is prepared by focused ion beam and consists of a micro pillar containing an entire contact hole filled with carbon nanotubes. On-axis rotation electron tomography allows us to study the complete network of as-grown carbon nanotubes inside the contact hole without missing wedge artefacts. This is of great importance when quantifying our results. A 3D view of a contact hole including the carbon nanotubes is shown in Fig. WP5.2b [13, 14]. These imaging techniques were applied to functionalized CNTs, Ti-based nanotubes and nanoribbons, hybrid CNT/TiO₂ films, and exfoliated graphite-based compounds.

2.3.2 Electronic properties of CNTs and sensing properties

CNTs are promising building blocks for the construction of nanosized electronic devices. KULeuven (P2) has successfully fabricated devices consisting of two crossing metallic DWNTs by attaching electrical contacts to both DWNTs [15]. It was found that the devices can operate as a pair of FETs due to the semiconductor-like behavior of the disturbed parts of the DWNTs near the crossing. The lower DWNT is used as a gate electrode, while the upper one forms the channel of the FET structure. Two regions of the channel that are located near the point where the upper CNT, which is attached to the substrate by Van der Waals forces, is lifted up from the surface by the lower DWNT, reveal strong SGM effects. The electrical switching behavior of the FETs is confirmed by the EFM images. STM imaging was used to visualize the atomic-scale distortions near a crossing, which may be responsible for the FET operation. The application of the crossed CNT devices with very short gate lengths allows to strongly reduce the parasitic capacitance and improve the high-frequency performance.

Electronic properties of CNTs were studied computationally by UCL (P3) [16]. Like in most materials, the presence of defects in carbon nanotube has been demonstrated experimentally. The modifications induced by such defects in the electronic properties of the carbon hexagonal network have been investigated using first-principles calculations. One of the most frequently observed defect is the mono-vacancy which consists in a single carbon atom removed from the graphene sheet. In this specific case, the remaining hole undergoes a Jahn-Teller distortion upon relaxation, where two of the atoms near the vacancy move closer, forming a pentagonlike structure while the third atom is displaced by 0.43 Å out of the plane, as illustrated in Fig. WP5.3a, and observed experimentally (Fig. WP5.3b). Indeed, due to the presence of a vacancy defect in the supercell, new flat bands (low electronic group velocity) arise near the Fermi level (E_F), predominantly resulting from the atoms located around the corresponding vacancy. All these electronic states of the single vacancies in graphene are strongly localized and yield typical defect states with sharp peaks located around E_F.

Computed constant-current STM images of this vacancy defect have been calculated within a tight-binding approach in order to facilitate the interpretation of STM images of defected carbon nanostructures [17]. Such a STM image (Fig WP5.3c) does not reveal any threefold symmetry due to the atomic reconstruction mentioned above. The largest protrusion is located on the sole two-
coordinated atom located in front of the pentagon with a long C–C bond produced by the reconstruction.

The trigonal symmetry of the image (Fig. WP5.3e) can be restored by invoking a dynamical Jahn-Teller effect, where the pentagon rotates by $\pm 2\pi/3$. This dynamic switching between degenerate structures is activated by a barrier of 0.13 eV. The image would then be an average of three structures equivalent to that of the nonreconstructed one rotated by $\pm 2\pi/3$ (Fig. WP5.3d). Finally, these vacancy defects should also play a key role in the chemical reactivity of carbon nanotubes. Indeed, the modulation of the conductance due to specific molecules adsorbed at the defected sites should be detectable thus suggesting nanotubes as potential candidates for sensing applications [16].

2.4 Other carbon materials

Finally, while not an initial objective within WP5, the theoretical first-time demonstration of the dynamical formation of endohedral Ni-metallofullerenes was accomplished by UA-PLASMANT (P4) in collaboration with IMEC [18, 19]. Using both classical and DFT MD simulations, it was shown how depending on impact energy and impact location various metallofullerene complexes can be formed by ion implantation, including exohedral Ni-C$_{60}$, endohedral Ni@C$_{60}$ and heterohedral Ni-C$_{59}$.

3. Main achievements in relation to the initial objectives

In the field of (ultra)nanocrystalline diamond, the main objectives can be summarized as follows: (i) accomplishing and understanding nucleation of nanocrystalline diamond (NCD) particles and subsequent film growth by a combination of experimental and simulation techniques; (ii) experimentally accomplishing biosensing by DNA functionalization of (U)NCD films; (iii) heavily B-doping of diamond particles and films to turn them p-type conducting and superconducting when sufficiently cooled down. Compared to the initial work programme, the use of Ar-rich plasmas to grow UNCD, i.e. renucleated diamond films, has been replaced with the continuous bias technique that also leads to very small grained films.

The objectives of WP5 regarding graphene can be summarized as follows: (i) the study of the structural, electronic and transport properties of graphene and multilayers of graphene by means of ab initio calculations; (ii) the study of the adsorption and absorption of small molecules on graphene and the targeted functionalization of graphene; (iii) the experimental growth and characterization of carbon nanowalls. The recent synthesis of graphene and the experimental observation of Dirac charge carriers have awaken an enormous interest in these systems. The unusual properties of carriers in graphene are a consequence of the gapless and approximately linear electron dispersion at the vicinity of the Fermi level at two inequivalent points of the Brillouin zone. In the low-energy limit the quasiparticles in these systems are described in term of massless chiral relativistic fermions governed by the Dirac equation.

The initial objectives in WP5 in the field of carbon nanotubes include: (i) the structural and electronic properties of individual multiwalled carbon nanotubes; (ii) the effect of defects on the electronic properties of carbon nanotubes; (iii) the sensing properties of ideal and defected carbon nanotubes; and (iv) the magnetic properties of carbon nanotubes decorated with metallic nanoclusters. Initially, also the simulated catalyzed growth of single walled carbon nanotubes by classical MD was an objective. However, test simulations showed that the interatomic potentials described in the literature are not sufficiently accurate to model the growth process. Therefore, this objective was temporarily set on hold. Using a very recently developed interatomic potential (2009), much more realistic results were recently obtained by UA-PLASMANT (P4).

The main objective within WP5 regarding other carbon materials (i.e., carbon materials other than (U)NCD, graphene and CNTs) was the study of the structural and electronic properties of amorphous carbon systems in particular the computational evaluation of electronic excitation spectra. Although not an initial objective, also the simulated formation of metallofullerenes was accomplished.
References

Section II. Research Results – WP5: Carbon nanotubes and related carbon materials
III. Networking

III. 1. Network Meetings

GENERAL IAP MEETINGS AND MEETINGS OF THE EXECUTIVE COMMITTEE

1st Meeting of the Executive Committee & WP Leaders, University of Antwerp, March 13, 2007.


1st General meeting and 2nd Meeting of the Executive Committee & WP Leaders, University of Liège, November 22, 2007.


2nd General Meeting and 4th Meeting of the Executive Committee & WP-Leaders, KU Leuven, November 25, 2008.

5th Meeting of the Executive Committee & WP-Leaders, UCL, June 3, 2009.

3rd General Meeting and 6th Meeting of the Executive Committee & WP-Leaders, UCL, November 25, 2009.

WORK PACKAGE MEETINGS

WP1: Metallic and oxide clusters:

- Workshop on Transport Phenomena in Dusty Plasmas (organised by UA-Plasmant (P4) & UA-NANO (P1)), University of Antwerp, April 3, 2008.
- Workshop on Metallic and Oxide Clusters (organised by KU Leuven (P2)), KU Leuven, February 16, 2009.
- Nanowal Day: Molecular and Nano-Electronics (organised by ULg (P5)) University of Liège, May 8, 2009.

WP2: Magnetic dots and wires

- Workshop on Spintronics (organised by UA-NANO (P1)) University of Antwerp, May 9, 2007.

WP3: Semiconductor quantum dots and wires

- “Brunch” Workshop on Semiconductor Nanoclusters (organised by UCL (P3)), UCL, November 3, 2008.
• “Brunch” Workshop on Semiconductor Nanowires (organized by UCL (P3)), UCL, June 3, 2009

WP4: Superconducting nanosystems

• Workshop on Superconducting Nanosystems (organised by KU Leuven (P2)), KU Leuven, July 24, 2008.
• Workshop on Nanostructured Superconductors (organised by UA-NANO (P1)), UA, February 10, 2009.
• Workshop on Vortex Dynamics in Mesoscopic Superconductors (organised by KU Leuven (P2)) KUL, July 14, 2009.

WP5: Carbon nanotubes and related carbon materials

• Workshop on Carbon Based Materials (organised by UA-NANO (P1) & U Hasselt (P6) & KU Leuven (P2)), KU Leuven, March 31, 2008.
• Symposium on Carbon Nanostructures (organised by UA-Plasmant (P4)), Congress centre ’t Elzenveld, Antwerp, September 15, 2008.
• Graphene Workshop (organised by UA-NANO (P1)), UA, November 24, 2008.

III. 2. Common use of equipment and exchange of researchers

List of the most important common use of equipment:
• Transmission electron microscopy (P1). This has lead to common publications with almost all partners.
• Scanning probe microscopy (P2, P3) has been used by several partners.
• Ab initio density functional based computer programme: ABINIT (P1, P3, P5). This program was developed by X. Gonze (P3) and is currently also used by P1 and P5. The importance of this type of modelling has increased over the years. In many papers these days experimental results are compared with ab initio calculations.

Specific examples of the common use of equipment are detailed in Sec. III. 3.

Exchange of researchers should be viewed as mobility because of the small distance between the partners (max. 120 km between the Belgian partners).

There have been regular work visits which have resulted in joint experiments, joint calculations and co-publications. IAP-researchers have met regularly at symposia organized by the different partners, at the WP-meetings and at the annual general IAP-meetings.

The PhD in progress of P. Vansweevelt (P6) has P. Wagner (P6) as PhD-adviser and C. Van Haesendonck (P2) as co-adviser. For the PhD in progress of T. Moorkens (P2) the advisor is C. Van Haesendonck (P2) and F. Peeters (P1) belongs to the advisory committee of this PhD. In several of the PhD committees the extern members were professors from the research groups belonging to the IAP network.

There has been an increase of important international mobility as a consequence of the multiple international collaborations. Several longer international stays were also realized.

Section III. Networking
III. 3. Joint experiments and joint calculations. Exchange of materials and tools

UA-NANO (P1), KUL (P2) and UHasselt (P6):

**WP4: Superconducting nanosystems**
- Joint experiments on the preparation and physical properties of nanoparticles made from superconductor (A15) materials.

**WP5: Carbon nanotubes and related carbon materials**
- Joint experiments on the electronic transport properties of graphene-based layers. *Results are prepared for publication.*
- Joint FWO project on electronic properties of biologically-modified, graphene-based layers.

UA-NANO (P1), UA-Plasmant (P4) and UHasselt (P6):

**WP5: Carbon nanotubes and related carbon materials**
- Joint experiments on the nucleation mechanism of nanograined diamond and characterization of nanocrystalline diamond (NCD) grown by continuous dc bias during plasma enhanced chemical vapour deposition. *Results are published in Proceedings of the Material Research Society Meeting, and a joint paper will be submitted soon.*
- Regular meetings between the partner groups on the comparison of experiments and computer modeling for (ultra)nanocrystalline diamond thin film growth.
- Joint FWO project proposal on the origin of nano- and microdiamond in exogenous objects and on the nucleation mechanism of nanograined diamond.

UA-NANO (P1), UCL (P3) and ULg (P5):

**WP3: Semiconductor quantum dots and wires**
- Joined calculations on the electronic structure of Si nanowires and possibilities for applications. *Results are submitted to Phys. Rev. B.*

UA-NANO (P1) – KUL (P2):

**WP1: Metallic and oxide clusters**
- Joint research on ZSM-48 zeolite family materials resulted in *publication in Chemistry of Materials.*
- Joint experiments on 3D imaging of nanoparticles in biomaterials.
- Cluster deposition and exposure to H₂ of Au and AuPd clusters and transmission electron microscopy (TEM).
- TEM experiments on Pb nanoclusters embedded in Si.

**WP2: Magnetic dots and wires**
- TEM experiments on spin torque systems (Co nanoclusters in Ag).
WP3: Semiconductor quantum dots and wires
- Joint research (experiment versus theory) on exciton confinement InAs/InP quantum wires and quantum wells. *Joint publication in Phys. Rev. B.*
- Collaborations on classification and control of photoluminescence of Si nanocrystals. *Results are published in Nature Nanotechnology.*

WP4: Superconducting nanosystems
- Experiments on the parameters of GaAs films which in contact with superconducting materials resulted in *joint publication in European Physical Journal B.*
- Transverse voltage measurements in Al transport bridges with different arrays of triangular-shaped pinning potentials and calculations of the effect of transverse vs. longitudinal ratchet.

WP5: Carbon nanotubes and related carbon materials
- Joint research on synthesis of few-layer graphene and carbon nanotubes using microwave plasma-enhanced chemical vapour deposition. *Publications in Nanotechnology and J. Optoelectronics and Advanced Materials.*
- Synthesis of methyl-functionalized Ti-MCM-41 nanoparticles and their catalytic properties. *Results are published in Journal of catalysis.*

UA-NANO (P1) – UCL (P3):

WP3: Semiconductor quantum dots and wires
- Transfer of scanning gate microscopy (SGM) data and initiate collaboration.

WP4: Superconducting nanosystems
- Experimental measurements (UCL) and theoretical modelling (UA-CMT) of transport properties on NbN superconducting strips resulted in *publications in Phys. Rev. B.*

UA-NANO (P1) – UA-Plasmant (P4):

WP1: Metallic and oxide clusters
- Modelling of chemical processes in the low pressure capacitively coupled RF discharges resulted in joint *publication in J. Appl. Phys.*
- Regular meetings on the comparison between experiments and computer modeling for the growth of complex oxide thin films and on molecular dynamics simulations for laser-induced melting and vaporization of metals.
WP5: Carbon nanotubes and related carbon materials
- UA-CMT and UA-Plasmant also collaborated on the DFT study of the mechanisms leading to the initial stages of carbon nanotube growth.

UA-NANO (P1) – UH (P6):

WP1: Metallic and oxide clusters
- Joint TEM experiments on the visualisation of nanoparticles in biomaterials.

WP5: Carbon nanotubes and related carbon materials
- Joint experiments on diamond nucleation by carbon transport from buried nanodiamond Ti sol-gel composites. *Publication in Advanced Materials.*
- TEM studies on molecularly imprinted polymers.
- TEM & Electron energy loss spectroscopy (EELS) investigations on sol-gel based nucleation layers for NCD.
- Joint experiments on the imaging of molecular imprints.

UA-NANO (P1) - U Paris (EU Partner):

WP1: Metallic and oxide clusters
- EMAT-UA (P1) collaborated with M.P. Pileni and I. Lisiecki (Paris, EU Partner) on the nature of Co and Co-O nanoparticles. *Results are published in EMC and Chemistry of Materials.*

KUL (P2) – UCL (P3):

WP2: Magnetic dots and wires
- Channeling experiments on membrane templates.
- Oxygen implantation in Co nanowires.
- Growth of Fe nanowires for Moessbauer experiments.

WP3: Semiconductor quantum dots and wires
- A. Volodin and V. Iancu (KUL) and M. S. Rodrigues (UCL) shared expertise on pulsed valve deposition techniques in ultra high vacuum (UHV), in view of experiments involving ultra-clean deposition of nanowires on semiconductor substrates.

WP4: Superconducting nanosystems

KUL (P2) – UH (P6):

WP1: Metallic and oxide clusters
- Collaborations on the study of thermal properties of CoSi and NiSi structures. *Results are published in J. Phys. D.*
- Joint experiments on the electronic properties of networks of Pd nanoparticles.

WP2: Magnetic dots and wires
- EXAFS synchrotron experiments on magnetic nanoparticles made by the micellar method.
- Neutron reflectivity experiments on multiferroic BiFeO3 films.
WP4: Superconducting nanosystems
- Joint FWO project on superconductivity in synthetic diamond.

WP5: Carbon nanotubes and related carbon materials
- Carbon nanowalls: biological modification with DNA strands and hybridization experiments with complementary and mismatched DNA. Results are published in Chem Phys. Lett.
- Development of electric contacting methods for graphene flakes.

UCL (P3) – Ulg (P5):

WP1: Metallic and oxide clusters
- Collaborations on electronic and structural properties of ferroelectric oxides. Publication in Phys. Rev. B.
- Calculations within first-principal density functional theory have been conducted to study the properties of GeTe clusters and nanowires and resulted in publications in Phys. Rev. B and Phys. Rev. Lett.

WP3: Semiconductor quantum dots and wires
- Joined calculations on typical ferroelectric perovskite oxides (like BaTiO$_3$ and PbTiO$_3$) which yielded the proposal of new B1 hybrid functional providing simultaneously correct structural, ferroelectric and electronic properties in this class of systems. Published in Phys. Rev. B.
- Exchange of information concerning simulations of the electronic properties of semiconductor nanowires and experimental techniques to measure their local electronic properties.

WP5: Carbon nanotubes and related carbon materials
- First-principles approach to material and nanosystems properties. Published in Computer Physics Communications.

UA-Plasmant (P4) – UH (P6):

WP5: Carbon nanotubes and related carbon materials
- Collaborations on the study of (ultra)nanocrystalline diamond thin film growth by microwave plasmas.
- Calculations on growth of NCD under continuous bias and comparison with experiment.

Section III. Networking
III. 4. Colloquia and workshops


“Engineering of Functional Interfaces EnFI 2008”, organized at *Aachen University of Applied Sciences* on June 12 – 13, 2008 by T. Doll (Johannes-Gutenburg University Mainz), M.J. Schöning (Aachen University of Applied Sciences) and P. Wagner (UHasselt).


Workshop on “Ion beams to tailor the magnetic properties of advanced materials at the nanometer scale”, *KULeuven*, February 24, 2010. Organizers: A. Vantomme (KUL) and K. Temst (KUL).


III. 5. Joint doctoral Schools and tutorials

Joint European Master Degree program FAME (Functional Advanced Materials Engineering, Erasmus Mundus I program) between ULg, UCL and other international partners (started in 2007).

Joint Complementary Master degree in “Nanoscience and Nanotechnology” between UCL, ULg and other Belgian partners (started in 2008).

“EMAT winter school on electron microscopy”: a dedicated course (4 weeks) in advanced electron microscopy organised by the EMAT group (P1) for IAP members as well as for foreign scientists.


III. 6. Internal communication

All the information relevant to the researchers of the IAP-project was put on the webpage: http://www.cmt.ua.ac.be/iap6/. Announcements of workshops and other events could also be found there. The latter information and non-IAP organized workshops and conferences relevant for the IAP-project, and new vacancies were regularly communicated electronically to the researchers of the network (at the kick-off meeting a list of email addresses of researchers involved in the IAP-project was asked and this emailing list is regularly updated).
III. 7. Follow-up committee

The follow-up committee consists of:

Prof. Dr. Marc Van Rossum (Imec, Leuven, Belgium)
Prof. Dr. Petra Rudolf (University of Groningen, Netherlands)
Prof. Dr. Josep Nogues (Institut Catala de Nanotecnologia, Barcelona, Spain)

They obtain each year the annual report and are asked for comments and suggestions to improve the IAP-project. They are invited to the annual “General IAP meeting”. To increase the involvement of the follow-up committee we decided last year to invite each year one member of the follow-up committee to present an invited talk at our annual meeting.

III. 8. Added value

III. 8. 1. Joint publications

Thanks to the network, existing collaborations were able to continue and new collaborations have been set up between researchers of the different partners. This has led to several joint publications between the partners. An overview of the joint publications over the period 2007-2009 is given in Table 2A. The separation over the different years is shown in Table 2B which gives an idea of the increase of the output resulting from such collaborations within the network.

Table 2A: Joint publication in the period 2007-2010

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Table 2B: Joint publication in 2007/2008/2009(+2010)

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III. 8. 2. Prizes and awards

1. IAP P6/42 Annual PhD Prize

In order to increase the visibility of the IAP P6/42 network an Annual PhD Prize for the best PhD thesis, which was defended at one of the teams of the network, was established. The PhD prize Committee consists of the WP team leaders, supplemented with one of the members of the follow up committee. The chairperson of the Committee rotates between the WP leaders. The recipients of this prize are listed in Sec. V.2.

2. Other prizes and awards

In Annex II we give a list of (i) awards and (ii) featured papers that were realized by the members of this IAP-network.

III. 8. 3. Specific examples

UA-NANO (P1)

Hartwin Peelaers was trained in the group of F. Peeters (UA-NANO, P1), mostly by his younger colleague B. Partoens, in \textit{ab initio} calculations of the electronic structure of quantum wires. This technique was new to UA-NANO, and therefore a new collaboration was set up with X. Gonze (UCL, P3) in order to obtain the necessary expertise in this area. Although the problem of \textit{ab initio} calculations of the electronic and vibrational properties of quantum wires turned out more difficult than anticipated, H. Peelaers was able to bring this work to a good success which resulted in two publications in Nano Letters (IF=10.37) and two in Applied Physics Letters (IF=3.73) and one paper in progress with X. Gonze (UCL, P3) and one with the group of Ph. Ghosez (ULg, P5). He defended his PhD thesis in December 2009 and was awarded the IAP PhD-prize. In the meantime he received a BAEF-fellowship for a one year postdoctoral research in the group of Prof. C. Van de Walle (Santa Barbara, USA).

Parallel with the work of Peelaers another student, O. Leenaerts, used the ABINIT code to study the interaction of molecules with graphene. This resulted: i) in a first publication in Physical Review B in 2008 which, within 2 years, has already 54 citations and, ii) in a new collaboration with the experimental group of Chris van Haesendonck (KUL, P2) on the workfunction of multilayers of graphene.

Thanks to the current IAP the group UA-NANO (P1) was able to obtain new expertise in the area of \textit{ab initio} calculations and to initiate new collaborations with theory groups from UCL (P3) and ULg (P5) and with an experimental group of KUL (P2). Furthermore, it lead to a successful application for a SBO project on 'In Silico Materials Design (ISIMADE) and experimental validation for novel optical coatings' (2009-2012) in which B. Partoens (UA-NANO, P1) and X. Gonze (UCL, P3) are participating. The expertise on computational modelling in Belgium was brought together in a FWO-WOG project (2009-2014) on 'Computational modelling of materials' coordinated by F. Peeters (UA-NANO, P1) and which includes groups from KUL (P2), UCL (P3), UA-Plasmant (P4), ULg (P5) and theory groups from FUNDP (Namur), ULB (Brussels), Delft (NL), MIT (Cambridge, USA) and Santa Barbara (CA, USA).
KU Leuven (P2)

Obviously there is an important and unique added value through the interaction with the different theory groups of the IAP consortium. In Leuven there are no condensed matter theorists, implying that the interaction is essential. Most developed is the interaction with UA-NANO (F.M. Peeters) and in particular the work with the group of V.V. Moshchalkov on nanostructured superconductors that has resulted in several common publications. Other interactions have more recently been started e.g. on the electronic and mechanical properties of few-layer graphene (C. Van Haesendonck) and should be valorized in terms of common publications in the near future.

Another clear added value is provided by the interaction with UA-NANO (G. Van Tendeloo), where essential information about the structural properties of nanowires and in particular nanoparticles could be obtained via high-resolution TEM. A striking example is a common publication in Nature Physics with the group of V.V. Moshchalkov on the photoluminescence from Si nanocrystals. There has also been a very successful and fruitful collaboration (common publications) on metallic clusters with the group of P. Lievens, where the atomic scale structure of the clusters could be linked to their specific functional properties (magnetic exchange bias, hydrogen uptake). With the group of C. Van Haesendonck a close collaboration has been initiated on self-assembled protein wires, revealing the complementary information that can be obtained from TEM and from AFM. Moreover, it could be clearly demonstrated that such wires can act as templates for forming metallic nanowires by electrochemical deposition. A manuscript has now been accepted for publication in Advanced Materials, where it is demonstrated how electron microscopy based tomography combined with AFM allows to investigate the helical arrangement of metallic nanoparticles during the initial growth of the metallic wires.

Diamond films, which are grown by the CVD technique and intensively investigated by the UHasselt partner, have provided a nice playing ground for the KULeuven researchers to explore in close collaboration with the UHasselt partner two unique physical properties (resulting in common publications). Using electrostatic force microscopy (EFM) the group of Chris Van Haesendonck could link the homogeneity at nanometer scale of the 2D hole gas, which is formed at the diamond film surface upon hydrogenation, to the hydrogenation procedure that was used by the UHasselt partner. On the other hand, the group of V.V. Moshchalkov relied on electrical transport measurements down to very low temperatures to investigate the superconducting properties of the boron-doped diamond films prepared by the UHasselt partner.

There has been a successful collaboration (with common publications) between UCL (L. Piraux) and the group of V.V. Moshchalkov on the vortex lattice in superconducting films that is affected by periodic pinning arrays. The appropriate pinning arrays are fabricated at UCL by electrodeposition into anodized aluminium oxide nanotemplates, while the vortex lattice properties (in particular matching effects) can be probed at low temperatures using electrical transport and magnetization measurements. It is clear that in the near future simulations based on DFT can also provide an important added value for the experimental research activities at KULeuven. Although there are no common publications at this point, there have been several interactions with the experts of UCL, ULg and UA-NANO to explore the many possibilities offered by these simulations. One very relevant example is the work on multiferroicity, where the experimentalists at UHasselt (M.K. Van Bael), who prepare multiferroic samples using chemical synthesis, have set up a close interaction with experimentalists of the KULeuven (M.J. Van Bael, K. Temst, A. Vantomme, C. Van Haesendonck) to investigate the electrical and magnetic properties as a function of temperature and applied electrical...
and magnetic fields. Here, the input of the ULg theorists may allow to establish the essential link between composition, structure and functional properties of the multiferroic samples.

**UCL (P3)**

All meetings within IAP network are highly instrumental in maintaining relationships, promoting information exchange, and adding value by starting new, major collaborations.

Since the start of the IAP, the group of L. Piraux at UCL has initiated a collaboration with the group of V. Moschalkov at KUL. UCL has a large expertise in nanofabrication using the nanotemplating approach, that makes possible to the preparation of well-ordered arrays of nanopores, bumps and nanowires with characteristic dimensions at the nanoscale. On the other side, the KUL team is recognised worldwide for its scientific expertise in vortex dynamics in superconductors and hybrid ferromagnetic/superconductor nanostructures. This collaboration gives rise to sharing of samples and experiments and exchange of researchers. Also, in this framework, 2 PhD thesis: Wim Vinckx (KUL-2007) and X. Hallet (UCL -scheduled in 2011) and six common publications during the period 2007-2009 (Physica C, Small, Applied Physics Letter).

On the occasion of the Summer School on Nanosciences in 24-28 August 2009, held in Leuven, the keynote speakers were Profs. J.-M. Lehn (Nobel Laureate) – Strasbourg, H. Manoharan – Stanford, and A. Rowan – Nijmegen. During the period of the Summer School, the group of Dr. S. Melinte and Prof. G.M. Rignanese from Louvain-la-Neuve had the opportunity to initiate a collaboration with the group of Prof. H. Manoharan. In this natural way, the association of the experimental work carried out on scanning tunnelling microscopy (STM) by the group of Dr. S. Melinte and the theoretical work of the team of Prof. G. M. Rignanese with the corresponding strategy followed at Stanford University by Prof. H. Manoharan offers a prospectus for a richer scientific output of the IAP network.

The main research theme of Prof. V. Bayot group within WP3 concerns the investigation of local-scale electron transport inside semiconductor nanodevices, using SGM. The development of this new technique relies on in-depth comparison between experimental and simulated data. In this framework, the groups of Profs. V. Bayot (UCL) and F. Peeters (UA) joined forces to uncover the detailed mechanisms giving rise to the contrast in SGM images in different regimes of electron transport (low and high magnetic field, ballistic and/or coherent transport, ...). In particular, members of both groups met several times and exchanged experimental data and simulations results concerning low temperature SGM on quantum rings. Different aspects were spotted, such as the search for the origin of concentric conductance fringes observed by SGM outside the area of the quantum rings, and the asymmetric behaviour of SGM data observed upon reversing the tip voltage. These meetings were at the origin of new ideas at the consortium level, both on the experimental side (e.g.: new device concepts and new measurement techniques) and on the theoretical side (e.g.: new simulations methods aiming at reproducing specific experimental configurations). Note that the simulations tools developed within the group of Prof. F. Peeters (UA) are complementary with those developed by Dr. M. Pala (Grenoble), which have already proven very efficient to explain the SGM contrast observed within the area of the quantum rings (see, e.g., the recent publications on this subject by M. Pala and members of Prof. V. Bayot group). Thanks to the IAP network, the teams of Dr. M. Pala and of Prof. F. Peeters have now started to collaborate on this topic.

Furthermore, low temperature STM is a technique that is currently developed within the group of Dr. S. Melinte, in view of future experiments on semiconductor nanowires. Developments in progress include a new pulsed valve system to deposit nanowires dispersed in various solvents onto a
reconstructed semiconductor substrate prepared in UHV. As the other IAP team involved in STM manipulation of clusters and nanowires (Prof. C. Van Haesendonck group, KUL) could also benefit from this new deposition system, members of both groups met several times in order to set up a protocol for transferring samples by keeping the UHV environment. Both UHV systems needed to be adapted in order to allow the connection of a mobile UHV system, equipped with an autonomous pumping setup. This first joint experimental step and first contacts were a prerequisite for future joint experiments, and for the creation of a versatile interuniversity platform for atomic-scale structural and spectroscopic characterization of nano-objects. The possibility to exchange samples between the only two low temperature UHV STM systems operated in Belgium and, therefore, to take advantage from the complementary tools attached to both microscopy systems is a clear added value gained through these networking activities.
Section III. Networking
IV. Position of the IAP Network

IV.1 Cutting-edge Research

IV.1.1 Scientific highlights of the network

The major scientific highlights can be listed as follows:

- New ways of controlling the reactivity of small gold clusters by selective atom doping.
- Novel imaging technique of the 3D characterization of the organisation of hybrid protein-NP complexes.
- First fully based ab initio explanation of environment and ligation charge transfer effects in hybrid gold NP.
- Using state-of-the-art lithography and nanomanipulation techniques, a conductive scanning probe tip was positioned on a single magnetic nanowire within a membrane, allowing measurements of the spin torque effect.
- The contribution of domain walls to the magnetoresistance was measured in magnetically modulated Fe films, in which controllably and reproducibly a periodic set of domain walls can be nucleated.
- Realization of an ultra-low temperature nano-scanning gate that can operate in a magnetic field up to 15 T.
- Extension of the ABINIT code to first principle approach of electronic, optical and vibrational spectroscopies.
- Using state-of-the-art ab initio techniques, detailed quantitative predictions have been made of potentially new multiferroic materials (e.g., in PbTiO$_3$/SrTiO$_3$), which will guide the experimentalists.
- Theoretical explanation of the enhancement of the superconducting critical temperature in nanowires.
- Visualization of frozen kinematic vortices.
- First direct visualization of symmetry induced giant vortex formation.
- Theoretical prediction and first direct visualization of pinning induced vortex clustering and giant vortex formation.
- Discovery of type-1.5 superconductivity.
- First-time realization of PECVD-growth of carbon nanowalls that consist of only a few atomic layers.
- Theoretical demonstration of electrical confined quantum dots in graphene bilayers.
- Theoretical prediction of the possible formation of endohedral Ni@C$_{60}$ metallofullerene.
- Experimental realization of state-of-the-art nucleation procedures for high-quality diamond growth.
- Realization of full 3D imaging of a complete network of as-grown CNTs by on-axis rotation electron tomography.

A more detailed explanation of the scientific highlights are organised below according to the different work packages. They are related to the mainstream in the specific scientific domain.
Section IV. Position of the IAP Network

WP1: Metallic and oxide clusters

In the field of the characterization of the properties of individual doped metallic clusters, the work of P2-KUL on the theoretical and experimental characterization of doped gold and copper clusters and of the effect of doping on catalytic properties that shows that the selective insertion of a single dopant atom can be used to control the chemical reactivity of gold and copper clusters lead to a publication in the prestigious journal Faraday Discussion together with a cover, which demonstrates the forefront character of this research.

Another important field where WP1 partners (P1 and P2) have carried out cutting edge research is the 3D characterization of nanoparticles by electron tomography coupled to TEM and XRD techniques. The joint work on the anchoring of silver nanoparticles on insulin fibrils is accepted for publication in the prestigious journal Advanced Materials. This is the first time that a biotemplated material is investigated in 3D. This was made possible by using advanced reconstruction techniques ("discrete electron tomography"). From a more general point of view, the use of state of the art imaging and near field spectroscopic techniques (TEM, STM, AFM) as the ones developed by P1 and P2 provides crucial understanding on the role of surface characteristics and of residual gases on the size distribution and self-organization of oxide and metallic NP’s. P1 in collaboration with P-EU and P6 (using XPS) showed how important fluctuations in size distributions and in composition affect the self-organization of magnetic nanoparticles. Ultimately, these characterization techniques should allow controlled patterning of surfaces with NP having catalytic or data storage properties.

P5 performed state of the art theoretical investigation of the effect of environment (ligand and solvent) and on the functionalization of metallic clusters. This work lead to an invitation to write an article for the special issue of the ACS Journal of Physical Chemistry C which will contain the work of two postdocs hired by P5 on the IAP, Dr. Ganga Periyasamy and Dr. Engin Durgun). These effects are essential for the use of these clusters as building blocks in intelligent sensors and nanoelectronics.

WP2: Magnetic dots and wires

a) Multiferroics

Multiferroics is a topic which is new for the network and which was not in the initial project work program. However, during the past few years, the worldwide interest in multiferroics (especially in nanostructured multiferroics and thin films) is exploding. It is clearly a hot topic from which rich physics is emerging, and which also attracts interest for its potential applications. It is also an appropriate topic for the network, since some of its most salient features are precisely related to a number of the goals of this work package, like e.g. the emergence of magnetism (in magneto-electric materials), the magnetic anisotropy in relation to the complex crystal structure of multiferroic compounds, the existence of exchange bias in multiferroic systems etc. It is also a topic to which many of the network partners can contribute with their specific expertise, e.g. advanced theory at the ULg, high-resolution transmission electron microscopy at the UA-NANO, magnetotransport and neutron scattering at the KUL. Around the topic of multiferroics, new and strong interactions have emerged with a young group which is not in the current network, i.e. the group of Marlies Van Bael and An Hardy at the UHasselt (which is interacting with the UA-NANO and with KUL on this topic). We consider all these interactions and research related to multiferroics as extremely promising.

b) Exchange bias

Exchange bias is a more established topic within the network and it is one in which the participating partners are clearly at the forefront of the field, as can be observed from the many publications on this topic in top journals. The network activities concerning exchange bias excel in terms of deeper understanding of the interfacial ferromagnetic/antiferromagnetic coupling (KUL), the exploration of new geometries in which exchange bias is observed (e.g. UCL with its work on nanowires and KUL...
with its work on nanocaps), and the exploration of new ways to generate exchange bias (KUL with its work on inducing exchange bias by oxygen implantation in Co films).

c) Magnetic nanowires
The network is very fortunate to have one of the world’s leading experts on the templated growth of (magnetic) nanowires as one of the partners: indeed, the UCL partner has unique and extensive expertise in this matter, allowing systematic probing of many different aspects of magnetic nanowires. Apart from the templated growth, one-dimensional magnetic structures are also prepared using glancing-angle deposition in MBE, lithography and ion beams. The precise control over the resulting geometry provided an advantage of the network over international competitors.

d) Spin torque effects
Spin torque effects are currently also a very hot topic, on the one hand because of its fundamental scientific challenges and on the other hand because of its potential applications. It is, technically, a difficult topic, because spin torque can only be observed in magnetic systems like nanowires, multilayer pillars or granular materials. Again the template-grown nanowires turn out to be a ‘natural geometry’ allowing systematic spin torque effect measurements.

e) Spectroscopy on magnetic islands
The elucidation of the electronic structure within small magnetic islands remains at the forefront of physics, because it provides direct information about confinement effects and the quantum nature of nanometer-sized (magnetic) islands. The detailed scanning tunneling microscopy and scanning tunneling spectroscopy experiments carried out within the network are absolutely state of the art and are systematically published in top-ranking journals.

WP3: Semiconductor quantum dots and wires
The development of first-principle formalisms, and the associated implementation efforts have a large impact on the scientific community. Many researchers use such tools daily. At the level of the ABINIT software, whose development is coordinated at the P3, and to which the P1 and P5 contribute, the main mailing list has at present more than 1300 registered addresses, while the article presenting the project, published in 2002 [X. Gonze et al., Comput. Materials Science 25, 478-492 (2002)] has been cited more than 1000 times, of which about 350 in the years 2008-2009. P3 focuses on the first-principle approach to spectroscopy, especially electronic, optical and vibrational spectroscopies. This IAP project introduced the challenge to adapt the theoretical tools suited for the study of bulk materials to the study of nanosystems.

In this respect, the use of many-body perturbation theory for the accurate computation of the electronic structure of nanosystems has been quite successful. To our knowledge, the full band structure of Si NWs, obtained in the GW approximation, will be the first one to be published. The study of the exciton-plasmon coupling and the associated introduction of a new algorithm to bypass the Tamm-Dancoff approximation is at the forefront of theoretical research in nanophysics [Exciton-plasmon states in nanoscale materials: breakdown of the Tamm-Dancoff approximation, M. Gruning, A. Marini, and X. Gonze, Nano Letters 9, 2820-2824 (2009)].

The P3 theory group, as well as nine other leading groups in the domain (altogether more than 200 researchers) have recently founded the “European Theoretical Spectroscopy Facility” (http://www.etsf.eu) of which P3 is the central node, and X. Gonze the president. By organizing formations, distributing software applications, and undertaking “user’s project”, the ETSF has a strong worldwide impact in theoretical spectroscopy. The work on GeTe nanoplatelets was the subject of an impressive synopsis: “Twisting left and right gives logic another turn” by D. Ucko. It has been recognized as the first evidence for polarization vortices obtained at a truly first-principles level. This is a major step forward in the modelling of ferroelectric nanoparticles [Polarization Vortices in

Complex oxides play an important role in various applications and their nanostructures are nowadays the subject of numerous researches in order to clarify the size-evolution of the properties but also the possibility of inducing new phenomena. The prestigious magazine Science classified recent discoveries at oxide interfaces as one of the top 10 scientific breakthroughs of 2007. In this context, P5 demonstrated that an artificial superlattice (Fig. WP3.6), which has a multilayer structure composed of alternating atomically thin layers of two different oxides (PbTiO₃ and SrTiO₃), possesses properties radically different to either of the two materials by themselves and behaves like an improper ferroelectric. The emergence improper ferroelectricity is a direct consequence of the artificially layered structure and is driven by interactions at the atomic scale at the interfaces between the layers. Besides the immediate applications that could be generated by the unusual dielectric properties of this artificial nanomaterial, this discovery opens a completely new field of investigation and the possibility of new functional QDs and NWs based on oxide materials engineered on the atomic scale. [E. Bousquet, M. Dawber, N. Stucki, C. Lichtensteiger, P. Hermet, S. Gariglio, J.-M. Triscone and Ph. Ghosez: Improper ferroelectricity in perovskite oxide artificial superlattices, Nature (London) 452, 732-736 (2008)].

On the experimental side, a new SGM system was built in a ³He/⁴He dilution fridge, equipped with a superconducting coil. The low temperature part of the dilution fridge insert (the mixing chamber) was modified and a home-made scanning probe system based on a piezoelectric (tuning fork) detection of the tip movement was added, below the sample holder anchored on the mixing chamber. With the scanning probe microscope, the base temperature of the system is in the range 80-100 mK. The topographical resolution is in the range 1-5 nm at low temperature, and the system can operate up to a magnetic field of 15 T. These ranges of operation make this SGM system unique of its kind. Spectacular experimental SGM data were obtained at 100 mK on a “quantum Hall interferometer”, a mesoscopic quantum ring driven in the quantum Hall regime. This work is under peer review at Nature Communications, and may have an important impact, as quantum Hall interferometers are possible building blocks of the proposed “topological quantum computers”.

WP4: Superconducting nanosystems

The first theoretical description of the experimental measured enhancement of the superconducting parameters in nanowires and nanofilms, was presented by P1. They showed that size-dependent oscillations of the critical temperature in single-crystalline nanofilms of lead on silicon can be well understood with a numerical solution of the Bogoliubov-de Gennes equations. This work is of particular importance because it is the first theoretical paper on the subject that becomes now a hot topic. Indeed, a year ago experimentalists demonstrated [S. Y. Qin, J. Kim, Q. Niu, and C. K. Shih, Science 324, 1314 (2009)] that superconductivity survives in two-atomic-layer thick nanofilms of Pb, which was the world's thinnest superconductor in 2009 [see, e.g., H. H. Weitering, Chem.Phys.Chem. 10, 3183 (2009)]. In the beginning of 2010, one-atomic-layer films of Pb and In were reported to be superconducting below 1.8 and 3.4 K, respectively [T. Zhang et al, Nature Phys. 6, 104 (2010)]. Thus, single-crystalline metallic nanofilms of atomic uniformity are attracting now much attention. What is so special about superconductivity in such nanosystems? In two words, it is the formation of multiple single-electron subbands due to the quantization of the perpendicular electron motion, i.e., a multiband superconductor induced by quantum confinement. Two years ago partner P1 was the first who understood the importance of this problem and tackled this problem theoretically.

Besides the pioneer work by P1 where a clear account on the importance of the electron scattering time (the intrinsic healing time to recover superconductivity) to develop phase slip lines has been presented, the most resonant result on non-equilibrium superconductivity has been the recent joint publication by P1 and P2. This manuscript concerns the direct visualization of frozen kinematic
vortices by fast thermal quenching. The presented results not only provide the first direct evidence of a counterintuitive vortex-vortex attraction when vortices are set in motion, but also shed new light on unravelling the basic ingredients behind the formation of relativistic vortices. As such, they link two apparently disconnected parts of superconductivity, Abrikosov vortices and phase slip lines. In addition, we believe that this investigation of the formation of flux stripe patterns due to competing repulsive and attractive interactions will be of interests to physicists, metallurgists, material scientists, and chemists, where similar phenomenology can be observed.

Ought to the diversity of the physics tackled within the subject devoted to the manipulation of vortices and S/F hybrid systems, it is difficult to highlight one single result. The international reputation of P1 and P2 on S/F hybrid structures is reflected in the recently invited review article (KUL, P2) which has been selected as a highlight 2009 of the Superconductor Science and Technology journal. This invited review article not only presents a thorough and comprehensive overview of the physics involved with electromagnetically coupled S/F hybrids systems, but it also complements previous review articles on this topic by discussing new aspects such as the limiting case of soft-ferromagnets.

Although not at the core of the current IAP project but without any doubt of primary relevance to the superconducting community is the newly discovered type 1.5 superconductors by partner P2 in collaboration with scientists from Switzerland. This genuine new type of superconductivity results from the coexistence of two order parameters, one of them exhibiting type I superconductivity whereas the other lies in the type II regime. This Type 1.5 superconductivity has been spotted in Physics World, Science, Wikipedia and other blogs and was selected for View Point and as an editors’ choice in Physical Review Letters in 2009. The formation of fluxon patterns in this type 1.5 superconductors is a fascinating topic which is related with the much broader physical phenomena of self-organization. The usually periodic patterns are often the result of competing interactions. One of the typical structures consists of stripe patterns, which are found in magnetic, colloidal, and biological systems.

In brief, there is no doubt that the current IAP project has not only contributed to strengthen and invigorate previously running collaboration among all partners, but has also established a solid link and helped to define common new objectives between theoretical and experimental groups. From an international perspective, the present research project is perfectly aligned with the European ESF Research Program Networking “Nanoscience and Engineering in Superconductivity-NES” directed by Prof. V. Moshchalkov. In addition, the research described in WP4 included the active participation of several international teams working in the field of superconductivity and magnetism such as Prof. R. Wijngaarden (Amsterdam, Magneto-optics), Prof. V. Metlushko (University of Illinois at Chicago, nanomagnets), Prof. S. Bending (Bath, Scanning Hall Probe Microscopy), Prof. H. Suderow (Madrid, Scanning Tunnel Microscopy), Prof. A. Buzdin (Bordeaux, BCS theory and S/F hybrids systems), Prof. C. Reichhardt (Los Alamos, molecular dynamics simulations), to name a few.

The current IAP project has contributed not only to strengthen and invigorate previously running collaboration among all partners involved in the WP4, but has also helped to define common new objectives between theoretical and experimental groups. More specifically, the combined effort of P1 and P2 on the study of superconductor-ferromagnet hybrid systems has situated these two partners as a world-wide recognized reference on this particular topic. The international reputation of P1 and P2 on S/F hybrid structures is reflected in a recently invited review article selected as a highlight 2009 of the Superconductor Science and Technology journal and a total of 35 publications during the last three years on the subject. In addition, the rapid development on the fabrication of high quality nanoporous templates by P3 in combination with the experimental expertise of P2 on superconductivity, has brought these two partners to a top international level as manifested by the quality of the publications and the numerous invited talks. We should also emphasize that the common interest by P1, P2, and P3 on the investigation of dissipative mechanisms in superconducting nanowires allowed us to build up a very solid national network which will undoubtedly bring these groups to the core of this fascinating field.
WP5: Carbon nanotubes and related carbon materials

The scientific highlights of the work accomplished in the framework of WP5 are quite diverse, given the number of topics covered in this WP. However, the most important highlights can be summarized as follows.

In the diamond-related work, the main highlight is the study of the nucleation of diamond and the different aspects of the three techniques mentioned in the scientific summary. This is particularly true regarding the collaborative nature of this work, with contributions from UA-NANO/EMAT (P1), UA-Plasmant (P4) and UHasselt (P6). The method based on the colloidal seeding, developed by UHasselt (P6), is state-of-the-art in nucleation procedures for diamond growth. This work has made clear for the first time the importance of using core diamond particle sizes of 5 nm or even lower. These particles must be fully deaggregated and stable in solution to give high nucleation densities. The diffusion-based model developed together with UA-NANO/EMAT (P1) is an interesting topic that leaves many questions unanswered. It has led to a new FWO project between two UHasselt (P6) promoters and one from UA-NANO/EMAT (P1). The results on nucleation and the fabrication of diamond nanoparticles from NCD films grown under continuous bias, are clearly at the utmost forefront of the field.

In the graphene-related work, different highlights must be mentioned.

The theoretical work performed by UA-NANO/CMT (P1) on the electronic and mechanical properties of graphene is groundbreaking, demonstrating the use of graphene as a sensitive gas sensor and its potential for fabrication of nanocages and nano-membranes.

The KU Leuven partner (P2) has succeeded for the first time to use PECVD to grow carbon nanowalls that consist of only a few atomic layers (down to 4 layers). The vertically oriented few-layer graphene sheets can be conveniently used for field emission applications. The high-density networks of few-layer graphene sheets have a very high surface to volume ratio that offers unique possibilities for various other applications. Furthermore, in collaboration with the UHasselt (P6) the networks were, e.g., successfully used for the detection of the binding between complementary single-stranded DNA fragments.

Using ab-initio calculations UCL (P3) demonstrated the possibility to tune the electronic properties of graphene, by absorption of lines and strips of H and K (donors) and F (acceptor) on graphene, H⁺ and OH⁻ functionalization of graphene nanoribbons, and especially the ozone functionalization of graphene, opening a route to the control of the metal-insulator transition in chemically modified nanographenes.

In the field of carbon nanotube-related work, various highlights can be distinguished.

UA-NANO/EMAT (P1) succeeded in the 3D quantification of carbon nanotube networks in interconnects by electron tomography, allowing the study of the complete network of as-grown carbon nanotubes inside a contact hole without missing wedge artefacts.

KU Leuven (P2) has been able to obtain for the DWNTs atomic-resolution topographical and spectroscopic images of superior quality that are comparable to the best results that have been reported worldwide, using STM and STS at liquid helium temperature. Furthermore, in close collaboration with the UCL (P3) partner the STM and STS results can now be compared in detail to simulations based on ab initio calculations. This allows to link the local electronic structure of the DWNTs to the presence of specific defects that range between bends in the tubes down to atomic size defects.

Using a combination of first-principles MD and tight-binding MC, UCL (P3) has demonstrated the possible coexistence of a closed-end tip growth mechanism with the usual root growth mechanism in the catalyzed growth of SWNTs.

In the field of other carbon materials, UA-Plasmant (P4) presented a first-time demonstration, both by classical MD and first-principles MD, of the possible formation mechanisms of exo- and endohedral Ni-metallofullerenes.
IV.1.2 Perspectives of the network’s research domain for the coming five to ten years

It is expected that nanotechnology will have a profound influence in the 21st century. The network research domain is nanomaterials which takes a materials science based approach to nanotechnology. Materials with morphological features on the nanoscale are fabricated and their properties are investigated. This study is still in its infancy and new nanomaterials and new systems are emerging regularly. Furthermore, combining materials leads to hybrids which is a fertile ground for increased functionality. Because this is a huge area, we focused the network towards the study of clusters and nanowires. The possibility to nano-engineer the size, shape, structure and composition of clusters and nanowires new effects and properties are discovered which can be useful in different applications. It is expected that this area will still be important over the next decades to come.

The perspective of the network’s research domain for the future is discussed below in more detail.

WP1: Metallic and oxide clusters

The three subjects: 1) characterization of the properties of individual doped metallic clusters, 2) 3D characterization of nanoparticles by electron tomography, and 3) the effect of environment on the functionalization of metallic clusters, will no doubt be the subject of intensive research in the next 5 to 10 years and are likely to lead to technological application in catalysis, hydrogen storage and nanotechnologies for data storage, advanced sensing and the realization of complex logic operations at the molecular and nanoscale. The characterization of the 3D structures by complementary spectroscopic means and the control of the composition of nanomaterials at the atomic scale is crucial for understanding the physical properties of nanostructures in comparison to their bulk and atomic counterparts. They are also essential for developing accurate theoretical and modeling tools at a scale where matter properties are not quite those of the atomic scale and neither those of the bulk. As exemplified by their results, the partners of WP1 clearly gather the critical mass for making an impact in this field at the international level.

WP2: Magnetic dots and wires

As main directions for nanomagnetism research in the next five to ten years, we can identify the following items:

Dynamics of magnetic nanostructures will become ever more important, not in the least because of the link with applications. Further progress in the research of the dynamics is closely linked with evolutions at third and fourth generation synchrotron and x-ray free electron sources, where it will be possible to study dynamics at the picosecond time scale.

Magnetism in hybrid inorganic/organic structures. Elucidation of induced magnetism in non-magnetic organic compounds. Creation of artificial magnetic ordering by stacking organic molecules which contain a magnetic metal ion.

Deeper understanding of non-linear effects in magneto-optics.

Magnetic oxides with atomic control of interfaces, e.g., creation of ferromagnetism at the interface between two non-magnetic oxides.

Understanding of confinement effects and their possible use, e.g. in cryptography.

Spin torque effects: deeper understanding and its realization with lower currents, enabling applications.

Multiferroics: deeper understanding and achieving predictive power of the cross-coupling between different ordering parameters.
Expected breakthrough in dilute magnetic semiconductors (especially those based on wide-gap semiconductors like ZnO): unequivocal evidence of establishing true ferromagnetism, elucidation of coupling mechanism between localized spins.

**WP3: Semiconductor quantum dots and wires**

The perspectives related to first-principles calculations within the 5-10 coming years are rather exciting. On the one hand, the capability to simulate larger systems will depend on the capability to parallelize the software better than nowadays, so that one can use petaflop machines efficiently. On the other hand, real challenges are the *accuracy* of first-principles calculations, and the capability to treat nanosystems in which *strong correlations* are present. In particular, the accuracy of standard approximations is not sufficient for predictions that can be unconditionally trusted. Recent progress has opened the opportunity of an order of magnitude improvement of the accuracy obtained on some of the spectroscopic properties (and also atomic positions and electronic structure). The development of new formalisms (e.g. based on the Luttinger-Ward class of functionals, or based on the Adiabatic-Connection and Fluctuation-Dissipation theorems) is to be pursued. Moreover, the couplings between vibrational, electronic, geometric degrees of freedom, that could be neglected previously, enter into the game.

One interesting perspective that will be explored in the future is the engineering of exotic phenomena at insulating *oxide interfaces*. Emergent phenomena at oxide interfaces have been recognized by Science Magazine as one of 2007’s top ten breakthroughs. Just as the engineering of physical properties at semiconductor interfaces was the crucial step in Si-based electronics, the next great advance might rely on the multiple novel functionalities of oxide interfaces. Our interest will focus on how to play at the nanoscale to design improved ferroelectric, piezoelectric and multiferroic materials. It will also concern the study of the two-dimensional electron gas and NWs at oxide interfaces. These activities will be pursued within the European project OxIDes coordinated by Ph. Ghosez (ULg).

The ongoing work about GeTe nanoparticles and NWs seems to open promising perspectives for *phase change* applications, and this will be further investigated by studying the properties of these nanosystems in the amorphous phase. Nanosystems with related chemical compositions will also be investigated in view of thermoelectric applications. This collaborative work will imply both the development of theoretical tools for the improved modelling of thermoelectric and the applications to selected systems.

Certainly, group IV semiconductor NWs will remain at the heart of nanotechnology and nanosciences for the coming 10 years and several participants are committed to follow a vigorous research on NWs. While the search for feasible interconnects in nanoelectronics are continuing, Si NWs have appeared to be an attractive 1D material because of the well-known Si based microelectronic fabrication technology and their use directly on Si-based chips. Si NWs display diversity of electronic properties depending on the number of Si atoms in their cross section. Rod-like, oxidation resistant SiNW can now be fabricated with small diameters (1-7 nm) and display diversity of interesting electronic properties. In particular, the band gap of semiconductor Si NWs varies with their diameters. The techniques developed within WP3 have been used to study the excited states of Si NWs, in a collaboration between P1, P3 and P5, and represent a strong asset for further collaborations.

The development of techniques such as SGM to study the local scale behaviour of charge carriers represents a new approach in the field of electron transport. Only a few groups in the world have developed the technical skills required to perform such experiments, and P3 is currently at the forefront thanks to its new SGM system operating down to 80 mK and 15 T. This equipment, combined with the versatile nanofabrication tools available within the P3 clean rooms offers various prospects in the short and long term. Moreover, SGM data offer a much more complete view of transport than “classical” macroscopic measurements, and, therefore, allow much more in-depth tests of simulation and theory results. One is now in the position to investigate the correspondence between

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the structure (including, e.g. the confinement geometry) and the functional properties, such as electron transport, of QDs and NWs. In this context, the SGM tool will be invaluable as it can both pinpoint the location of individual defects in the confined geometry and directly observe the effect of such defects on electron transport.

The perspectives related to scanning probe microscopy of electron transport within the 5-10 coming years are highly promising. First, the challenge is to obtain experimentally a full structural description of the investigated system, and to correlate it to its transport properties. In this respect, the next step is to combine SGM with STM, which gives access to the local atomic structure of nanoobjects. Such a combination would be extremely useful: for example, it would allow to identify the atomic position and nature of a particular dopant within a semiconductor nanodevice, and to examine its influence both on the LDOS and on carrier flow in its vicinity. It would also lead to a very complete and precise comparison between experimental data and ab-initio simulation results. Furthermore, one can also envision experiments involving other types of local-scale perturbations of a nanodevice using AFM cantilevers. Local-scale perturbations of different types (stress/strain, localized charges, localized spins, ...) are ubiquitous in nanodevices, and strongly affect their transport properties.

**WP4: Superconducting Nanosystems**

Even though the confinement of superconductivity at nanoscale dimensions has attracted substantial attention during the last decade, still many fundamental questions remain open. Among the most interesting topics is the enhancement of the superconducting critical parameters, particularly the critical temperature, of small nanoparticles and nanofilms. A large amount of theoretical research by P1 has been devoted to this topic, but little experimental results have been achieved due in part to the difficulties inherent to the rapid aging of small particles and the detection of weak superconducting signals.

Concerning the manipulation of fluxons, nowadays the mechanisms ruling the behavior of fluxons at nanoscale both, statically and dynamically are fairly well understood. However, some of the simplest theoretically envisaged systems such as vortex concentrators, flux lenses, and step motors, have not yet been realized experimentally. In addition, in order to make the topic of fluxonics more attractive from the applications point of view, it is necessary to explore new superconducting materials of technological relevance such as YBCO or coated conductors. The extension to these systems is far from trivial. On the one hand, it involves a combination of much more delicate multistage sample deposition than the processes followed to obtain conventional superconductors. On the other hand, the pinning mechanisms needed in high-$T_c$ materials require improving the current nanolithography technique at least an order of magnitude or even reroute completely the fabrication techniques towards bottom-up (or all chemical) approaches. A clear effort following the latter vein has been pursued by several labs (Cambridge, Barcelona, and Los Alamos), and in the coming years it is expected that these investigations will profit from the knowledge gained at submicron scale (P1, P2, P3). An example of this trend is the current interest in superconducting cables where the introduction of ferromagnetic particles is a possible way to increase the critical current (i.e., the dissipationless regime).

All in all, it is crucial to continue the struggle to comprehend the physics of superconductor/ferromagnet hybrids. Among the most fascinating points that need to be addressed during the next decade are (i) an extension of the magnetic pinning theory within a more realistic theoretical formalism such as time dependent Ginzburg-Landau model, (ii) exploration of the thermodynamic properties (specific heat, thermal conductivity) of these hybrid systems, (iii) fabricate more controlled devices where the ferromagnetic subsystem is replaced by a micro-electromagnetic component. We believe that these investigations will inspire further developments in this area of solid state physics and perhaps motivate new applications of technological relevance.
It is also worth noticing that most of the research performed so far has focused on simple BCS type of superconductors. This approach allows one to build up the basic knowledge and understanding in the topic before tackling richer and more exciting systems such as triplet superconductivity (SrRuO), multicomponent superconductors (MgB$_2$) or ferromagnet-based superconductors (pnictides). Without any doubt this particular topic concerning the manipulation of vortices will be a very active line of theoretical and experiment research during the coming decade.

**WP5: Carbon nanotubes and related carbon materials**

While it is obviously a very difficult task to predict in which directions any field might evolve, several perspectives are envisaged for the coming years.

Currently, the most promising role for **nanodiamond particles and films** is to serve as a biocompatible material that has a surface that can be functionalised, and that can serve (in the case of particles) as a drug delivery agent. The surface properties of the film will be intensively studied and used to form heterostructures with other types of material, like small molecules, organic material, etc., for fundamental studies in e.g. charge transfer. Also, there remain many unsolved fundamental questions on size effects in small nanodiamond particles related to doping (superconducting effects), defects, luminescent properties and the relation to the surface termination, etc.

Of fundamental importance remains the unraveling of the exact growth mechanism of (U)NCD films. While much progress has already been made (as evidenced by the results shown in the scientific summary), many questions still remain. Advanced simulation techniques such as those developed and employed by UA-Plasmant (P4) will therefore continue to be an important research direction in the coming years.

The DNA-functionalization of graphene flakes and (U)NCD films will only gain more attention and importance, indicating the forefront position of the research conducted by UHasselt (P6) in this field of WP5.

All **graphene-based** nanostructures are expected to display the extraordinary electronic, thermal and mechanical properties of graphene and are thus promising candidates for a wide range of nanoscience and nanotechnology applications. Some experiments have shown an interesting dependence of the work function of multilayer graphene on the number of layers. Using density functional theory, UA-NANO (P1) will investigate the dependence of the work function on the number of graphene layers, on strain and the effect of adsorbed molecules. The KUL partner (P2) will perform Kelvin probe force microscopy to locally probe the work function of graphene and multi-layer graphene. The effects of strain on the electronic properties will also be investigated.

The UCL node (P3) plans to continue to investigate theoretically carbon-based nanostructures, including both carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) Although these systems share similar graphene electronic structure, confinement effects are playing a crucial role. Indeed, the lateral confinement of charge carriers could create an energy gap near the charge neutrality point, depending on the width of the ribbon, the nanotube diameter, the stacking of the carbon layers regarding the different crystallographic orientations involved. Their unusual electronic and transport properties promote these carbon nanomaterials as promising candidates for new building blocks in a future carbon-based nanoelectronics, thus opening alternatives to present silicon-based electronics devices.

Also in the **carbon nanotube field**, various perspectives can be distinguished. Indeed, despite intensive research efforts worldwide, linking at the atomic level the local electronic properties and the electrical conductivity to the presence of specific defects in carbon nanotubes and other nanostructures remains a big challenge. During the next few years the KULeuven (P2) partner will investigate this link by performing STM measurements in UHV and at low temperatures in the presence of a transport current (“atomic scale potentiometry”). This requires to deposit nanotubes on insulating substrates and to
attach to a nanotube electrical contacts that are within nanometer distance from each other and connect the nanotube to large predefined metallic contact pads. This may be achieved using STM based nanolithographic patterning techniques that obviously need to be applied “in situ” under UHV conditions. Through a collaboration with Prof. Markus Ahlskog at the University of Jyväskyla the KULeuven (P2) partner has access to a wide variety of high-quality carbon nanotubes that are prepared by different methods (arc discharge, laser ablation, chemical vapor deposition (CVD)). Furthermore, a new collaboration has also been initiated between UCL (P3) and KULeuven (P2) on the magnetic properties of randomly decorated CNTs (SQUID measurements versus theory prediction). However, only preliminary results are presently available.

Finally, one of the initial objectives in WP5 was the simulated catalyzed growth of SWNTs by classical MD. However, due to the lack of quality of the available interatomic potentials, this system could not yet be modeled accurately, and hence this topic was temporarily set on hold. However, very recently a new collaboration was initiated by UA-Plasmant (P4) with Prof. Adri van Duin at the Pennsylvania State University on this topic. The first preliminary results are very encouraging, and hold promise for the future realistic modeling of SWNT growth at the atomic scale.

IV.1.3 Build-up of critical mass

The present IAP project concerns the study of the structural, optical, magnetic, electrical and reactive properties of clusters and nanowires made up of different materials and combination of materials. Because of the versatility of the different materials and systems studied and the wide range of investigated properties a large range of fabrication, characterization and modelling tools are required. As demonstrated in Sec. I.3.2, where a list of the available instrumentation is given, a critical mass of equipment is available on the network. This is further supplemented by instrumentation that is available to several of the research groups through their international collaborations (e.g., synchrotron, neutron reactors, … ).

The pooling of the complementary expertise of a large number of research teams (note the 3 partners consist each of different research teams) has brought a critical mass of more than 300 highly qualified personnel (i.e., 31 permanent researchers, 153 postdocs and 140 PhD-students) collaborating on the same project.

The build-up of critical mass within the different work packages will now be discussed.

WP1: Metallic and oxide clusters

The partners in WP1 gather a wide expertise, ranging from the experimental characterization of the properties of isolated NP, i.e., size, size distributions, composition, composition fluctuations, optical, magnetic, electronic spectra, the effect on these properties of their functionalization and of their environment, the imaging of their self-organisation on surfaces and on 3D biotemplates to state-of-the-art ab initio quantum and classical computations.

Due to the complementarity of their expertise, the partners in WP1 have built a critical mass that allows them to tackle challenging and multi-scale problems in a competitive way at the international level, from the level of the controlled synthesis of isolated nanoparticles to the control of their self-organisation on various templates in view of catalysis and data storage applications.

WP2: Magnetic dots and wires

A number of the partners in WP2 have long-standing expertise in magnetic studies, but there was very limited overlap between the actual systems that are studied. The interactions that were catalyzed by the network have stimulated mutual interest and have triggered synergy between the existing expertise. For instance, the magnetic nanowires traditionally prepared at UCL are being ion-implanted
using the expertise that KUL built up on thin films. The development of tomographic capacities at UA-NANO are being employed to visualize the distribution of magnetic nanoparticles used in spin torque systems. Finally, another nice example is the common experimental interest in multiferroic materials (UH, UA-NANO, KUL) and the guiding role of theory (ULg) in synthesizing new multiferroics. These new synergies take some time to come to fruition but it is clear that the network played a strong role in making it happen and this will result in joint papers from groups that so far did not publish jointly. The number of groups that is now forging together their expertise in magnetism is now indeed such that a true critical mass has been reached.

WP3: Semiconductor quantum dots and wires

The collaborations within the present IAP have been very fruitful and the pooling of expertise in the IAP network certainly built a critical mass recognised at national and international level. On the theoretical front, collaborations between P3 (X. Gonze), P1 (B. Partoens, F. Peeters) and P5 (Ph. Ghosez, J.-Y. Raty) have been quite intense during the 2007-2009 period. While many joint publications are still in preparation, several common publications between the different partners have already appeared. On one side, the application of the first-principles techniques to the study of GeTe NWs and nanoplatelets, in collaboration between P3 – P5, have lead to several publications. The collaboration between P3 – P1 yields now publications, so it has been slower to start than the above-mentioned collaboration, but the interplay between methodological developments and associated implementations, from P3, and the applications done mostly by P1 is the strongest there. The P5 – P1 side of the collaboration is equally producing results.

At the technical level, the collaboration between P1, P3, and P5 allowed these partners to combine expertise in order to compare explicitly different approaches (LDA, GW, BSE, hybrid B1) for the modelling of Si NWs. Additionally, B. Partoens, from P1, has been member of a jury of a student in engineering at P3, while X. Gonze, from P3, and Ph. Ghosez, from P5, have been members of the jury of the PhD thesis of H. Peelaerts, from P1, both working on Si NWs.

The collaborations between the experimentalists and theory groups are also on the agenda of WP3. At the start of this project, the interpretation of the experiments performed by P2 on the embedded self-assembled quantum dots were supported by the calculations of the P1 group. This has lead to several joint publications. P1 started to perform simulations with different techniques to reproduce different aspects of the SGM experimental results obtained by the P3 group. In particular, the contrast observed when the tip scans away from quantum rings is investigated. The simulations will determine, e.g., if this contrast results from the effect of the tip perturbation potential on the phase acquired by electrons along the arm of a quantum ring, or from changes in electron semiclassical trajectories. Different visits have been lead to exchange data and to follow the progress of simulations and experiments. The code co-developed by Dr. M. Pala and P3 was also transmitted to P1. P1 also provides simulation support for the recent experimental results on quantum Hall interferometry by P3. Currently, P3 fruitfully collaborates with P2 on the development of scanning probe techniques. Specifically, both groups are adapting their STM systems and develop a protocol to allow for sample exchanges under ultra-high vacuum environment, which is expected to be validated in the near future. This is the first step towards future joint experiments taking advantage of the complementary tools attached to both systems, and to combine STM with SGM in the next 5-10 years.

WP4: Superconducting Nanosystems

The current IAP project has contributed not only to strengthen and invigorate previously running collaboration among all partners involved in the WP4, but has also helped to define common new objectives between theoretical and experimental groups. More specifically, the combined effort of P1 and P2 on the study of superconductor-ferromagnet hybrid systems has situated these two partners as a world-wide recognized reference on this particular topic. The international reputation of P1 and P2 on
S/F hybrid structures is reflected in a recently invited review article selected as a highlight 2009 of the Superconductor Science and Technology journal and a total of 35 publications during the last three years on the subject. In addition, the rapid development on the fabrication of high quality nanoporous templates by P3 in combination with the experimental expertise of P2 on superconductivity, has brought these two partners to a top international level as manifested by the quality of the publications and the numerous invited talks. We should also emphasize that the common interest by P1, P2, and P3 on the investigation of dissipative mechanisms in superconducting nanowires allowed us to build up a very solid national network which will undoubtedly bring these groups to the core of this fascinating field.

WP5: Carbon nanotubes and related carbon materials

The work performed in WP5 consists of various subtopics, ranging from quantum transport in graphene nanoribbons to the experimental fabrication of macrosized graphene multilayers, which are investigated by a host of both experimental and simulation techniques, as conducted by six different contributing partners. However, as evidenced by the number of joint papers and the journals these papers are published in, there is a strong collaborative drive in this WP. As a result, the various topics are tackled by a combination of techniques, resulting in a scientific output enhanced both in number and quality. As this scientific output is published in the field’s most authoritative journals, it is fair to say that the pooling of expertise in WP5 has indeed built a critical mass, both on the national and on the international level.

IV.2 International role

IV.2.1 Collaboration with European Partner within the Network

At the kick-off meeting (25 March 2007) the EU-partner presented an overview of the research of her group. A delegation of the IAP network visited the laboratory of Prof. M.-P. Pilieni in 2007. There were several visits of Dr. I. Lisiecki (collaborator of Prof. Pilieni) to the laboratory EMAT (UA-NANO, P1) and of researchers from EMAT to Paris. At the IAP general meeting of 25 November 2009, Prof. Pilieni gave an invited talk on “Intrinsic properties due to nanocrystals ordering in 2D superlattices and in 3D supra crystals: A new class of materials for a new physics”.

The collaboration with the Université Pierre et Marie Curie led to the following publications:


Prof. Pilieni was also a jury member for the Ph.D thesis of Stuart Turner (UA).

It was planned to appoint Dr. E. Klecha (a postdoc with Pilieni) to the IAP network in the EMAT group (UA-NANO, P1) starting from September 2009. Unfortunately, she decided to leave academia.

At present the budget for the EU-partner was used only for travel between some of the IAP partners (mostly between Paris and UA-NANO (P1)) and Paris. The European partner has complementary techniques to fabricate nanoparticles and arrays of nanoparticles. It is based on self-assembly driven by chemical interactions. The IAP network obtained samples from the EU-partner. The original aim was to transfer some of those techniques to some of the experimental groups of the IAP. It turned out that this

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was more difficult than expected. Currently, most of the contacts are limited to UA-NANO (P1) and UHasselt (P6).

At present, we are actively looking for a postdoc who will collaborate directly with Paris.

**IV.2.2 International activities**

**IV.2.2.1 Participation in European and international research projects**

**UA-NANO (P1)**

- G. Van Tendeloo obtained an “ERC advanced grant” in 2009.
- G. Van Tendeloo obtained an integrated FP7 project (IFOX) in 2009.
- Participation in the following ESF-networks:
  - Exploring the Physics of Small Devices (2009-2014)
  - Arrays of quantum dots and Josephson Junctions (AQDJJ) (2004-2009)
- Joint research project within the framework of the cooperation SECyT - FWO-VI: “Static and dynamic properties of mesoscopic and nanostructured superconductors”, (2009-2010).
- Joint research project within the framework of the cooperation CNPq (Brazil) - FWO-VI: “Theoretical study of nano-materials” (2010-2011).

**KU Leuven (P2)**

- FWO CPNq (Brazil) bilateral project with Universidade Federal do Espírito Santo, Vitoria, Brazilie: “Exchange Bias and Interlayer Coupling in the Fe/Mn/Fe system: Spin Structure, Interface Disorder and Coupling Mechanisms” (promotors: K. Temst, A. Vantomme, E. Passamani), 2010-2012.
- SPIRIT: support of public and industrial research using ion beam technology Integrated Infrastructure Initiative (I3) funded by the European Commission (promoter: A. Vantomme), 2009-2013.

*Section IV. Position of the IAP Network*
UCL (P3)


UA-Plasmant (P4)


ULg (P5)

- F. Remacle : coordinator of the FET NANO-ICT project MOLOC (Molecular Logic circuits), (2008-2011).
- Ph. Ghosez : coordinator of the European project OxIDes (Engineering Exotic properties at oxide interfaces, NMP, FP7), (2009-2012).
- F. Remacle. External member of the Chemistry evaluation Committee of the National Science and Engineering Research Council (NSERC) of Canada (2010-2013).
- Ph. Ghosez : General Secretary of the European Multifunctional Materials Institute (EMMI-AISBL)

UHasselt (P6)

IV.2.2.2 Organization of international symposia

UA-NANO (P1)


KU Leuven (P2)

- SyNeW (Synchrotron and Neutron Workshop), Brussel, 23 April 2009.
- Light at the forefront of Physics, Brussels, 19 September 2009.

UCL (P3)

- Organisation of the Ninth International Conference on the Science and Application of Nanotubes (NT08), Montpellier, France, 29/6-4/7/2008 (http://www.cnrs-imn.fr/NT08/), (UCL - J.-C. Charlier).
- X. Gonze : Organizer of the CECAM Tutorial "Theoretical spectroscopy lectures : theory and codes" (Lyon, France, December 10-14, 2007).
- X. Gonze : Organizer of the CECAM Tutorial "Basic techniques and tools for development and maintenance of atomic-scale softwares" (Lyon, France, February 11-15, 2008).
- X. Gonze : Organizer of the "International school on vibrational spectroscopies" (Cinvestav-Queretaro, Queretaro, Mexico, March 30 - April 5, 2008).
- X. Gonze : Organizer of the meeting "European Theoretical Spectroscopy Facility : the emergence of a research infrastructure" (Louvain-la-neuve, Belgium, November 28, 2008).
- X. Gonze : Organizer of the CECAM Tutorial "Theoretical spectroscopy lectures : theory and codes" (Zurich, Switzerland, May 25-29, 2009).
- CECAM tutorial: “Linear and non-linear responses of solids with the ABINIT software”, April 26-30 2010, Organizers R. Caracas (ENS), Ph. Ghosez (ULg) and X. Gonze (UCL).

ULg (P5)

• 20th International Symposium on Integrated Ferroelectrics (ISIF-2008), Singapore, June 2008, session “Theory” co-organized by A. Levanyuk (Madrid) and Ph. Ghosez.
• Fall Meeting of the Materials Research Society (MRS), Boston (MA, USA), November 2008: Symposium on Theory and Applications of Ferroelectric and Multiferroic Materials co-organized by Ch. Ahn (Yale), Ph. Ghosez (ULg), M. Kawasaki (Tohoku), D. Schlom (PennState) et J.-M. Triscone (Geneva).
• Linear and non-linear responses of solids with the ABINIT software, CECAM Tutorial; April 26-30 2010, Organizers R. Caracas, Ph. Ghosez and X. Gonze.

UHasselt-IMO (P6)

• Joint General Scientific Meeting of the Belgian Physical and Biophysical Societies, Antwerp University, Antwerpen, Belgium, May 30 1, 2007. (Co-organizer: P. Wagner-UHasselt).
• General Scientific Meeting of the Belgian Physical Society, Université Libre de Bruxelles, Brussels, Belgium, May 21, 2008. (Co-organizer: P. Wagner-UHasselt).
• Engineering of Functional Interfaces EnFI 08, Aachen University of Applied Sciences, Jülich, Germany, June 12-13, 2008. (Co-organizer: P. Wagner-UHasselt).
• Joint General Scientific Meeting of the Belgian Physical and Biophysical Societies, Hasselt University, Hasselt, Belgium, April 1, 2009. (Organizer: P. Wagner-UHasselt).
IV.2.2.3 Invitation to give lectures at prestigious international conferences

Here 10 selected invited lectures are listed. A complete list of invited lectures at international conferences can be found in Annex 3.

*International Conference CIASEM*
Rosario, Argentina, 25-28 October 2009
G. Van Tendeloo: “Possibilities of EM for the analysis of nanomaterials” (plenary lecture)

*CECAM-Workshop: Structural, electronic and transport properties of quantum wires*
Lyon (France), 9-12 June 2008.
F. M. Peeters: “Impurities in self-assembled free-standing semiconductor nanowires”

*12th European Conference on Applications of Surface and Interface Analysis (ECASIA ’07)*
Brussels, Belgium, September 2007
C. Van Haesendonck: “Imaging nanoscale magnetism with scanning probe microscopy”

*7th European Conference on Applied Superconductivity*
Brussels, Belgium, 17-20 September 2007
V. V. Moshchalkov: “Pinning by nanoengineered periodic arrays of antidots”

*2008 Winter Conference on Plasma Spectrochemistry*
Temecula, California, USA, January 7-12, 2008
A. Bogaerts: “PLASMANT: Plasma, Laser Ablation and Surface Modeling- ANTwerp”

*2009 European Winter Conference on Plasma Spectrochemistry*
Graz, Austria, February 15-20, 2009
A. Bogaerts: “Modeling of laser ablation processes for plasma spectrochemistry: Different pieces of the puzzle”

*2008 International Magnetics Conference (INTERMAG 2008)*
Madrid, Spain (2008)
L. Piraux: “Low Temperature Magnetoeelastic Effects in Template Grown Ferromagnetic Nanowires”

*International Conference on Carbon Nanoscience and Nanotechnoloy (NanoteC07)*
University of Sussex, Brighton, UK, 29/8-1/9/2007
J.-C. Charlier: “Defects in carbon nanotubes: from atomic structures to quantum transport”

*18th European Conference on Diamond, Diamond-like Materials, Carbon Nanotubes, and Nitrides*
Berlin, Germany, September 9-14, 2007
O.A. Williams, K. Haenen, *et al.*, “Growth and electronic properties of nanodiamond”

*International Conference on Particle Synthesis, Characterization, and Particle-Based Advanced Materials (PARTICLES 2008), Orlando, Florida, May 12, 2008*
H.-G. Boyen, “Nanoparticles for magnetic recording: the prospects and drawbacks of self-assembly”
IV.3. Durability of the IAP

From a scientific point of view the output of the network in terms of successful interactions and common publications certainly justifies that the network is continued in the next phase. There are obvious many synergies possible, where complementary expertise and approaches (experimental techniques as well as theoretical approaches) provide an important added value for the research of the different groups. The instrumentation that has been built up over the years is another clear asset for future collaboration.

For the future network we envisage on the one hand a continuation of subjects where there is an existing international leadership like, e.g., nanostructured superconductivity, and on the other hand new subjects where already in the present network we made some inroads as: multiferroics (P1, P2 and P5), graphene (P1, P2, P3, P4 and P6) and interaction of nanoparticles with bio-molecules (P1, P2 and P5).

With respect to multiferrocity, the first experimental activities within the IAP network are only emerging at this point. For future research it looks very challenging to focus on hybrid systems consisting of nanoparticles and nanowires that are embedded in a matrix or deposited on a surface to induce interrelated functionalities that are governed by the created interfaces.

The investigated interaction between biomolecular templates and nanoparticles offers interesting opportunities for creating self-assembled metamaterials with new optical and optoelectronic functionalities.

In relationship with the current activity in WP1, a thematic of the network that is very promising is the characterization of hybrid oxide and metallic clusters, interacting with organic, functional ligands. The IAP network has considerable expertise in characterizing these structures that are building block for novel materials in catalysis, sensing and molecular electronics at the nanoscale.

With the available theoretical and experimental knowledge it should be feasible to create hybrid materials consisting of graphene layers with deposited nanoparticles that have specific functionalities (magnetic, superconducting, … ). This way it may be possible to add these functionalities to graphene without destroying its excellent electronic properties.

On the level of instrumentation new progress is envisaged. Note that we are now facing an era where visualization techniques have improved drastically. This is permitting us to directly image individual vortices, test the applicability of the existing theories, and discover fascinating new results. The future combination of SGM with STM will lead to complementary information on the same type of nano-objects. While STM yields extremely detailed information about the electronic structure of the object surface, SGM data can be directly linked to local-scale electronic transport inside nano-objects, and can also lead to pinpoint electron scattering centers or dopants. The proposed combination would allow to correlate the atomic structure and spectroscopic properties of surface electrons with carrier transport properties. This conjecture would be extremely valuable: for example, it would be possible to examine the influence of a particular dopant both on the local electron density of states and on carrier flow in its vicinity. It would also lead to a very complete and precise comparison between experimental data with ab-initio simulation results.

Our IAP network has a quite long history. Originally, it contained the many different research activities of most of the Belgian groups that are active in condensed matter physics. When preparing the proposal for the presently running IAP, we tried to put more focus and organised the project around five work packages that focused on different systems. There is overlap between work packages through the scientific personnel that contributes to different work packages and through, e.g., the used instrumentation and the modelling techniques. The hybrid systems provided a natural way for communication between different work packages.
Next time the network should be focused more on very specific, challenging research questions, and where one relies on the complementary expertise of the partners to tackle (for a very restricted number of systems) the different aspects of the research questions in the different work packages. This will inevitably imply that partners will have to (re)orient their research in a different (new) direction.

Concerning the organization, we believe it would be good to rely even more upon the WP leaders in view of the scientific coherence. Since this requires considerably more effort from the WP leaders, one may for instance establish for each of the WPs a small supervisory committee that consists of representatives from the partners that have a major contribution in the WP.
V. Output

V.1. IAP publications

List of the 10 most relevant publications related to the achievements of the IAP project (IF = impact factor of journal; CI = number of citations; source: ISI Web of Knowledge):

*Imaging Electron Wave Functions Inside Open Quantum Rings*
(UCL)

S. Godefroo, M. Hayne, M. Jivanescu, A. Stesmans, M. Zacharias, O. I. Lebedev, G. Van Tendeloo, and V.V. Moshchalkov
*Classification and control of the origin of photoluminescence from Si nanocrystals*
(KUL and UA-NANO)

O. Leenaerts, B. Partoens, and F. M. Peeters
*Adsorption of H$_2$O, NH$_3$, CO, NO$_2$ and NO on graphene: A first-principles study*
(UA-NANO)

*Diamond nucleation by carbon transport from buried nanodiamond TiO$_2$ sol-gel composites*
Advanced materials 21, 670 (2009). **IF 8.191, CI 2**
(UHasselt and UA-NANO)

I. Lisiecki, S. Turner, S. Bals, M. Pileni, and G. Van Tendeloo
*The remarkable and intriguing resistance to oxidation of 2D ordered hcp Co nanocrystals: a new intrinsic property*
Chemistry of materials 21, 2335 (2009). **IF 5.046, CI 1**
(UA-NANO and EU)

X. Hallet, M. Mátéfi-Tempfli, S. Michotte, L. Piraux, J. Vanacken, V. V. Moshchalkov and S. Mátéfi-Tempfli
*Quasi-hexagonal vortex pinning lattice using anodized aluminum oxyde nanotemplates*
Small 5, 2413 (2009). **IF 6.525, CI 1**
(UCL and KUL)

E. Durgun, Ph. Ghosez, R. Shaltaf, X. Gonze and J.-Y. Raty
*Polarization Vortices in Germanium Telluride Nanoplatelets: A Theoretical Study*
Phys. Rev. Lett. 103, 247601 (2009). **IF 7.18, CI 0**
(ULg and UCL)
E. C. Neyts and A. Bogaerts
*Formation of endohedral Ni@C_{60} and exohedral Ni-C_{60} metallofullerene complexes by simulated ion implantation*
Carbon 47, 1028 (2009). **IF 4.373, CI 1**
(UA-Plasmant)

*Formation of Stripelike Flux Patterns Obtained by Freezing Kinematic Vortices in a Superconducting Pb Film*
Phys. Rev. Let. 104, 017001 (2010). **IF 7.18, CI 0**
(KUL and UA-NANO)

F. Leroux, M. Gysemans, S. Bals, J. Batenburg, J. Snauwaert, T. Verbiest, C. V. Haesendonck, G. van Tendeloo,
*3D characterisation of helical silver nanochains mediated by protein assemblies*
Advanced Materials (2010), accepted. **IF 8.191, CI 0**
(KUL and UA-NANO)

**Fig. 1:** Number of publications realized within the IAP network versus the journal impact factor. The publications are grouped in 5 categories according to the impact of the journal. This figure illustrates the increased productivity over the years and the increase in journal impact factor of the realized publications.
V.2. Appeal of the IAP

1) The **IAP network logo** is:

![IAP network logo](image)

which integrates the Belgian Science Policy logo with the abbreviations of our network: QCN Quantum effects in Clusters and Nanowires. “Q”: quantum effects in the common theme in the study of clusters and nanowires.

2) The **updated website** can be found at: [http://www.cmt.ua.ac.be/iap6/](http://www.cmt.ua.ac.be/iap6/). Part of the website is accessible to the outside world and contains information of the participants, a short description of the scientific themes of the IAP-network, a list of organized workshops and the available positions in the network. Another part of the website is password protected and has the following information: i) the coordinates of the members of the follow-up committee, ii) a detailed description of the 5 work packages, iii) the agenda of the meetings of the executive committee and work package leaders and of the IAP general meetings, iv) a list of the publications, v) the PhD prize with copies of the submitted theses, and vi) the annual reports.

3) The IAP-network organizes an **annual prize** for the best PhD thesis for the given year.

**2007**: The following candidates were nominated for the prize: Golibjon Berdiyorov (UA, P1), Steven Brems (KU Leuven, P2), Sebastien Faniel (UCL, P3) and Joris Van de Vondel (KU Leuven, P2).

Dr. Joris Van de Vondel (KUL, P2) received the Annual PhD Prize 2007 for his PhD Thesis: “Vortex dynamics and rectification effects in superconducting films with periodic asymmetric pinning” (Promoters: Prof. V. Moshchalkov, Prof. C. de Souza Silva).

**2008**: The following candidates were nominated for the prize: Eric Bousquet (Universite de Liege, P5), Koen Schouteden (KU Leuven, P2), Sylvia Wenmackers (U Hasselt, P6) and Werner Gillijns (KU Leuven, P2).

The PhD Prize Committee awarded the prize to: Dr. Werner Gillijns (KUL, P2) for his PhD Thesis: “Nucleation of superconductivity and vortexmatter in superconductor - ferromagnethybrid nanosystems” (Promoters: Prof. V. V. Moshchalkov, Dr. A. V. Silhanek).

**2009**: The following candidates were nominated for the prize: Stefan Decoster (KU Leuven, P2) and Hartwin Peelaers (UA, P1).

The PhD Prize Committee awarded the prize to: Dr. Hartwin Peelaers (UA, P1) for his PhD Thesis: “An ab initio study of the electronic and dynamical properties of Si, Ge and Si/Ge nanowires.” (Promoter: Prof. B. Partoens, co-promoter: Prof. F.M. Peeters).

4) On 29 April 2010, Prof. A. Geim received an **honorary doctorate** from the University of Antwerp for the 'Discovery of graphene and his fundamental contributions to different areas in mesoscopic physics'.
V.3. PhD and postdoc training

PhD students are encouraged to participate in the different tutorials and doctoral schools (see Sec. III). The goal is that on the average each PhD student participates at least once a year in an international event outside Belgium. Junior postdocs take actively part in the supervision of bachelor and master theses. Postdocs are encouraged to actively participate in the organization of the research and the training of PhD students. Two of the work packages (i.e., WP4 and WP5) are run by senior postdocs. The follow-up of the day-to-day organization and reporting is done by Dr. V. Misko, a senior postdoc of UA-NANO. In the organization of several of the WP-meetings PhD students and postdocs were closely involved. Several of the PhD students and postdocs actively participate, a limited amount of their time, in didactic assignments.

Examples of IAP trained PhD students and postdocs that went abroad (this is not an exhaustive list):
- V. Mlinar (UA-NANO, P1) did a postdoc with Dr. A. Zunger at NREL (National renewable energy laboratory) (CO, USA).
- H. Peelaers (UA-NANO, P1) will do a postdoc with Prof. C. Van de Walle (Computational Materials Group, University of California, Santa Barbara, CA, USA).
- Erik Neyts (UA-Plasmant, P4) made two postdoc stays at the University of Tokyo (Japan) in October-December 2008 and January-March 2010.
- Kristof Paredis (KU Leuven, P2) is currently doing a postdoc with Prof. Beatriz Roldan at the University of Central Florida, where the research focus is on the experimental investigation of size- and shape-selected nanostructures.

Table 3. The number of PhD students and postdoc researchers.

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<thead>
<tr>
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<th>IAP financed</th>
<th>Non IAP financed</th>
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<tbody>
<tr>
<td></td>
<td>PhD students</td>
<td>Postdocs</td>
</tr>
<tr>
<td>P1 UA-NANO</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>P2 KU Leuven</td>
<td>4</td>
<td>5</td>
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<tr>
<td>P3 UCL</td>
<td>5</td>
<td>6</td>
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<tr>
<td>P4 UA-Plasmant</td>
<td>2</td>
<td>4</td>
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<tr>
<td>P5 ULg</td>
<td>0</td>
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<td>P6 UHasselt</td>
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Examples of some training success stories

Dr. Kristof Paredis and Dr. Koen Schouteden

Kristof Paredis obtained his PhD from the K.U.Leuven in September 2008 (Promoter was A. Vantomme) with a thesis on "The formation of iron silicide nanostructures on noble metal induced superstructures on Si(111) surfaces". The research activities of Krisitof Paredis were closely related to WP1 and WP2. Koen Schouteden obtained his PhD from the K.U.Leuven in October 2008 (Promoters were C. Van Haesendonck and P. Lievens) with a thesis on "Tunneling microscopy and spectroscopy of metallic and magnetic nanoclusters on atomically flat surfaces". The research activities of Koen
Schouteden were also closely related to WP1 and WP2. Both Kristof Paredis and Koen Schouteden successfully implemented and optimized scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) with atomic resolution. STM and STS, which can now be applied "in situ" in ultra-high vacuum and down to low temperatures, provide unique opportunities for the K.U.Leuven partner for investigating quantum confinement effects at the level of individual particles and wires with nanometer dimensions. Both Kristof Paredis and Koen Schouteden continue their STM and STS based research as postdocs. Kristof Paredis has obtained a postdoc position at the University of Central Florida starting from January 2010. Koen Schouteden has been selected as a postdoctoral researcher of the Science Foundation - Flanders starting from October 2009 and continues to be closely involved in the IAP.

**Dr. Sebastien Faniel**

Being trained in the groups of Prof. V. Bayot and Dr. S. Melinte, S. Faniel has been one of the 10 participants of the IAP PhD prize contest over the first three years of activity of the network and the unique participant from UCL. During his doctoral work, he investigated the low-temperature magnetotransport properties of p-type GaAs open quantum dots. After developing a fabrication process for p-type nanostructures, he succeeded to observe, for the first time, conductance fluctuations and weak anti-localization in hole quantum dots below 500 mK, which provided a clear evidence of coherent transport in hole quantum dots. From these observations, he obtained a temperature dependence for the holes' dephasing time together with an upper limit for the spin-orbit scattering time. He found that the fabricated dots are in the strong spin-orbit interaction regime and that the absolute value of the holes' dephasing time is approximately one order of magnitude smaller than that reported for electrons in similar system.

Right after his PhD thesis, he continued his activity at UCL as a post-doctoral researcher for few months. During this short period, he contributed to the development of new local probe microscopy systems in the group. This includes (i) the installation of the low temperature STM and the study of the electronic structure of ZnO(0001) surfaces with Dr. J. Dumont (FUNDP) and Dr. B. Hackens (UCL) and (ii) the design of a low temperature (<100 mK) measurement system accommodating a SGM setup with Dr. B. Hackens (UCL). These activities were accomplished within the WP3 framework. They offered him the possibility to become familiar with the experimental tools involved in the IAP 6/42 network and to meet the other research groups collaborating within this project.

Presently he is a post-doctoral fellow at Hokkaido University, Japan, where he continues to accumulate key experience in the specific field of spintronics, a topic of peculiar importance for the present and forthcoming activities in the nanophysics network. At the end of this post-doctoral stay he plans to return to UCL and to re-integrate the teams of Dr. S. Melinte and Prof. V. Bayot and to apply for a “Chargé de Recherche” position. S. Faniel is finishing a postdoc with Prof. T. Koga at Hokkaido University (Japan).

**Dr. Frederico Martins**

Dr. Frederico Martins worked as a postdoc during two years in the group of Prof. V. Bayot, after obtaining his PhD degree at the “Institut Néel”, in Grenoble, France. His research activities in Grenoble were mostly focused on the combination of AFM with electrical measurements. He used the AFM in two different approaches, both aiming at studying the local-scale properties of few-electron systems: the first approach was focused on detecting and measuring local charges on semiconductor substrates, and the second aspect of his research concerned low temperature SGM.
During his stay in UCL, he first developed his expertise in SGM. His project was to probe electron transport in the quantum Hall regime. To achieve this goal he contributed (with Dr. B. Hackens and Dr. S. Faniel) to build a unique ultra-low temperature SGM system, operating inside a He\textsuperscript{3}/He\textsuperscript{4} dilution refrigerator equipped with a superconducting coil. The conception of the equipment was extremely challenging, and therefore represented an excellent training to measurement techniques in “extreme” cryogenic environments. He obtained experimental results demonstrating the ability of this technique to reveal the spatial structure of transport inside a quantum ring in the quantum Hall regime, and to find the precise location of localized electron islands within the device (these results have been recently submitted for publication). His results are spectacular and represent a breakthrough in the field of quantum Hall interferometry, which is at the focus of intense scientific activity due to recent theoretical proposals of topological quantum computers involving localized electron states in the quantum Hall regime.

Moreover, he was also trained in nanofabrication techniques in the UCL clean room environment. In particular, he participated in the fabrication of quantum rings on semiconductor heterostructure samples. Thanks to this training, he could find a postdoctoral position at IEMN, Lille, France where he is currently working on the development of a new semiconductor device process based on InP substrates. He recently applied for a “Chargé de Recherche” position within the group of Prof. V. Bayot (UCL).

Dr. Joaquin De La Torre Medina

Joaquin was hired by the IAP project during the last 3 years and has successfully defended his PhD in September 2009. His research was focused on the investigation of the magnetic properties of arrays of ferromagnetic nanowires that were fabricated by electrodeposition into nanoporous templates. Understanding the fundamental properties of magnetic nanostructures is a central issue in magnetic materials due to its importance in a large range of technological applications. Considering different approaches to investigate the magnetic properties of arrays of magnetic nanowires, Joaquin has proved that ferromagnetic resonance (FMR) is a very powerful technique that can be used as a tool for the characterization of magnetic properties and dipolar interaction in arrays of magnetic nanowires. Arrays of single domain magnetic nanowires (NWs) are a model system for studying magnetic interactions and switching behavior and have been proposed as candidates for ultrahigh storage densities. In addition, Joaquin has demonstrated the importance of composite materials based on nanowire arrays into porous templates as potential candidates for technological applications in various domains including microwave devices.

Over the last 4 years, Joaquin has published about 12 papers in journals such as Phys. Rev. B, Applied Physics Letters and J. Applied Physics. He occupies a post-doc position in the group of L. Piraux at UCL since 6 months and he probably will obtain a permanent position at the University San Luis Potosi (Mexico).

V. 4. Young emerging research teams

UA-Plasmant (P4) and UHasselt (P6) can be considered as “young emerging research teams”. Both partners are integrated quite well in the network, as evidenced by the number of collaborations by both groups and the other partners. Indeed, UA-Plasmant (P4) has ongoing collaborations with UA-NANO (P1) and UHasselt (P6), while UHasselt has collaborations with all contributing partners to WP5.
UHasselt effectively plays a forerunner role in the field of (U)NCD in WP5. UA-Plasmant (P4) – which was previously not involved in the topics covered by WP5 – has benefited significantly from the collaborations with the other partners, especially regarding knowledge about first-principles simulation techniques (with P1, P3 and P5) and the possibility to compare theoretical results with experimental results and has furthermore also contributed to various joint publications (several are still in progress).

Examples of new young emerging research teams within the partners of the IAP project
They can be considered as subteams within larger existing teams.

Sara Bals of EMAT (P1): she was hired recently as professor at UA and is building up a group on nano-TEM with emphasis on soft-hard matter interphases.

Bart Partoens of CMT (P1): Over the last 4 years he has build a new group around ab initio calculations of electronic structure with application to e.g., nanowires, graphene and graphene-based materials.

Milorad Milosevic of CMT (P1): after his Marie Curie postdoc at Bath (UK) he was hired at UA and is starting to build up his own theory group. Topics are: superconductivity and molecular dynamics simulations.

H.-G. Boyen (P6) was hired as professor at the University Hasselt. He brings new expertise on colloidal nanoparticles and functionalization of surfaces.

The KULeuven (P2) recently hired Carmen Bartic as a professor. Before she was a staff member at IMEC. She is now building up her own research group on bioelectronics and will be actively involved in the IAP related research collaboration (UA-NANO and KUL) on the interaction of biopolymers and metallic nanoparticles.

The IAP project has worked as a catalyst for these young teams which have already been able to secure their own funding. For example, there exist already a joint FWO (Flemish Science Foundation) project between Bals (P1), Milosevic (P1) and Van Haesendonck (P2) and a SBO (Strategic basic research)-project with Partoens (P1), X. Gonze (P3) and others. Joint projects have recently been submitted between Bals (P1) and Partoens (P1) and between Milosevic (P1) and Moshchalkov (P2).
Section V. Output
Annex 1: Publications 2009-2010

A. Joint publications

UA-NANO (P1), UA-Plasmant (P4) & UHasselt – IMO (P6)

Characterization of nanocrystalline diamond films grown by continuous DC bias during plasma enhanced chemical vapor deposition.

UA-NANO (P1) & Paris LM2N (EU)

I. Lisiecki, S. Turner, S. Bals, M. P. Pileni, and G. Van Tendeloo
The remarkable and intriguing resistance to oxidation of 2D ordered hcp Co nanocrystals: a new intrinsic property
Chemistry of materials 21, 2335 (2009).

UA-NANO (P1) & KUL (P2)

Ordered end-member of ZSM-48 zeolite family

Direct room-temperature synthesis of methyl-functionalized Ti-MCM-41 nanoparticles and their catalytic performance in epoxidation

S. Bals, J. Batenburg, D. Liang, O. Lebedev, G. van Tendeloo, A. Aerts, J. A. Martens, and C. E. Kirschhock
Quantitative three-dimensional modeling of zeolite through discrete electron tomography

M. Di Vece, S. Bals, J. Verbeeck, P. Lievens, and G. van Tendeloo
Compositional changes of Pd-Au bimetallic nanoclusters upon hydrogenation

M.V. Milosevic, W. Gilljins, A.V. Silhanek, A. Libal, F.M. Peeters, and V.V. Moshchalkov
Guided nucleation of superconductivity on a graded magnetic substrate

*Formation of Stripelike Flux Patterns Obtained by Freezing Kinematic Vortices in a Superconducting Pb Film*


F. Leroux, M. Gysemans, S. Bals, J. Batenburg, J. Snaeuwaert, T. Verbiest, C. V. Haesendonck, G. van Tendeloo,

*3D characterisation of helical silver nanochains mediated by protein assemblies*

Accepted to Adv. Mat.

**UA-NANO (P1) & UCL (P3)**

C. Kerner, B. Hackens, D. S. Golubovic, S. Poli, S. Faniel, W. Magnus, W. Schoenmaker, V. Bayot and H. Maes

*Control and readout of current-induced magnetic flux quantization in a superconducting transformer*


**UA-NANO (P1) & UA-Plasmant (P4)**

V. Georgieva, M. Saraiva, N. Jehanathan, O. Lebedev, D. Depla, and A. Bogaerts

*Sputter-deposited Mg-Al-O thin films: linking molecular dynamics simulations to experiments*


D. A. Ariskin, I. V. Schweigert, A. L. Alexandrov, A. Bogaerts, and F. M. Peeters

*Modeling of chemical processes in the low pressure capacitively coupled RF discharges in a mixture of Ar/C2H2*


W. Wendelen, A. Dzhurakhalov, F. Peeters, and A. Bogaerts,

*Combined molecular dynamics – continuum study of phase transitions in bulk metals under ultrashort pulsed laser irradiation.*


**UA-NANO (P1) & UHasselt – IMO (P6)**


*Diamond nucleation by carbon transport from buried nanodiamond TiO2 sol-gel composites*


*Characterization of nano-crystalline diamond films grown by continuous DC bias during plasma enhanced chemical vapor deposition*

**KUL (P2) & UCL (P3)**

X. Hallet, M. Mátéfi-Tempfli, S. Michotte, L. Piraux, J. Vanacken, V. V. Moshchalkov, and S. Mátéfi-Tempfli

*Quasi-hexagonal vortex pinning lattice using anodized aluminum oxyde nanotemplates*  

X. Hallet, M. Mátéfi-Tempfli, S. Michotte, L. Piraux, J. Vanacken, V. V. Moshchalkov, and S. Mátéfi-Tempfli

*High magnetic field matching effects in NbN films induced by template grown dense ferromagnetic nanowires arrays*  

X. Hallet, S. Mátéfi-Tempfli, M. Mátéfi-Tempfli, S. Michotte, L. Piraux, J. Vanacken, and V. V. Moshchalkov

*Artificial pinning centers using the barrier layer of ordered nanoporous alumina templates*  

**KUL (P2) & UH (P6)**

B. L. Willems, G. Zhang, J. Vanacken, V. V. Moshchalkov, S. D. Janssens, O. A. Williams, K. Haenen, and P. Wagner

*Negative magnetoresistance in boron-doped nanocrystalline diamond films*  


*Intrinsic granularity in nanocrystalline boron-doped diamond films measured by scanning tunneling microscopy*  


*Biological modification of carbon nanowalls with DNA strands and hybridization experiments with complementary and mismatched DNA*  

B. L. Willems, G. Zhang, J. Vanacken, V. V. Moshchalkov, S. D. Janssens, K. Haenen, P. Wagner, I. Guillamón, H. Suderow, and P. Vieira,

*Granular superconductivity in metallic and insulating nanocrystalline boron-doped diamond films*  

B. L. Willems, G. Zhang, J. Vanacken, V. V. Moshchalkov, H. Suderow, S. D. Janssens, K. Haenen, and P. Wagner,

*In/extrinsic granularity in superconducting boron-doped diamond*  
accepted for Physica C (2010).
UCL (P3) & ULg (P5)


*ABINIT: first-principles approach to material and nanosystem properties*


E. Durgun, Ph. Ghosez, R. Shaltaf, X. Gonze and J.-Y. Raty

*Polarization Vortices in Germanium Telluride Nanoplatelets: A Theoretical Study*


R Shaltaf, E. Durgun, J.Y. Raty, P. Ghosez and X. Gonze

*Dynamical, dielectric, and elastic properties of GeTe investigated with first-principles density functional theory*


B. Publications

UA-NANO (P1) (EMAT)

S. Turner, O. Lebedev, O. Shenderova, I. Vlasov, J. Verbeeck, and G. Van Tendeloo

* Determination of Size, Morphology, and Nitrogen Impurity Location in Treated Detonation Nanodiamond by Transmission Electron Microscopy*


*End-to-end assembly of shape-controlled nanocrystals via a nanowelding approach mediated by gold domains*


*Nanodiamond photoemitters based on strong narrow-band luminescence from silicon-vacancy defects*


Yang Xiao-Yu, Li Yu, G. van Tendeloo, Xiao Feng-Shou, Su Bao-Lian

*One-pot synthesis of catalytically stable and active nanoreactors: encapsulation of size-controlled nanoparticles within a hierarchically macroporous core@ordered mesoporous shell system*

E. Beyers, E. Biermans, S. Ribbens, K. de Witte, M. Mertens, V. Meynen, S. Bals, G. Van Tendeloo, E. Vansant, and P. Cool
Combined TiO$_2$/SiO$_2$ mesoporous photocatalysts with location and phase controllable TiO$_2$ nanoparticles

C. Gorlé, J. van Beeck, P. Rambaud, and G. van Tendeloo
CFD modelling of small particle dispersion: the influence of the turbulence kinetic energy in the atmospheric boundary layer

J. T. Titantah, D. Lamoen, M. Schowalter, and A. Rosenauer
Density-functional theory calculations of the electron energy-loss near-edge structure of Li-intercalated graphite

I. M. Afanasov, O. N. Shornikova, V. V. Avdeev, O. Lebedev, G. Van Tendeloo, and A. T. Matveev
Expanded graphite as a support for Ni/carbon composites
Carbon 47, 513 (2009).

I. M. Afanasov, V. A. Morozov, A. V. Kepman, S. G. Ionov, A. N. Seleznev, G. Van Tendeloo, and V. V. Avdeev
Preparation, electrical and thermal properties of new exfoliated graphite-based composites

Probing the interaction between gold nanoparticles and oxygen functionalized carbon nanotubes
Carbon 47, 1549 (2009).

P. Verlooy, A. Aerts, O. Lebedev, G. van Tendeloo, C. Kirschhock, and J. A. Martens
Synthesis of highly stable pure-silica thin-walled hexagonally ordered mesoporous material

V. Caignaert, A. Abakumov, D. Pelloquin, V. Pralong, A. Maignan, G. van Tendeloo, and R. Raveau
A new mixed-valence ferrite with a cubic structure, YBaFe$_4$O$_7$: spin-glass-like behavior
Chemistry of materials 21, 1116 (2009).

J. Hadermann, A. Abakumov, S. van Rompaey, A. S. Mankevich, and I. E. Korsakov
Comment on ALaMn$_2$O$_{6-y}$ (A = K, Rb): novel ferromagnetic manganites exhibiting negative giant magnetoresistance

J. F. Colomer, R. Marega, H. Traboulsi, M. Meneghetti, G. van Tendeloo, D. Bonifazi
T. G. Parsons, H. D’Hondt, J. Hadermann, and M. A. Hayward
*Synthesis and Structural Characterization of La(1-x)A(x)MnO(2.5) (A = Ba, Sr, Ca) Phases: Mapping the Variants of the Brownmillerite Structure*

N. Pop, V. Pralong, V. Caignaert, J. F. Colin, S. Malo, and G. van Tendeloo
*Topotactic Transformation of the Cationic Conductor Li4Mo5O17 into a Rock Salt Type Oxide Li12Mo5O17.*

C. Bittencourt, G. van Lier, X. Ke, I. Suarez-Martinez, A. Felten, J. Ghijsen, G. van Tendeloo, and O Ewels Christopher
*Spectroscopy and defect identification for fluorinated carbon nanotubes*

*The role of oxygen at the interface between titanium and carbon nanotubes*

V. Djokovic, R. Krsmanovic, D. K. Bozanic, M. McPherson, G. van Tendeloo and P. S.Nair
*Adsorption of sulfur onto a surface of silver nanoparticles stabilized with sago starch biopolymer*
Colloids and Surfaces B-BioInterfaces **73**, 30 (2009).

*Multi-Functional Copper Oxide Nanosystems for H2 Sustainable Production and Sensing*

D. Esken, X. Zhang, O. Lebedev, F. Schröder, R. A. Fischer
*Pd@MOF-5: limitations of gas-phase infiltration and solution impregnation of [Zn4O(bdc)3] (MOF-5) with metalorganic palladium precursors for loading with Pd nanoparticles*

G. van Tendeloo, J. Hadermann, A. M. Abakumov, E. V. Antipov
*Advanced electron microscopy and its possibilities to solve complex structures: application to transition metal oxides*

G. Smeulders, V. Meynen, G. van Baelen, M. Mertens, O. Lebedev, G. van Tendeloo, B. Maest, and P. Cool
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M. Eckert, E. Neyts, A. Bogaerts,
Modeling adatom surface processes during crystal growth: A new implementation of the Metropolis Monte Carlo algorithm.

N. Baguer, V. Georgieva, L. Calderin, I. T. Todorov, S. Van Gils and A. Bogaerts
Study of the nucleation and growth of TiO2 and ZnO thin films by means of molecular dynamics simulations.

E. Neyts and A. Bogaerts
Modeling of PECVD growth of nanostructured carbon materials.

E. Neyts, M. Eckert, M. Mao and A. Bogaerts
Modeling of hydrocarbon plasmas for nanoparticle formation and the growth of carbon nanostructures.

V. Georgieva, I. T. Todorov and A. Bogaerts
Molecular dynamics simulation of thin film growth: importance of the interatomic interaction potential.

E. Neyts, Y. Shibuta and A. Bogaerts
Bond switching regimes in nickel and nickel-carbon nanostructures.

ULg (P5)

G. Periyasamy, A. Sour, J. P. Collin, J. P. Sauvage, and F. Remacle
Computational, Structural and Mechanistic analysis of the electrochemically driven pirouetting motion of a copper rotaxane

G. Periyasamy and F. Remacle,
Ligand and solvation effects on the Electronic Properties of Au55 clusters: a DFT study
NanoLett. 9, 3007 (2009).

G. Periyasamy, R. D. Levine, and F. Remacle,
Electronic wave packet motion in water dimer cation: A many electron description,

G. Periyasamy, J.-P. Collin, J. P. Sauvage, R. D. Levine, and F. Remacle,  
Electrochemically driven sequential machine: an implementation on copper rotaxanes,  

G. J. Long, S. Tanase, F. Remacle, G. Periyasamy, and F. Grandjean,  
Combined Moessbauer Spectral and Density Functional Theory Determination of the Magnetic Easy-Axis in Two High-Spin Iron(II) 2-Pyrazinecarboxylate Complexes,  

R. Pekoz and J.Y. Raty  
*From bare Ge nanowire to Ge/Si core/shell nanowires: A first-principles study*  

C. Otjacques, J.Y. Raty, MV. Coulet, M. Johnosn; M. Schober, C. Bichara and J.P. Gaspard  
Dynamics of the Negative Thermal Expansion in Tellurium Based Liquid Alloys  

R Shaltaf, E. Durgun, J.Y. Raty, P. Ghosez et X. Gonze,  
Dynamical, dielectric, and elastic properties of GeTe investigated with first-principles density functional theory  

E. Durgun, Ph. Ghosez, R. Shaltaf, X. Gonze and J.-Y. Raty,  
Polarization Vortices in Germanium Telluride Nanoplatelets: ATheoretical Study  

S. Bhattacharjee, E. Bousquet and Ph. Ghosez  
Engineering multiferroism in CaMnO3  

M. Goffinet, P. Hermet, D. Bilc and Ph. Ghosez  
Hybrid functional study of prototypical multiferroic bismuth ferrite  

G. Periyasamy, E. Durgun, J.-Y. Raty, and F. Remacle,  
DFT Studies of Solvation Effects on the Nanosize Bare, Thiolated, and Redox Active Ligated Au55 Cluster  

**UHasselt-IMO (P6)**

M. Bäcker, A. Poghossian, M.H. Abouzar, S. Wenmackers, S.D. Janssens, K. Haenen, P. Wagner, M.J. Schöning,  
Capacitive field-effect (bio-)chemical sensors based on nanocrystalline diamond films


Annex 2: Awards and Featured papers

A. Awards

See also Sec. V.2 for the IAP-network annual prize for the best PhD thesis.

2007

Dr. Vladan Mlinar (CMT-UA, P1) received the 2nd prize in the 2007 EU-NoE: SANDiE competition for his PhD thesis: “Electronic Structure Calculation of Single and Coupled Self-Assembled Quantum Dots” (Promoter: Prof. F. Peeters).

Dr. Milorad Milosevic (CMT-UA, P1) received the Prize of the UA Research Council 2007: "Prijs van de Onderzoeksaad Frans VERBEURE".

Dr. Vyacheslav Misko (CMT-UA, P1) received a Marie Curie International Fellowship (24 months research at the UA).

Dr. Vyacheslav Misko (CMT-UA, P1) received an “Odysseus” award (Type II) – the “Odysseus” Program of Flemish Government and the FWO-Flanders: http://www.fwo.be/en/FWOOdysseus.aspx

Dr. Johan Vanacken (KUL, P2) received the “Hubei Chime Bell Award” 2007 for Economic and Scientific Development in the Hubei Province – Special prize issued by the Hubei government (Hubei province, China).


Dr. Kristof Paredis (KUL, P2) is currently doing a postdoc with Prof. Beatriz Roldan at the University of Central Florida, where the research focus is on the experimental investigation of size- and shape-selected nanostructures.

2008

Dr. Dries Smeets (KUL, P2) received the Award Patrick Gas & François d’Heurle for his PhD dissertation on “Nucleation, diffusion and texture during growth of CoNi-silicides” (promoter Prof. Dr. André Vantomme). With this biannual award, the Institut Matériaux, Microélectronique et Nanosciences de Provence (IM2NP-CNRS) in Marseille recognizes an outstanding experimental PhD thesis about diffusion and/or phase transformation with diffusion. This price is awarded in memory of Patrick Gas en François d’Heurle, two pioneers in the field of solid state diffusion.

Dr. Erik Neyts (UA-Plasmant, P4) received the prize for the best oral presentation at the “10th High Temperature Plasma Processes Conference”, Patras, Greece, 7-11 July, 2008.

Prof. Annemie Bogaerts (UA-Plasmant, P4) received the “Lester W. Strock Award of the New England Section of the Society for Applied Spectroscopy”, in recognition for “Outstanding contributions in the

Annex 2. Awards and Featured Papers
areas of plasma and surface modeling”. The award was presented at the FACSS Conference, Reno, US, 30 September 2008.

E. Bousquet (ULg, P5) - "Silver PhD Student Award" from the MRS (Boston, December 2008)


Eric Bousquet and Philippe Ghosez (ULg, P5) – “Prix La Recherche 2008” (awarded by La Recherche Magazine) in the field of “Sciences of communication and Information Technologies”.

Eric Bousquet (ULg, P5) – MRS Graduate Student Silver Award, (Boston, USA).

2009

G. Van Tendeloo (UA-NANO, P1) obtained an “ERC advanced grant” in 2009.

A. Bogaerts (UA-Plasmant, P4) obtained Winter Plasma Award 2009, in recognition for “Outstanding contributions in the field of laser ablation modeling”

F. Peeters (UA-NANO, P1) was awarded the title of 'Doctor Honoris Causa' by the University of Szeged (Hungary) on November 11, 2009.

F. Remacle (ULg, P5) – Fellow of the APS.

2010

Hartwin Peelaers (UA-NANO, P1) received a BAEF (Belgian American Educational Foundation) fellowship to perform research at the University of California, Santa Barbara.

N. Lin (UA-NANO, P1) received the “Master thesis prize” from the Belgian Physical Society for his thesis “Vortex dynamics in mesoscopic superconducting Corbino disks”, promoters: Dr. V.R. Misko (“Odysseus” program) and Prof. Dr. F. M. Peeters.

Eric Bousquet (ULg, P5) – Prix Des Amis de l'ULg, (Liège, Belgium).

Eric Bousquet (ULg, P5) received “Prix Des Amis de l'ULg”, (Liège, Belgium) and has been a “Selected Participant” to the 60th Interdisciplinary Meeting of Nobel Laureates, (Lindau, Germany).
B. Featured papers

2007


2008


Annex 2. Awards and Featured Papers
UH (P6)

**UA-Plasmant (P4):** The paper “Diamond, a material for acoustic devices”, by Mortet, O.A. Williams, K. Haenen, *physica status solidi (a)* **205**, 1009-1020 (2008), was featured as “Invited Feature Article”.

2009


2010


**UA-NANO (P1):** The paper: “Transport detection of quantum Hall fluctuations in grapheme” by S. Branchaud, A. Kam, P. Zawadzki, F.M. Peeters, and A.S. Sachrajda Phys. Rev. B **81**, 121406(R) (2010) was selected by the editors of PRB to be an Editors' Suggestion.

Annex 3: Invited lectures at international conferences

UA-NANO (P1)

F. Peeters: “Electronic structure calculation of self-assembled quantum dots and molecules”.

F. Peeters: “The three vortex loop state in superconductors with a magnetic core”.

The 6th Int. Conf. on Materials Processing, Properties and Performance, Beijing (China), 14-16 September 2007.
F. Peeters: “Tuning the superconducting properties of nanomaterials”.

The 6th Int. Conf. on Low Dimensional Structures and Devices (LDSD 2007), San Andres (Columbia), 15-20 April 2007.
F. Peeters: “Resonant tunneling in graphene microstructures”.

F. Peeters: “Electronic structure calculation of self-assembled quantum dots and molecules”.

Workshop: Recent trends in nanomagnetism, Leuven (Belgium), 5 February 2008.
F. M. Peeters: “Magnetic quantum dots”.

NES-Workshop: Probing superconductivity at the nanoscale, Alicante (Spain), 4-7 June 2008.
F. M. Peeters: “Superconducting nanowires: Andreev states and magnetic field induced transistions”.

F. M. Peeters: “Impurities in self-assembled free-standing semiconductor nanowires”.

CECAM-Workshop: Computational approaches to semiconductor, carbon and magnetic nanostructures, Lyon (France), 16-19 June 2008.
F. M. Peeters: “Graphene quantum dots”.

Graphene Canada 08 – Workshop, Banff (Canada), 14-19 September 2008.
F. M. Peeters: “Interaction of molecules with graphene: a first principles study”.

NATO-Workshop: Recent Advances in Nonlinear Dynamics and Complex System Physics
Tashkent (Uzbekistan), 6-11 October 2008.
F. M. Peeters: “Tuning the superconducting properties of nanomaterials”.

VII Brazilian School of Superconductivity and Workshop on Frontiers of Superconductivity and Magnetism - Materials, Mechanisms and Applications, Muro Alto (Pernambuco, Brazil), 8-12 December 2008.
F. M. Peeters: “Vortex flow and phase slip phenomena in mesoscopic superconductors”.

10th International Conference on Quasicrystals (ICQ10), Zürich (Switzerland), July 6-11, 2008
V. R. Misko: “Critical currents in quasiperiodic pinning arrays: Chains and Penrose lattices”.

Annex 3. Invited Lectures
International Conference on Superconductivity and Magnetism (ICSM-2008), Ankara University in Side-Antalya (Turkey), 25-29 August 2008.
V. R. Misko: “Shape and pinning induced vortex states in mesoscopic superconductors”.

International Conference on Superconductivity and Magnetism (ICSM-2008), Ankara University in Side-Antalya (Turkey), 25-29 August 2008.
M. V. Milosevic: “Fluxonic cellular automata”.

International Conference on Superconductivity and Magnetism (ICSM-2008), Ankara University in Side-Antalya (Turkey), 25-29 August 2008.
A. A. Shanenko: “Nanoscale Andreev-type states induced by quantum confinement”.

V. R. Misko: “Dynamics of Vortex Shells in Mesoscopic Superconducting Corbino Disks”.

A. A. Shanenko: “Superconducting nanowires: transverse quantization and quantum-size cascades”.

EMAG 2009, Sheffield (UK), (9-11 September 2009).
G. Van Tendeloo: Plenary lecture: “Quantitative imaging in 2D and 3D”.

Spanish-Portuguese EM meeting, Segovia (Spain), (16-19 June 2009).
G. Van Tendeloo: Plenary lecture: “Imaging nanostructures”.

Workshop on “Limits to characterisation and modelling of atomic scale processes and defects” (18-20 May 2009), Bernkastel (Germany).
G. Van Tendeloo: Invited lecture: “Limitation and EM characterisation of ceramic multilayers”.

CIASEM (25-28 October 2009), Rosario (Argentina).
G. Van Tendeloo: Plenary lecture: “Possibilities of EM for the analysis of nanomaterials”.

MRS, Boston (USA), (1-4 December 2009).
G. Van Tendeloo: “Imaging interfaces”

MRS spring meeting, San Francisco, CA, USA, April 2009.

J. Hadermann: “Structure determination of complex oxides”.

S. Van Aert: “Atomic resolution mapping using quantitative high-angle annular dark field scanning transmission electron microscopy”.

MRS spring meeting, San Fransisco, CA, USA, April 16, 2009.

32nd international symposium on dynamical properties of solids, Dyproso XXXII, Antwerp, Belgium, September 15, 2009.
J. Verbeeck: “Characterising nanostructures with EELS”.

Annex 3. Invited Lectures
J. Verbeeck: “Model based quantification of core loss and low loss electron energy loss spectra”.

J. Verbeeck: “Control of the high temperature transport properties of GdBaCo_2O_5+x epitaxial films by inducing microstructural defects”.

F. Peeters: “Graphene quantum dots”.

14th Brazilian Workshop on Semiconductor Physics, Curitiba (PR, Brazil), 23-27 March 2009.
F. Peeters: “Graphene nanostructures”.

International Conference on Superconductivity and Magnetism (ICSM2010)
Antalya, Turkey, 25-30 April 2010.
F. Peeters: “Tuning superconductivity in nanomaterials”.

International Conference on Superconductivity and Magnetism (ICSM2010)
Antalya, Turkey, 25-30 April 2010.
A. Shanenko: “Nanosized superconductors: A new type of the BCS-BEC crossover induced by quantum-size effects”.

International Conference on Superconductivity and Magnetism (ICSM2010)
Antalya, Turkey, 25-30 April 2010.
V. R. Misko: “Unconventional dynamics of vortex shells in mesoscopic superconducting Corbino disk”.

International Conference on Superconductivity and Magnetism (ICSM2010)
Antalya, Turkey, 25-30 April 2010.
M. Milosevic: “Vortex matter in two-band mesoscopic superconductors”.

International Conference on Superconductivity and Magnetism (ICSM2010)
Antalya, Turkey, 25-30 April 2010.
V. R. Misko: “Controlling the critical current in superconductors with quasiperiodic pinning arrays”.

KU Leuven (P2)

The Capri Spring School on Transport in Nanostructures, Villa Orlandi, Anacapri, Italy, March 2007.
C. Van Haesendonck: “Scanning probe microscopy for measuring local electrical and magnetic properties (2 lectures)”.

12th European Conference on Applications of Surface and Interface Analysis (ECASIA ’07),
C. Van Haesendonck: “Imaging nanoscale magnetism with scanning probe microscopy”.

P. Lievens: “Physical and chemical properties of binary clusters”.

P. Lievens: “Size and composition dependent magnetism in small binary clusters”.

Annex 3. Invited Lectures
A. Vantomme: “Structural analysis of thin films, surfaces and interfaces using ion beams”.

A. Vantomme: “Growth of nanostructured systems”.

A. Vantomme: “Introduction to RBS channelling”.

International Conference on Nanophysics and Nanoelectronics, Nizhny Novgorod, Russia, 10-15 March 2007.
V.V. Moshchalkov: “Vortex ratchets in nanosuperconductors”.

V.V. Moshchalkov: “Superconductor/Ferromagnet hybrid nanostructures”.

5th International Conference on Vortex Matter, Rhodes, Greece, 8-14 September 2007.
V.V. Moshchalkov: “Vortex manipulation in the S/F hybrid nanostructures”.

V.V. Moshchalkov: “Pinning by nanoengineered periodic arrays of antidots”.

International Conference on Clusters at Surfaces, Warnemünde, Germany, 25-29 May 2008.
Peter Lievens: “Scanning probe microscopy investigations of cobalt clusters on gold surfaces”.

Peter Lievens: “Clusters, nanopuzzles of atoms”.

IMM – Radboud Universiteit Nijmegen, 8 April 2008, Nederland.
Peter Lievens: “Tuning magnetism in small binary clusters”.

Peter Lievens: “Size and composition dependent geometric and electronic structure of bimetallic clusters”.

Peter Lievens: “Scanning probe microscopy investigations of cobalt clusters on Au(111)”.

A. Vantomme: “Introduction to RBS channeling”.

Annual Meeting of the DPG and DPG Spring Meeting of the Condensed Matter Division, Berlin, Germany, 25-29 February 2008.
A. Vantomme: “Rare earth doping of GaN”.

LACAME08, the Latin-American Conference on the Applications of the Mössbauer Effect, La Plata, Argentina, 10-14 November 2008.
A. Vantomme: “Get perpendicular: the spin microstructure in Fe-FePt bilayers”.

Prix Patrick Gas et François d’Heurle, Marseille, France, 23 October 2008.
D. Smeets: “Nucleation, diffusion and texture during growth of CoNi-silicides”.

Annex 3. Invited Lectures
20th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas USA, 10-15 August 2008.

D. Smeets: “Instantaneous analysis of real-time RBS data using Artificial Neural Networks”.

K. Temst: “Growth and characterization of nanostructured systems”.

K. Temst: “Neutron Scattering”.

International Conference on Superconductivity and Magnetism (ICSM-2008), Ankara University in Side-Antalya (Turkey), 25-29 August 2008.
A.V. Silhanek: “Superconductors with magnetic pinning landscape”

A.V. Silhanek: “Interplay between geometric and magnetic confinement of superconductivity in S/F hybrids”

European Conference Physics of Magnetism 2008 (PM’08), Adam Mickiewicz University, Poznan, Poland, June 2008.
Chris Van Haesendonck: “Resistance of domain walls induced by spatial modulation of exchange bias and surface roughness”.

Chris Van Haesendonck: “Finite-size effects in the CoO/Co exchange bias system”.

P. Lievens: “Binary clusters and the electronic shell model (part 1 and part 2)”.

Gordon Research Conference on Clusters, Nanocrystals & Nanostructures, Mount Holyoke College, South Hadley, USA, 19-24 July 2009.
P. Lievens: “Kondo-Like Screening of Magnetic Moments in Fe- and Co-Doped Ag Clusters”.

Symposium on Size-Selected Clusters, Brand, Austria, 8-12 March 2009.
P. Lievens: “Size-dependent Kondo screening in small Fe- and Co-doped Ag clusters”.

Genesis Research Institute Symposium 2 on Cluster Science (Toyota Technological Institute), Nagoya, Japan, 24-26 February 2009.
P. Lievens: “Endohedrally Doped Clusters”.

A. Vantomme: “Thin film studies by the application of complementary techniques in real time”.

International Conference on the Applications of the Mössbauer Effect, Vienna, Austria, 2009.
A. Vantomme: “The spin microstructure in perpendicularly magnetized L10-FePt and Fe-FePt bilayers”.

Annex 3. Invited Lectures
A. Vantomme: “Introduction to RBS channelling”.

K. Temst: “Introduction to Neutron Scattering - application to nanostructures”.

UPBL03 Brainstorm Meeting, ESRF, Grenoble, France, 9-10 February 2009.
K. Temst: “Future challenges for NRS in low-dimensional correlated electron systems”.

Department of Physics and Astronomy Seminar, University of Canterbury, Christchurch, New Zealand, 13 March 2009.
K. Temst: “Exchange Bias in magnetic nanostructures”.

Nanomagnetism probed by X-rays and Neutrons, Ruhr-Universitaet Bochum, Germany, 12-13 June 2009.
K. Temst: “PNR Studies of exchange biased Co/CoO nanostructures”.

K. Temst: “Get perpendicular: the spin structure in perpendicular magnetized Fe-FePt bilayers”.

V.V. Moshchalkov (keynote invited speaker): “Type 1.5 Superconductivity”.

Joint ESF and JSPS workshop on Nanoscience and Engineering in Superconductivity. Tsukuba (Japan), March 2009.
A.V. Silhanek: “Direct Visualization of magnetic pinning”

A.V. Silhanek: “Self-Organized mode lock-in effects in Superconductor/Ferromagnet hybrids”.

UCL (P3)

Luc Piraux: “Template-grown magnetic nanowires for spin transfer devices”.

István Mátéfi-Tempfli: “Nanowires and nanostructures fabrication using template methods: A step forward to real devices combining electrochemical synthesis with lithographic techniques”.

István Mátéfi-Tempfli: “Fabrication of nanowires and nanostructures. Measurements and applications”.

J.-C. Charlier (Plenary Talk): “Atomic scale modelling of carbon nanotubes: from structures to quantum transport”.

J.-C. Charlier  (Invited Communication): “Quantum transport in carbon nanotubes”.

J.-C. Charlier (Invited Communication): “Defects in carbon nanotubes : from atomic structures to quantum transport”

J.-C. Charlier (Invited Lecture): “Quantum transport in carbon nanotubes”.

J.-C. Charlier  (Invited Communication): “Using defects in carbon nanotubes”.

*Third international workshop on DFT applied to metals and alloys*, Oran, Algeria, 2-4 May (2007).
X. Gonze: “The ABINIT project : modern software engineering techniques for simulation of materials and nanosystems”.

X. Gonze: “Modern software engineering techniques applied to the simulation of materials and nanosystems: the ABINIT project”.

X. Gonze: “The ABINIT project : simulation of materials and nanosystems, from software engineering techniques to high performance computing”.

X. Gonze: “First-principles computation of dynamical properties of solids and nanostructures with ABINIT”.

L. Piraux: Magnetic nanowires for spintronics purposes.

L. Piraux: “Magnetotransport on single magnetic nanowires”.

*Journées C’nanoNO*, Poitiers, France (2008).
L. Piraux: Les nanofils magnétiques en spintronique.

L. Piraux: Template-grown magnetic nanowires for spin transfer devices.

La "magnétorésistance géante" et le prix Nobel de Physique 2007
*Ecole doctorale thématique: Physique et Astrophysique*
Louvain-la-Neuve, Belgium (2008)
L. Piraux


Annex 3. Invited Lectures
L. Piraux: Nanofils ferromagnétiques pour applications hyperfréquences.

J.-C. Charlier: “*Ab initio* quantum transport in carbon nanotubes”.

J.-C. Charlier: “Gas sensors based on defective carbon nanotubes”.

J.-C. Charlier: Spin transport in graphene nanoribbons: the crucial effect of point defects.

*Trends in Nanotechnology (TNT2008)*, Oviedo, Spain, 01-05/9/2008.
J.-C. Charlier: “Quantum transport in carbon nanostructures”.

J.-C. Charlier: Gas sensors based on defective carbon nanotubes.

J.-C. Charlier: “Electronic transport in zigzag graphene nanoribbons”.

G.-M. Rignanese: “First-Principles Investigation of High-K Dielectrics”.

B. Hackens: “Imaging electron local density of states inside mesoscopic quantum rings”.

B. Hackens: “Imaging confined semiconductor systems”.

*29*\textsuperscript{th} *International conference on the physics of semiconductors (ICPS29)*, Rio de Janeiro (2008).
B. Hackens: Imaging the electron local density of states inside buried semiconductor quantum rings.

Luc Piraux: “Magnetotransport on single magnetic nanowires”.

Luc Piraux: “Magnetic nanowires for spintronics purposes”.

B. Hackens: “Imaging confined semiconductor systems”.

J.-C. Charlier (Invited Tutorial Talk): “*Ab initio* quantum transport in carbon nanotubes”.

*Trends in Nanotechnology (TNT2008)*, Oviedo, Spain, 01-05/9/2008.
J.-C. Charlier (Invited Lecture): “Quantum transport in carbon nanostructures”.

J.-C. Charlier (Invited Talk): “Quantum transport in carbon nanostructures”.

Annex 3. Invited Lectures
14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste (Italy), 8-10 January 2009.
G.-M. Rignanese: “Band Offsets From Many Body Perturbation Theory”.

CALPHAD XXXVII, Prague (Czech Republic), May 18-22 (2009).
X. Gonze: “First-principles computation of phonon spectra and thermodynamical properties”.

Seventh International Conference on Computational Methods in Science and Engineering, Rhodes (Greece), September 29 – October 4 (2009).
X. Gonze: “The ABINIT Project : Software Engineering Techniques Meet Simulation of Materials and Nanosystems”

"From Basic Concepts to Real Materials", Santa Barbara CA (USA), November 2-6 (2009).
X. Gonze: “The ABINIT Project : Software Engineering Techniques Meet Simulation of Materials and Nanosystems”.

**UA-Plasmant (P4)**

A. Bogaerts: “Laser ablation and sample transport: the heartbeat and blood circuit of LA-ICPMS”.

A. Bogaerts: “Plasma modeling: The type of discharge dictates the best model to be used”.

E. Neyts and A. Bogaerts: “Reaction mechanisms and thin a-C:H film growth from low energy hydrocarbon radicals”.

A. Bogaerts: “Computer simulations of gas discharges for a better understanding of the plasma behaviour”.

A. Bogaerts: “Computer modeling of etch plasmas: capacitively coupled and inductively coupled rf Discharges”.

*“GLADNET Training Course” (in framework of a European Marie Curie Research Training Network), September 11, 2007, Antwerpen, Belgium.*
A. Bogaerts: “Modeling of analytical glow discharges”.

*“Colloquium Spectroscopicum Internationale XXXV”, September 23-27, 2007, Xiamen, China.*
A. Bogaerts: “From the laser-solid interaction till the aerosol transport to the ICP: a simulation tour of laser ablation”.

*“12th European Summer School “Low Temp Plasma Physics”: Master Class “Physical Vapor Deposition”, October 6-13, 2007, Bad Honnef, Germany.*
A. Bogaerts: “Introduction to magnetron sputtering: Basic Physical Processes and Mechanisms”.

E. Neyts and A. Bogaerts: “Numerical modeling of plasmas and plasma-surface interactions”.

Annex 3. Invited Lectures
A. Bogaerts: “Modeling of a dielectric barrier discharge used as a flowing chemical reactor”.

5th International Conference on Laser-Induced Breakdown Spectroscopy, September 22-26, 2008, Berlin, Germany.
A. Bogaerts: “Numerical modeling of laser induced vaporization, plume expansion and plasma formation”.

35th Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Conference, September 28 - October 2, 2008, Reno, NV, USA.
A. Bogaerts: “Modeling of plasmas, plasma-solid and laser-solid interaction”.

Invited plenary lecture at the “2008 Winter Conference on Plasma Spectrochemistry”, January 7-12, 2008, Temecula, California, USA.

A. Bogaerts: “Overview of plasma modelling”.

A. Bogaerts: “Computer simulations of processing plasmas”.

A. Bogaerts: “Modeling of laser ablation processes for plasma spectrochemistry: Different pieces of the puzzle”.

E. Neyts: “Modeling plasma-surface interactions”.

“Society of Vacuum Coaters Plasma Processing Conference”, May 9-14, 2009, Santa Clara, CA, USA.
E. Neyts and A. Bogaerts: “Modeling of plasmas and plasma-surface interactions for the synthesis of carbon nanostructures”.

E. Neyts and A. Bogaerts: “Modeling of hydrocarbon plasmas for nanoparticle formation and growth of carbon nanostructures”.

“29th International Conference on Physics of Ionized Gases”, July 12-17, 2009, Cancun, Mexico.
S. Paulussen and A. Bogaerts: “Plasma assisted conversion of greenhouse gases to value-added chemicals”.

E. Neyts and A. Bogaerts: “Modeling of plasmas and plasma growth of carbon nanostructured materials”.

A. Bogaerts: “Plasma modelling”.

Annex 3. Invited Lectures
A. Bogaerts: “Modeling of the plasma chemistry and plasma-surface interactions in reactive plasmas”.

A. Bogaerts: “Computer modeling for plasmas and plasma-surface interactions”.

A. Bogaerts: “Computer modeling for predicting the effects of nitrogen addition to argon glow discharges”.

A. Bogaerts: “Computer simulations for plasma etching applications”.

E. Neyts and A. Bogaerts: “Theoretical formation of exo- and endohedral complexes and nanostructures”.

“Symposium of the Discussion Group for Plasma Spectrochemistry in Japan”, October 9, 2009, Tokyo, Japan.
A. Bogaerts: “Modeling of laser ablation for ICP-MS”.

A. Bogaerts: “Modeling of low-temperature plasmas: some case studies of different modeling approaches”.

“36th Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Conference”, October 18-22, 2009, Louisville, KY, USA.
J. Pisonero, H. Lindner, A. Bogaerts and D. Günther: “Did we learn something in LA-ICP-MS?”

A. Bogaerts: “Computer modeling of plasmas and plasma-surface interactions”.

**Ulg (P5)**

F. Remacle: (a) First Attochemistry Symposium : ‘Ultrafast hole migration modular molecules from small peptides to hydrogen bonded clusters’, (b) Switching Devices Symposium : ‘Implementation of an all electrochemically driven cyclable set-reset machine on copper rotaxanes’.

*MRS Spring Meeting, San Francisco, USA, 14-18/04/2009.*
F. Remacle: “Atomic and electronic structure of Ge-Sb-Te Phase Change materials”.

*APS March Meeting, 16-20/03/2009, Pittsburgh USA.*
F. Remacle: “Polarization Patterns In GeTe From Bulk To Ferroelectric Nanoclusters”.

*APS March Meeting, New Orleans (USA), Mar 10-14, 2008.*
F. Remacle: “Mechanism of GeSbTe phase change materials: an ab initio molecular dynamics study”.

*MRS spring meeting, San Francisco, USA, 24-28/03/2008.*
F. Remacle: “Structural and Vibrational Properties of Tellurium Based Materials”.

*Annex 3. Invited Lectures*
UH (P6)

IGAS Symposium Berlin, Germany, November 10, 2008.
P. Wagner: “Bio- and chemosensors based on CVD-diamond films”.

P. Wagner: Functionalisation of diamond with organic linker molecules and DNA.

ISAS seminar, Institute for Analytical Sciences, Berlin, Germany, April 7, 2008,

Nanocarbon and Nanodiamond 2008, Saint-Petersburg, Russia, July 1-4, 2008.

Jahrestagung des AK-BioMST e.V., Technologiezentrum Dortmund, Dortmund, Germany, June 19, 2007.

O.A. Williams, K. Haenen, et al., “Biological applications of nanocrystalline diamond”.

H.G. Boyen, “A micellar approach to magnetic ultra-high density data storage media”.

O.A. Williams, K. Haenen, et al., “Growth and electronic properties of nanodiamond”.


World Congress on Biosensors, Shangai, China, May 14-16, 2008.
S. Wenmackers, V. Vermeeren, K. Roodenko, S.D. Silaghi, N. Esser, P. Wagner, Optical conformation studies on DNA layers covalently bound to diamond-based sensors.


Engineering of Functional Interfaces EnFI 08, Jülich, Germany, June 12-13 2008.
S. Wenmackers, V. Vermeeren, K. Roodenko, S.D. Pop, N. Esser, P. Wagner, „Functionalisation of diamond with organic linker molecules and DNA“.


Annex 3. Invited Lectures

H.-G. Boyen, “Assembly of molecular junctions: Evidence for chemical interactions between a metal overlayer and its molecular support”.

*Max-Bergmann-Symposium*, Dresden, Germany, November 4-6, 2008.
P. Wagner, “Nanocrystalline diamond as a platform for label-free real-time DNA sensors”.

H.-G. Boyen, *Noble dwarfs - insights into the fascinating world of nanostructures*.

H.-G. Boyen, *Ordered nanoparticle arrays from block-copolymer templates*.


*Summerschool on Nanoscience and Nanotechnology*, Leuven, Belgium, August 24-28, 2009.
H.-G. Boyen, “Self-assembled nanostructures at surfaces – from fundamental aspects to applications”.


*MRS 2009 Fall Meeting*, Hynes Convention Center & Sheraton Boston Hotel, Boston, MA, USA, November 30-December 4, 2009.

K. Haenen, “Recent progress in phosphorus doping of CVD diamond on (110)-oriented substrates”.

Annex 3. Invited Lectures