HUMAN RESOURCES AND MOBILITY (HRM) ACTIVITY

MARIE CURIE ACTIONS
Host fellowships for Early Stage Research Training (EST)

PART B

'NANOCAGE'

PARTNER 1 (co-ordinator): Nanoscience group,
University of Nottingham, UK (NOTTM)

PARTNER 2: Institut für Schichten und Grenzflaechen,
Forschugszentrum Jülich GmbH (FZJ)

PARTNER 3: Computational Modelling Group,
National Microelectronics Research Centre (NMRC), Ireland

PARTNER 4: Fullerene Group,
Queen Mary, University of London (QM)

B1 SCIENTIFIC QUALITY OF THE RESEARCH TRAINING AREA

B1.1 Motivation and Focus of Proposal

The European Commission (in common with practically all other national and international scientific funding agencies) recognises the key importance of nanometre scale physics in the development of future information and communication technologies (ICTs). This is keenly demonstrated by the specific targeting of an entire thematic area in FP6 on nanometre scale science. *The NANOCAGE project we propose is exceptionally well aligned with the nanoscience-related priorities of the Commission and involves the development of protocols to study, manipulate and tune the properties of an exotic form of nanostructured matter: endohedral fullerenes (endofullerenes)* [1] *(Fig. 1).*

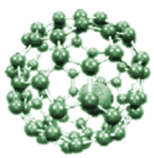

Fig.1 *Illustration of an endofullerene*

Fullerenes can be considered as molecules almost ‘custom built’ for nanoscience: a hollow carbon cage of the order of 1 nm in diameter, they are employed in very many areas of fundamental and applied nanoscience [2]. Endofullerenes - where an atom or cluster of atoms is encapsulated inside the fullerene cage - represent a subset of the fullerene family with particular potential in the development of novel functionalities within molecular electronics [3]. The *NANOCAGE* project brings together four key European groups - namely the *Nottingham Nanoscience group* (NOTTM), the *Institute of Thin Films and Interfaces (ISG), Forshcungszentrum, Jülich* (FZJ), the *Computational Modelling group, National Microelectronics Centre, Ireland* (NMRC), and the *Fullerene Group, Queen Mary, University of London* (QM) - in the areas of scanning probe microscopy and spectroscopy, fullerene science, and synchrotron-based spectroscopies to provide unprecedented insights into the physiochemical properties of adsorbed endofullerene molecules. The proposed research programme is *essential* if the potential of endofullerene systems as key elements of quantum computing [4] or molecular electronics technologies is to be realised.

The proposed *NANOCAGE* project establishes a multi-host early stage training project focussed on a research problem which involves scientific problems and questions at the leading edge of international nanoscientific research. *This represents an extremely exciting opportunity for postgraduate students, involving training in a broad range of cross-disciplinary experimental and theoretical methods which form the basis of state-of-the-art nanometre scale science.* Furthermore, the research project is related to the study and manipulation of a materials system that, despite having immense potential in nanoscale and molecular electronics, is currently poorly understood. There is thus particular scope for the production of high impact research results. It is important to note that two hosts within the project, Nottingham and NMRC, were awarded Marie Curie training site status under Framework 5. The EST project we propose will enable us to build on this success, securing closer collaborative links and thus promoting enhanced research integration within the European Research Area (ERA). Only with the combined expertise associated with integrating research in this manner is it possible to address the types of cutting edge scientific questions at the heart of the *NANOCAGE* project.

B1. 2 Beyond the state of the art: Innovative aspects of the research and training programmes

The key breakthrough associated with the NANOCAGE project is the extension of the state of the art in molecular electronics to encompass control of the electronic and physiochemical properties of caged atoms on surfaces.

Fullerenes have played a central role in the development of a variety of single molecule techniques and spectroscopies, each of which is currently an intensely active sub-field of nanoscience and nanotechnology. These include: single molecule manipulation (Fig. 2, [2, 5,6]), single molecule electronic [7] and optical [8] microscopy, and monomolecular electronic devices [9]. The novelty of the endofullerene species arises from the encapsulation of an atom or clsuter within the carbon cage. There are very many fundamental questions:

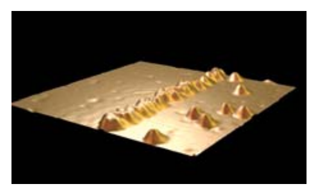

Fig. 2 *STM-fabricated 1D fullerene wire [2]*

- How is the encapsulated atom coupled to the fullerene cage?
- Is it possible to address the caged atom and change its electronic state?
- Are the magnetic properties of the endofullerene similarly addressable or tunable?
- How are the intramolecular dynamics (the motion of the caged atom(s)) affected by distortions of the fullerene cage?
- Might a prototypical experimental electronic device based on endofullerenes be fabricated using single molecule positioning techniques similar to those demonstrated for the archetypal fullerene, C_{60} [5,6]?

None of the questions listed on the previous page have yet been answered for adsorbed endofullerenes: this is the fundamental scientific motivation underlying the NANOCAGE proposal.

In the development of a viable molecular electronics technology the molecule-surface interaction is an exceptionally important parameter that not only determines the spatial distribution of the molecular units but also strongly affects their structural and electronic properties. Yet, despite the recent exciting proposals for novel functional devices based on endofullerenes [4], *the basic issues related to our ability to measure, exploit and control the properties of the caged atom remain unaddressed*. As noted above the primary outcome of the project will therefore be extending the state of the art in molecular and nanoscale electronics to encompass the control of atoms encaged in molecules.

In addition to the inherent novelty of the scientific questions to be addressed within the *NANOCAGE* EST network, the combination of host institutions involves a unique blend of expertise which will play an essential role in achieving the objectives of the project. The combination of key European groups in the areas of fullerene synthesis and spectroscopy (Dennis et al., Queen Mary), scanning probe microscopy (Julich and Nottingham), density functional theory of fullerene systems (Greer et al., NMRC), and synchrotron spectroscopy (Nottingham) provides a multi-faceted and interdisciplinary approach to addressing the challenging scientific problems listed above. We reiterate that this approach represents an extremely attractive, exciting and comprehensive training programme for postgraduate researchers in nanoscience.

B1. 3 Benefit of Research Programme to the European Research Area (ERA)

Nanoscale science is a burgeoning influence on almost every area of 21st century science and technology. The Commission has recognised for some time the importance of investment in nanoscience and this is reflected in the wide variety of nanometre scale science-based projects that have been funded under COST, ESPRIT and IST programmes in the 4th and 5th frameworks. That FP6 involves an entire thematic area (associated with total funding of €1.3 billion) devoted specifically to nanoscience and related fields, pays testament to the widely perceived potential of nanoscience in the coming decades. In addition, it is important to realise that under FP6 nanoscience is not restricted to a single thematic area. As might be expected from the intensely cross-disciplinary nature of the field, nanotechnology features in many other thematic priorities.

A recent report on nanoscience and nanotechnology in the European Commission programmes[†] has highlighted the very strong position of the EU in nanotechnology: European scientists are at the forefront, producing 34% of the total number of publications in the field (compared to US: 24%, and Japan: 14%)[‡]. There are a considerable number of European Networks of Excellence involving strong nanoscience elements (for example, the Nottingham group is part of the *PHANTOMS* network on mesoscopic systems and both FZJ). Indeed, a total of 86 nanoscience-related networks bringing together over 2000 groups were operational at the beginning of 2002[†]. However, it is important to bear in mind that the US remains the dominant force in the Information and Communication Technologies (ICT) sector of which nanoscience forms a large component. It is therefore essential to continue to ensure provision of high quality postgraduate training in Europe (such as that detailed in the following sections) to both build on the EU's predominant scientific position in nanoscale science and to counter the 'drift' of talented students and researchers to the US. In the longer term, the establishment of training projects and networks such as *NANOCAGE* will promote further close integration of research teams within the ERA, strengthening in turn the European nanoscience base. A particularly noteworthy aspect of the proposed EST project is that it not only builds on previous collaborations (Nottingham – Queen Mary, Nottingham – NMRC) but introduces important new links between Julich and the other institutions (Nottingham, Queen Mary, and NMRC).

B1.4 The Research Programme: Objectives and Deliverables

An overarching theme of the *NANOCAGE* project is the exploration of the correlations that exist between the structural, electronic, vibrational, and transport properties of atoms encaged in endofullerenes. In the following, we list the key research and training objectives contributing to this overall theme. It is very important to note that although, as outlined below, there is a division between the research and training components, a key focus throughout the project is the provision of internationally leading PhD training in cutting edge nanoscience. Thus, the research and training objectives throughout the project will necessitate careful timing and coordination (as described in detail in Section B4).

[†] *www.cordis.lu/nanotechnology, www.cordis.lu/rtd2002*

[‡] *A. Hullmann, Nanotechnology: Europe on Top in Nanoscience, in Indinews 2, Internal Newsletter on S&T&I Indicators, EC, 2001, fig.2*

Research objectives

1. To ascertain the effects of chemisorption on the properties of encapsulates in a variety of endofullerene molecules in order to develop protocols for tuning the electronic structure of the caged atom or cluster;
2. To probe whether chemisorption induces changes in the position of the encapsulated atom(s) and, if so, how those structural changes affect Objective 1;
3. To probe the electronic spin state of caged atoms in endofullerenes in order to determine their potential as qubits;
4. To determine the intramolecular vibrational modes of chemisorbed endofullerenes;
5. To establish the role of the valency and vibrations of a caged atom in determining the electrical transport properties of an endofullerene molecule. Similarly, to establish the role of cage distortion in electrical transport;
6. To construct small endofullerene assemblies using molecular manipulation and to explore the temperature-dependent dynamics of those assemblies using variable temperature STM;
7. To construct prototypical monomolecular and bimolecular electronic devices based on endofullerenes.

Training Objectives

- provision of comprehensive, cross-host training in a variety of core and novel nanoscientific experimental and theoretical methods (some of which only available within the *EST* network we propose);
- development of postgraduates' nanoscientific knowledge base through attendance at seminars, group meetings, workshops and Summer schools organised by the EST network;
- expansion and broadening of scientific thinking due to exposure to a wide range of new concepts and ideas;
- development of transferable skills through attendance at Graduate School courses and network-related activities;
- a strengthening of the ability of European researchers in nanoscience to undertake cross-disciplinary research;
- development of written and oral communication, team-working and time management skills;
- improvement of written and spoken English/German;
- a general increase in the 'scientific confidence' of postgraduate researchers through: (i) close interaction and discussion with a range of researchers in the EST project host institutions, and (ii) via presentation at/ participation in internal seminars and (inter)national conferences;

B1.5 The Requirement for Multi-site activity

Having defined the key objectives of the project, we outline in Table I on the following page the primary deliverables and milestones related to the proposed research and training programme. It is important to stress at this point that the grouping of host institutions involved in the project represents a critical mass in terms of addressing the particular scientific problems and questions of interest. Specifically, the project comprises four groups with expertise spanning synthesis (QMW), imaging, manipulation and spectroscopy (Nottingham/ Julich), and theory (NMRC). The collective expertise of this particular combination of groups spans a very broad range of areas at the core of state-of-the-art nanoscience, *viz.* scanning tunnelling microscopy and spectroscopy (STM); single molecule vibrational spectroscopy/ inelastic tunnelling spectroscopy (IETS); molecular positioning and manipulation; atomic force microscopy; near field optical microscopy; synchrotron radiation spectroscopies (SRS) including photoelectron spectroscopy and X-ray absorption spectroscopy; Hartree Fock (HF) and density functional theory (DFT); and fullerene synthesis and related spectroscopies. (See Section B3 for a discussion of the hosts' track record and research highlights in these areas). It is precisely this combination of skills that is required to comprehensively fulfil the objectives of the research programme listed above – an EST project involving only a single site simply would not have the requisite breadth of expertise nor the necessary interdisciplinary character. The wide breadth of expertise also makes a very significant contribution to the extremely high quality of PhD training that will be provided.

B 1.6 The requirement for PhD training in this area

From the perspective of both the ERA and the career progression of the Marie Curie fellows, the importance of high quality PhD training in nanoscience cannot be understated. Given the arguments related to the predominance of the EU in nanoscience outlined above, it is essential that increased integration within the ERA is employed both to strengthen the world leading position of the EU in this area and to promote a research environment where the European scientific community might challenge the US in ICT. It is particularly important that students from, for example, less favoured EU states should have the opportunity to transfer knowledge from internationally leading European groups to their home countries. An important method of facilitating this type of dissemination of nanoscientific research skills is via an EST multi-site project such as that proposed here. A multi-site project also has the important advantage that it maximises the impact of the research programme across a number of member states.

Programme, Deliverables and Milestones

The project research programme, deliverables and milestones are shown below in Chart B1_1 and Chart B1_2..

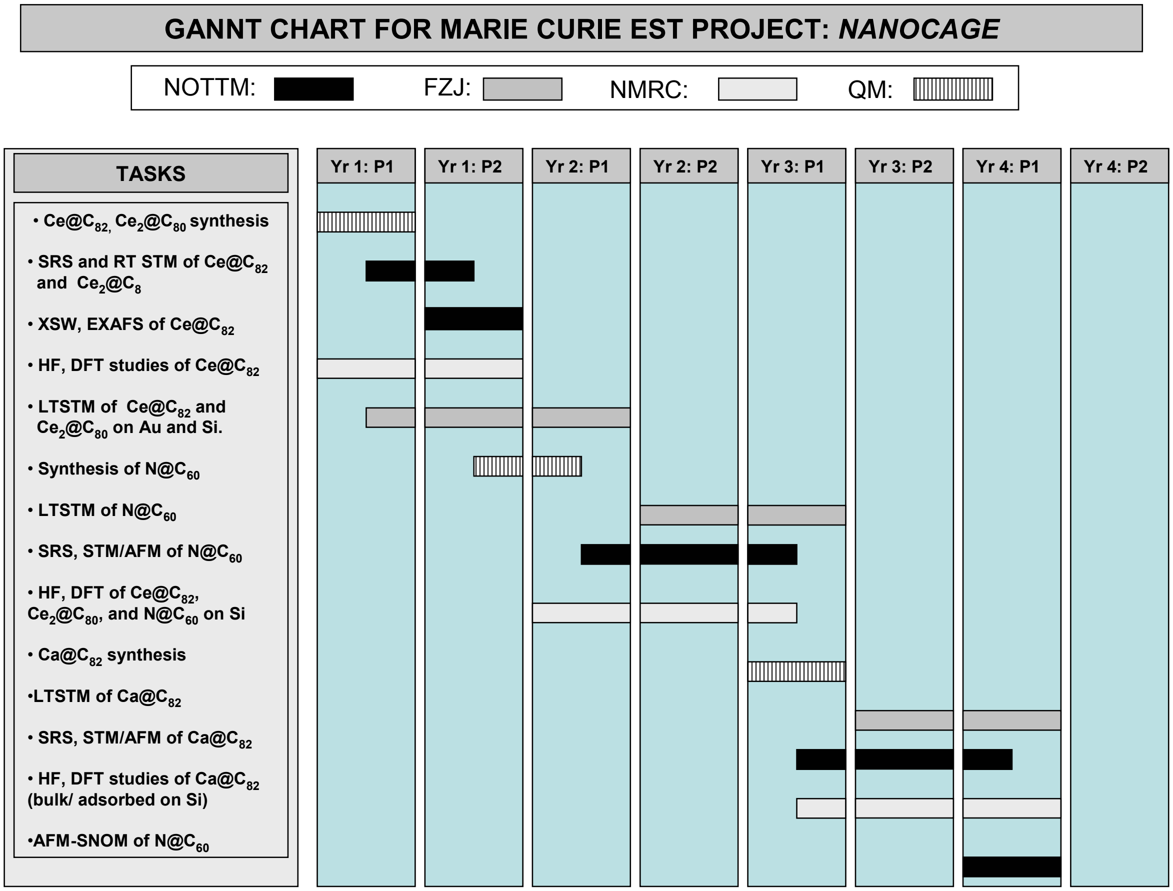

***Chart B1_1**: Gannt chart for NANOCAGE project (for acronym explanations see caption for Table B1). Consideration of training objectives (in particular, inter-host transfer of early stage researchers) has informed the scheduling. Note that Yr 1: P1 stands for "Year 1, Period 1" and represents the first six months of the project. Similar 1abelling is used throughout. Under 'Tasks', 'synthesis' also takes into account chromatography, ESR and NMR spectroscopy.*

RESEARCH DELIVERABLES

END OF YEAR 1

•Acquisition of PES, XAS, XSW, IETS and tunnelling spectra of $Ce@C_{82}$ and $Ce_2@C_{80}$ on Si and Au surfaces.

•Completion of theoretical analysisof $Ce@C_{82}$.

•Intercomparison of experimental and theoretical data: elucidation of effects of adsorption.

END OF YEAR 2

•Completion of LTSTM manipulation of Ce@C82 and $Ce_2@C_{80}$: fabrication of nanostructures and analysis of kinetics of assemblies.

•Construction of proptypical monomolecular device: compression of endofullerene

•Elucidation of effects of compression and manipulation on (inelastic) tunnelling spectra.

• RT STM, AFM, and PES of $N@C_{60}$.

END OF YEAR 3

•Completion of theoretical analysis of $N@C_{60}$ and $Ce_2@C_{80}$

•Acquisition of SRS, STM images and IETS for $N@C_{60}$ molecules on Si and Au.

•Intercomparison of experimental and theoretical data for $Ce@C_{82}$, $Ce_2@C_{80}$, $N@C_{60}$: elucidation of intramolecular dynamics and bonding.

END OF YEAR 4

•Completion of theoretical studies of $Ca@C_{82}$.

•Intercomparison of theoretical and experimental vibrational spectra for $Ca@C_{82}$ and $Ce@C_{82}$: elucidation of role of size /valence of caged atom.

•Synthesis of 'bimolecular device' comprising tip-endofullerene-endofullerene-substrate system.

•Completion of final report.

***Table B1_1:** Deliverables and milestones for the NANOCAGE project. Note that the following acronyms have been used for both Chart B1_1 and Table B1_1: SRS - synchrotron radiation spectroscopy; PES – photoemission spectroscopy, XAS – X-ray absorption spectroscopy, XSW – X-ray standing wave spectroscopy, IETS – inelastic tunnelling spectroscopy, HF – Hartree Fock, DFT – density functional theory.*

Note that each of the deliverables maps directly onto one or more of the specific research objectives given on p. 3.

B2 QUALITY OF THE TRAINING ACTIVITIES

B2. 1 Requirement for Graduate Training in Nanoscience

Arguably the single most important feature of nanometre scale science is that it involves a convergence of the traditional scientific disciplines at the nanometre level [2]. Consequently, nanoscience pervades almost every area of 21st century science and technology. The key strategic importance of nanotechnology is recognised across all scientific communities, at national, European, and worldwide levels. For example, a recent briefing document on the state of UK science notes the significance of the EU's approach to funding under FP6 and, in particular, recognises that FP6 involves a focus of effort on a limited number of key technologies where the EU is well placed to compete on the world stage, namely biosciences, e-science, aeronautics, *and nanoscience*. Similarly, the following quote by Commissioner Busquin is taken from the proceedings of an EC/NSF workshop towards the end of 2001:

"Today, at the beginning of the 21st century, research in the life sciences, the information technologies, and the materials sciences converges upon a commonality: the domain of the nanometer, and the manipulation of atoms and molecules. Continued technological progress becomes dependent upon achieving control of materials at the nanoscale".[†]

<u>The EST project we propose involves precisely these objectives:</u> the manipulation and control of elements of a novel molecular system. This goal is in turn very well aligned with the Commission's statement regarding the aims and objectives of Thematic Priority Area 3 ("Nanotechnology and Nanoscience, Knowledge-based Multifunctional Materials and New Production Processes and Devices"): "*to stimulate breakthroughs, which can lead to entirely new materials, new devices, new products and new industries".* Furthermore, from the perspective of researcher training, it is essential that European students are educated in the cutting edge experimental and theoretical nanoscience methods, techniques, and instrumentation that underlie the *NANOCAGE* research programme. This will not only ensure that the EU maintains its predominance in this area and counter the transfer of scientists from Europe to the US or Japan but, with sufficiently exciting and innovative nano-related projects, we will attract many talented researchers *into* the ERA. Finally, a key objective of our graduate training programme is to ensure, by providing an intellectually challenging and rewarding scientific environment, that as many doctoral graduates as possible pursue research careers following their PhD studies.

B2. 2 Research Training Activities under the 'NANOCAGE' Early Stage Training project

Postgraduate research training within the EST network will be subdivided into four key areas:

- (i) individual 'hands on' research training;
- (ii) graduate courses and seminars;
- (iii) multi-host activities;
- (iv) transferable and complementary skills.

Table B2_1 on the following page provides a graphical synopsis of the research training programme to be provided under the *NANOCAGE* project: each of the areas outlined in Table B2_1 is described in some detail in the following sections. It is important to reiterate at this point that both the project coordinator (NOTTM) and NMRC have been designated as Marie Curie training sites under Framework 5. The Nottingham Nanoscience group (and, indeed, the School of Physics & Astronomy in which the group is based) also has a strong history of cross-European collaboration (see Sections B3 and B7). Finally, the Nottingham group is lead coordinator of a recently established (Feb. 2003) University of Nottingham *Interdisciplinary Doctoral Training Centre* which involves research groups across a broad range of disciplines (Physics & Astronomy, Chemistry, Pharmaceutical Sciences, Biomedical Sciences, and Genetics).

Other hosts within the EST project similarly have strong track records in both national and international graduate training. Each year, FZJ hosts more than 700 visiting scientists from over 50 countries and therefore the institute has a particularly strong portfolio of collaborative research projects. NMRC has supported research at a European level as a large scale facility (LSF) under the 4th and 5th Framework and as a Host Site for the 5th Framework Marie Curie Fellowships programme

[†] *EC Commissioner Busquin Proceedings EC/NSF workshop Toulouse, Oct. 2001Office for Official Publications, ISBN 92-894-0793-X*

TABLE B2_1: Research Training Activities under the NANOCAGE Early Stage Training Project

Host 1: NOTTM	HOST 2: FZJ	HOST 3: NMRC	HOST 4: QMW
No. of early stage researchers			
• *2 x 36 months* • *24 man-months of visiting researchers*	• *2 x 36 months* • *12 man-months of visiting researchers*	• *2 x 36 months* • *12 man-months of visiting researchers*	• *1 x 36 months* • *6 man-months of visiting researchers*
Individual 'hands on' technical training			
• *UHV techniques* • *SPM imaging* • *Molecular manipulation* • *Fullerene deposition* • *XPS, UPS* • *Synchrotron spectroscopy* • *Near field optics*	• *Cryogenic techniques* • *LT STM* • *STS and IETS* • *Single molecule spectroscopy* • *LT molecular manipulation* • *UHV techniques* • *Monte Carlo simulations.*	• *Computational chemistry* • *Hartree Fock methods* • *Density functional theory* • *Theoretical approaches to treat molecular conduction*	• *(Endo)fullerene synthesis* • *NMR spectroscopy* • *Electron spin resonance* • *High performance liquid chromatography* • *General analytical chemistry competencies*
Graduate courses, modules and seminars			
• *Dedicated nanoscience modules provided through IDTC*[†]*.* • *Weekly group meetings/ journal club.* • *Nanoscience seminar programme.* • *Departmental colloquia.* • *National and international conference attendance.*	• *Annual postgraduate school* • *National and international conference attendance.* • *Departmental seminars*	• *IT and programming courses* • *National and international conference attendance.* • *Departmental seminars*	• *National and international conference attendance.* • *Departmental (Chemistry) seminars and colloquia*
Transferable/ complementary skills			
• *University of Nottingham Graduate School courses* • *Ethics and Good Research Practice (IDTC)* • *University of Nottingham Centre for English Language Education* • *Safety issues in research* • *Workshop training* • *Undergraduate teaching*	• *Language courses* • *Presentation of work at national/ international conference.*	• *Language courses* • *Presentation of work at national/international conference* • *Information technology skills* • *Computer aided design*	• *Language courses* • *Presentation of work at national/international conference*

Multi-host training activities

- *All students will carry out at least 25% of their training activity in hosts other than the home institution.*
- *An Early Stage Researcher 'mini-conference' will take place at the end of Year 3 of the project.*
- *The following workshops will be organised (1 per year):*
    - *Exploiting Synchrotron Spectroscopies in Molecular and Nanoscale Science (NOTTM)*
    - *Low temperature Scanning Tunnelling Microscopy and Spectroscopy (FZJ)*
    - *Computational Techniques for Nanoscience (NMRC)*
    - *Fullerene science (QMW)*
- *All fellows will be expected to join the Marie Curie Fellowship Association (MCFA), through which wider societal issues may be explored and debated.*

† IDTC : Interdisciplinary Doctoral Training Centre.

B2.3 Training: Benefits of a multi-host project and role of each host

Benefits of multi-host project

Before describing in detail the contributions of each institution to the training programme (which are also briefly outlined in Table B2_1), we outline the key additional research training benefits arising from the particular *combination* of hosts chosen for the *NANOCAGE* EST network. Nottingham and Queen Mary have a strong history of collaboration on fullerene-related problems. Indeed, the Queen Mary group leader (Dennis) and the coordinator (Moriarty) are co-investigators on a major UK EPSRC grant whose focus is the study of fullerene-surface interactions using a combination of synchrotron techniques. We note at this point that the analysis of adsorbed fullerenes is a component of that grant and, very recently (Dec. '02 / Jan. '03) we have succeeded in carrying out the first preliminary photoemission and X-ray absorption measurements of the interaction of endofullerene molecules with a Si surface. The *NANOCAGE* project will not only extend this preliminary work to a much wider range of endofullerenes and substrates but will involve measurements and manipulation (eg inelastic tunneling spectroscopy, low temperature STM imaging and manipulation) which are simply not possible without the expertise and instrumentation of the Julich group. Furthermore, the recent involvement of Nottingham and NMRC in a 5th Framework RTN (see Section B7), has prompted the strengthening of that collaboration (in particular involving a greater degree experiment/theory overlap) within the proposed *NANOCAGE* project.

To summarise, the benefits of our multi-host approach are:

- The collective expertise of the EST project four host network spans synthesis, imaging and spectroscopy, and theory. This breadth of expertise is simply not possible with a single host project. Furthermore, the four host approach represents the smallest critical mass of researchers capable of comprehensively addressing the research problem.
- The broad instrumentation base required to complete the project is not available in a single institution.
- Developing the experimental expertise of early stage researchers across both chemistry (QM) and physics (NOTTM, FZJ) disciplines is a key feature of the training programme. Nanoscience, in particular, requires researchers who have received cross-disciplinary training if the field is to fully realise its immense potential.
- In addition to the question of cross-disciplinary training in experimental nanoscience, we are strongly of the opinion that the experiment – theory divide in science should be narrowed. The multi-host training programme we propose is geared towards ensuring that early stage researchers receive training in both experimental and theoretical methods.

Host 1: Nanoscience Group, University of Nottingham, UK (NOTTM)

As co-ordinator of the project Nottingham will play a leading role in project management (see Section B4) and the provision of complementary skills training. The Nanoscience group offers training in a very broad range of techniques used extensively in cutting edge nanoscale and condensed matter science. The techniques of relevance to the *NANOCAGE* project are as follows:

- *Scanning probe microscopy (SPM)* STM; STM-based single molecule manipulation; contact, non-contact and tapping mode AFM; force-distance spectroscopy; scanning capacitance microscopy (SCM); scanning near field optical microscopy (SNOM); electric force microscopy (EFM); magnetic force microscopy (MFM).
- *Ultra high vacuum techniques and technology*.
- *Photoelectron spectroscopy* (the group has access to a high performance X-ray/ ultraviolet photoelectron spectroscopy system as part of a multidisciplinary consortium of University of Nottingham schools that was successful in securing €900K for the instrument from the UK Engineering & Physical Sciences Research Council).
- *Synchrotron-based spectroscopies*: photoemission, resonant photoemission, near edge X-ray absorption spectroscopy (NEXAFS), extended X-ray absorption fine structure (EXAFS), X-ray standing wave (XSW).
- *Low level optical measurements*. The group has recently been funded to develop a novel combined UHV SNOM-AFM system and work on a near-field Raman microscope system is underway.
- An important aspect of the group's research is that while a large number of commercial instruments are available, we have successfully designed and constructed novel scanning probe systems. Furthermore, a number of the commercial instruments are user-configurable. Thus, in addition to training in conventional scanning probe methods, there is significant potential for students to get involved with "custom designed" and thus highly innovative scanning probe experiments.
- The research profile of the Nottingham group is considerably enhanced by the large number of national and international collaborations in which it is involved. See Section B7 for a list of current and previous EU support which involves the majority of our European collaborators.

Doctoral Training
Training of Ph.D. students in the School of Physics & Astronomy includes subject-specific advanced lecture courses, problem solving and communication skills and is responsive to the policies of the research councils. The recent establishment of the University of Nottingham *Interdisciplinary Doctoral Training Centre* (IDTC) will provide a range of graduate modules on topical aspects of nanoscience including: *Atomic and Molecular Manipulation*; *Self-assembly in Polymer, Molecular and Nanoparticle Systems;, Near-field Optic;,* and *Synchrotron-based Spectroscopies*. The fellow will be expected to attend at least one of the modules most relevant to his/her research project – the precise modules to be taken by the fellow will be agreed prior to the start of the fellow's training programme. In addition, a novel laboratory-based postgraduate module involving training in the industry standard *LabVIEW* interfacing and graphical programming environment has been established. This module will prove particularly beneficial to those students who have had little training in implementing modern computer-based laboratory measurement techniques or designing computerised experiments – a key feature of innovative nanoscience experimental work. The School also runs a number of courses related to safety issues in research and a short introduction to standard workshop techniques and practice. The former will be mandatory for all fellows.

The Nanoscience group runs a seminar programme where speakers from other universities and other Schools within the University of Nottingham give talks on current exciting (and largely interdisciplinary) research areas (see www.nottingham.ac.uk/physics/research/nano/seminars). We consider attendance at these seminars an important facet of a student's doctoral training. In addition, the group holds weekly meetings where each week a graduate student presents a short (10 minute) presentation on their work to the rest of the group. This makes an important contribution to developing both the clarity and quality of student presentations.

The University of Nottingham Graduate School Research Training Programme
Complementing the research project-specific training described above, all fellows will be expected to attend training courses provided by the University of Nottingham Graduate School. The UK Research Councils and industry have, over the past few years, emphasised the importance of providing postgraduate research students with a much broader range of research-related and transferable (e.g. written and oral presentation) skills. The University of Nottingham, via the Graduate School, responded to this need by initiating the Research Training Programme in October 1996. This University-wide programme is open to all postgraduate research students, providing courses in topics ranging from Research Management to Scientific Writing, Communication & Presentation Skills, and is now into its fifth year of operation. Visiting fellows will be expected to enrol for relevant modules. In addition, visiting postgraduates who did not have English as a first language would be required to have an IELTS score of 6.0 (or equivalent) or attend English language courses in the University's Centre for English Language Education.

Justification for number of early stage researcher man-months requested: The Nottingham group requests two 3 year researchers and a total of 24 man months funding to support visiting doctoral students. In addition to the time spent at the other host institutions (25%), each researcher will be expected to work with a very broad range of experimental techniques within Nottingham (see list above). Given the high levels of technical training required to carry out the experiments, and the necessity for similarly comprehensive complementary skills training, two 3 year early stage researchers represent the absolute minimum manpower required. We will also invite applications from doctoral students pursuing their studies in other member, associated or 3rd states to work on the *NANOCAGE* project for periods between 6 months and 12 months. We are particularly keen to receive applications from doctoral students working on related novel fullerene or nanotube systems.

Host 2: Forschungzentrum Julich, Germany (FZJ)
FZJ provides technical expertise and training in the following areas: *variable temperature and low temperature STM*, *cryogenics*, *UHV techniques*, *Monte Carlo simulations*, and *kinetic processes in growth and adsorption*.

This expertise complements that of the Nottingham group exceptionally well. In particular, low temperature STM and (inelastic) tunnelling spectroscopy measurements are core elements of the *NANOCAGE* research project. The additional stability of a low temperature - as compared to a room temperature - STM in terms of, for example, significantly reduced thermal drift, enables a wide variety of exciting experiments that are simply not feasible at higher temperatures. Among these are the following: (i) acquisition of single molecule vibrational spectra using inelastic tunneling spectroscopy, (ii) single molecule distortion (via tip induced compression), lateral and vertical manipulation of individual molecules, (iii) STM tip-assisted assembly of weakly adsorbed endofullerene assemblies (on, for example, passivated Si surfaces); (iv) elucidating the temperature dependent dynamics of the endofullerene molecule (through, for example, a study of the stochastic 'disassembly' of an STM-fabricated assembly as the temperature is slowly increased from ~ 4 K); (v) probing intramolecular dynamics through the acquisition of inelastic tunneling spectra across a (narrow) range of temperatures near 4 K.

In addition to their expertise in variable and low temperature STM, *FZJ* has a very strong track record in the study of kinetic processes on semiconductor surfaces (see Section B3). An important part of this work has been the use of Monte Carlo simulations to provide insights into the relevant diffusion mechanisms. Monte Carlo simulations will also be used in the context of the *NANOCAGE* project in order to elucidate the endofullerere-surface interactions via the estimation of quantities such as the molecular hopping rate and the associated diffusion barrier height. The parameters derived from the simulations will be directly compared to those measured using STM at variable temperatures. Due to the technically demanding nature of the experiments, FZJ has a similar requirement to Nottingham in terms of early stage researcher man-months. However, somewhat less time is requested for visiting researchers due to the necessity to ensure extended periods of research time are available on the single low temperature STM system available in the group.

Related Areas of Doctoral Training
In addition to the provision of technical skills training, FZJ will make strong contributions to the training programmes of early stage researchers through the organization of a *NANOCAGE* workshop on STM and tunneling spectroscopy methods. Julich runs an annual postgraduate school and therefore has particular experience in tailoring workshops to researchers' training requirements. Furthermore, complementary skills training in scientific presentation and communication for those researchers whose first language is not English or German will be carried out through FZJ language courses and via the presentation of research at internal meetings, national and international conferences.

Host 3:Computational Modelling group, National Microelectronics Research Centre, Ireland (NMRC)
NMRC brings extensive expertise in electronic structure and transport calculations to the NANOCAGE project (see Section B3). They will employ Hartree Fock and density functional methods to the study of the ground state geometry, electronic and vibrational properties, and total energy of both free and adsorbed endofullerene molecules. NMRC will interact closely with the experimental groups in the EST project - this will be facilitated by the exchange of early stage researchers between hosts. Note that although NMRC have previously studied both $N@C_{60}$ and $P@C_{60}$ as isolated molecules, NANOCAGE represents a significant broadening of their theoretical work with regard to both the complexity of the endofullerenes to be studied (eg $Ce@C_{82}$ and $Ce_2@C_{80}$) and the necessity to include a substrate or additional chemical groups bonded to the outer shell of the fullerene. The complexity of the calculations makes this a challenging early stage training project and funding for 2 three year fellowships is therefore requested. A slightly lower number of visiting researcher man months (12, as compared to Nottingham's 24) is requested due to the computationally expensive, and thus 'resource-hungry', nature of the calculations.

Host 4:Fullerene Group, Department of Chemistry, Queen Mary's, University of London, UK (QM)
The Fullerene Group is world-leading in the synthesis of novel fullerene systems (see Section B3). In addition to synthesis and purification using liquid chromatography methods, the group has a very strong track record in the use of NMR and ESR spectroscopies as characterisation tools. Early stage researchers will be trained in the synthesis, purification, and spectroscopy of the endofullerene molecules used throughout the *NANOCAGE* project. As the focus in the *NANOCAGE* proposal is on addressing and tuning the properties of endofullerenes whose synthesis is well-established within the QM group, a slightly lower amount of researcher man month funding is requested (one 3 year researcher and 6 man-months of visiting researchers). It is important to note, however, that the fullerene fabrication and spectroscopic expertise of QM represent important additions to the cross-disciplinary character of the early stage researcher's skills base.

B2.4 Impact of the 'NANOCAGE' Project on Nanoscience at National and International Levels

The NANOCAGE project will extend the worldwide state-of-the-art in both molecular electronics and fullerene science to encompass the understanding and control of the properties of atoms caged within adsorbed fullerenes. The host network assembled for the project represents a unique combination of expertise and research instrumentation/ infrastructure and, as such, there is particular potential for key breakthroughs: to date, no other group in the world has attempted to spectroscopically explore the properties of endofullerenes adsorbed on semiconductors.

B3 QUALITY/ CAPACITY OF THE HOSTS

In the following sections we outline the research and training track records of the four hosts comprising the EST network. A particularly important feature of the *NANOCAGE* project is the complementary and interdisciplinary nature of the host institutions' expertise. As described in Section B2, this will form an integral component of the training of early stage researchers. Hence, the complementary character of the hosts' expertise is highlighted in the following sections.

B3.1 Host 1 (co-ordinator): Nanoscience group, University of Nottingham (NOTTM)

A member of the elite Russell Group of research-driven universities, the University of Nottingham is a prestigious British higher education institution with the highest number of undergraduate applications per place in the UK. The University has over 22,000 students (originating from more than 100 different countries), 2,000 academic staff and an annual total income of €287M. The value of externally funded research contracts and grants for the 2001/2002 academic year was €124M . There are nearly 5,600 places in halls of residence and self-catering accommodation on or close to the main campus (where the Nanoscience group is located). The University has an extremely well-developed infrastructure for hosting students from outside the UK, co-ordinated by the International Office. A well-staffed Accommodation Office provides information and advice on accommodation for fellows who wish to live off-campus.

Nottingham Nanoscience Group: Infrastructure, Research and Training Track Record

The School of Physics & Astronomy in which the Nanoscience group is based provides a dynamic research environment with rapidly rising postgraduate student numbers and an annual research income of ~ €4.5M (the total value of active grants is approximately €15M). The Nanoscience group is housed in a suite of ten laboratories which have recently been refurbished (via national infrastructure grants totaling €750K) and contain an excellent equipment base comprising three UHV STMs, three air/liquid AFMs, and a low temperature (not UHV) tuning fork-based AFM. A novel UHV scanning near field optical microscope (SNOM)-AFM hybrid instrument is also under construction. The group is also pursuing the development of a near field Raman microscope. Furthermore, a high performance XPS/UPS system is available to the group for 12 weeks per year. The group was designated as a Marie Curie training site under Framework 5 and therefore the provision of high quality interdisciplinary research training within the group is recognised by the Commission.

The current composition of the Nanoscience group is as follows: four academic staff[†], four postdoctoral researchers (three non-UK nationals), 11 full time postgraduate students (of whom three are international students), and – at any given time – one or more Marie Curie fellows supported on a Fifth Framework Training Site contract. Over 80 papers (including a major invited review article on nanostructured materials [2]) have been published since the establishment of the group in 1995 and combined funding over that time has totalled over €4M. The group has been particularly successful in securing beamtime at national and international synchrotron sources. For example, the project coordinator (Moriarty) currently holds a UK EPSRC grant worth €1.05M whose focus is the application of synchrotron spectroscopies to the analysis of fullerene systems. Recent awards of beamtime at EU synchrotrons include 14 days at MaxLAB (Jan 2003) and 7 days at the ESRF (July 2003). The group's expertise with regard to synchrotron-based research has been recognised through Moriarty's appointment as Chair of the UK Synchrotron Users Surface Science specialist group, and the recent invitation to present a plenary lecture at the upcoming UK Synchrotron Radiation Users Meeting (Sept. 2003). Key research highlights of the group include: (i) Nottingham was the first group in the world to carry out controlled single molecule manipulation and positioning at room temperature [5], (ii) the elucidation of fullerene-silicon interactions [10-12], (iii) the construction of a specialised SPM controller [13], (iv) far from equilibrium pattern formation in nanoparticle systems [14,15], and (v) the synthesis of hydrogen-bonded molecular templates [16]. Indicators of the quality of this research include invitations to present talks at a considerable number of national/ international conferences.

Nanoscience in Nottingham: Strategy and Training

The Nanoscience group's success in appointing fellows on the Fifth Framework Training Site contract (NANONOTT) held since Mar. 2002 (3 fellowships awarded, with 3 applications pending) indicates that Nottingham is already seen as a particularly attractive host for training in nanometer scale science. A number of recent developments have further strengthened the nanoscience research base within the University. Nanoscience was identified as a research area of particular strategic importance and thus a *Centre for Nanoscience and Technology (CNT)* was set up in Dec. 2002. Closely aligned with

[†] Other lectureships in Nanoscience in the School of Physics & Astronomy have recently been advertised.

the objectives of the CNT, a recently established (Jan. 2003) University *Interdisciplinary Doctoral Training Centre (IDTC)* will contribute greatly to the quality of graduate training in the *NANOCAGE* network through the provision of taught modules in topical areas of nanoscience, training in research presentation and ethics, and cross-disciplinary integration of research projects. As discussed in Section B2, the University's Graduate School programme also plays an integral and essential role in ensuring the provision of high quality nanoscale science and nanotechnology training.

B3.2 Host 2: Institute of thin films and interfaces (ISG), Forshcungszentrum, Jülich (FZJ)

The status and quality of Forshcungszentrum, Julich (FZJ)

The Research Centre Julich (FZJ) is a German government laboratory employing 4200 staff who work on a broad spectrum of research topics. Of the 4,200 staff, approximately 1100 are research scientists, 400 are PhD students, 150 are undergraduates, and 350 are trainees. A particularly important feature of the research strategy of FZJ – and an approach closely aligned with the Commission's policies – is the development of cooperation and collaboration beyond the boundaries of particular disciplines. The total institutional funding income of FZJ in the last financial year was €230M with additional funding of €51M coming from sources such as public resources, the European Union, third-party funds from industry, and income from royalties. FZJ hosts more than 700 visiting scientists from over 50 countries each year and consequently *the Centre has particular experience and expertise in dealing with European (non-national) students.* As a large institution, facilities such as a guest house, free language courses, and accommodation services are provided. The Centre has a strong history of encouraging increased female participation in science including actively promoting its scientific training programmes to potential young researchers (including school leavers).

Institute of Thin Films and Interfaces (ISG): Research and Training Track Record

Dr. Voigtländer's group within the ISG has an extremely strong track record in the area of microscopic studies of nanostructure formation and growth in semiconductor systems. A particularly important component of the group's work has been the elucidation of the roles of kinetic processes and instabilities – in addition to thermodynamics – in the assembly of a variety of novel nanostructures [17-19]. This work has resulted in the publication of 20 papers in the last 5 years including two *Physical Review Letters* and an *Applied Physics Letter*. The impact of the Voigtlander group's work on the nanoscience and semiconductor research communities is clear both from the high number of citations per paper and the publication of an invited review article in *Surface Science Reports* in 2001.Particular research highlights include the contribution of a detailed understanding of the role of strain and surfactants in semiconductor growth [20], the observation and detailed explanation of the self-limited growth of Ge nanostructures on Si(100) [18], and the fabrication of 'magic number' islands on Si(111) [19]. International researchers play a central role in the group's research programmes: at present two Humboldt fellows (from Prague and Russia) and two Japanese guest scientists are employed in the Voigtlander group.

Although the primary experimental tool used throughout the Voigtlander group's work has been UHV STM, their research training expertise differs from and complements that of Nottingham (where scanning probe systems are also extensively used). This is because the work in Julich involves variable temperature, high temperature, and – most recently – low temperature STM measurements. In particular, a very recent unpublished result of particular significance to the *NANOCAGE* project has been the acquisition of single molecule (CO) vibrational spectra via inelastic electron tunneling in a LT STM. The Nottingham group does not have the appropriate equipment or requisite expertise to carry out variable/ low temperature STM and LT tunnelling spectroscopy. *The Julich group's complementary expertise in low temperature STM and kinetic processes will play a vital role in the NANOCAGE project***.** As discussed in Section B2, tunneling spectroscopy, STM imaging, and molecular manipulation at low temperature are techniques that are at the very heart of the *NANOCAGE* research programme and are essential for the success of the project. Furthermore, LTSTM and, in particular IETS are increasingly important tools in nanoscience and it is thus essential that early stage researchers are trained in these techniques.

B3.3 Host 3:Computational Modelling Group, National Microelectronics Research Centre (NMRC)

The status and quality of the National Microelectronics Centre, Cork, Ireland (NMRC)

NMRC is Ireland's largest research centre and was established to provide the infrastructure necessary to assist the development of microelectronic and microsystems industry in Ireland. The research undertaken at NMRC is divided into four areas: Microtechnology, Nanotechnology, Bio/ICT, and Photonics. During 1999, the Irish government designated the NMRC as the National Nanofabrication Facility with a subsequent investment of over €30M for nanotechnology equipment. *The NMRC has supported research at a European level as a large scale facility (LSF) under the 4th and 5th Framework programmes and as Host Site for the 5th Framework Marie Curie Fellowships programme.* As Ireland's largest engineering postgraduate school, the NMRC hosts over 60 postgraduates with typically greater than 40% of these students being non-Irish nationals. The support infrastructure for hosting European and international students is well established. Students take part in a taught component presented by NMRC staff for both the Masters and PhD degrees and the NMRC's state-of-the-art fabrication and computational facilities are available for all postgraduate projects. NMRC has established partnerships with University College Cork academic departments to allow students to pursue degrees in engineering or science, as appropriate to their specific research topics.

Computational Modelling Group: Research Track Record

The Computational Modelling Group consists of five permanent researchers, six postdoctoral researchers, and six to eight postgraduate students. Research within the groups spans continuum modelling of thermomechanical problems, computational materials science, and electronic structure theory. The group works with major companies such as IBM, Motorola, Philips, and Infineon on basic research for IT. The co-ordinator of the group (Greer) is chairman of the Theory & Modelling Working Group of the European Union's Nanoscale Information Devices research inititative and has acted as a consultant on future research directions in nanotechnology at national and European levels. He has also acted as a special issue editor for Materials Science in Semiconductor Processing, Microelectronic Engineering, and Computational Materials Science, and is on the editorial board of Microelectronic Engineering. Greer has also acted as a reviewer for the European Union, Enterprise Ireland, and the European Science Foundation, and has successfully supervised Masters and PhD students for both science and engineering degrees. Furthermore, he has acted as an external PhD examiner for a number of European universities. He is a senior member of the IEEE, and a member of both the Institute of Chemistry of Ireland and the German Physical Society. Key research highlights include the determination of the electronic structure of isolated (i.e. non-adsorbed) $N@C_{60}$ and $P@C_{60}$ molecules [4a, 4b] and the study of electron transport in molecular wires [21].

Computational Modelling Group: Training Provision

All postgraduate researchers are fully integrated into the Computational Modelling Group at NMRC. The NMRC operates to an ISO 9001 standard, and all group monthly meetings, maintenance of research notebooks, simulation documentation and files are handled according to ISO procedures. This sets the minimum standard for research supervision and documentation. All postgraduate students must comply with the requirements of their host department and NMRC for postgraduate study, including: submission of project plans and periodic updates, satisfactory completion of the taught component of their degree programme (where required), mid-term review by an external examiner, final oral examination and submission of thesis. Supervisors, in addition to ISO requirements, are required to act according to the "Guidelines for Postgraduate Supervision" as determined by the University College Cork inter-faculty committee. Postgraduate students work closely with postdoctoral and permanent research staff, and a lively environment for discussion and debate exists. Supervisors meet frequently with postgraduate students on a weekly, if not daily, basis.

Queen Mary University of London

B3.4 Host 2: Fullerene group, Department of Chemistry, Queen Mary, University of London (QM)

Queen Mary and Westfield College is a major component of the University of London, the United Kingdom's largest university. The fullerene group (headed by Dr. John Dennis) within the Department of Chemistry is a world leader in the isolation and spectroscopic characterisation of fullerenes and endohedral fullerenes. This group possesses two Japan Analytical Industry LC908 recycling High Performance Liquid Chromatography machines. Coupling each of these machines to fully reparative (20 mm diameter) Cosmosil 5PYE columns gives the group the most efficient HPLC capability dedicated to fullerene research outside Japan. Within the Department of Chemistry, the fullerene group has excellent access to a high-resolution ESR spectrometer and a 600 MHz multinuclear NMR spectrometer for temperature-dependent characterisation of both diamagnetic and paramagnetic fullerenes, endohedral fullerenes, and carbon peapods. John Dennis received his D.Phil. from the University of Sussex (1993), and subsequently has received internationally competitive research fellowships from the Australian Research Council, the Japan Society for the Promotion of Science, and the Humboldt Foundation. In 1999, he was appointed as a lecturer in physical chemistry at Queen Mary and Westfield College, University of London. He has published over 50 highly cited primary reefed journal articles (*average of ca. 60 citations/paper*), and *was the first to purify 15 of the 19 fullerenes so far completely isolated, and ca. ¼ of all endohedral fullerenes (including the only successful isolation of the nitrogen-containing endohedral fullerene* iNC_{60}*).*

B4 MANAGEMENT AND FEASIBILITY

B4.1 Organisational Management

A Management Board will be established comprising the four group leaders (namely, Moriarty, Nottingham; Voigtlander, Julich; Greer, NMRC; Dennis, QM) and will be chaired by the co-ordinator (Moriarty). The Board will be responsible for both co-ordinating the overall progress of the project and ensuring that each early stage researcher follows the appropriate training programme. In particular, the board will take decisions related to the following issues:

- Coordination of research training programmes: ensuring that appropriate levels of technical and complementary skills training are reached by each student.
- Ensuring appropriate levels of publicity for vacancies and for key research results.
- Financial and administrative organisation of the EST project.
- Management of project finance, legal issues and any conflicts which may arise.
- Coordination and organisation of information interchange and transfer for all cross-host meetings.
- Scheduling and organisation of workshops and 'mini conference'.
- Communication with the Commission, coordination of legal issues.
- Management of aspects of dissemination, exploitation and IPR
- Promotion of societal issues.

In addition, members of the management board will be designated specific responsibilities. These are outlined in Chart B4_1 below and discussed in detail in the following sections.

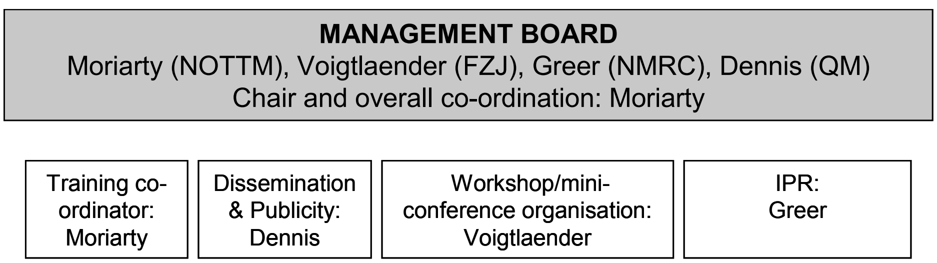

Chart B4_1. *Overview of management board and responsibilities of members*

Suitability of participants

All of the participants have experience of managing project based, goal-oriented research and are highly successful in their technical fields (as discussed in detail in Section B3). They are therefore well suited to these tasks and have a proven track record of commitment to long term research.

B4.2 Practical Measures to Implement the Training *(see Chart B4_2 on following page)*

The chair of the Management Board will also act as Training Co-ordinator. Although another member of the Board could be appointed as Training Co-ordinator we believe that this would substantially add to the administrative burden. Following recruitment of an early stage researcher, the supervisor in the appropriate host institution will be required to contact the Training Co-ordinator to discuss the personal career development programme planned for the student. The Training Co-ordinator will in turn contact the other members of the management board to confirm the proposed career development plan (see Chart B4_2).

The progress of individual early stage researchers with regard to formal University or Institution procedures (e.g. completion of formal monthly meeting reports, as is required of all Nottingham graduate students) will be the responsibility of individual supervisors in each of the host institutions. However, at the end of each year of the project two members of the board (the primary supervisor and one other) will assess the (mandatory) end of year reports for all early stage researchers employed on the *NANOCAGE* project. Successful completion of the end of year report will be essential in order for a student to progress to the next year of their training programme. In the event of poor student performance, the Board Chair will liaise with the Board members and the Commission to minimise the impact on the research programme. The Board will therefore play an important role in quality control, ensuring that the early stage researchers' scientific competence reaches an appropriate level. As noted in Section B2, the students will be formally assessed on both their written and their oral end-of-year reports. The oral report will be delivered as part of a ½ day meeting held at the end of each of the workshops in Years 1 – 4 of the project. Student presentations during the one day mini-conference in Year 3 of the project will also be formally assessed by the board members.

Facilities provided for the Fellows

All appointed fellows will be allocated a desk in a dedicated postgraduate office with access to a telephone. Each fellow will also have access to either a desktop or laptop personal computer with appropriate data analysis, word-processing and presentation software and internet facilities (e-mail, world wide web). A standard introduction package related to research and training in the 'NANOCAGE' network will be prepared by the coordinator and mailed to all successful applicants prior to the start of their fellowship. This will be in addition to the information on postgraduate studies provided by the Graduate School/ Office of the relevant host.

Research co-ordination and strategy for ongoing project assessment

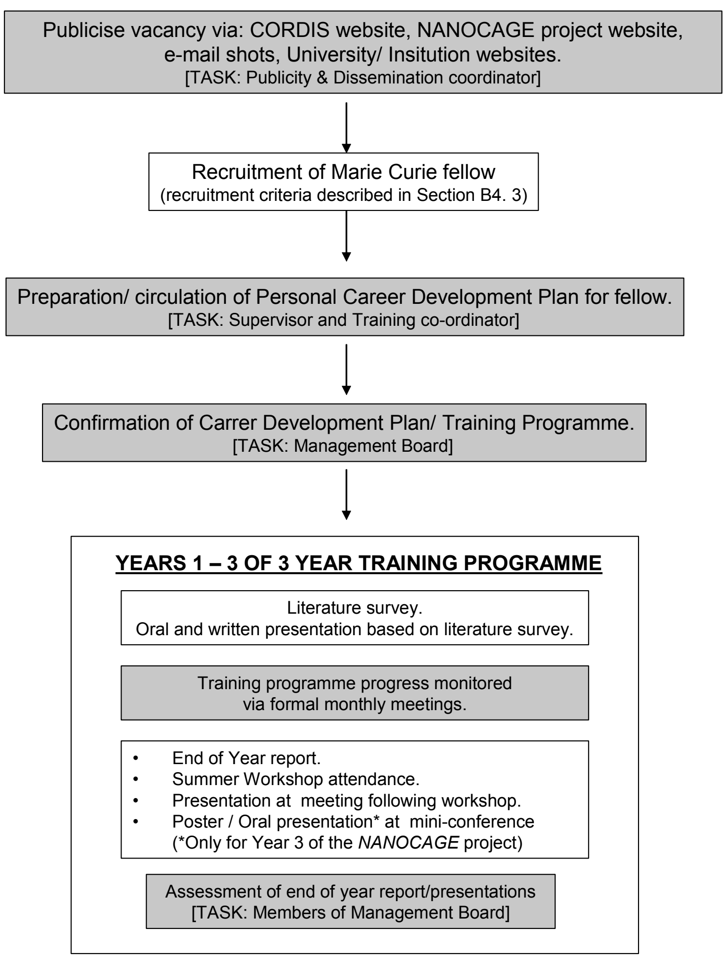

Chart B4_2*: A sample organization and monitoring strategy for a 3 year early stage training project.*

A particular role of the Management Board will be the regular re-assessment of project goals in the light of progress within the project as well as the inter-relationship of the deliverables which have been identified. It is possible that estimated timetables for progress for different aspects of the programme may depart from the actual times required for particular activities. A particular concern would be progress which is slower/faster than anticipated which will result in a knock-on effect to associated aspects of the project in terms of both training and research objectives. Also of significance will be the possibility that some processes developed within the consortium might offer sufficient enhanced prospects of breakthrough that might lead to a revision of the priorities of the project. The Management Board will provide a forum for the debate of such issues.

Meeting Timetable

To effectively co-ordinate the project the following formal meetings will be held:

- Management Board video-conferencing or web-based communication (every 3 months)
- Board meeting following Summer workshops at the end of Years 1 - 4.

These formal meetings will of course be supplemented by rather more frequent inter-host communication which will be via e-mail and telephone. Conflicts of views between different partners regarding the appropriate response to any situation which might arise will be settled by Management Board debate and, if necessary, voting.

Monitoring and Reporting Progress: Access to Supervisors
A strategy introduced by the Graduate School in the University of Nottingham to provide effective monitoring of student progress is to hold formal, *documented* monthly meetings between the supervisor and the postgraduate researcher. These meetings are of course not the sole contact mechanism – indeed, for the training hosts comprising the *NANOCAGE* network it is most likely that students will generally have the opportunity to consult with the research supervisor on a daily basis. However, the provision of a documented meeting at the end of each month is a useful mechanism for the supervisor to ensure that the early stage researcher's project is progressing satisfactorily and, from the researcher's point of view, to raise in a formal setting any issues that might concern them. We propose to adopt this scheme in order to monitor research and training progress within the *NANOCAGE* project. As the project involves four hosts with substantial transfer of researchers between institutions, these documented meetings will be an essential component of project management. In the event of unsatisfactory student progress at the end of Year 1, the monthly report documentation will be considered at the Board's annual meeting.

Research progress will also be monitored via meetings of early stage researchers, postdoctoral researchers associated with the project, and supervisors following the Summer workshops. (Note that the postdoctoral researchers will be funded via other national and/or EU schemes). These meetings will involve the presentation of early stage researcher reports on work carried out to date. Furthermore, the 'mini conference' in Year 3 of the project will not only act as a useful training platform to enhance the complementary/transferable skills of the early stage researchers employed on the *NANOCAGE* contract, but it will also serve to focus the direction of the network on the key outstanding issues remaining for the final year of the project.

B4.3 Recruitment

Positions will be advertised in high impact scientific journals such as *Science* and *Nature*, on the *CORDIS* website, on the host institutions' websites, on the *NANOCAGE* project website, and via e-mail 'shots' to colleagues worldwide. It is interesting to note that applicants for the current Marie Curie positions within the Nottingham group (i.e. for the 5th framework *NANONOTT* training site) have largely been made aware of the vacancies either through the *CORDIS* website or via the group's homepage. Particular effort will therefore be expended in constructing a user friendly *NANOCAGE* project website. This will be the responsibility of the Publicity & Dissemination co-ordinator (Dennis, QM).

The choice of fellows will be dictated by the following criteria:

- Quality – a key criterion must obviously be the academic quality of the candidate;
- Academic references;
- Interdisciplinarity – we are particularly keen to attract students whose first degree is not in a physics-based discipline;
- Gender balance – we will promote the societal objectives of Framework 6 through the monitoring and promotion of gender equality via recruitment within the project. It is worth noting that of the three Marie Curie fellows thus far appointed on the Fifth Framework training site contract in Nottingham, two have been female and their 1st degree is in a discipline other than Physics (Chemistry, Medical Bioengineering).

B4.4 Dissemination and Publicity

Effective dissemination of the output of the project will also be realised through the *NANOCAGE* web page which, in addition to being used for recruitment purposes, will act as a bulletin board for project activities as well as a gateway for further information such as scientific publications. Links on the website to the CORDIS website, the Marie Curie Actions homepage, and the Marie Curie Fellowship Association will be provided. The web site will also act as a focus for attracting SMEs who might potentially be interested in commercialising appropriate outputs of the project.

Final versions of early stage researcher end-of-year reports will be posted on the website but initially made available only to the four members of the management board. Following publication of any research results related to the reports, they will be made generally publicly available. The web-based availability of end-of-year reports will, in addition to the supply of the research deliverables detailed in Section B2, provide an important mechanism of evaluating the overall progress of the EST project in terms of its training objectives.

We will target high impact factor journals such as *Nature, Physical Review Letters, Physical Review B, Applied Physics Letters, J. Chem. Physics,* and *Nanoletters* when publishing the results associated with the project. We find that the *Virtual Journal of Nanoscale Physics* is an effective medium in which to promote exciting nanoscale research – publication in the afore-mentioned journals tends to ensure inclusion in the Virtual Journal (a number of the publications of the host institutions have previously been selected for inclusion). Early stage researchers will be actively encouraged to present their results at high profile international conferences such as the international STM and NANO meetings, ECOSS, EPS meetings, and the annual American Vacuum Society (or MRS) conference. Furthermore, results will be submitted to appropriate nanoscience and condensed matter-related national conferences, workshops and meetings. The Marie Curie EST programme and the appropriate contract number will be cited in all publications and presentations.

Each of the institutions involved in the *NANOCAGE* project makes particular efforts to communicate the importance and excitement of their research to the general public. For example, the overall coordinator (Moriarty) has given a number of public lectures on the topic of nanoscience for the Institute of Physics in the UK and recently delivered a series of invited lectures in a number of key Irish higher education institutions for the Institute of Physics in Ireland. Furthermore, all host institutions in the *NANOCAGE* project will continue to host open days and deliver lectures for schoolchildren, schoolteachers, and the general public.

B4.5 Management of IPR

An IPR officer (Greer, NMRC) will co-ordinate aspects of the project related to IPR. Note that Greer has particular expertise related to interactions with major IT and microelectronics companies and is thus well versed in issues related to the protection of intellectual property. In addition, the host institutions comprising the EST network each have Research Support Offices with which the IPR officer will liaise to ensure appropriate protection of intellectual property arising from the project.

B4.6 Financial management plan

The funds arising from the project will be managed centrally by the Coordinator to ensure effective control and timely disbursement. To further ensure optimum timeliness of the distribution of funds, the Coordinator will forward the relevant sums in respect of Fellows as and when they are appointed. The 3% of total EU contribution to the project in respect of management costs will be made available to the partners, up to their ceiling amounts, on receipt by the Coordinator of fully documented eligible expenses such as audit certificates etc., thus ensuring further control and monitoring of this important budgetary element. Any remaining funds, in addition to the Coordinators' own share, will be applied to the project by the Coordinator to ensure an effective central financial management regime and smooth running of the project to the ultimate benefit of the Commission and the partners.

The contribution to the research expenses of the Host will be managed centrally to ensure control and eligibility of expenses applied fairly across the partnership, and will be made available upon recruitment. Expenses related to the recruitment of researchers by partners may of course be distributed in advance depending on requirements. Similar provisions will apply to those expenses unique to multisites. Overhead will be claimed by all partners on actual expenditure only, in the usual way. In all cases the equitable distribution of funds will be agreed upon by the Management Board in compliance with all contractual obligations and proper accounting conventions.

B5 RELEVANCE TO THE OBJECTIVES OF THE ACTIVITY

B5.1 Benefit of proposed training project to European research integration

Nanoscience is a rapidly expanding field at the very heart of scientific research across the world. In the context of the European Research Area (ERA), nanotechnology is of exceptional importance in that it forms one of the primary disciplines in which Europe plays a leading role. Not only does nanoscience offer exciting opportunities in fundamental basic science (arising largely from the convergence of traditional disciplines that the field represents), but the Commission recognises the potential for nano-related innovation, applications, and economic opportunities across many industrial sectors. To translate the European lead in fundamental nanoscience into a competitive advantage for European industry (in particular in the ICT arena), two key objectives must be achieved[†]: the creation of an RTD-intensive nanotechnology-related industry, and the promotion of the uptake of nanotechnology in existing industrial sectors.

Attraction of talented early stage researchers into nanoscience via high quality, exciting, and innovative projects will play a central role in fulfilling these two objectives. Provision of internationally leading training is of tantamount importance. We believe that the *NANOCAGE* project described in this proposal soundly addresses both these issues. Furthermore, assembling a network of hosts focussed on a topical problem in nanoscale science – as is again the case for the EST project we propose – is an integral component of structuring the ERA and promoting the dissemination of research results throughout Europe. This, in turn, will enhance the position of European research in an area where it is already a world leader.

It is important to note that the proposed EST project builds on previous collaborative work between a number of host institutions comprising the training network. In addition to national collaborative links between NOTTM and QM, the Nottingham Nanoscience group was previously involved in a Fifth Framework RTN (*Quantum Information Processing Device using Doped Fullerenes (QIPDDF*)) with Greer's group in NMRC. Although the proposed *NANOCAGE* project involves a similar materials system (fullerenes), the research carried out under the *QIPDDF* contract had significantly different research objectives and deliverables. Furthermore, the training components associated with *NANOCAGE* are radically different from those under the QIPDDF contract. In particular, the *NANOCAGE* EST programme not only involves a much broader training programme (in terms of the technical and complementary skills each researcher will acquire) but places particular emphasis on the provision of cross-disciplinary training and the integration of experimental and theoretical methods.

The continued collaboration of the NMRC and Nottingham groups is a key benefit of the proposed training project both in terms of value to the individual host institutions and with regard to the improved structuring of the ERA. Broadening of the NMRC-NOTTM collaboration to include close links with QM and FZJ similarly helps realise the Commission's strategic goal of developing increased integration under the ERA. We are also confident that the inter-host links developed within the *NANOCAGE* project will, as is demonstrably the case for the previous EU contract noted above (and indeed is true of many other European collaborations in which the host institutions are involved), promote extensive continued future collaboration. In particular, we are hopeful that the EST multi-host project we propose will lead to significant prospects for the submission of future collaborative European grant proposals.

B5.2 Benefit of proposed training project to early stage researchers

The *NANOCAGE* project training objectives are specifically focussed on the provision of:

- proficiency in a broad range of specific nanoscientific and nanotechnological techniques;
- the structured development of complementary/ transferable skills such as written and oral communication, team-working, and time management.

As stressed a considerable number of times throughout this proposal, a combination of cross-disciplinary and multi-faceted training in nanometre scale science and technology represents a particularly attractive skills base for an early stage researcher to acquire. There is a strong need for the training programme we propose, due to the ever-increasing reliance of European

[†] *EC proposal for Council decision, Specific Programme implementing FP6 COM(2001)279*

industry and academia on research tools such as scanning probes, density functional theory, high flux X-ray spectroscopies, and novel synthetic/ physical chemistry methods. The NANOCAGE project not only involves a very significant proportion of the gamut of modern nanoscience tools and techniques available to a scientist, but will also give early stage researchers the opportunity to develop novel approaches to a number of problems at the forefront of nanoscience (for example, exploiting the electronic state of a caged atom in a prototypical monomolecular device).

The development of expertise within the multi-host environment we propose will not only enable each early stage researcher to develop scientific collaborations early in their career but will promote an awareness of the key significance collaborative efforts play in the development of cutting edge science. As co-ordinators, we are hopeful that this awareness will in turn lead to a willingness of early stage researchers to foster and develop collaborative work in their careers beyond the EST project. Fostering European collaboration is of course especially important for researchers from less favoured nations. We are also confident that the exciting scientific project, the multi-host environment, and the opportunity to carry out cross-disciplinary research involving an intermix of experiment and theory will each serve to attract talented researchers into a research career in nanometre scale science.

B5.3 Benefit of proposed training project to host institutions

Section B5.1 touched on a number of significant benefits that the proposed training project will provide for the hosts in terms of collaboration within the ERA. We both reiterate those benefits in the following list and include a number of other key advantages associated with the training project.

- Development of new collaborations and strengthening of existing collaborative links;
- Broadening of the instrumentation and expertise base, significantly enhancing the research and training opportunities available to each host;
- Integrating experimental and theoretical research via inter-host mobility of early stage researchers;
- Early stage researcher training within multihost networks provides a highly qualified pool of postdoctoral researchers in nanoscience;
- Solving a complex, leading edge problem in nanoscience and thus enhancing the scientific reputation of the hosts (which, in turn, will stimulate further collaborative ventures);

B5.4 Contribution to international recognition of training programme/ qualification.

The integration of research training within a multi-host project, as we propose, is an important stepping stone towards the development of consistency in the standards associated with the award of PhD across Europe. This goal is not unrelated to the Bologna declaration which is particularly concerned with *"the readability and comparability of European higher education degrees worldwide",* noting that these *"should be enhanced by the development of a common framework of qualifications, as well as by coherent quality assurance and accreditation mechanisms"*. We believe that the project we propose will produce high profile research results which, when disseminated to the community through publication in high impact factor journals and presentation at key international conferences, will play a substantial role in contributing to international recognition of the training programme.

B6 ADDED VALUE TO THE COMMUNITY

The 3rd *European Report on Science & Technology* † notes that 2.14 million graduates and PhDs were conferred in Europe in 2000 as compared to 2.07 million in the US, and 1.1 million in Japan. However, fewer researchers are employed in Europe, there is less investment in research and development (R & D), and the so-called 'brain drain' of qualified, talented postdoctoral researchers and graduate students from Europe to the US continues to increase. As pointed out by Research Commissioner Philippe Busquin, "*increasingly, our researchers look first to the US before considering what is available for them here in Europe*". Although, as pointed out in earlier sections of this proposal, Europe currently holds a leading position in nanoscience-related research, it is essential that the objectives of the ERA given below (and taken from the *European Research Area* website at *http://europa.eu.int/comm/research/era/index_en.html*) are met if this position is to be maintained and strengthened. In particular, the eventual 'conversion' of nanoscience-related basic research into applied R & D in the ICT sector will require these (and other) objectives to be met. For each point listed below we describe how the *NANOCAGE* proposal we propose meets the particular objective of the ERA.

- *Stimulating and supporting joint activities at national or regional level, as well as among European organisations: development of a common knowledge base*

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NANOCAGE involves not only national collaboration (QM and NOTTM) but collaborative activities spanning 3 member states (UK, Ireland, and Germany). The project both builds on previous research links (NOTTM-NMRC, NOTTM-QM) and involves the establishment of a wholly new collaborative effort between FZJ, NOTTM, QM, and NMRC. The four host training scheme proposed contains a combination of researchers which represents a 'critical mass' with respect to the research objectives of the project.

- *More abundant and more mobile human resources involving the introduction of a European dimension to scientific careers*

For the reasons outlined in Section B5, we have specifically designed the research training programme to ensure considerable mobility of early stage researchers between the host institutions. We are confident that the collaborative links between the host institutions in the training programme we propose will bolster the willingness of early stage researchers to maintain European mobility and to foster strong European collaborations in their own research careers. Furthermore, we are keen for researchers from less favoured areas of the EU to apply for early stage researcher positions and will actively encourage students from these areas to apply.

- *More prominence to the role of women in research*

Female scientists are unfortunately still under-represented in key scientific and research positions†. We will strive at all times to maintain an appropriate gender balance and, as described in Section B4, female participation will be actively encouraged with regard to recruitment. Particular attention will be paid to issues related to maternity leave and family mobility allowance. We will encourage all fellows to join the Marie Curie Fellowship Association – this will provide a useful pathway for female researchers to influence the direction of the Marie Curie programme. In particular, the cross-disciplinary nature of nanoscience provides an important pathway by which female early stage researchers might be recruited. It is noteworthy that two out of three of the Marie Curie fellowships awarded by the Nottingham group to date have been to female researchers in other disciplines (Chemistry and Biomedical Engineering). Furthermore, the synchrotron-based programme of research carried out by the NOTTM-QM collaboration has been driven by two exceptionally talented female researchers: Dr. Karina Schulte, a postdoctoral associate of Dutch nationality, and a graduate student, Ms. Mito Kanai (of Japanese nationality).

- "*Need for more basic research contributing to innovation in the long run*"

This objective is of particular relevance to the *NANOCAGE* project which, although largely involving fundamental, basic research, has particular significance to applied nanoscience due to the focus on the electronic and electrical transport properties of novel molecular units.

† http://www.cordis.lu/rtd2002/indicators/

- *Improving the attraction of Europe for researchers from the rest of the world.*

  We are of the opinion that this objective is best addressed by the provision of high quality training programmes which involve a variety of institutions focused on an exciting, novel, and intellectually challenging research project. The *NANOCAGE* project fulfils this role. It is also firmly based in an area in which the EU is world-leading. A particularly important element of the training programme we suggest is the high degree of inter-host mobility, leading to enhanced multidisciplinary and cross-boundary (eg experiment/theory) training for early stage researchers. Similarly, the broad range of complementary skills training makes a strong contribution to the attractiveness of the project.

- *Need for improved marketing of research to motivate students to invest in scientific careers.*

  The *NANOCAGE* EST project incorporates an exciting and novel research programme in cutting edge nanoscience. In our experience, web-based advertisement of research and training positions is a particularly effective method of attracting students and personnel. Particular effort will therefore be expended on the construction of a user friendly, attractive, and functional website related to the project in order to advertise vacancies and to disseminate key results related to the project. Vacancies will also be advertised in leading international journals (*Nature, Science*).

- *Stimulating young people's taste for research and careers in science*

  We are hopeful that the spectrum of workshops, graduate courses, inter-host activities, and conferences which form a core element of the training programme we propose will provide a stimulating scientific training environment. Furthermore, although all early stage researchers will receive high levels of supervision and support (see Section B4), we will strive to ensure that they have the opportunity throughout the training programme to suggest and follow (approved) lines of research in which they have a particular interest. This is particularly important from the point of view of 'ownership' of a particular scientific project – it is important that the student feels that they are making an important contribution to the progress of the research. Following a research problem from the formulation of the question to the derivation of a detailed understanding of the underlying science is a large component of what makes scientific research a deeply satisfying career option: if we are to ensure the progression of graduate students to long-term research careers, this component of the early stage training process should not be neglected.

B7 PREVIOUS EU PROPOSALS AND CONTRACTS

Nanoscience group, Nottingham (NOTTM)

NANONOTT, Marie Curie Training Site Host contract HPMT-CT-2001-00407.
Start: October 2001. End: September 2005

SUSANA, Fifth Framework 5 research training network contract HPRN-CT-2002-00185 (coordinated by Dublin City University. Start: September 2002. End: March 2006)

NANOSPECTRA, Framework 5 research training network contract HPRN-RTN2-2001-00311 (coordinated by ISEN, France). Start: September 2002 End: March 2006)

QIPD-DF, IST-1999-11617 (coordinated by Maynooth College, Ireland). Start: January 2000. End: March 2002.

Computational Modelling group, National Microelectronics Research Centre (NMRC)

Nanoscale Integrated Circuit Engineering (NICE), IST-1999-29111, 01-Aug-2000 to 29-Feb-2004

QIPD-DF, IST-1999-11617, 01-Jan-2000 to 31-Dec-2001

Read Out of Single Spins (ROSES), IST-2001-37150
01-Jan-2003 to 31-Dec-2004

ATOMCAD , HPRN CT-1999-00048, 01-Feb-2000 to 31-Jan-2004

Marie Curie Site Development Host: Microelectronics Research Site at NMRC, HPMT-2000-00091

Institute of thin films and interfaces (ISG), Forshcungszentrum, Jülich (FZJ)

Application for FP6 Network of Excellence (*Dynano*) pending.

B8 OTHER ISSUES

- *Ethics*

Although supposed potential ethical issues related to nanotechnology have recently been discussed in the popular scientific press – for example, the use of 'nanobots' or 'assemblers' to direct and control biological processes – these issues remain at present firmly within the realm of science fiction[†]. There are no ethical concerns related to experimental protocol or sample synthesis within the proposed early stage training project.

- *Safety*

Safety issues include the use of cryogenic liquids, high voltages (particularly those associated with ultra high vacuum ion pumps which are typically of the order of 5 – 7 kV), X-ray sources (both in the host institutions and, more importantly, at European synchrotrons), lasers (e.g. those used for Raman spectroscopy), and chemistry laboratory methods. Safety training and associated protocols are in place within the host institutions and a fellow will not be permitted to commence their research training programme without first completing the relevant safety courses and submitting the appropriate documentation. Particularly stringent safety procedures are associated with research work at synchrotrons.

- *Gender balance*

We will strive to make a strong contribution to redressing the gender balance in science. As noted in Section B6, the Nottingham group has recently had considerable success in recruiting highly talented female graduate students, postdoctoral researchers, and Marie Curie fellows and we are keen to build on this success. All fellows (whether male or female) will be encouraged to join the Marie Curie Fellowship Association (MCFA) which – as also noted in the preceeding sections – provides a forum for debate on a range of scientific and societal issues including the issue of female participation in science. For example, during the Fifth Framework programme the MCFA played a pivotal role in disseminating information related to a European Commission conference whose goal was to establish links with networks of women scientists and to sustain and optimise the networking efficiency (see the MCFA website at http://www.mariecurie.org/, and, in particular, http://www.mariecurie.org/src/press/ womensciencereport.html)

- *Dissemination and the Public Perception of Science*

A user-friendly, informative and aesthetically pleasing website will be used to disseminate information not only to the nanoscience research community but to the general public. Each of the host institutions involved in the NANOCAGE project is involved in schemes to ensure more effective communication of scientific research to the general public. (Indeed, the UK research councils recently introduced a specific funding mechanism for precisely this purpose). For example, the Nottingham group is involved in a number of University and national schemes which are dedicated to explaining exciting areas of state-of-the-art research in higher education institutions to schoolchildren/ schoolteachers. These include programmes aimed at encouraging students in local schools to consider careers in science. In addition, the School of Physics and Astronomy will host an Institute of Physics (UK) *Physics Update* course in July 2003. These courses make schoolteachers aware of recent developments and innovations in University teaching and research.

The project coordinator (Moriarty) has given general talks on Nanoscience at previous Physics Update events, to A-level (secondary school) students, and at University open days. Similarly, FZJ has a strong history of promoting its scientific training programmes to high school students and provides a comprehensive programme of vocational training. Both the University of London (QM) and NMRC also make strong efforts to promote their scientific research to the general public. Throughout the duration of the *NANOCAGE* project (and beyond), we will ensure that significant efforts are made in communicating key research breakthroughs to the public. This may involve the generation of press releases and we will liaise with the host institutions' respective Research Support Offices as to the protocols involved. (The co-ordinator has some experience of liasing with press offices as the Nottingham group's work has been featured on BBC Radio 4, BBC Radio 5, and in the national press).

[†] For a detailed and convincing rebuttal of many of the more outlandish claims associated with nanoscale science and technology, see the September 2001 edition of *Scientific American*.

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