Project No. FP7 – 212348

NFFA

Nanoscience Foundry and Fine Analysis

D3.1

Design of the NFFA Infrastructure

Work Package	**No.3**
Work Package Title	**Design study of NFFA-RI centres, technical layout of instrumentation and tools**
Activity Type	**RTD**
Lead Beneficiary	**1 CNR-IOM**
Estimated P/Ms	**15**
Nature	**Report**
Dissemination level	**Public**
Delivery Date	**Contractual M30 Actual M32**
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Delivery Slip

	Partner/Activity	Date	Signature
From	CNR-IOM	30/01/10	Tormen
Reviewed by	PSI	31/01/10	Gobrecht
Approved by	COORDINATION BOARD	31/01/11	All

Document Log

Issue	Date	Comment	Author
1-0	30/01/10	Deliverable first version	Tormen
1-1	31/01/10	Check first version	Gobrecht
2-0	09/12/10	Inclusion of theory part	Fabris
2-1	13/12/10	Approved upon addition of executive summary	CB
2-3	12/01/11	Consistency check	Rossi, Africh, Orani
2-3	18/01/11	Modifications requested by AC&SP	Sartori, Africh

Document Change Record

Issue	Item	Reason Change

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Deliverable D3.1: Design of the NFFA Infrastructure

1. INTRODUCTION

1.1. Purpose of the document

The purpose of this document is to describe the general aspects of the NFFA infrastructure, which will represent the European platform for promoting the scientific understanding and the technological exploitation of nanoscience to unprecedented levels.

More specifically, the document deals with the objectives and main constructive criteria to be adopted for the realization of the EU distributed infrastructure of Nanoscience Foundry and Fine Analysis centres.

1.2. Application Area

The targets of this document are the members of the NFFA Project, the EC Project Officers, and the general public.

1.3. References

Description of Work (DoW). See at web site:
http://www.nffa.eu/UserFiles/file/Annex_I_DoW.pdf

The design study is based on an effort of imagination aimed at forecasting the needs and the challenges that scientists in the domain of nanoscience and nanotechnology will have to face by 2020.

The exercise of extrapolating the future emerging needs in nanoscience and nanotechnology is supported by the knowledge of the present state of the art available in the NFFA consortium, and stimulated by the expectations and desiderata of scientists presently working with the edge-cutting techniques in different nanoscience domains.

The information shared by NFFA partner facilities was obtained during brain-storming sessions and in discussions with representatives from several other institutions in Europe and USA.

In particular the DoE Nano-centres in Berkeley, Brookhaven, Argonne and Sandia were visited and analyzed in their structure and operation as reference facilities in a context of research that is nevertheless quite different with respect to the European Research Area.

1.3.1. Objective of Work Package 3

The Objective of WP3 is the design study of NFFA-RI centres, the technical layout of instrumentation and tools.

1.3.2. Description of work broken down into tasks

The following tasks are defined in WP3:

T3.1) Design study of the overall infrastructure: experimental and theoretical facilities

T3.2) Design study of a nanolithography station within the facility

T3.3) Design study of user-oriented material growth facilities

T3.4) Design study of user-oriented metrology facilities

T3.5) Design study of a molecule and nano-particle manipulation lab

T3.6) Design study of nano-bio labs

T3.7) Assessment of the possible contribution of existing facilities that could be integrated in NFFA-RI

2. EXECUTIVE SUMMARY

This deliverable within the workpackage 3 “Design study of NFFA-RI Centres, technical layout of instrumentation and tools” describes the basic elements of the laboratories to be incorporated in future NFFA centres. The planned NFFA-RI Centres, organized in a network of three to six bodies, will be capable of combining state of the art nanofabrication and complementary analysis methods with the full exploitation of fine analysis enabled by radiation source methods offered by large scale research facilities (LSFs). This combination, not represented among the available European public research infrastructures, will bring as added value the overcoming of barriers for the emerging of a more mature stage of development and the removal of bottlenecks in the European competitiveness in medium-long term research programs on nano-functional materials and nano-systems with special implications on ENERGY, HEALTH and ENVIRONMENTAL issues. The infrastructure will offer European scientists a unique access to advanced instrumentation covering the synthesis and nanofabrication, to advanced nano-metrology and characterization, and to all relevant fine analysis methods by co-locating the NFFA centres with the most relevant radiation sources Large Scale Facilities. It is the aim to provide mature, standardized micro- and nanotechnological processes in the broadest sense with unrivalled levels of reliability and reproducibility. Each centre will be co-located and well connected to a relevant radiation source (SR, FEL, lasers, neutrons), offering a wide opportunity of exploiting materials definition and fine properties. Each centre shall present common characteristics in terms of basic instrumentation platform and organization, such as the division into seven internal facilities (nanofabrication, material growth, metrology, handling of molecular and nanoscale objects, nano-bio, theoretical modelling, fine analysis and instrumentation), as well as peculiarities connected to the type of radiation source operating on the same site, and other complementary existing infrastructures or special local competences. NFFA centres aim to provide to European scientists a novel infrastructure that can support basic science at the nanoscale as well as with atomic precision along with innovative applications that explore beyond the short to medium term issues of electronics industry and current nano-bio applications.

Most of the activities of each centre will be devoted to user support. However, for the scientists in the centres about 50% of their time should be available for in-house research to make the centres attractive for the brightest people and to further develop methods and instruments. The basic experimental infrastructure in each centre will be the same, in order to safeguard compatibility between the centres and an optimal level of redundancy. Moreover, each centre may be specialized in a specific direction requiring special equipment, e.g. in terms of materials and/or applications, e.g. IT, Bio, Energy etc. This specialisation of cause will be closely correlated to the in-house science program and the mission of the parent institution.

In longer term, the centres will aim for a visionary concept of a “total characterization line”. This will be a standardized, highly automated system giving a complete, non-destructive characterisation of user’s samples in order to make sure that the sample really has the properties assumed by the user before it is analyzed in the LSFs. This will require a high level of standardisation in handling and sample geometries.

Typical NFFA centres should have an approximate total size of 6300 m^2 plus access to a guest house (~1000m^2) for the users who, in contrast to sojourns at normal LSFs, may have to stay several weeks or even months. The core lab of each centre will consist of a state of the art clean room of about 1900m^2 with various classes of cleanliness. The layout will be “finger-type” which has proven to be the most effective and flexible one. About 4000m^2 are necessary for conventional labs, workshops, offices, meeting rooms etc. The average initial investment of an NFFA building when started from the green field is estimated to 35 M€. This amount of cause can vary with the type of specialisation of the centre and with local circumstances (land prices, labour cost etc.). The necessary staff for operation is estimated to about 70 people. Apart from the direct running cost an amount of about 10% of the initial investments for equipment should be budgeted annually in order to keep the laboratories up to date.

The most advanced top-down micro- nanofabrication technologies down to the molecular scale will require high resolution lithography, material growth and pattern transfer processes, which will have to be installed in the clean room labs. For ultimate resolution pattern definition special “noise-free” clean room cells have to be realized which are properly isolated from any external mechanical (vibrations, sound) influences and electromagnetic interferences. Apart from standard, e.g. metal deposition processes the material deposition techniques may be subject to the specialisation of the individual centre. The focus may be on semiconducting, metallic, dielectric or organic materials. The necessary equipment, its approximate cost and the necessary resources for operation are summarized in tables in the delivery report. The design of a complete nano-bio laboratory in a specialized centre is suggested in the report as are various aspects of handling and manipulation of nanomaterials and nanoparticles.

A very important aspect of the NFFA centres is a standardized metrology. Reliable metrological techniques have to be in place for all relevant physical, chemical or biological parameters of the user’s samples to be processed. Extensive exchange of information between the different NFFA centres is mandatory in this area, also interaction with the national standards authorities is recommended.

In the appendix of the deliverable report some existing nanotechnology centres in Europe and in the USA are briefly described which are neighbouring large scale facilities but are not necessarily in the same organisation with them. European facilities are only described who are not partners in the NFFA design study.

3. MOTIVATION

During the past two decades, nanoscience and nanotechnology have involved a growing community of researchers with competences in materials science, surface science, chemistry, biology, electrical engineering and photonics that has developed a highly interdisciplinary method of work in order to attempt mastering both the fabrication and the functional control of nanostructures. The creativity of this community has lead to new concepts in science at the nanoscale, to the invention of approaches and methods for synthesis and analysis, and to the development of new materials and functional systems suitable for innovative applications.

As it often happens to a young scientific discipline, the first development stage is driven by the excitement and by the creative exploration of the new “land”. In fact, in two decades the vastness of nanoscience and nanotechnology territory has been explored in many directions, often chaotically and not always with the necessary accuracy and criticism. In this stage many relevant demonstration experiments have been performed leading to the evidence that control of material synthesis, nanofabrication, and proper characterization of dimensions and functionalities were performed. Now, a more mature stage must follow, in which the discoveries will be more carefully tested and critically analyzed, before being confirmed or discarded, refined and generalized – and, most important, being developed into highly reproducible protocols suitable for repetition of experiments and development of practical applications, finally generating value for the economy.

In order to drive nanoscience and nanotechnology towards maturity a higher level of metrological control in all relevant stages of synthesis, nanofabrication and characterization is mandatory and requires the adoption of the most advanced methods of measuring the properties of matter at the nanoscale and at the short time scale. Much of this can be achieved by the methods of probing matter that are based on brilliant, or short-pulsed, or highly monochromatic radiation sources as found at synchrotrons (storage rings), free electron lasers, and neutron sources provided a suitable environment is created for integrating synthesis and nanofabrication laboratories with atomic resolution microscopies, high energy resolution spectroscopies, high time resolution structural and dynamical probes. Such environment is not available in nano-foundry type laboratories that are typically built around clean rooms with no or limited access to fine analysis methods, nor at radiation sources where the sample preparation and control are often the limiting factors in the research, due to inadequate infrastructure for materials synthesis and nanofabrication. In this respect, the lack of an infrastructure capable of combining state of the art nanofabrication and complementary analysis methods with the full exploitation of fine analysis enabled by radiation source methods represents a barrier for the emerging of this more mature stage of development and a bottleneck in the European competitiveness in medium-long term research programs on nano-functional materials and nano-systems with special implications on ENERGY, HEALTH and ENVIRONMENTAL issues. Similar analyses were developed in Nanoscience/Nanotechnology Roadmaps, NMP documents and the GENNESYS exercise.

The purpose of the NFFA design study is to provide a clear vision and a concrete action plan for the implementation of an infrastructure that would contribute effectively to filling this gap, by offering the European scientists a unique access to advanced instrumentation covering the synthesis and nanofabrication, to advanced nano-metrology and characterization, and to all relevant fine analysis methods by co-locating the NFFA centres with the most relevant radiation sources Large Scale Facilities).

Science is based on the fact that to be acceptable results need to be reproducible. Irreproducible experiments are useless in the scientific endeavour. Materials whose “wonderful” properties depend on the “finger” of the experimenter will never enter in a technology roadmap. Doubtful or incomplete characterizations of nanoscale materials may be of little help to the advance of knowledge, and possibly misleading for further investigations. Similarly, advanced analysis and characterization demonstrated on reference samples must be fully exploited on innovative materials and systems in order to realize the added value of the new methods.

That is why the NFFA project aims for designing infrastructures where researchers can rely on reproducible techniques of synthesis, nanostructuring, and characterization, the prerequisite for further advancing the field of nanoscience and nanotechnology. Providing a scientific service helping to solve this issue represents the mission of the NFFA RI.

4. BASIC STRUCTURE AND OPERATION OF THE NFFA CENTRES.

NFFA aims to become “the European infrastructure for nanoscience research with integrated access to fine analysis method and instrumentation”. In order to achieve this goal a structure of several centres has to be designed, each one co-located and well connected to a relevant radiation source (SR, FEL, lasers, neutrons), offering a wide opportunity of exploiting materials definition and fine properties. Each centre shall present common characteristics in terms of basic instrumentation platform and organization, as well as peculiarities connected to the type of radiation source operating on the same site, and other complementary existing infrastructures or special local competences.

A research proposal for work at NFFA might span from one that can be carried out at one given centre, or at any of the NFFA centres, perhaps only needing a subset of the facility methods to others that will need the special features of two or more centres and radiation sources for being performed.

The structure of the proposed NFFA centres is designed to implement and support this long term strategy of providing stronger foundations to nanoscience, favouring a deeper level of understanding – by the set of equipments, the proximity to LSFs where advanced characterization methods are available, the bidirectional benefit in the interaction between NFFA centre and LSF, the selection criteria for the scientific and technical staff and the internal organization. Although diversified by their dominant research field and specialisation, all NFFA centres will share a common basic structure, articulated into a set of internal user-oriented facilities of:

- **Nanolithography**
- **Material synthesis**
- **Metrology and Advanced Analysis**

- **Handling of molecular and nanoscale objects**
- **Nano-Bio**
- **Theoretical modelling and simulations, theoretical spectroscopy**
- **Possible Fine analysis endstations and/or instrumentation**

The centres will be organized with the facilities occupying adequate space and environment, in a highly intercommunicating structure, made of proper architecture of the centres and careful description of the job-profiles for scientists, engineers, technical and administrative staff and management.

The architecture of the ideal, green field filling, NFFA centre will include state of the art clean rooms, wet chemistry laboratories, inorganic synthesis labs (including atomic manipulation in UHV), nano-bio laboratories, nanofabrication by litographies, etching, beam assisted chemical deposition, properly integrated electron microscopy laboratories, advanced analysis laboratories, and possibly end stations and beamlines exploiting the radiation sources, in cooperation with the radiation source facilities. Theoretical research and support to data analysis will be transversal to all activities, including intelligent synthesis design, total energy analysis of nanostructured matter, quantum behaviour of realistic nano-objects, theoretical analysis of spectroscopies and simulation of microscopies and time resolved measurements. The infrastructure for theory may include local computing power mostly for code development and connection to high power computing networks (PRACE) for simulation/modellization projects. The infrastructure for data handling will include archiving and open access protocols.

Office, meeting space will be available to users and users groups/networks, in addition to the facility meeting rooms and seminar rooms. User's residency may exceed a few days and, in particular for PhD students or Post Doctoral fellows it may imply several months or years residency (part time or full time) at the NFFA centre. In such case it is mandatory that a work-place is reserved for users, in open-space or small office architectures. Also some storage/small laboratory space could be reserved to long term users under appropriate conditions. The possibility of contractual research by industry or other private bodies may include renting of laboratory and office space, under properly regulated circumstances. The general layout of the centre should favour both optimal location of special equipment (e.g. anti-vibration bases for TEM and high resolution lithography machines, at ground or underground level) and meeting of staff, management and users even if not implied in the same projects at a given time.

The general organization of the work will put on equal footing the activity of the NFFA RI for supporting user's science (50% of NFFA scientist work time, 85%-100% of NFFA engineers and 100% technical staff dedicated to users activities, including training on instruments and security, and technical facility management) and for carrying out own scientific programmes involving also 50% of work time by the NFFA scientists and possibly a quotas for engineers (up to 15%).

Both user's proposals and in-house research will generally involve several or all the facilities of each centre. NFFA scientists will be most successful when they will implement or develop cross-disciplinary competences and skills, such to assist or lead the users to the integration of radiation methods, or theory, or microscopy or any of the relevant approaches to their own research programme.

Each one of the (up to seven) facilities of a NFFA centre will be outfitted with an adequate set of state-of-the-art equipment. The different NFFA centres will share a common basic scheme of structure. However, only general purpose basic tools will be duplicated in all centres (e.g. FEG SEM with frequent cross calibration between all centres to a common standard), otherwise the NFFA centres would be a bare duplication of each other.

A first goal is to define the basic structure and equipment of general relevance for supporting advanced research at the nanoscale, with optimal access to such equipment from the specific facilities (bio, synthesis etc.) that may need it. The layout of cleanrooms could in fact include direct doors to other facility environments where appropriate, including analytical facilities. In one reference case, the Argonne DoE centre, a synchrotron radiation beamline is extended from the storage ring inside the nanocentre building. Such arrangement could be useful, but may not be possible or needed in some cases. It is very relevant that a transfer system for samples from the NFFA laboratories to the fine-analysis instruments is designed and implemented with the needed characteristics (UHV, cryogenic or high temperature, controlled atmosphere, fields). It is very important that the instrumentation on the beamlines is adapted to receive the samples from NFFA.

The specialization of each NFFA centre will be consequence of the focus of the science program (internal research plus main user groups if present) and the structure of the scientific teams will be optimized for the priorities (i.e. scientific and industrial environment) of each individual site where the NFFA centre will be co-located with existing radiation sources and other research and/or development facilities.

The role of distributed facility implies that work done at different centres is fully complementary and that an ***optimal level of redundancy*** in the available instrumentation and methods is provided both as basic of all centres and as backbone of the common metrology system to be developed and implemented. Any of the accepted users' projects may be carried out, at least in part, in any of the centres, possibly requiring special facilities that are not ubiquitous for economical or technical reasons. It will be the job of the NFFA coordination headquarters to address the proposals to the most appropriate centre in terms of equipment, competences of the scientific/technical staff, and characteristics of the co-located radiation source where relevant. More centres may be involved in a single proposal or long term research programme, as well as in internal research programmes. This implies that the part of work that can be done equivalently in different centres is metrologically characterized in such a detail that reproducibility is effectively warranted. This is an obvious goal, but it is far from being trivial to implement. Round robins of calibration can be done on many instruments, but a special general protocol of nano-metrology must be developed and simultaneously adopted by all NFFA centres in order to reach the goal of the full reproducibility of nano-objects and analysis. Besides increasing the science productivity of NFFA the reproducibility certified by advanced metrology will be important in order to reduce to the optimum redundancy, and the duplication of costs (personnel and instrumentation), to preserve the resources for covering a wider and more differentiated front of advanced technological and scientific developments.

The general aim is to make the instrumentation available to users (hands on) qualified after a training course that will be provided by the NFFA centre for all the specific tools needed by the project for which the cost/benefit balance is advantageous both to the users and the facility management. In fact, depending on the complexity and cost of the instrumentation, as well as of the duration and extension of the users project, the access modality will be different. A basic set of tools and methods will be directly operated by all the users in self-service mode (open hands on access). More complex instrumentation will also be available for direct operation by pre-qualified users with frequent and/or prolonged permanence in a centre (limited hands on access). Finally, some instrumentation due to their high degree of sensitivity and risk of damages, will be normally operated by the dedicated scientific and technical staff (hands off access). This has practical implications since the scheduling of some facilities in high demand may be easier if staff operators run them. Also in some cases (e.g. high resolution TEM) the training of users may be too heavy and could be justified only for long term residency in a centre (phD students), whilst acquisition of TEM images in regular, shorter term, proposals should be done in collaboration with the NFFA scientists.

NFFA will not be a duplication of existing electronics industry oriented facilities. Well established, industrial research facilities (such as for example LETI in Europe) exist and cover well the technological issues of silicon-based nanoelectronics. However, owing to their narrow domain and focused industrial objectives, these expensive facilities lack the flexibility to cover the vastness of materials, methods, concepts and applications of nanoscience and nanotechnology, and are anyhow unsuited to serve as open-access user's facilities.

NFFA aims to provide to European scientists a novel infrastructure that can support basic science at the nanoscale as well as with atomic precision along with innovative applications that explore beyond the short to medium term issues of electronics industry and current nano-bio applications.

The science program for the NFFA centres will consist of two synergic activities: the in-house research projects under the responsibility of NFFA staff and associated scientists, and the users' scientific projects (see D2.2). The duty for the scientific staff to conduct in-house research for 50% of their working time is, as recognized by other scientific service institutions (e.g. the five DoE Nanocentres) essential to attract world-class scientists in the leading positions in the centres. Moreover, a good internal science program is a mean to train NFFA centre staffs to high level scientific competence which will better support the user access and programs (see D2.2).

The in-house science programme of NFFA will be coordinated (see D2.2, D4.3), but each centre will develop its own science programme chapter, according to its technical characteristics and also to its main founding agency policy and/or local partner institutions. What is common to all NFFA is that the scientific personnel will be selected to have (or will be trained to develop) multidisciplinary skills and multi method/technique competences and approaches across the relevant facilities, including beamlines on the radiation sources.

The staff scientist will be the effective actor in introducing the fine analysis methods in projects by scientists that are not acquainted to them, or similarly the modelling/simulation numerical methods or the theoretical spectroscopy analysis tools.

5. POTENTIAL OF THE FACILITIES

The major issue that nanoscience and nanotechnology have to face entering a stage that may well be defined "maturity" is related to the availability of reliable, reproducible and possibly fast techniques by which nanomaterials and nanosystems (inorganic, organic, biological or combined) can be 1) "designed" 2) synthesised, 3) processed, 4) manipulated and 5) characterised.

The overall structure of any of the NFFA facilities is designed for providing support to nanoscience and nanotechnology related experimental activities based on state-of-the-art equipment, in such a way that the outcome of the research carried out here and in conjunction with complementary LSF techniques could represent solid scientific milestones.

The open access, on the basis of the scientific merit of the research proposals, to NFFA will represent a major step forward in the effective operation of the ERA and a unique opportunity for European scientists to perform advanced research with shared instrumentation and methods at the state of the art. More scientists will become users of the LSF and more users of the LSF will perform highly reproducible and advanced research thanks to access to NFFA centres.

5.1 A new challenging initiative involving all NFFA centres: "the total characterisation line".

A major obstacle to the scientific progress in nanoscience and nanotechnology is represented by the difficulty of obtaining exhaustive and accurate information about the systems (nanosystems, nanomaterials, nanodevices, etc.) under investigation. In fact, characterising a system in many respects - i.e. physical (optical, electronic, mechanical, thermodynamic, etc.), chemical (composition, atomic structure, defects), morphological (shape, surface structure, interfaces, etc.) - employing a broad range of measurement techniques, increases the possibility of a deeper comprehension of its properties and of all their correlations. However, gaining thorough information about a system through highly accurate and exhaustive characterisations is in general difficult for two main factors.

In small to medium scale laboratories usually only a limited number of characterisation tools is available; often the different equipments belong to different groups having distinct interests and fields of activity, and are therefore not available as a service to other groups. Organising and performing systematically a wide campaign of characterisations is a very labour intensive activity that is often not done

NFFA will develop and implement as a backbone of its centres and operation mode a “total characterization line”. This concept is somewhat inspired to the industrial assembly line, but applied to the elaboration of nanomaterials. The idea is essentially that of a “line” in which an object with nanometric dimensions (sample) undergoes a full metrological check-up (a long series of characterisations as automatised as possible) while proceeding from consecutive synthesis/nanofabrication/measurements stages to “metrology stations” in a suitable environment (vacuum/UHV line).

Schematically: a batch of samples are queued, each associated with its own measurement protocol. This is defined (even remotely on an online template) by the researcher, or selected from a list of standard protocols available for each category of materials or systems, and prescribes the parameters to be applied in the characterisations (such as the sampling wavelength range in spectroscopic techniques, the size of the AFM field scans, the coordinates at which maps have to be performed, etc.).

All measurement stations are operating at the same time on different samples. Once the longest measurement ends, all samples move one step forward in the total characterisation line. Assuming no time loss, the throughput of the “total characterisation line” will be determined by the longest characterization step (unless the latter is split and performed alternatively in two or more branch lines with the same equipment).

The implementation of such a concept seems technically feasible, though various aspects may be very challenging, such as interfacing all characterization instruments to the same pipeline, bypassing a measurement station in case of a failure or for its maintenance, or the transfer of samples from growth, synthesis, etching, and lithography tools to the “metrology line”, and transfer to the beamlines of the LSF under UHV conditions (if necessary).

Some techniques may be rather straightforward to implement into the metrology line. Others, in particular those that usually require a more direct and frequent interaction of the operator on the tool, may be more complex. It will be challenging to develop some skills of Artificial Intelligence in order for the equipment to manage situations in which some level of “understanding” of the situation is required, such as finding the optimal measurement conditions. A list of possible techniques for the “metrology line” includes AFM, MFM, STM, Kelving probe microscopy, mechanical and optical profilometry, hardness measurement, photoluminescence, ellipsometry, absorbance, reflectance, RHEED, Raman, FTIR, X-ray diffraction, four point electrical measurements, SIMS, FIB sectioning, top-view and cross-section view SEM microscopy for in plane and cross inspection, EDX, SPA-LEED, XPS. Care must, however, be taken to apply only techniques whose interaction with the sample does not influence the results of another measurement. The primary use, initially, will therefore be for classes of samples with known sensitivity, similar properties and characterisation needs, like e.g. inorganic thin films of similar materials.

A record containing all the results of the measurements relative to any sample (raw data, elaborated data, maps, plots, images, etc.) will be automatically generated as entry into the data/metadata management system and made available to the experimenters, as well as an element of the data repository (see D4.9).

Adopting and adapting the assembly line concept to metrology will increase dramatically the productivity and the reproducibility of the measurement procedures. The additional benefits of implementing such a metrology line would be the following:

- Providing a more systematic way of determining correlations between any two properties of the same material, or of the entire set of properties at two different times (to study for example aging of materials).
- Gaining at least one order of magnitude in the speed by which a thorough characterisation can be obtained.
- Making possible the certification (perhaps even with legal validity) of most relevant material properties for any samples.

- Providing a universal sample holder, avoiding loss of time in mounting samples onto different sample holders and into different setups.
- Saving the experimenter time of the operations that can be automated.
- Avoiding possible procedural biases and random errors introduced by the experimenter.

A particular advantage of a full characterization of a sample within a very short time, would consist in the possibility for users to come to a LSF with their own samples or to prepare them on-site and have them fully characterised, before going into the specialised measurement techniques available at the beamlines of LSFs or TEM or other fine analysis methods.

In the development of such a “total characterisation line” the world’s most prominent toolmakers will be invited to participate to tenders for development and adaptation of their instruments jointly to the total characterization line development team.

It has to be said that the presence of the “characterization line” is ancillary to the creative part of the research work. It is a goal in order to certify and store in repository the conditions of samples after every step of treatment therefore helping in the definition of accurate protocols that, after the discovery/development might become easier and reliable to be reproduced many times and in different laboratories. Stand-alone, man operated, metrology and characterisation tools will be also present in the metrology and advanced analysis facility of each NFFA centre, both in the development time of the “line” as well as in the long term (see D3.4).

We can take as a reference the examples of what has happened in biology, where the advent of DNA sequencing has significantly accelerated biological research and discovery, we can infer that, an improvement that might be considered just quantitative, is eventually leading to new qualitatively different possibilities, such as the high throughput DNA-sequencing systems did for genome research.

Both, characterisation measurements on tools with human-interface and automated high throughput 'metrology lines', should, however, be an answer to a well defined scientific question and individually motivated in the proposal, to provide an efficient use of resources & instrument time.

6. NFFA INFRASTRUCTURE

A reference infrastructure of an NFFA centre, to be built on a green field next to a large scale analytical facility, should consist of a single building of around 6000 m^2 total effective area. Additionally, a guesthouse for the NFFA users should be available in the neighbourhoods.

Depending on the different ground conditions, town planning rules, and other possible constraints, the architectural design of each building will depend on the specific location of the centre. The projects for the NFFA buildings should be object of a European Tender for contract and evaluated by a commission of architects, engineers, and scientists with respect to the following criteria:

- Scientific functionality
- Flexibility (equipment maintenance, ease of equipment relocation, etc.)
- Possibility to direct connection to the LSF experimental hall
- Possibility of further extensions
- Environmental Impact and energy efficiency
- Aesthetics
- Cost

The building will tentatively accommodate the items listed in the table 1.

Deviations from the above common structure may be considered in order to accommodate specific needs linked to the individual specialization of each NFFA centre.

The main constructive constraints are set by technical specifications of the different laboratories. With the exception of the Nanobio laboratory and part of the laboratories of the

Metrology and Advanced Characterization facility, all other laboratories will be in cleanrooms, with different specifications relatively to class of cleanliness, temperature and humidity control, presence or absence of antivibration floor, shielding from electromagnetic fields and stray magnetic fields.

	Area (m^2)		Area (m^2)		Area (m^2)		Area (m^2)
Laboratories		**Administration**		**Internal services**		**Other**	
Nanolithography	400	User Office	60	Entrance-hall & reception	100	Corridors	940
Material synthesis	350	Offices	240	Library	150	Rest rooms	100
Metrology and Advanced Analysis	350	Archive	50	Seminar room (120 seats)	170	Kitchen	60
Molecule & nanoparticle manipulation	150	*Partial 1*	350	Three meeting rooms with video conference.	130	Warehouse	200
Wetlab	300						
NanoBio	400	**Guesthouse**		Computation centre	5 0	*Partial 2*	1300
Total characterization line	150	Separate building with 30 rooms.	1000	Mechanical workshop	250	**External utilities**	
Theory facility	60						
Offices for technical and scientific staff	790			Electronics Workshop	150	Bunker for process gases	35
Offices for users (computer and internet access)	250			Advanced equipment development & test laboratory	150	Nitrogen tank enclosure	25
Empty space for lab expansion.	200					Waste storage	40
Total 1	3400	*Total 2*	1350	*Total 3*	1150	*Total 4*	1400

Table 1. Total area: 7300 m^2 (including 1000 m^2 of guesthouse).

The most severe constraints are related to the nanolithography and to part of the metrology labs (considering also the total characterization line in that). The need for anti-vibrating, low e.m. noise, low stray magnetic field, suggests to reserve the ground floor of the building to these laboratories. Also the molecule and nanoparticle manipulation, and the atomic resolution microscopy lab requires anti-vibrating floor. Therefore, at least 1000 square meters in the ground floor are reserved to laboratories. Additionally, the best fitting of the entrance hall, the warehouse would also be in the ground floor. This brings to 1500 m^2 the lower bound for the surface area.

A possible choice would be to arrange the ~6300 m^2 of the centre in a 4 level building or to increase further the foot area of the building to 2100 m^2 and 3 levels. In the latter case (which seems to be the most appropriate) the building could be distributed as follows:

-1. **Basement.** Technical building infrastructure such as compressors for cooling water, air conditioning units, water purification plant, chemical waste treatment/neutralization etc., warehouse, mechanical workshop. The possibility to move at least part of these activities in an adjacent prefabricated building will be evaluated case by case according to the specific characteristic of the site.

0. **Ground floor.** Entrance hall and reception. The laboratories of nanolithography, material growth, metrology, total characterization line, molecule and nano-object manipulation. Corridors and rest rooms. Outside: Bunker for process gases, Nitrogen tank enclosure, Storage of wastes.
1. **First floor**. Laboratories of NanoBio, with a space left empty for lab expansion/upgrades. Library. Theory Laboratory. One meeting room with video-conference. Electronics Workshop, Advanced equipment development & test laboratory. Administration: User Office, Offices, Archive. (Corridors and rest rooms).
2. **Second Floor.** The offices of scientific and technical staff. Seminar room (120 seats). Two meeting rooms with videoconference. Computation centre. Kitchen. (Corridors and rest rooms).

Overall cost of the building: a rough estimation of the cost of the building can be obtained assuming an average price of 4 k€/m^2 of the non-technical areas, 6 k€/m^2 for the technical ones, and 8 k€/m^2 for the cleanroom. This first estimation would set the cost of an NFFA facility building to 35 M€. State-of-the-art construction for maximum flexibility would include 50 cm high technical space below the floor of higher floors, accessible from above, to distribute services and basic fluid facilities, allowing for reposition outlets as a function of evolving needs. This implies less than 10% initial cost in the construction and basically eliminates disruptive and costly reconfigurations during the 20 years operation of the facility, and beyond.

Operating cost of an NFFA centre has to cover the salaries of the persons employed there plus other running costs plus – this is very important – an annual investment budget allowing the renewal of the centre's equipment within less than 10 years. Only under these conditions a NFFA centre can stay a "state of the art" lab.

6.1 Laboratories

The detailed description of each laboratory is covered by other documents (see deliverables D3.2, D3.3, D3.4, D3.5, D3.6). In the following we provide a brief description of their main features of the scientific parts of the facility, as an overview.

A universal sample holder compatible with all experimental systems might be developed to fully exploit the potential of proposals involving more than one NFFA facility. In addition to it, a versatile and universal system (which could become a standard) for transferring in UHV conditions the samples on their sample holder among the facilities and to the LSF for the most specialized characterizations should be engineered.

6.1.1 The cleanroom

All NFFA laboratories, with the exception of Nanobio and Theory, need to be at least partially installed in environments cleaner or much cleaner than just normal rooms where no precaution is taken to minimize the number of dust particles contained in the air. In the case of the NanoBio lab, regulations according to Biosafety law have to be applied; an installation of a cell culture lab will require additional precautions against contamination of the cultures. In the case of Theory lab, assuming the installation of some local computing power, a suitable machine room with air cooling and acoustic insulation shall be provided, as well as operator office space. Table 2 displays the basic specifications the different laboratories need to comply with, in order to ensure the correct operation conditions to the equipments therein.

	Surface Area (m^2)	Clean-liness (ISO 14644-1)	Thermal Control (°C)	Humidity Control (%)	Antivibration floor Y/N	Shielding e.m. noise Y/N	Shielding stray magnetic field Y/N
Laboratories							
Nanolith. I	**150**	**ISO4**	**21 ± 0.1**	**45 ± 5**	**Y**	**Y**	**< 1 mGauss (0 – 100 Hz)**
Nanolith. II	**250**	**ISO5**	**21 ± 0.5**	**45 ± 5**	**Y**	**Y**	**N**
Material Synthesis I	**100**	**ISO6**	**21 ± 3**	**N**	**N**	**N**	**N**
Material Synthesis II	**250**	**no special requirements**	**21 ± 3**	**to be evaluated**	**N**	**N**	**N**
Metrology and Advanced Analysis I*	**200**	**ISO7**	**21 ± 1**	**Y**	**Y**	**Y**	**< 1 mGauss (0 – 100 Hz)**
Metrology and Advanced Analysis II	**300**	**no special requirements**	**21 ± 1**	**to be evaluated**	**to be evaluated**	**y**	**to be evaluated**
Manipulation of molecules and nano-particles	**150**	**to be evaluated**	**21 ± 2**	**N**	**Y**	**Y**	**Y**
NanoBio I:	**360**	**S1**	**21 ± 2**	**N**	**N**	**N**	**N**
Nanobio II: Two cell culture rooms.	**30**	**Classification according to genetics safety law.**	**21 ± 2**	**N**	**Y**	**N**	**Y**
Nanobio III: Cold room	**10**	**As above**	**4 ± 1**	**N**	**N**	**N**	**N**
Wetlab	**300**	**to be evaluated**	**21 ± 2**	**Y**	**N**	**N**	**N**
Theory Lab.	**60**	**Not applicable**					**N**
Total	**2160**						

*including the Total Characterisation Line

Table 2. Laboratories with estimate of the necessary surface area and the most fundamental conditions in relation to cleanliness, e.m. field, stray magnetic field, temperature and humidity.

The specifications for the various laboratories are the result of a compromise between various aspects: if the process performed by given equipments is not affected by temperature/humidity conditions which fall outside of human comfort ranges, it is convenient not to specify tight tolerances. Tight tolerance will result in unnecessary costs, and lower ease in the use of the equipments by the operator. It should be mentioned here that the need for low particle counts in the air of a lab is originating from semiconductor manufacturing. There, particle concentration directly influences the device yield and thus ultimately the commercial success of the company. This justifies the huge investments and operating cost of ISO 4 and below environments. In research *reproducibility* of sample preparation is more important than yield. Therefore in an NFFA clean room control over temperature, humidity, vibrations etc. will be more important than particle count.

Class	Maximum particles/m^3						FED STD 209E equivalent
	≥0.1 µm	≥0.2 µm	≥0.3 µm	≥0.5 µm	≥1 µm	≥5 µm	
ISO 1	10	2					
ISO 2	100	24	10	4			
ISO 3	1,000	237	102	35	8		Class 1
ISO 4	10,000	2,370	1,020	352	83		Class 10
ISO 5	100,000	23,700	10,200	3,520	832	29	Class 100
ISO 6	1,000,000	237,000	102,000	35,200	8,320	293	Class 1,000
ISO 7				352,000	83,200	2,930	Class 10,000
ISO 8				3,520,000	832,000	29,300	Class 100,000
ISO 9				35,200,000	8,320,000	293,000	Room Air

Table 3. *Number of particles per unit volume of air for the different classes in the* ***ISO 14644-1*** *and in the* ***FED STD 209E*** *standards.*

The laboratories will be organized in such a way that robotics may develop as a major option in sample handling for sequences of nanofabrication / characterisation steps, connecting synthesis, patterning, metrology line, delivery to beamline ancillary equipments or, in some cases, to beamlines themselves.

The NFFA cleanroom should be organized as a modern modular cleanroom facility, in which service rooms are interposed between two consecutive rooms. In this manner the equipments can be installed with the operator interface on the side of the cleanroom while the rear part is facing the gray room from which it is accessed for maintenance and repair.

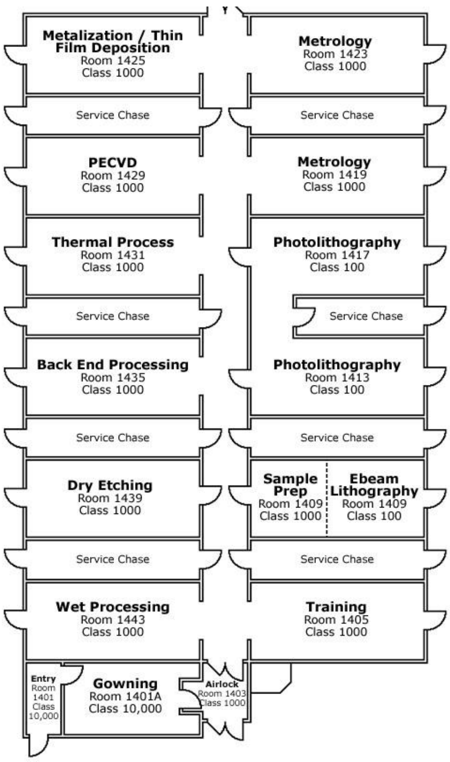

Fig. 1. Typical arrangement of working areas in a modern cleanroom (the present scheme is only an example and the number, size and destination of the rooms has to be adapted to the scopes of the facility); an important feature consists in the presence of “gray rooms” (service chase) interposed between two consecutive rooms, for placing the equipments “through the wall”, i.e. with the rear in areas accessible to personnel in charge of their maintenance, and the front accessible by the operator. The rooms are arranged at opposite sides of a corridor which allow the cleanroom staff to move from an equipment to the next according to the chain of processes and characterisations they need to perform. The layout of the NFFA cleanrooms should follow essentially this scheme, which a kind of “Darwinian” evolution has selected as the most efficient arrangement of fabrication-oriented laboratories.

The NFFA might require specific design, taking into account the need of dividing user access areas from internal staff only areas.

A summary of the scope and of the characteristics of each internal laboratory is presented in the following. A more detailed description of each of them is contained in the deliverable D3.2-D3.3-D3.4-D3.5-D3.6.

6.1.2 Nanolithography

In a near future, the production of the most technologically advanced materials will not only be ensured by the methods of chemical/physical synthesis. New functional materials may be produced by contribution of top-down nanofabrication technologies. Thanks to the maturity of the present technology, nanofabrication enables the structuring of materials at scales comparable to some intrinsic physical dimensions (e.g. the mean free path of the charge carriers, the wavelength of optical, acoustical, plasmonic or excitonic modes). Very frequently, these dimensions are on the scale between a few nanometres and a few tens of nanometres.

Having reached, with lithographic capabilities, the scale at which some physical phenomena take place in materials, will allow the exploitation of nanofabrication as a material synthesis technique, conferring to materials new properties departing from those inherited from the chemical/physical synthesis.

Among those new artificial materials, engineered by means of nanofabrication, we find for example photonic crystals, metamaterials, nanomagnets of a single domain, superhydrophobic surfaces, special optical materials able to alter the polarization and the orbital angular momentum of the e.m. radiation.

To enable a research program on the wide range of advanced topics in nanoscience, the NFFA network will host the following instrumentations: high-end Gaussian beam systems, Nanoimprint Lithography systems, Dual Beam (FIB+SEM) with pattern generator, different scanning probe lithographies (STM, AFM and Dip Pen), photolithography (mask aligners), spin-coaters. In addition, one X-ray Interference Lithography, one X-ray (proximity) Lithography and one Injection molding system should be available in the NFFA network. A list of other equipments that the nanolithography laboratories in the NFFA centres comprises, gloveboxes, electroplating station, UHV evaporators and sputtering. A range of pattern transfer techniques, based on reactive plasmas will be available, such as Inductive Coupled Plasma (ICP) etchers for silicon for III-V semiconductors, Deep Reactive Ion Etching, chromium etchers and a Ion milling system. Finally, an area of the facility will be equipped for Soft lithography methods.

Considering the different specifications and access regulations of different equipments, the cleanroom should be divided in two main areas, Nanolith I and Nanolith II.

Nanolith I will contain EBL (High-end Gaussian beam system), UV-Nanoimprinting, laminar flow hood with spin-coater and hot plate, and will have tight specifications for cleanliness (ISO4), Thermal control (21± 0.1 °C), antivibration floor and shielding for e.m. and stray magnetic field. The use of EBL and UV-NIL will be restricted to scientific/technical staff.

Nanolith II will contain all other instrumentations and will be open to users after proper training.

6.1.3 Material synthesis

NFFA facilities dedicated to material synthesis should provide standardized and reproducible processes focalized towards the preparation of various forms of materials (single crystals, thin films, nanoparticles, supramolecular aggregates, etc.).

NFFA synthesis facility will take advantage of the proximity of the Metrology and Advanced Analysis Facility: each sample produced in the Synthesis facility can undergo a set of measurements defining principal parameters, by using standard characterization techniques present in the neighbouring facility (Transmission Electron Microscopy, Scanning Electron Microscopy, X-Ray

Diffraction, Scanning Tunnelling Microscopy, Atomic Force Microscopy, X-ray Photoelectron Spectroscopy, μ-Raman, etc.).

One of the main tasks of NFFA material synthesis will be to improve the *in-situ* characterization of the synthesis process, including characterisation tools into synthesis chambers or directly connecting the latter to advanced analysis chambers, and also taking advantage of the fine analysis techniques at the neighbouring LSF (see D3.3 for possible technical solutions).

One of the main problems when accessing synchrotron radiation facilities is the limited time available to prepare samples, a preparation that has to be usually done during beam time. This is in general a serious drawback and a waste of precious beam time. Ideally, one should be able to prepare and characterize samples close to LSFs prior to the measurements. This is a critical point that is not being adequately addressed in most cases and dedicated NFFA centres close to LSFs would greatly help in this direction.

A strategy to be developed is that of producing sample libraries, e.g. alloys or metal oxide compounds as obtained by cross wedge depositions on a substrate or other gradient concentration techniques that will produce a continuous variation of composition/crystalline/stress/strain properties of a class of samples all grown on a common substrate and separated laterally by tens of micrometers. At NFFA it will be possible to “scan” these samples also by exploiting micro-beams of X-rays or soft X-rays to probe structure or magnetic properties for example. An automated scan of these properties will quickly identify the “regions” of interest for further investigation and speed up considerably the material science/nanoscience analysis.

There is a fundamental aspect to be considered in the planning of the material synthesis laboratory that induces to make a rather different type of choice as compared to the nanolithography lab. In fact, while most lithographic techniques can be performed on different materials using the same tools (lithography is performed on most cases on organic polymeric materials acting as sacrificial layers, or as in the case of FIB by direct physical milling, process that can be applied to most materials), with the deposition techniques, for the sake of high quality and purity of the materials, it is important to have different systems for different materials or class of materials. In this sense the lithographic processing is more universally applicable than the deposition technologies. Therefore a rather large number of systems is necessary to cover the range of most advanced materials. However each NFFA facility will be specialised in specific subjects and collaborate with the rest of centres, optimizing the important investment, by sharing equipment and know-how.

Part of the Material synthesis facility could be located in an ISO6 cleanroom. Most of the processing for material growth will be in dedicated chambers, therefore there is not a critical need for pushing the cleanliness to the limit. However, in many cases the materials may serve as the starting point for the fabrication of nanodevices and artificial materials, which requires instead high cleanliness standards. It follows that this environment has to be sufficiently clean, even though after the growth process the materials “see” the environment conditions for a short time.

We refer here to the deliverable D3.3 “User-oriented Material Synthesis Facilities” for a general description of both conventional and cutting edge preparation techniques. We briefly introduce the techniques that should be available at the NFFA-facilities. The different methods are divided into five main categories, i.e. Physical Vapour Deposition (PVD), Chemical Vapour Deposition (CVD), Chemical Solution Deposition (CSD), Single Crystal Growth and Sol-Gel.

PVD involves purely physical processes such as thermal vacuum evaporation or plasma sputter bombardment rather than involving a chemical reaction at the surface to be coated as in CVD(see below). PVD includes thermal, electron beam, sputtering, cathodic arc and pulsed laser deposition.

CVD includes a variety of chemical processes used for the growth of high quality deposits of materials such as silicon, carbon fibers, carbon nanofibers, filaments, carbon nanotubes, SiO_2, silicon-germanium, tungsten, silicon carbide, silicon nitride, silicon oxynitride, titanium nitride, high-k dielectrics as well as synthetic diamonds. Gaseous precursors of the constituent materials are transported by a carrier gas (typically helium or argon) to a mixing zone where they react, and then to the deposition zone. To this class of processes belong Plasma-Enhanced CVD (PECVD), Rapid thermal CVD (RTCVD), and Atomic layer deposition (ALD).

CSD includes very common methods to coat surfaces with films of molecules or polymers such as Spin and Dip Coating, Self-Assembled Monolayers (SAMs) and Langmuir-Blodgett techniques.

Single Crystal growth of inorganic materials is extremely relevant to modern technology. Inorganic single crystals can be prepared by different methods such as the Czochralski and Bridgman techniques, various floating zone methods, and hydrothermal growth. Organic single crystals can be prepared from solution using a large variety of methods, such as simply preparing a solution of the molecule and letting the solvent evaporate slowly so the molecules have time to interact between them and crystallize.

The Sol-Gel technique is based on the hydrolysis of liquid precursors and formation of colloidal sols. It is a cheap and low-temperature technique that allows for the fine control of the product's chemical composition.

The NFFA-facilities will provide access to all five categories of material preparation techniques. However, every NFFA centre will have its own focus, resulting in a different range of equipments installed at each site.

6.1.4 Metrology and Advanced Analysis

Ensuring the reproducibility of material synthesis, nanofabrication and their metrological characterisation is the specific target of the entire NFFA project. The idea behind it is that only on solid results nanoscience and nanotechnology can progress further than the present status of development. The first natural way of ensuring that this ambitious objective is within reach of an NFFA network (and once reached maintained and set as a new standard in nanoscience), will be provided by internal cross-checks between the different NFFA centres.

For this purpose, the NFFA centres will develop and provide a common well-defined metrology. For the same reason, the metrology facility will offer a common set of instrumentation whose performance will be continuously calibrated. In this view, NFFA internal protocols will have the capacity of contributing to the definition of new standards for nanoscience.

In addition, the facility will offer access to a set of state of the art tools for high-level science in advanced analysis experiments, with instrumentation that is typically only available in few academic laboratories.

Finally, as discussed in the paragraph 3.1 of the present document, a need for a more complete sample characterisation will be addressed by launching an initiative to develop a fully automated "total characterisation line", in which batch of carefully prepared samples will be characterised in most of the possible ways, in a short time and limiting the intervention of the experimenter, who will obtain at the end a complete report on the characterised sample. This will increase the knowledge, by strongly increasing the throughput of characterisation techniques, making easier the correlation of all most relevant properties of a system under investigation. The project for the development of the total characterisation line will take several years of effort by the entire NFFA infrastructure together with equipment manufacturers, experts of automation and vacuum technology, and worldwide established companies. The cost will be high, but it will enable the scientific community to make a jump to a higher level of understanding of nanoscience, paving also the way towards a more reliable use of nanosystems in technology.

As part of the in-house activity, particular attention will be dedicated to the development of new cutting-edge instrumentation that will be open to user's access as soon as sufficiently tested by the NFFA staff.

Metrology and Advanced Analysis facilities will be closely connected to the other facilities in each NFFA centre. The facility will contribute to a better and faster characterisation of the samples before the beamtimes at the LSFs or other experiments, and to the development of high-level joint scientific proposals. Furhtermore, a section of the metrology and advanced analysis facility will be located inside the neighbouring LSF, with NFFA staff personnel working on specific beamlines together with LSF scientists as a bridge between NFFA and LSF competences. The collaboration will extend to the development of new instrumentation combining typical LSF techniques with classic lab characterisation tools. The list of equipments installed in the metrology laboratory will be divided into different sections:

- Microscopy Section, with Electron Microscopes, Scanning Probe Microscopes, Emerging Microscopes
- Structural, Optical and Elemental analysis Section, with X-Ray laboratory, Optics laboratory, Surface analysis and Compositional Analysis
- Magnetic Characterisation Section
- Thermal and Mechanical characterisation Section
- Transport properties Section
- LSF Located Section

6.1.5 Molecule and nano-particle manipulation

Nanomanipulation, or positional and/or force control at the nanometre scale, is a key enabling technology for nanotechnology by filling the gap between top-down and bottom-up strategies. Presently, nanomanipulation can be applied to the scientific exploration of mesoscopic physical phenomena, biology, and the construction of prototype nanodevices. A growing interest is reserved to bio-materials and bio-nanotechnology to solve these problems specifically for experiments associated to LSFs (Large Scale Facilities). The linking of the macroscopic world to the nano-world of single molecules, nanoparticles and functional nanostructures in devices which match the LSFs beamlines constraints (e.g. microbeam, limited space and time) represents a technological challenge. Various manipulation techniques have to be made accessible to researchers involved in fine analysis at LSFs. A range of technologies and their main features is reported in Table 4.

	Contact-less manipulation				*Contact manipulation*		
	Optical Manipulation		***Magnetic Tweezers***	***Dielectro-phoretic Tweezers***	***Scanning Probe Microscopy Manipulation***		***Microgripper***
	Optical Tweezers	***Optical Leviation***			***STM***	***AFM***	
Resolution	*Medium/high*	*Medium/high*	*Medium/high Medium/high*	*Medium*	*Very high*	*Very High*	*High/VeryHigh*
Environment	*Liquid*	*Air/Vacuum*	*Liquid*	*Liquid*	*Vacuum*	*Air/Liquid/Vacuum*	*Air/Liquid/Vacuum*
Freedom Degrees	*3D+force measurement*	*3D*	*3D+force measurement*	*2D*	*2D*	*2D+force measurement*	*3D*
Flexibility	*Very high*	*High*	*Medium*	*Medium*	*Low*	*Medium*	*High*
Robustness	*High*	*High*	*High*	*Medium*	*Low*	*Medium*	*Medium*

Table 4. Different manipulation tools that will be available at NFFA centres with most relevant properties.

Based on the main technical characteristics reported in Table 4, the manipulation techniques (MTs), classified in contact and contact-less will offer a wide range of possibilities for assembling nanosystems as well as for manipulation (controlling position and orientation) in front of a beam for fine analysis experiments. The entire range of manipulation techniques will be implemented taking into account the concrete need for manipulation of materials, samples and nanodevices at large scale facilities. A special regard will be given to contact-less techniques which provide more flexibility than the contact techniques in terms of the manipulation freedom degrees and the environment in which they can be implemented, and more specifically to setups of optical tweezers and optical levitation.

6.1.6 NanoBio

The facilities for biological research will be equipped according to the specialization and research focus of the NFFA site. The offered infrastructure will range from a Biolab user facility (as already provided by some LSFs) with basic equipment (CO_2 incubator, sterile working bench, cryo-microtome) for sample preparation and storage and access to characterization techniques, to a NanoBio facility with ambitious scientific program and advanced instrumentation. Those sites should be developed considering possible collaborations with the scientific environment of the LSF and, most important, synergies with other NFFA facilities at the site (material growth, thin film, nanopatterning, lithography facilities), that will be one of the characteristic benefits of the NFFA-concept. Nanobiological research themes with increasing significance, strong synergy potential and a strong LSF - affinity are: - Biointerfaces, Biomimetics, Biosensor devices, Nanomedicine, Toxicology, Proteomics, Protein crystallography.

Besides instrumentation that can be shared in the frame of the general Metrology facility at the site, a NanoBio-lab (irrespective of the size) will also need access to Support labs, that will to some extent also be necessary or useful for other facilities:

Chemical lab: a chemistry lab with standard equipment and a chemical synthesis facility (fume hood, pH-meters, heating/stirring plates, microcentrifuges, ultrasonic processor, microscope with CCD camera, glove box with controlled atmosphere, precision balance, standard chemical lab supply) will be available at every NFFA site.

Microfluidics lab: Stopped-flow- / rapid mixing equipment, automated, high throughput facilities for biological samples. Recent practical experience suggest also to consider the need for the presence of a clean area for microdevices assembly.

Bio-lab: Standard equipment includes a biological safety cabinet, laminar-flow box, CO_2-Incubator with inverse microscope with CCD camera, autoclave. The basic layout of the Biolab should provide sufficient space/infrastructure to allow an upgrade of the biological safety level and the installation of additional equipment.

Many characterization tools that will be provided by the general Metrology facility for other research areas will require only some adaptability, some precautions and suitable environmental conditions to be also useable for biological tasks. At specialised NanoBio-facilities, analytical techniques that are most frequently used by this facility will be installed directly inside the BioNano lab area. A duplication will only be necessary if the danger of (mutual) contamination or other conflicts related to kind or frequency of use make sharing unpractical.

Instrumentation of general use, that will be very frequently used for NanoBio research and should be located inside the biolab:

- Spectroscopy: Spectroscopy (μ-Raman, UV-VIS, IR,)
- (Fluorescence) Microscopy and Imaging
- Environmental Scanning Electron Microscopy (FE-SEM)
- Mass spectrometry, HPLC

Methods that are also interesting for other facilities and that would profit from further development by dedicated research groups:

- Cryo lab: Cryo- Electron microscopy / -tomography
- NMR spectroscopy
- Optical tweezers, Single particle chemistry on biological macromolecules

A specialised NanoBio facility could also be installed to do research at the S3 safety level, requiring infrastructure for storage, handling and disposal of highly infectious or biohazardous material. This would require a strong interest also from the associated LSF, because it would require investment and safety adaptation also from this side. The most probable location for such a facility would be at a LSF that is already involved in such research.

6.1.7 Materials Modelling and Simulation

The NFFA theory facility for materials modelling and simulation will provide numerical and theoretical support to the users by assisting and complementing the characterisation and fabrication activities carried out in the NFFA centres. As a result, this theory facility will be transversal to the NFFA centres and should be designed to cover a large spectrum of competences ranging from phenomenology, nanobiology, theoretical materials science, physics and chemistry, down to algorithmics and software engineering. As such it is a valuable component of the “total characterisation line” that is pursued by the NFFA project.

The general goal of the theoretical facility is to provide the detailed and fundamental atomistic insight into materials' properties that allows for optimising their functional properties and for guiding a more efficient and controlled bottom-up assembly. To this end, a coordinated interconnection with the experimental advanced characterization (spectroscopy and microscopy) and nanofabrication NFFA facilities should be envisaged. The example of similar existing theoretical facilities that are well inserted into large-scale experimental infrastructures (see appendix A), shows that the scientific and technological achievements resulting from this coordinated collaborations can demonstrably be way superior to the sum of the outputs from the individual disciplines.

The NFFA theoretical facility will develop and apply multiscale computational techniques for the numerical materials' simulation. Its main **objectives** include:

* <u>providing theoretical support</u> to the NFFA users. This can be achieved by the research staff, who will perform quantitative numerical simulations necessary to complement the selected experimental analysis. However, we stress that the most efficient and fruitful working scheme has been shown to be the one in which the users themselves perform the numerical modelling with the resources of the facility (see next point), with the assistance and guidance of the research staff. Ideally, the theory facility should offer theoretical support both to experimental groups already performing an approved experiment in one NFFA centre, as well as to external theory groups;

* <u>providing computational resources</u> (scientific software, in house computing cluster, and access to massively parallelized external computing resources) necessary to carry out the numerical calculations described above. The theory facility should aim at promoting the remote use of the computational resources from the users, thus minimizing the necessity for their actual presence on the NFFA site. This can be achieved by the development of software tools and web portals that allow the users to submit and manage computational jobs to complex hardware architectures (even distributed, such as grids) remotely, via a web interface. For the non-expert users the interface should be designed so as to select automatically and transparently most of technical and hardware-specific parameters. At the same time the interface should allow the expert user to customize and fine-tune the simulation run;

* <u>providing training and assistance</u> to the users who request access to the computational resources, both with direct, dedicated supervision as well as by organizing technical hands-on workshops and tutorials dedicated to the specific computational tools and methods offered at the facility;

* <u>developing novel theoretical approaches and methodologies</u> as well as optimizing the available implementations. Besides the software solutions for facilitating and automating the remote management of advanced computational facilities (see above), the theory facility should be a reference point for the development of new theoretical, numerical, and computational methods for the more efficient and accurate calculation of the spectroscopies and microscopies available in the NFFA centres. The most challenging and urgent issues on which the theory facility should focus include the accurate description of the excited states of molecular compounds or of complex nanostructures systems (starting from the gas phase but aiming at the complexity of liquid solutions), ultrafast spectroscopies, multiscale simulations with embedding or for accelerating rare events, and

molecular dynamics of excited states. We remark that, at present, there is no scientific network or project that address these issues in a coordinated way. We believe that the theory NFFA facility would be among the ideal candidates for such developments, which could be accelerated and stimulated by the close and intense interaction with experimental users and the materials' modelling community;

* developing a scientific program of in house research in selected scientific fields relevant to the NFFA centres. The research staff should be selected among the internationally recognized leaders in these fields so as to stimulate the interest of users to the facility.

The NFFA facility should be organized around a **multidisciplinary research group** of 4-5 independent staff members with diverse expertise and background. Their scientific profiles should cover the wide spectrum of NFFA research applications, and could be tentatively identified as

- nanoscale materials science and engineering / solid state physics / surface science;
- method development/ computational spectroscopy / many body theoretical physics;
- quantum chemistry / computational chemical physics;
- soft matter/statistical and biological physics/polymer theory;
- scientific software engineering.

Selected interest fields should include (but not be limited to) nanomechanics, nanoelectronics, materials for energy harvesting and conversion, soft matter and biological systems, self-assembly at surfaces and in solution, heterogeneous and homogeneous catalysis.

In analogy to the other NFFA facilities, the working time of the staff members should be distributed on equal footing between collaborative projects with specific users of approved projects (50%) and internal research programmes (50%). The users of the theory facility will be selected with the same procedures set up for the other facilities, which should be based on the review of external referees. On the basis of the information obtained from EU and USA theory facilities (European Theoretical Spectroscopy Facility, Molecular Foundry, Centre for Functional Nanomaterials, Brookhaven National Lab) as well as from our experience as theory group at a synchrotron laboratory, this NFFA theoretical facility could be expected to complete between five and ten users projects per year.

The **general methodology approach** of the computational facility will be multiscalar and multilevel, with a particular emphasis on the atomic level. The facility will therefore offer and use a variety of computational methods and approaches. These should allow for quantitative predictions of materials' properties at time and length scales as different as i) the optical electronic transitions in photo-excited heterogeneous nanostructures (requiring many-body perturbation theories), ii) the electronic ground states of large collections of independent atoms -from several tens up to hundreds (requiring Density Functional Theory approaches), iii) the kinetic and dynamical properties of materials such as molecular self-assembly (involving molecular dynamics with DFT or empirical forces), iv) rare events such as thermally activated processes and chemical reactions (requiring the use of accelerated dynamics), etc.. All of this for periodic crystals and disordered systems, complex heterogeneous materials such as molecular aggregates at surfaces or in solution, heterogeneous catalysts, low-dimensional nanostructures (nanotubes, nanowires or graphene), junctions, etc. Particularly relevant to the NFFA project will be the possibility to calculate spectroscopies (such as core-level photoemission, X-ray absorption, UV photoemission, Electron Energy Loss, Raman and Infra Red spectroscopies, also in the ultrafast regime), as well as to simulate Scanning Tunneling or High-resolution Transmission Electron Microscopy images. The accurate simulation of several of these spectroscpies and microscopies is already possible with the present status of theory and approximations. However, other cases, particularly those involving excited states or ultrafast dynamics, are still in their infancy and require theory and method development (see below).

In particular, **computational techniques** based on DFT, in combination with the Car-Parrinello (CP) first-principles molecular dynamics (MD), will be the central computational techniques of the NFFA theory facility. This approach is extremely popular both in the solid-state/material science, as well as in the soft matter/biophysics community, and is likely to provide the main core of the users support. In addition, one should have a scheme of integrating these approaches in higher levels of theory, for example when requiring a quantitative description of photoemission spectra or electron level alignment (in this case employing approaches based on many-body perturbation theory, such as the GW). Another example is a better estimate of reaction transition states and activation theories that can be achieved by employing quantum-chemistry methods. The methodology present in the NFFA facility should however also allow for lowering the level of theory with respect to the DFT one, by coarse graining the description of the system or considering empirical force fields. Finally it would also be desirable to combine different levels of theory, such as in hybrid QM/MM approaches.

One of the computational collaborative projects capable to offer this flexibility is the QUANTUM ESPRESSO project (www.quantum-espresso.org), coordinated by the CNR-IOM DEMOCRITOS centre in the premises of the NFFA headquarters. Its open access, modularity structure, dedicated software development environment (http://qe-forge.org), high diffusion in the community, performance and scalability on diverse high-performance parallel computers, as well as facility of use (also to the non specialist) make it the best candidate to be the computational pillar of the NFFA theory unit.

The **QUANTUM ESPRESSO** (QE) is an integrated suite of computer codes for electronic-structure calculations and materials modelling based on density-functional theory, plane waves basis sets and pseudopotentials to represent electron–ion interactions. QUANTUM ESPRESSO is free, open-source software distributed under the terms of the GNU General Public License. The basic computations/simulations that can be performed include: a) calculation of the Kohn–Sham orbitals and energies for isolated or extended/periodic systems, and of their ground-state energies; b) complete structural optimizations of the microscopic (atomic coordinates) and macroscopic (unit cell) degrees of freedom, using Hellmann–Feynman forces and stresses; c) ground state of magnetic or spin-polarized systems, including spin–orbit coupling and noncollinear magnetism; d) *ab initio* molecular dynamics, using either the Car–Parrinello Lagrangian or the Hellmann–Feynman forces calculated on the Born–Oppenheimer surface, in a variety of thermodynamical ensembles, including N P T variable-cell; f) density-functional perturbation theory (DFPT), to calculate second and third derivatives of the total energy at any arbitrary wavelength, providing phonon dispersions, electron–phonon and phonon–phonon interactions, and static response functions (dielectric tensors, Born effective charges, infrared spectra, Raman tensors); f) location of saddle points and transition states via transition-path optimization using the nudged elastic band method; g) ballistic conductance within the Landauer–Buttiker theory using the scattering approach; h) generation of maximally localized Wannier functions and related quantities; i) calculation of nuclear magnetic resonance and electronic paramagnetic resonance parameters; l) calculation of K-edge x-ray absorption spectra. The main components of the QUANTUM ESPRESSO distribution are designed to be expanded and integrated in a modular form. They can efficiently exploit massively parallel architectures by distributing both data and computations in a hierarchical way across available processors, ending up with multiple parallelization levels that can be tuned to the specific application and to the specific architecture. This remarkable characteristic makes it possible for the main codes of the distribution to run in parallel on most or all parallel machines with very good performance in all cases.

We remark that the **development of simulation packages and scientific software** is a recognized strength of the EU computational community with respect to the USA and Asian counterparts. Therefore, we consider particularly important for the success of the theory facility that it develops close links with existing and well-developed computational projects for the modelling of materials, such as QE. Ideally the NFFA theory facility should also aim at promoting the interoperability between different computational codes/approaches. For example by interfacing data obtained with one code (for example the QE package mentioned above) with others based on different principles (such as the CP2K project, http://cp2k.berlios.de/) or distributed by the European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu). In addition, it is desirable an active involvement of the NFFA theory facility into the relevant EU networks in the field of numerical simulation of materials, such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM, www.cecam.org), the ETSF, or the Psi-K network (www.psi-k.org).

The users and in-house research will require dedicated **resources for high-performance**, high-throughput, parallel computing. The precise requirement of computer power will be highly dependent on the specific projects. The resources will partly come from a local high-performance computing cluster (to be used for code and theory developing, for tuning the computational parameters, as well as for performing the preliminary routine/preparatory calculations). The production runs will instead be performed on massively parallelized computing resources to be negotiated with the main European supercomputing centres/networks/grids. On the basis of the present available technologies, a reasonable estimate for the local cluster consists of about 100 computational cores (each node with multiple motherboards containing multiple core processors) summing to about 1600-2000 computational cores.

NFFA theory facilities specifications:

- ~60 m^2 of technical room suitable for installing an initial set of 5 racks (3 dedicated to the computational nodes, 2 for the necessary switches, and 1 for the data storage). This dimension considers an expansion during the lifetime of the facility up to about 8-9 racks. The room should be equipped with facilities for its thermal control.
- A local high-performance parallel cluster of about 100 computational cores (each node with multiple motherboards containing multiple core processors) summing to about 1600-2000 computational cores.
- Office space for the 5 staff members and ~10 desks in an open space for the users/collaborators.

6.1.8 Instrumentation development

NFFA will develop instrumentation for nanoscience by prototyping, validating and adopting in its suite of methods original instrumentation. The tip enhancement of EM field is expected to allow for nanoscale sensitivity of extremely powerful diagnostics based on Raman spectroscopy for example. Tip control and shaping methods for STM/STS is also a key improvement for both atomic precision manufacturing as well as for atomic resolution analysis. Combination of space and time resolution in microscopy for example, based on fs laser pump sources and coupling to FEL analysis is expected to open fundamentally new possibilities of science.

These methods could be developed by NFFA and by NFFA users also thanks to design and manufacturing capability of the NFFA centres. Electronic, photonic and mechanic workshop along with design engineering and software support are to be included in the laboratory.

Instrumentation development will be one of the well defined topic of collaboration with industry, aiming both at the fabrication of innovative instruments and to their certification and proposal to become standard reference instruments in the field.

7. NFFA STAFF

A first estimation of the staff needed for a single NFFA centre is of about 70 people.

Additionally Ph.D.s and master students will be admitted to the centres for medium-long periods to perform their thesis work or specific science projects.

The facilities scientific staff has a twofold task: providing technical assistance and support to external users, and performing the in-house research programme. Training and assistance of active and potential users in the designing and performing the experiments and further developing the methods and instruments are included in the job profile of the NFFA researcher and, to a limited extent, engineers.

8. APPENDIX

How an NFFA facility compares to other centres as to the size of the laboratories and the staff?

As a comparison we mention here some key-figures, relative to few examples of existing facilities related to nanoscience and technology, but having different targets and mission with respect to the service to the scientific community and themes of main focus.

At one extreme we find in Europe the case of LETI.

LETI (http://www-leti.cea.fr/en) operates 8,000 m² state-of-the-art clean rooms, in 24/7 mode, on 200 mm and 300 mm wafer standards. With 1,200 employees, Leti trains more than 150 Ph.D. students and hosts 200 assignees from partner companies. Strongly committed to the creation of value for the industry, Leti puts a strong emphasis on Intellectual Property and owns more than 1,400 patent families. In 2008, contractual income covered more than 75% of its budget worth 205 M€. Comment: the huge size of the LETI facility derives from the fact that it is conceived mainly as a R&D centre reproducing industrial process has they are found in production facilities. The equipments are essentially the same as those in present in semiconductor production lines for 200 and 300 mm. We clarify here that this is a totally different target which leads to different size and cost of the facility compared to an NFFA centre.

Molecular foundry

Founded in 2006 by the Department of Energy (DOE), the Molecular Foundry,Berkeley, Ca, (http://foundry.lbl.gov), is a critical part of the DOE's National Nanotechnology Initiative, a multi-agency framework designed to improve human health, economic well-being and national security through leadership in nanotechnology. The Foundry supports broad nanoscience research efforts in both "hard" nanomaterials (nanocrystals, tubes and lithographically patterned structures) and "soft" nanomaterials (polymers, dendrimers, DNA, proteins and whole cells), as well as in the design, fabrication and study of multi-component, complex, functional assemblies of such materials.

Molecular Foundry, includes approximately 4,800 square feet of Class 100 cleanroom space, with a smaller Class 10 area for nanofabrication/lithography and clean measurement, and a 5,500 square-foot low vibration, low-electromagnetic-field laboratory housing state-of-the-art imaging and manipulation tools.

As a Scientific User Facility, the Molecular Foundry provides outside researchers ("Users") with the instrumentation, in-house expertise and multidisciplinary environment necessary to pursue research that can benefit from or contribute to nanoscience. From biologists, chemists and physicists, to biochemists, engineers and optics and photonics researchers, scientists from all over the world utilize the Foundry's state-of-the-art facilities at no cost, advancing research in critical fields in medicine, energy, computing and many other disciplines.

The **Centre for Nanoscale Materials** (CNM) (http://nano.anl.gov/) at Argonne National Laboratory is a premier user facility, providing expertise, instruments, and infrastructure for interdisciplinary nanoscience and nanotechnology research. Academic, industrial, and international researchers can access the centre through its user program for both non proprietary and proprietary research. The centre's goal is to support basic research and the development of advanced instrumentation that will help generate new scientific insights and create innovative materials with novel properties. The scientific portfolio includes energy-related research and development programs. The CNM is one of five U.S. Department of Energy (DOE) Office of Science Nanoscale Science Research Centres (NSRCs) dedicated to nanoscience and nanotechnology. It was constructed under a joint partnership between the DOE and the State of Illinois, as part of DOE's Nanoscale Science Research Centre program. Together the NSRCs comprise a suite of complementary facilities that provide researchers with state-of-the-art capabilities to fabricate, process, characterize, and model nanoscale materials, and they constitute the largest infrastructure investment of the National Nanotechnology Initiative. The laboratory is articulated into 5 internal facilities (http://nano.anl.gov/facilities/index.html) of: 1) Materials Synthesis. 2) Nanofabrication Research (controlled synthesis and directed assembly of nanomaterials; lithographically assisted patterning etc.) 3) Proximal Probes. 4) Dedicated Hard X-Ray Beamline at the APS In this facility 5) Computational Nanoscience

The **Centre for Functional Nanomaterials** (CFN) (http://www.bnl.gov/cfn/) at Brookhaven National Laboratory provides state-of-the-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions. The CFN is a science-based user facility, simultaneously developing strong scientific programs while offering broad access to its capabilities and collaboration through an active user program. The overarching scientific theme of the CFN is the development and understanding of nanoscale materials that address the Nation's challenges in energy security, consistent with the Department of Energy mission.

The centrepiece of the facility is composed of five state-of-the-art groups of laboratories called Laboratory Facilities, a Theory and Computational Centre, and a set of advanced endstations on beamlines at the NSLS. The Laboratory Facilities include forefront capabilities in nanopatterning, transmission electron microscopy, nanomaterials synthesis, ultrafast laser sources, and powerful probes to image atomic and molecular structure, together with clean rooms and other support instrumentation. Access is also offered to the Laser Electron Accelerator Facility (LEAF).

The Cornell **NanoScale Science & Technology Facility (CNF)** **(**http://www.cnf.cornell.edu/**)** is a national user facility that supports a broad range of nanoscale science and technology projects by providing state-of-the-art resources coupled with expert staff support. 2007 marked our 30th year in operation. Research at CNF encompasses physical sciences, engineering, and life sciences, and has a strong inter-disciplinary emphasis. Over 700 users per year (50% of whom come from outside Cornell) use the fabrication, synthesis, computation, characterization, and integration resources of CNF to build structures, devices, and systems from atomic to complex length-scales.

The Cornell Nanofabrication Facility is located in the Knight Laboratory on the Cornell University campus. The Knight Laboratory is a 20,000 square-foot building which was specifically designed and constructed by Cornell for the facility in late 1981. All of the instruments in the facility, with the exception of the computing equipment, are in the cleanroom. The cleanroom occupies 7,500 square-feet and is approximately Class 1000. Local processing benches within that cleanroom are Class 10. Careful consideration was given to the facilities for advanced lithography. Each of the rooms housing the electron-beam lithography systems are on concrete slabs isolated from the rest of the building foundation. Furthermore, the walls of these rooms are constructed with no embedded metal. The resulting environment has very low vibration (<50 nm at 3 Hz) and electromagnetic interference (<2 mG at 60 Hz). Extensive automatic safety systems are employed in the areas of the facility where hazardous gases are used.

Karlsruhe Nano Micro Facility (KNMF) (http://www.knmf.kit.edu/) is a high-tech platform for structuring and characterising a multitude of functional materials at the micro- and nanoscale.

The facility is focused on providing open and (for public work) free access to multimaterial state-of-the-art micro and nano technologies for users from industry and academia, either national or international.

The facility offers a laboratory for Micro- and Nanostructuring, a laboratory for Microscopy and Spectroscopy, laboratory for Synchrotron Characterisation, 22 technology clusters, 32 technology experts.

The range of nanolithography technologies includes: electron beam lithography deep x-ray lithography, laser material processing, injection moulding, hot embossing, focused ion beam, dip-pen nanolithography, thin film technologies, atomic layer deposition, dry etching cluster, nanoimprint lithography.

The range of Microscopy and Spectroscopy techniques includes: scanning electron microscopy, transmission electron microscopy, X-ray photoelectron spectroscopy, Auger electron microscopy, bulk and trace analysis of nanomaterials, electron micro-probe analysis, Laser ablation ICPMS, thin film characterisation methods, scanning probe technologies, atom probe tomography, NMR spectroscopy, atomic force microscopy cluster.

The synthesis and characterization laboratory includes: Hard x-ray microscopy and 3D tomographic imaging, High resolution synchrotron small angle x-ray scattering (SAXS), Infrared micro and nanospectroscopy, In-situ powder diffraction, Laboratory diffractometry under non-ambient conditions, Soft x-ray spectroscopy, microscopy, and spectromicroscopy.