NMP4-CT-2004-500198

Nanoquanta

Nanoscale Quantum Simulation for Nanostructures and Advanced Materials

Executive Summary

Year Three

Instrument: *Network of Excellence*

Thematic Priority: *Nanotechnology and nanosciences, knowledge-based multifunctional materials and new production processes and devices (NMP)*

Period covered: from 1st June 2006 to 31st May 2007 Date of Preparation: 15th July, 2007

Start date of project: 1st June, 2004 Duration of project: 4 years

Co-ordinator: Professor Rex Godby, University of York

Section 0

Executive Summary

In its third year, the *Nanoquanta* NoE has made substantial progress in its major integration objective of the establishment of the European Theoretical Spectroscopy Facility (ETSF), including the successful completion of the first call for proposals from ETSF users, and the initiation of the resulting selected pilot projects. *Nanoquanta* has also continued its strong tradition of integrated scientific activity with significant scientific results published in all its scientific areas. Training and career development for young researchers has continued apace at both local and network-wide level, with our community of researchers becoming strongly integrated, not just at the strategic level of individual research groups, but also at the level of individual researchers. The network has made progress in the field of code integration, code distribution, interoperability and user interfaces – crucial for both the network's own future research and the operation of the ETSF – and the network's employment of full-time programming specialists is bearing fruit. Three major funding proposals for the continuation of the ETSF's operation and our scientific activity have been submitted, in addition to several smaller projects at national or regional level.

The network encompasses 120 scientists in ten research teams, together with a small number of Associate Members who are former members of network groups continuing to work with us on Nanoquanta work packages. Scientifically, the network employs a wide range of theoretical and computational methods to study electrons in nanostructures and materials and their interaction with light, particularly density-functional theory and many-body perturbation theory.

The work is divided into nine work packages, with each contractor contributing to the planning of every work package, and to the delivery of most work packages. Each work package corresponds to an "Integration Team", drawn from several contractors, which manages the work package. The contractors are:

- University of York (United Kingdom)
- Fritz-Haber-Institut, Berlin (Germany)
- Freie Universität, Berlin (Germany)
- Friedrich-Schiller-Universität, Jena (Germany)
- Université Catholique de Louvain (Belgium)
- Lunds Universitet (Sweden)
- Universitá degli Studi di Milano (Italy)
- Laboratoire des Solides Irradiés (France) [1]

[1] "Unité mixte de recherche" of the three contractors Centre National de la Recherche Scientifique, Commissariat á l'Energie Atomique and École Polytechnique.

- Istituto Nazionale per la Fisica della Materia (Rome "Tor Vergata", Italy)
- Universidad del País Vasco / Euskal Herriko Unibertsitatea (Spain)

The ETSF is a major intended outcome of the network. The ETSF is intended to become the worldwide reference centre for the theory of spectroscopies in condensed matter. Two of our integration teams, IT1 and IT3, are dedicated to the development of the ETSF and the fostering of external scientific relations through the vehicle of the ETSF.

Integration Team 1, "Establishing the Infrastructure of the ETSF", has as its objectives to identify the scope, role and target audience for the European theoretical spectroscopy facility (ETSF); explore possible structures for the ETSF and their implementation; ensure the legal, administrative and financial support from industry, research facilities and academic institutions; secure internal and external funding for the ETSF; set up the elementary infrastructure for an efficient implementation of the ETSF; and create an efficient intra-network information source related to this IT. Progress towards these objectives has proceeded well. Following an intensive publicity campaign directed at potential ETSF users, which included production of an attractive leaflet, creation of the new ETSF web site, and publicity in several spectroscopy-oriented newsletters and bulletins, we launched the ETSF's first call for proposals in March 2007, and selected several pilot projects from among the 54 proposals received. In addition, IT1 has spearheaded the preparation of three major EU funding proposals: an e-infrastructure I3 proposal which will continue to make the ETSF accessible and suited to the needs of users[2], and two ITN proposals to continue the ETSF's and *Nanoquanta*'s strong record in training PhD students[3]. Further ETSF-related funding has been applied for, and obtained, by individual *Nanoquanta* nodes. All this IT1 activity has been made possible by intensive activity, including fortnightly audioconferences of the Integration Team, and the appointment of a full-time administrator for IT1 to help operate and plan the ETSF.

The other ETSF-related integration team is Integration Team 3, "External relations", whose objectives are to promote the impact of the NoE, its targets and activities as one integration instrument in the new European Research Area; to design a strategy to interact with experimental and industrial entities; to monitor the needs and interests of SMEs and establish links with existing industrial networks; to bridge the gap between existing competence in the NoE and needs of experimental groups and industrial companies; to promote training and formation of industrial staff; to promote the transfer of young researchers of the NoE to industry and large scale European infrastructures; to publicise and disseminate activities in research, support and training of the ETSF; and to be aware of ongoing work in similar fields, and to promote the NoE work outside Europe. We recognise that all these matters are best pursued through the vehicle of the ETSF, and so the operation of IT1 and IT3 have been combined.

The principal objectives of Integration Team 2, "Training and Reach- Out", are the development of technical platforms and the stimulation of communication within the network, the training and enhanced mobility of researchers as well as the external promotion of network activities through scientific meetings and public dialogue. In this way, the network contributes to the qualification and growth of the community of scientists working in nanoscience in Europe. At the same time, it encourages collaborative efforts and actively spreads the results of network research both within scientific circles and the general public. In Year 3, *Nanoquanta* has organised or sponsored three training events: a major hands-on school in Benasque, a CECAM tutorial and the Epioptics-9 school. The network has organised its major annual scientific workshop in Houffalize and its now annual Young Researchers' Meeting in San Sebastián. Communication between network researchers has continued at a high level, through a regular newsletter, a fortnightly scientific bulletin, active members' web sites and mailing lists, and above all the now

[2]We have recently learnt that this e-infrastructure I3 proposal has been successful.

[3]We have recently learned that one of these proposals is to proceed to the second stage of application.

very marked coherence of our researchers as an integrated unit (most clearly visible, perhaps, in the excellent cooperative scientific spirit exhibited at the Young Researchers' Meetings, extending not only to the establishment of new research collaborations but also to ideas about the strategic organisation and role of the ETSF).

The objective of Integration Team 4, "Social issues", are to create an effective policy on social issues in general and particularly with regard to young scientists appointed by the nodes. This policy, as developed in the *Nanoquanta* Network will also determine our long-term strategy for social issues for the future ETSF. The aim is to forge the ETSF into a centre which sets an example of a humanistic approach to science and research. The *Nanoquanta* active social policy, including the mentoring scheme, continues to prove successful and forms a model which plays a central role in ETSF planning.

Integration Team 5, "Isolate a Zero-Dimensional Structure and Conquer its Environment", has as its objectives to describe and understand zero-dimensional systems of biological and technological interest, and to investigate their interaction with the environment. This has resulted in 47 publications produced in Year 3, in the following main areas: Towards biological molecules, Photo-Technology, Transport, and Electron-ion dynamics.

Integration Team 6, "One-dimensional Systems and their Composites", has produced 34 publications in Year 3 in the following areas: quantum transport theory; phonon and electron-phonon interaction in 1D structures; study and characterization of magnetic response; calculation of the electronic structure and spectroscopic properties of 1D structures, their composites, and the role of environment; and formulation of a dynamical formalism for the description of excited-state chemical reactivity in bio-structures.

Integration Team 7, "Computing Total Energy and Excited States at Surfaces and Interfaces", has produced 41 publications in Year 3 in pursuance of the following objectives: improving total energy methods; *ab initio* methods for excited states; nanowires on nanostructured surfaces; organic overlayers on surfaces; dynamics of chemical reactions at surfaces; interfaces and grain boundaries; and electronic excitations in thin films.

Integration Team 8, "Fundamental Knowledge for Advanced Materials", aims to investigate ground state and in particular excited state properties of advanced materials, including magnetic materials and superconductors, as well as materials with stronger electronic correlation. This has resulted in 55 publications in Year 3, including the Rome node's study of liquid water, which is the first *ab initio* application of many-body perturbation theory to a liquid.

The work of Integration Team 9, "Integration of theory and code developments", aims to realise an integration of the work of the different nodes at the level of theory developments as well as code developments. Specific objectives for the work packages are to standardise the input and output files, to allow data exchange between different programs; to elaborate coding standards, also for documentation, that allow cross-checking and integration of routines from different programs; and to foster the integration of theory developments within the network, and the transfer between theory and code development. In Year 3 a mini-workshop on standardization of input and output files was held in San Sebastián. Most importantly, this resulted in a detailed NetCDF-based specification of a *Nanoquanta* file format for exchange of wavefunctions, densities and other critical data, and this has been implemented in most of our main codes. Further code interfaces have been completed. There have been numerous advances related to new implementations of theory in the different codes. The allocated funds for the employment of three professional programmers to assist with preparing various codes for easy usability within the context of the future ETSF is bearing fruit in the shape of the usability and power of several of our codes. IT9 has designed a Linux-based "live CD" for free distribution which allows 6 of the ETSF/Nanoquanta codes to be run on any PC. The workpackage also produced 9 publications in Year 3.

The network has detailed provisions to ensure that Intellectual Property (IP) generated by the project is properly and fairly disseminated and/or exploited. The network regularly reviews the status of IP generation and works with participant institutions to encourage dissemination and/or exploitation, consistent with the Consortium Agreement. Once proper regard has been had for protection of IP, our research is widely disseminated in the international scientific literature, at international conferences, at our network conferences and schools, and through our *Nanoquanta* web site. Several of the network's computer programs are already available under cost-free or commercial licences.

The overall scientific achievements of *Nanoquanta* may be measured by the following statistics for Year 3:

- 157 publications, including 49 joint publications (two or more *Nanoquanta* nodes) (31% of total)
- 15 papers in Physical Review Letters and 2 in Applied Physics Letters
- 140 invited talks

Nanoquanta Network of Excellence web site: `http://www.nanoquanta.eu/`
ETSF web site: `http://www.etsf.eu/`

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