NMP4-CT-2004-500198

Nanoquanta

Nanoscale Quantum Simulation for Nanostructures and Advanced Materials

Final Report

Publishable Summary

Instrument: *Network of Excellence*

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

Period covered: 1st June 2004 - 30th November 2008 Date of Preparation: 14th January, 2009

Start date of project: 1st June, 2004 Duration of project: 4½ years

Co-ordinator: Professor Rex Godby, University of York

Contents

Section 1

Project execution

The *Nanoquanta* Network of Excellence (1 June 2004 - 30 November 2008) has completed its work with major achievements, integrating the research of ten European groups in the theory and simulation of excited electrons in matter. The European Theoretical Spectroscopy Facility (ETSF), which is now in full operation, interacting strongly with users in experimental science and industry, was a major objective of the network. *Nanoquanta* has also achieved many significant scientific research results published in leading journals. Training and career development for young researchers has been a high priority at both local and network-wide level, with our community of researchers now strongly integrated, not just at the strategic level of research groups, but also at the level of individual researchers. The network has achieved important developments in the field of code integration, code distribution, interoperability and user interfaces, all of which are crucial for both the network's own future research and the operation of the ETSF. A major "e-Infrastructure" grant within the seventh Framework Programme for the continuation of the ETSF's user-facing operation has been successfully started, in addition to several smaller projects at national or regional level.

The network encompassed 150 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 employed 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. Over the course of *Nanoquanta*, the *ab initio* theory of electron spectroscopies has been in rapid development and expansion internationally, and *Nanoquanta* has made a very prominent contribution to this, both in terms of applications and in terms of development of the underlying theory and software. In many-body perturbation theory, our main techniques (the GW method for the one-particle spectral function and the BSE method for the optical absorption and EELS spectra) have moved from exotic theories being applied to simple prototype systems to powerful daily workhorses that can be applied to rather complex molecules, nanostructures and advanced materials. The other main technique used in *Nanoquanta*, time-dependent density-functional theory (TDDFT), has burgeoned, with many successful applications to response functions, optical properties and time-dependent phenomena of all kinds.

The contractors were:

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

The ETSF is a major achievement of the network. The ETSF aims to be the worldwide reference centre for the theory of spectroscopies in condensed matter. In addition to integrating leading research groups, its innovative feature is a new model for the interaction of theoretical research with the needs of experimental and industrial users, through regular calls for project proposals from those users. Over the course of *Nanoquanta*, the ETSF has been created and has bloomed into a fully operational facility, including three successful calls for user projects, attracting over 100 proposals, with the necessary scientific, management, administrative and user-liaison support structures in place and highly developed. The ETSF now has a formally designated Central Node, the Université Catholique de Louvain in Louvain-la-Neuve, which brings with it substantial financial support for the user-facing operation of the ETSF from the UCL and the Walloon Region, including the establishment of a senior Chief Executive position and a further administrative position. New ETSF Associate Nodes have been added. Further ETSF-related funding, including for permanent positions, has been applied for, and obtained, by individual ETSF nodes. An e-Infrastructure project, funded by FP7, is in operation (2008-10), and this is allowing the ETSF to continue and expand its service to users through regular calls for proposals. All this activity has been made possible by intense activity, including fortnightly ETSF administrative audioconferences.

The ETSF has achieved substantial publicity among potential users (in science and industry) and the broader scientific community and public, which have contributed to the three successful calls for user proposals. Also, the ETSF has a comprehensive and accessible web site has been totally redesigned and improved, with new underlying databases providing a sound basis for future expansion, especially regarding the submission and monitoring of user projects.

Training and Reach-Out has also been a key theme of *Nanoquanta*. 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. *Nanoquanta* has organised a total of eleven training schools, together with many more scientific conferences and workshops (including the innovative annual *Nanoquanta*/ETSF Young Researchers' Meeting). Internal communication has been vigorous, through e-mail lists, newsletters, bulletins, and the internal web sites. Over 50 PhD students have been trained collaboratively within the network's own groups: a supply of such skilled researchers who are used to working collaboratively across Europe is of great importance for the future of scientific research in general, and the future operation of the ETSF in particular.

The *Nanoquanta* Network has taken an active stance on social issues, developing a progressive policy on social issues in general and particularly with regard to young scientists appointed by the nodes. This policy also determines our long-term strategy for social issues for the ETSF. Examples include rules for recruitment strategy, provision of a créche at all scientific meetings, and a cross-node mentoring scheme for all young researchers.

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

Integration of theory and code developments has been an important theme, to ensure that the ETSF is able to offer an integrated suite of software to users that is as powerful as possible. This work aims to realise the 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. The main ETSF codes are available under the GNU Public License through the ETSF web site.

Closely linked to the creation and operation of the ETSF, of course, has been continued scientific progress and collaboration at the forefront of research between the ten *Nanoquanta* groups, overseen by the network's four scientific integration teams. The network has published 602 publications, including 176 joint publications (two or more *Nanoquanta* nodes) (29% of total). These include 74 papers in Physical Review Letters (plus two accepted), 10 in Applied Physics Letters, 1 in Nature and 1 in Nature Materials. *Nanoquanta* members have given 576 invited talks at conferences, meetings and external institutions on network research. Among the scientific highlights are work on electronic excitations in biological-related systems, photo-technology, transport in finite systems and electron-ion dynamics, 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, excited-state chemical reactivity in bio-structures, 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, electronic excitations in thin films, extension of many-body perturbation theory beyond the GW level, inclusion of phonon effects on the electronic spectra, using many-body perturbation theory to benefit the TDDFT description of optical spectra of matter, defects in silicon carbide, and optical properties of liquid water.

The *Nanoquanta* collaboration moves confidently into its next phase of development, under the banner of the ETSF, as a closely integrated scientific force operating at the international forefront of theoretical research, with a unique commitment to responsiveness to the needs of experimental and industrial scientists, together with a strong tradition in training and the development of its young researchers.

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

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Section 2

Publishable results

The major results of the project are published in the form of the many scientific papers already published, listed below. In addition, software, information and training material produced by the *Nanoquanta* project is publicly available for download through the ETSF web site[1], through which proposals for future ETSF user projects may also be submitted.

References labelled "NQ*" are jointly-produced, those labelled "NQ" are not.
This list shows all *Nanoquanta* papers published during the project; not all have necessarily been cited in reports.

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