



EUROPEAN COMMISSION  
RESEARCH DG HUMAN RESOURCES  
AND MOBILITY

RTN Periodic Activity Report

**Project No.:** 506842

**Project Acronym:** NANOQUANT

**Project Full Name:** Understanding Nano-Materials From the  
Quantum Perspective

## Marie Curie Actions

# RTN Periodic Activity Report

**Period covered:** from 01/04/2005 to 31/03/2006

**Date of preparation:** 12/05/2006

**Period number:** 2nd

**Start date of project:** 01/04/2004

**Date of submission (SESAM):**  
12/05/2006 13:04:46 CET

**Project coordinator name:**  
Prof. Hans Ågren

**Duration:** 36

**Project coordinator organisation name:**  
KUNGLIGA TEKNISKA HOEGSKOLAN

**Version:** 1

# Marie Curie Actions

## RTN Periodic Activity Report

### GENERAL INFORMATION

<b>Project No.:</b>	506842
<b>Project acronym:</b>	NANOQUANT
<b>Project full name:</b>	Understanding Nano-Materials From the Quantum Perspective
<b>Period number:</b>	2nd
<b>Period covered - start date:</b>	01/04/2005
<b>Period covered - end date:</b>	31/03/2006
<b>Project start date:</b>	01/04/2004
<b>Project duration [months]:</b>	36
<b>Project coordinator name:</b>	Prof. Hans Ågren
<b>Project coordinator organisation name:</b>	KUNGLIGA TEKNISKA HOEGSKOLAN
<b>Date of submission:</b>	12/05/2006

## SUMMARY OF THE RECRUITMENT DURING THE REPORTING PERIOD

**Contractor:** KUNGLIGA TEKNISKA HOEGSKOLAN

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Cornel Oprea	ESR (<4 years)	RO-Romania	No	Male	01/04/2004	31/03/2007	12
Guangde Tu	ESR (<4 years)	CN-China (People's Republic of)	No	Male	01/10/2004	31/03/2007	12
Jun Jiang	ESR (<4 years)	CN-China (People's Republic of)	No	Male	01/12/2005	30/11/2006	4

**Contractor:** SYDDANSK UNIVERSITET

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Emanuel Rubensson	ESR (<4 years)	SE-Sweden	Yes	Male	01/10/2005	30/09/2006	6
Ville Weijo	ESR (<4 years)	FI-Finland	Yes	Male	01/01/2006	31/12/2006	3

**Contractor:** UNIVERSITETET I OSLO

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Erik Tellgren	ESR (<4 years)	SE-Sweden	Yes	Male	11/11/2004	31/03/2007	12
Alex Cavallini	ESR (<4 years)	IT-Italy	Yes	Male	11/03/2005	10/10/2005	7

**Contractor:** UNIVERSITY OF HELSINKI

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Ying-Chan Lin	ESR (<4 years)	TW-Taiwan	No	Female	01/04/2004	30/09/2006	12

**Contractor:** JOHANNES GUTENBERG UNIVERSITAET MAINZ

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Rafal Adam Bachorz	ESR (<4 years)	PL-Poland	Yes	Male	01/10/2005	31/03/2007	6

**Contractor: CONSIGLIO NAZIONALE DELLE RICERCHE**

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Angelika Baranowska	ESR (<4 years)	PL-Poland	Yes	Female	01/07/2004	30/06/2005	3
Branislav Jansik	ER (4-10 years)	SK-Slovakia	Yes	Male	01/08/2004	31/01/2006	10

**Contractor: UNIVERSIDADE DE SANTIAGO DE COMPOSTELA**

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Jonathan Keith Vincent	ER (4-10 years)	UK-United Kingdom	Yes	Male	01/10/2004	31/12/2004	0
Sankha Ghosh	ESR (<4 years)	IN-India	No	Male	01/12/2004	30/06/2005	3

**Contractor: UNIVERSITY OF TARTU**

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Dana Martin	ESR (<4 years)	RO-Romania	No	Female	01/03/2005	31/03/2007	12
Maxim Bespalov	ESR (<4 years)	RU-Russian Federation	No	Male	01/02/2006	31/12/2006	2

**Contractor: INSTITUTE OF ORGANIC CHEMISTRY - POLISH ACADEMY OF SCIENCES**

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Andrej Antusek	ER (4-10 years)	SK-Slovakia	Yes	Male	01/09/2004	28/02/2006	11

**Contractor: THE UNIVERSITY OF WARWICK**

Name of the Researcher (as stated at time of selection)	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months covered by this recruitment during this reporting period
		Country	LFR				
Elias Rudberg	ESR (<4 years)	SE-Sweden	Yes	Male	15/11/2005	14/11/2006	4
Espen Tangen	ESR (<4 years)	NO-Norway	Yes	Male	21/11/2005	20/07/2006	4
Natalie Gilka	ESR (<4 years)	DE-Germany	No	Female	01/03/2006	14/11/2006	1

## SUMMARY OF THE EMPLOYMENT FORECAST FOR THE NEXT REPORTING PERIOD

**Contractor:** KUNGLIGA TEKNISKA HOEGSKOLAN

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Cornel Oprea	ESR (<4 years)	RO-Romania	No	Male	01/04/2004	31/03/2007	12
Guangde Tu	ESR (<4 years)	CN-China (People's Republic of)	No	Male	01/10/2004	31/03/2007	12
Jun Jiang	ESR (<4 years)	CN-China (People's Republic of)	No	Female	01/12/2005	30/11/2006	8

**Contractor:** SYDDANSK UNIVERSITET

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Emanuel Rubensson	ESR (<4 years)	SE-Sweden	Yes	Male	01/10/2005	30/09/2006	6
Ville Weijlo	ESR (<4 years)	FI-Finland	Yes	Male	01/01/2006	31/12/2006	9
Kestutis Aidias	ESR (<4 years)	LT-Lithuania	Yes	Male	01/07/2006	31/03/2007	9

**Contractor:** UNIVERSITETET I OSLO

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
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Erik Tellgren	ESR (<4 years)	SE-Sweden	Yes	Male	11/11/2004	31/03/2007	12
Alex Cavallini	ESR (<4 years)	IT-Italy	Yes	Male	11/03/2005	10/10/2005	0

**Contractor:** UNIVERSITY OF HELSINKI

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
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Ying-Chan Lin	ESR (<4 years)	TW-Taiwan	No	Female	01/04/2004	31/03/2007	12

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Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Attila Tajti	ESR (<4 years)	HU-Hungary	Yes	Male	01/10/2006	31/12/2006	3
Tommy Vänskä	ESR (<4 years)	FI-Finland	Yes	Male	01/09/2006	28/02/2007	6

**Contractor:** CONSIGLIO NAZIONALE DELLE RICERCHE

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
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Angelika Baranowska	ESR (<4 years)	PL-Poland	Yes	Female	01/07/2004	30/06/2005	0
Branislav Jansik	ER (4-10 years)	CZ-Czech Republic	Yes	Male	01/08/2004	31/12/2005	0

**Contractor: UNIVERSIDADE DE SANTIAGO DE COMPOSTELA**

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Siham Naima Derrar	ESR (<4 years)	DZ-Algeria	No	Female	01/05/2006	31/10/2006	6
Juan Pablo Senosiain	ER (4-10 years)	MX-Mexico	No	Male	01/09/2006	04/04/2007	7
Stefan Bilan	ESR (<4 years)	RO-Romania	No	Male	01/05/2006	30/11/2006	7

**Contractor: UNIVERSITY OF TARTU**

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Dana Martin	ESR (<4 years)	RO-Romania	No	Female	01/03/2005	31/03/2007	12
Maxim Bepalov	ESR (<4 years)	RU-Russian Federation	No	Male	01/02/2006	31/12/2006	9

**Contractor: INSTITUTE OF ORGANIC CHEMISTRY - POLISH ACADEMY OF SCIENCES**

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
		Country	LFR				
Andrej Antusek	ER (4-10 years)	SK-Slovakia	Yes	Male	01/09/2004	31/08/2005	0

**Contractor: THE UNIVERSITY OF WARWICK**

Name of the Researcher	Type	Origin		Gender	Start date of recruitment (dd/mm/yy)	End date of recruitment (dd/mm/yy)	No. of full-time equivalent months in the next reporting period
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Elias Rudberg	ESR (<4 years)	SE-Sweden	Yes	Male	15/11/2005	14/11/2006	8
Natalie Gilka	ESR (<4 years)	DE-Germany	Yes	Female	01/03/2006	31/10/2006	7

# PROJECT ACHIEVEMENTS DURING THE REPORTING PERIOD

## Research Achievements

### Scientific Achievements

During the second year the NANOQUANT project has been widened both with respect to the basic science objectives and the applications. We have continued with the development of the rigorous electronic-structure toolbox, applicable at the nanoscale and intended for the prediction of properties, for the interpretation of properties, and for testing simpler models with wider ranges of applicability. Our goal has been to act as an active modelling unit, providing theoretical support to experimental activities such as synthesis, materials characterization, and the "design of devices". The project objectives of the NANOQUANT network was formulated in terms of mathematical simulations of materials in order to describe their properties, spectra, reactions, and interactions which has become an increasingly viable approach in contemporary research, covering a wide range of phenomena of technical as well as fundamental importance. Adhering to the general philosophy of such modelling, the ultimate goal of the present project was to model and understand nanomaterials from a rigorous quantum perspective. This understanding is to be accomplished by transcending the traditional boundaries of rigorous electronic-structure simulations, from the scale where each atom makes a difference to the scale where the bulk properties can be derived. In doing so, materials fabricated at the nanoscale will be covered. All these ambitions have been well honoured during the second year of the network.

Considering nanoscale quantum modelling an essential objective of the network is to transfer the scale of quantum modelling from the atomic domain into the nano domain. Without its fulfilment, we cannot hope to reach the other objectives of understanding nanomaterials from a quantum perspective and of modelling materials of technological interest. A primary target of the network was therefore to consolidate the linear-scaling techniques (i.e., techniques with a cost proportional to the system size) developed under our previous FP5 network MOLPROP, extending their applicability range into the nano regime, beyond 10.000 atoms. This cannot be achieved merely by utilizing high-performance computing technology; it also depends critically on the development and adaptation of new computational schemes.

For example, although we already have the technology necessary for calculating the potential generated by thousands of atoms in density-functional theory (DFT), we are not yet in a position to solve efficiently the self-consistent field equations that these potentials give rise to for more than a few hundred atoms. To eliminate the diagonalization bottleneck in self-consistent field theories such as Kohn-Sham (KS) DFT and Hartree-Fock (HF) theory, we propose to optimize the one-electron density matrix directly, invoking an exponential ansatz for the atomic-orbital density matrix. Moreover, although the routine energy optimization for several thousand atoms is essential to our development of a scale-extensive technology, its potential can only be fully realized by the development of a companion technology for properties such as forces, excitation energies, frequency-dependent polarizabilities, and magnetic-resonance parameters. For large systems, these properties will be calculated using the exponential density-matrix ansatz.

We aimed to develop methods that enable a mixed classical/quantum-mechanical description of the processes in homogeneous and heterogeneous solution and biological systems by combining the quantum-mechanics/molecular-mechanics (QM/MM) model with models of heterogeneous and homogeneous solvation, thereby enabling the study of nonlinear processes of molecular systems solvated or attached to metal surfaces and nanoparticles. In these calculations, the electronic structure of the solvated compound is rigorously described by ab initio or DFT electronic-structure theory, with the polarization of the surrounding medium included in the quantum-mechanical equations.

We have reached considerable achievement in this area, central to the network: We have developed and improved existing routines for fast multiple moment technology for the evaluation of Coulomb interaction: A concomitant algorithm for linear scaling of the exchange interaction has been developed and will soon be put into operation: A so-called density purification scheme has been implemented and made efficient for diagonalization - free optimization, thereby removing an

essential bottleneck for very large systems: Sparse matrix algebra, enabling maintenance of linear scaling on large systems beyond 100 atoms: Implementation of elongation method for very large (50 1000 nm) quasi 1-dimensional systems, with applications in electronics.

In all this has put us in a position to study linear and non-linear properties for systems with up to 1000 atoms. Applications have been made on various optical, magnetic, electric and structural properties of large molecules. For instance we have studied an artificial so-called affibody complex that mimics the functionality of common protein antibodies. The linear scaling code has been applied for a variety of new density functional, some of them developed within the network (CAMB3LYP).

The large-scale developments of high-level correlation methods have the goal to enable rigorous calculations of molecular properties to chemical accuracy, they are also important in that they provide capabilities for benchmarking and tests of DFT. Such benchmarking will be actively pursued in the present project. In ab initio theory, work towards reduced scaling of computational cost focuses on coupled-cluster theory, including the use of Cholesky decomposition, Laplace transforms, and resolution-of-identity (density-fitting) techniques} as well as the exploration of local correlation schemes with integral pre-screening. In addition, new cost-efficient techniques with explicit inclusion of the interelectronic distances within the framework of coupled-cluster theory will be developed for both closed- and open-shell systems. Such methods are essential for the achievement of chemical accuracy for any but the smallest systems.

During the second year the development of coupled cluster schemes for larger molecules has been made possible by implementation of a  $N^6$  scheme for the CCSD(T) method using orbital-energy decomposition techniques. Various decomposition schemes have been used; the Cholesky decomposition suggested in the literature decompositions based on a rational approximations. A first parallel version of the CCSD(T) code (within the quantum chemistry program package aces has been completed which extends the applicability of the CCSD(T) approach further. Thus, calculations with more than 800 basis functions have become possible and calculations with more than 1000 basis functions are currently planned.

Multi-configurational relativistic DFT has been pursued during the second year in order to study and develop the basic aspects of electronic-structure theory. In particular, our aim was to focus on the role of spin and spin states in open-shell systems, which is of fundamental importance for processes involving radical species such as enzyme catalysis, for transition-state approaches and chemical reactions in general. A formulation of an orbital-restricted spin-dependent DFT with rigorous spin-dependent density functional is therefore a prime goal in NANOQUANT. An associated, closely related, goal is the development of a general correlation approach that combines the dynamical correlation recovered by DFT} with the near-degeneracy correlation recovered by multi-configurational reference expansions. This versatile approach to electron correlation is to be implemented in such a manner that it accommodates other important elements in the network---that is, four-component relativistic electronic-structure theory, the fourth-order property toolbox, and the techniques of linear scaling.

During the second year we have derived, implemented and presented the first applications of the generalized restricted-unrestricted method based on the density functional - Kohn-Sham - formalism. By using a spin-restricted Kohn-Sham representation for the reference state the well-known spin contamination problem is avoided, while the unrestricted representation of the perturbation response retains a proper description of spin polarization. This solves, to a large extent, the notorious problem of computing properties in open-shell systems using density functional theory, which we consider to be a major achievement in line with the proposed network goals. This, we believe, will in conjunction with the linear scaling technology have a large impact on the use of modelled magnetic resonance parameters to derive structure of biological molecules.

With NANOQUANT we want to pursue the work of the previous network MOLPROP - Molecular properties and Molecular Materials - and compute general properties of Nano-sized systems. This follows from the fact that it is through the measured properties than molecules and materials are characterized, and it is therefore important to make the theoretical models - e.g. linear scaling methods - applicable for properties. For instance, the internal molecular field such as those generated

by spinning nuclei and electrons, although exceedingly weak, provides numerous possibilities for diagnostics of materials by spectroscopy. Simulations of the magnetic resonance parameters generate indispensable information about materials such as their conformational structure and chemical bonding. NANOQUANT research is aimed to focus on the modelling of various magnetic resonance processes---namely, nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and optically detected magnetic resonance (ODMR). Modelling of spectroscopic processes in other regions of the electromagnetic spectrum was also projected: vibrational Raman optical activity (VROA) in the infrared region, natural and magnetically induced circular dichroism in the optical region, and Raman scattering in the X-ray region. Many theoretical and computational studies have been performed during 2nd year of static and frequency dependent molecular properties connected to various types of optical processes, birefringences and dichroisms induced by external fields at different levels of theory (Coupled Cluster, Density Functional Theory etc.). Projects involving several YRs hired by the network. Studies of Linear and nonlinear response to magnetic perturbations, hypermagnetisabilities, nuclear magnetic shielding, nuclear spin-spin coupling have been carried out. Much work has involved calculations of spin-rotation constants using coupled-cluster techniques. A novel approach to calculate magnetically induced current densities in molecular systems have been developed and applied to fullerenes. A new computational method was also developed for efficient real-space calculations of electrostatic potentials. Furthermore, studies and theoretical simulations of spectroscopes using synchrotron radiation aimed at supporting the interpretation of results obtained by experimental techniques (XPS, NEXAFS, AUGER, resonant AUGER) particularly convenient to study films of organic molecules, polymers and peptides on metallic surfaces, that are considered important classes of new "nano-materials" (Project involving the YR). All this work has been accomplished in tight collaboration between various node partners, most of them also involving hired YRs.

"Molecular and nano-electronics" and "molecular and nano-photonics" have formed the two most important high end goals of NANOQUANT. During year 2 we have accomplished a considerable advancement in these two important areas. A long-standing goal of molecular electronics has been to replace semiconductors by individual molecules so that electronic devices can be produced orders of magnitude smaller than their current semiconductor counterparts. Recent years, in particular, have witnessed a rapid development in the fabrication of nanosized molecular devices based on the use of single molecules or molecular strands. The physical principles underlying these devices are, nevertheless, largely unknown. The goal of the NANOQUANT work in this area was to gain more of the necessary understanding of the physical and chemical processes involved, to develop efficient computational approaches to simulate the electron transportation in molecular devices, and ultimately to use these techniques to improve device performance. The necessary tools and techniques for this work were to be integrated into our existing toolbox. A goal was to predict the optimal size and shape for metal contacts and molecular bridges of devices such as switches and transistors. A particular emphasis was put on conductivity of nanotubes and biological molecules. Within the network we have developed new first-principles computational methods that enabled to effectively treat very large nano-scale systems (elongation method). This has made it possible to address electronic structures and the coherent electron transport properties of these systems, and the prediction of entirely new physical and chemical phenomena. This generalized quantum chemical approach for electron transport has allowed treating the devices where metal and molecule are chemically or physically bonded on equal footing. Effects of molecular length, hydrogen bonding and inter-molecular charge transfer on the I-V characteristics of molecular devices have been studied. The approach can also provide accurate predictions of inelastic electron tunnelling spectroscopy of molecular junctions. Studies have included self-assembled conjugated polymers, carbon nanotubes, and DNA molecules that are several hundred nanometer long, containing more than 100,000 electrons.

Concerning molecular and nano-photonics, a task of the proposed NANOQUANT network has been to consolidate and extend the functionality of the existing fourth-order toolbox for electromagnetic properties to the nanoscale regime, involving the adaptation of density-matrix based HF and KS response theory. Subsequently, this toolbox is to be augmented with a program for the study of the propagation of electromagnetic pulses in nonlinear media. During the second year we have been able to merge the quantum-mechanical electronic-structure methodology with classical dynamical theory of pulse propagation into a versatile toolbox for simulations of the influence of laser characteristics on the properties of materials in general and of photonic devices in particular. These simulations

highlight the roles of pulse duration, dephasing, and resonant conditions on the transient cross sections, as well as the interplay between coherent one-step and incoherent many-step contributions. Applications have been conducted with optical power limiting, photobleaching (3D write), photodynamic therapy processes, up converted lasing, and multiphoton excitation processes in general. A related effort has concerned quantum modelling of quantum dots. These have been designed in combination with multi-photon excitation which offers unique advantages over one-photon excitation for use in biological and medical studies. The high spatial confinement and the ability of adjustment of the fundamental photon wavelengths for optimum penetration are key factors in producing high resolution multi-photon imaging. While the great majority of multi-photon studies are carried out with molecular chromophores, one has increasingly become aware of the intriguing possibilities offered by semiconductor quantum dots (QDs) for multi-photon bio-imaging owing to their high fluorescence yields and low bleaching capability. We have shown that the dynamics of the multi-photon processes in QDs can be well described by solving the time-dependent Schrodinger equation non-perturbatively. The ab initio computational methods to study semiconductor quantum dots have been extended to include also coupled-cluster models.

## Training and ToK

### SCHOOLS:

The following schools have received NANOQUANT YR attendance:

SOSTRUP Summer School on Molecular Properties, organized and staffed by members of the network (Odense and Oslo nodes), provided two weeks of intense training, through lectures and exercises, which bring the students up to the research level in the field. Fifty students attended the last summer school, of which the great majority were from the European countries. 7 NANOQUANT students have attended the school.

The European Summer School in Quantum Chemistry runs also biannually but every odd year. 3 NANOQUANT students.

The Finnish Winter school in Theoretical Chemistry}, organized by the Helsinki partner, is focused around a set of invited research talks on a current topic in theoretical chemistry. About 50 students participate in the school, where they also get the opportunity to present their own work. 8 NANOQUANT students have attended this school.

The Shanghai Winter School in Optical, Electronic, and Magnetic properties of Matter, Shanghai, January 7-15, 2006. Organized and staffed by the KTH node. 5 NANOQUANT students attended.

### TWINNING PROGRAM

The mobility among the present members of the nodes is already quite high, and has been further encouraged by a twinning program in which the students get the opportunity to work and train at more than one node. So far 3 such twinning actions have taken place (see home page for details).

### TRANSFER of KNOWLEDGE

Transfer of knowledge has been conducted through:

Contacts with Computer Centers

Contacts with Companies

Contacts with other EU networks

Policy of assigning ERs

Final network meeting

Transfer of Knowledge through softwares has involved continuous updating, maintaining and documenting world-leading softwares: DALTON, DIRAC, ACES~II, TURBOMOLE, with very wide distribution networks. The training of researchers in all these softwares has also been instrumental for this purpose. This has led to an immediate transfer of knowledge to thousands of ESRs and ERs throughout Europe. Two major releases (Dalton. 2.0, Dirac04) has been obtained during the network period.

DALTON 2.0 as example. Released March 04. 537 Licences ~ 1300 Users, 52 Countries.

Transfer of knowledge through connections with other EU networks. We identify ni particular contacts with EU-STREP project ODEON: Design and fabrication of optoelectronic devices based on innovative second-order nonlinear organic nanomaterials.

## VISITS

The visit program has been intense comprising 54 node-to-node visits by senior and junior researchers (see <http://www.theochem.kth.se/nanoquant/>).

## CAREER DEVELOPMENT

The KTH computational Science and engineering centre arranged a 2-day workshop (December 8-9 2005), in Stockholm, inviting a large number of industrial researchers within the area of computational science and a number of PhD students. The goal of the meeting was to provide career information and opportunities for students with speciality in computational modelling within the industrial sector after fulfilment of PhD studies. The meeting was organized as a series of general presentations of the industrial persons on the role of computing, the policy for recruitment and for collaboration with academia. This was augmented by groups discussions in a rotating scheme were groups of students could interview the industrial representatives. The results of the group discussions were presented by selected students and discussed.

The following companies were represented, FCC Chalmers, Astra Zeneca AB, ABB, SAAB, Scania, BioVitrum, Ericsson, Sandvik, featuring various branches (Power technology, trucks, pharmaceuticals, telecommunications, steel). 5 NANOQUANT students were present and were given the opportunity to take full part in these activities.

Two company representatives devoted extra time to the NANOQUANT students- Dr Carmen medina from Biovitrum AB and Dr. Timothy Powell from Astra Zeneca AB. A decision on a follow up by study visits at some selected companies.

## Management

### MANAGEMENT

The organisation has been structured into three tiers: coordinator node, core nodes, network nodes. The 20-year collaboration between the Scandinavian partners has guaranteed a seamless management of the network by the core, without this management being burdensome. The coordinator has beared full financial responsibility, and additionally has the overall responsibility for all network activities: training, science and administration, but consultation has been shared with the core. The high level of integration of the network has ensured that the coordination technique essentially remains informal as concerns matters for the seniors, while coordination remain structured concerning ESR and ER matters.

The financial management has essentially followed the one practiced in the FP5 network MOLRPOP. Thus the advanced payment was immediately be distributed to the nodes in proportion to the contracted amount. The yearly payment is regulated according to the most pressing criterion, namely the delivery of man-moths in the hiring. If these criteria are fulfilled the yearly payments to a node will directly follow its share of the contracted amount. If a node faces problem with hiring in

such a way that it is clear that it will not produce the contracted amount, the responsibility, and the appropriate financing for that, will be shifted to another node. This has happened in one case (transfer Mainz to Warsaw).

## DISSEMINATION

Dissemination of results has taken place using: Normal academic channels, through publications, conferences and smaller meetings. Network partners have been frequently invited to international conferences where they have taken the opportunity to display network results: NANOQUANT home page with bulletin board for scientific results. A summary of results is also given at the (linked) Cordis home page. The DALTON home page is used for more technical results concerning software development: Direct contact with potential end-users of results, experimentalists, companies (ie.g. BioVitrum AB), computer centres (e.g. CSC Helsinki, PDC Stockholm).

## NETWORKING

A home page has been set up (<http://www.theochem.kth.se/nanoquant/>) containing Network Data: Vacancies, Partners, Objectives, Applications, Collaborations, Publications, Training, Results and Achievements. Network Events: Employments, Organized meetings, Attendance of Meetings and Schools, Visits,

## ORGANIZED MEETINGS

The Stockholm, coordinator, node organized the first meeting for NANOQUANT leaders in Sandbjerg Estate, Soenderborg, Denmark May 4, 2004, dealing with organizational issues.

Prof. Trygve Helgaker (Oslo) organized the 8th Sostrup Summer School on Quantum Chemistry and Molecular Properties, Denmark, June 20 - July 2, 2004 (together with Prof. Poul Joergensen and Ass. Prof. Jeppe Olsen (Odense)

Prof. Kenneth Ruud (Oslo) organized, together with Hans Ågren (Stockholm) and Vincenzo Carravetta (Pisa), the Italian-Norwegian-Swedish Workshop on Quantum Molecular Sciences September 17-20 2004 give the number

The Helsinki node organized the Helsinki Winter School in Theoretical Chemistry entitled A Frontier of Chemistry: New Species, December 13th-16th, 2004.

The Helsinki node organized the Helsinki Winter School in Theoretical Chemistry entitled Nanophotonics, December 7th-9th, 2005.

The Mainz node (Prof. Wim Klopper) arranged the conference "Computational Tools for Molecules, Clusters and Nanostructures, at Karlsruhe, 23 - 26 January 2005. 10 principal NANOQUANT researchers attended.

MIDTERM Young Researcher Meeting, February 11, 2006, Oslo, organized by Oslo node.  
ARRANGED MANAGEMENT MEETINGS

The coordinator organized the first meeting for NANOQUANT leaders in Sandbjerg Estate, Soenderborg, Denmark May 4, 2004, dealing with organizational issues.

2) The coordinator node, organized a node leader management meeting on 2005-01-24 in Karlsruhe, Germany, discussing the present status of the NANOQUANT network.

3) MIDTERM review meeting, February 10 2006, Oslo.

Attended Conferences and Meetings

Conferences and Workshops: 24 Oral presentations, 13 poster presentations of which 20 were invited.

Publications (full duration): 87 Joint NANOQUANT papers, 25 NANOQUANT papers with involvement of young researchers.

## **DEVIATIONS/MODIFICATIONS TO THE ORIGINAL WORK PROGRAMME**

**Please indicate if the project**

b) has/will required some minor deviations/modifications to the original plan

**If you answered b) or c) please include a detailed description of the modifications in the report (one page)**

So far we have produced 192 man-months and which is 30 less than the projected 222 at year 2 in the work plan. This owes to late hiring during the first year. This has now been fully compensated and with the present hiring scheme we will well fulfil the contracted amount of 344 months, and even exceed this number by 20 months.

## **ADDITIONAL INFORMATION**

**Please indicate any additional information, which may be considered useful to assess the work done during the reporting period.**

<b>Attachments</b>	
<b>Name</b>	
<b>Date</b>	
<b>Signature</b>	