

12th Nanoquanta Workshop on Electronic Excitations: Time-Dependent Density-Functional Theory, Advances and Prospects. Aussois (Rhone-Alpes, France), September 18-22 2007.

ABSTRACT

We propose a five-day workshop whose aim is to assess the present status, the latest achievements and future perspectives of first principles approaches for the calculation of spectroscopic properties in solids, nanostructures, systems with increasing complexity, and materials of technological and biological interest. More specifically, this workshop will focus on Time-Dependent Density-Functional Theory (TDDFT) and its most recent developments that have made it a valid alternative to the Bethe-Salpeter Equation (BSE) approach for the accurate calculation of optical and dielectric spectra. Open questions, achievements, advantages, and drawbacks of TDDFT will be contrasted with those of other approaches, specifically the BSE, in order to stimulate discussions about the future of the field and to bring together scientists from different communities related to electronic excitations.

1. SCIENTIFIC SUMMARY

Spectroscopy, whether photonic or electronic, constitutes an essential diagnostic tool for characterizing materials properties. While structural properties of materials are mainly determined by their static electronic ground state, the response to external probes in modern spectroscopies can often only be explained in terms of dynamic excitations. A thorough understanding of excited state properties is therefore essential not only for their fundamental importance in Condensed Matter Physics and in Nanosciences, but also for their role in practical applications like the design of new materials with technological or biological interest. The theoretical foundations of this field are well established, and have been accompanied by physically well-motivated approximations suitable for ab-initio calculations in real materials. For the prediction of single-particle spectra and quasiparticle lifetimes for example many-body-perturbation-theory (MBPT) in Hedin's GW approximation[1] has proven to be highly successful [2]. The GW method is also used as a first step in an ab initio many-body approach to two-particle excitations through the solution of the Bethe-Salpeter Equation (BSE), which yields a correct description of photoabsorption spectra [3,4]. Time-dependent density-functional theory (TDDFT)[5], on the other hand, provides an alternative route to calculate optical and dielectric spectra. It has the important advantage of being computationally more efficient and also more amenable for practical simplifications than MBPT-based schemes [4]. The disadvantage of TDDFT is - like in DFT - the uncertainty associated with the essentially unknown exchange-correlation functional. Both the MBPT and the TDDFT approach have been applied to a wide variety of systems, ranging from simple atoms to systems with prospective technological application. Combined, they provide a reliable interpretation of experiments such as photoemission, photoabsorption, electron-energy-loss spectroscopy, inelastic X-ray scattering, quantum transport or scanning-tunneling microscopy [2,4].

The proposed workshop is intended to provide a forum to discuss the advances in the theoretical and computational treatment of optical/dielectric spectroscopy and quantum transport properties. The focus will be devoted to time-dependent density-functional theory, which has emerged as the most

convenient approach for describing neutral excitations in the last years. An important issue of current debate is certainly the accuracy of certain inevitable approximations and the domain of applicability. In TDDFT the time-dependent density replaces the static density of DFT as the fundamental variable, which makes TDDFT computationally much more efficient than the Green's function based Bethe-Salpeter Equation scheme, and thus potentially more suitable for applications to large and complex systems. While TDDFT is in principle exact for neutral excitations, its accuracy and predictive power depend crucially on the quality of the exchange-correlation kernel. For this reason much recent development has been devoted to the search for improved approximations to the exchange-correlation kernel. Of particular importance are here effects arising from the electron-hole interaction, so called excitons or excitonic effects, which determine the optical properties of semiconductors and insulators as well as nanostructures and molecules. An inherent drawback of TDDFT in this respect is, that it does not presently allow for an immediate interpretation of the computed quantities in terms of neutral excitation energies and excitonic wavefunctions as this is the case in the BSE approach, even though excitonic effects are correctly accounted for in the final observable spectra. It is also important to note in this context that most of the recent progress on TDDFT, especially on the design of new approximations to the exchange-correlation kernel, has resulted from a comparison with BSE and the concepts of many-body perturbation theory (MBPT). Interestingly the reverse is also true and concepts from the realm of TDDFT are now being applied in the context of MBPT. It remains to be noted that these excited states methods have, until now, been mostly applied to stationary nuclei. The extension to excited states molecular dynamics and electron-phonon coupling is an important current development. To put TDDFT into context attention will also be paid to recent developments in static DFT, like the development of novel functionals, and current issues in many-body perturbation theory, such as exact-exchange based GW calculations, self-consistency, vertex corrections or core-valence exchange.

In the light of these recent developments it appears timely to bring together researchers in this and related fields in one workshop to review the state of the art and to discuss future perspectives.

Summary of the motivation for the organization of this workshop:

- i) to provide a forum for discussions between researchers with different areas of expertise and points of view;
- ii) to assess the latest achievements and the perspectives of first principles spectroscopy methods (within the realm of both TDDFT and MBPT);
- iii) to attract young researchers to this developing field in order to increase the number of scientists involved in activities of this kind
- iv) to foster links between different research groups working on electronic excitations from first-principles.

To realize these objectives we propose a meeting with a broad scope. It is our aim to stimulate the scientific discourse between scientists from different communities and to promote the application of ab-initio methods to systems with immediate interest, beyond those of fundamental research. With regards to the latter, we regard participation from experimental groups as important contribution.

2. MEETING PROGRAMME AND FORMAT

Proposed topics to be covered:

- Fundamental theorems of TDDFT

- approximations to the exchange-correlation kernel
- recent developments
- ab-initio implementations of TDDFT: space-time versus frequency-reciprocal space
- new domains of application for TDDFT, in particular Quantum Transport
- application of TDDFT to new systems and new materials (with special emphasis on, nanostructures and bio-molecules)
- advantages and disadvantages of TDDFT in particular in comparison with BSE, but also with quantum chemical methods
- recent advances in many-body perturbation theory
- recent advances in spectroscopy and quantum transport
- other recent developments in electronic structure theory

The format of the workshop will be similar to the previous workshops listed in section 5, since this has been proven the best way to trigger discussions between participants and provide an informal environment. We are however in the need to increase the total number of days allocated to the event, from 4 to 5. This is caused by the increase in the number of participants and consequently, of the number of presented works, which now do not any more fit comfortably in a 4-day format workshop. A 5-day format is required to give the right space to informal side discussions and debriefings which characterized our primeval restricted successful Lyon events and unfortunately, with the increasing size of the events, lost most of their space. Each day of the conference will be divided into a morning session (9:00--12.40) and an afternoon session (15:30--20:00). Invited talks are allocated up to 40 minutes plus 10 minutes reserved for the discussion. In addition, up to 90 minutes will be reserved for one round-table discussion.

3. SCIENTIFIC ORGANIZERS CV and MOST RELEVANT PUBLICATIONS

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Valerio Olevano (VO) obtained his “Laurea” (degree in Physics) in 1993 with a thesis on “computer simulations of the QCD Theory on Lattice”, thus demonstrating since the beginning an interest to Computational Physics. After a stage in Experimental Condensed Matter Physics (Photoemission Spectroscopy), he started his PhD in 1996 working in Condensed Matter Theory. His PhD thesis was dedicated to the study of the electronic structure by the GW approximation and of the dielectric and optical properties by TDDFT. After completing his PhD (in 1999), he moved to the Laboratoire des Solides Irradieés (Palaiseau, France) for a two years Post-Doc in which he studied the other approach to optical and EELS spectroscopies, namely the BSE. In 2000, he got a permanent position (Chargé de Recherche) in the CNRS, the French national research council. Since then, his works focused on

the weight of local-field and excitonic effects in the dielectric and optical spectra of insulator and semiconductors by BSE and TDDFT; to the development of the theory toward new approximations for the exchange and correlation kernel beyond LDA (accounting of long-range effects, BSE derived approximations to the TDDFT); to the application of the above mentioned theories to complex, technologically interesting systems like superlattices and nanotubes; finally to the development of the MBPT beyond the GW approximation through vertex local corrections.

He is among the authors of the codes DP (linear-response TDDFT in plane waves), EXC (Bethe-Salpeter code), ABINIT-GW and TAU (inelastic lifetimes). He organised two schools in Palaiseau on the use of some of these codes and the underlying theory.

Very early, during his experimental Condensed Matter Physics stage, he took part to the organisation of a large event (more than 200 participants): the 6th International Conference on Electron Spectroscopy, held in Rome, on June 16-23, 1995. In that occasion he was mainly in charge of practical aspects. Then in 2004, he was one of the three local organisers of the XII International Workshop on Computational Physics and Material Science, held in Gif sur Yvette (France) on January 8-10, 2004 (90 participants). He took part both into the decisions of the scientific committee and into all the practical aspects, from the search for financing to the organisation of the sessions, lodging, meals, conference book, collect of participants, budgetary aspects. He also participated to the organizing and programme committee of a Miniworkshop in the 2006 edition of the French national conference Journées de la Matière Condensée and to NANOQUANTA '06.

Scientific output (from <http://wos.isiknowledge.com>):

24 articles in international peer-reviewed journals (leading to 205 citations)

Five most relevant publications in the last 5 years:

- F. Bruneval, F. Sottile, V. Olevano, R. Del Sole and L. Reining
Many-body perturbation theory using the density-functional concept: beyond the GW approximation
Phys. Rev. Lett .94, 186402 (2005)
- M. Bruno, M. Palumbo, A. Marini, R. Del Sole V. Olevano, A.N. Kholod and S. Ossicini
Excitons in Germanium Nanowires: Quantum Confinement, Orientation and Anisotropy Effects within a First-Principles Approach
Vir. J. Nan. Sci. & Tech., October 31, 2005; Phys. Rev. B 72, 153310 (2005).
- F. Sottile, V. Olevano and L. Reining
Parameter-free calculation of response function in TDDFT
Phys. Rev. Lett 91, 056402 (2003)
- L. Reining, V. Olevano, A. Rubio and G. Onida
Excitonic effects in solids described by TDDFT
Phys. Rev. Lett 88, 066404 (2002)
- V. Olevano and L. Reining
Excitonic effects on the Silicon Plasmon Resonance
Phys. Rev. Lett 86, 5962 (2001)

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Gian-Marco Rignanese (GMR) earned his degree in Engineering Physics (French “Ingénieur Civil Physicien”) from the Université Catholique de Louvain (UCL) in 1994 defending a thesis on various aspects of the *ab initio* study of silicon. The work included the parallelisation of a program for the calculation of response functions in the framework of Density Function Perturbation Theory. He started his PhD in 1994 at UCL under the supervision of Prof. X. Gonze, as a Research Fellow of the National Fund for Scientific Research (FNRS-Belgium). His work aimed at studying the SiO₂ surface and its interface with Si with first-principles. During his PhD, he spent nine months in the group of Prof. R. Car at the Ecole Polytechnique Fédérale de Lausanne, where he was also appointed as software development consultant by Cray Research. After finishing his PhD in 1998, he joined the group of Prof. S. G. Louie at the University of California at Berkeley, as Firmin Van Brée Fellow of the Hoover Foundation of the Belgian American Educational Foundation and grantee of the Fulbright Program of the Commission for Educational exchange. He developed parallel programs for electronic structure calculations by the GW approximation and the BSE in the framework of MBPT. From 2000 to 2003, he started to work on the dielectric properties of new materials for nanoelectronics in the group of Prof. X. Gonze at UCL as Post-doctoral Researcher of the FNRS-Belgium. In 2003, he obtained a permanent position as Research Associate of the FNRS-Belgium and Assistant Professor (Chargé de Cours) at UCL. Since then, his work has focused on electronic, dielectric, and transport properties of new materials for nanoelectronics.

Through his work, he earned a strong expertise in computational physics, with a special interest in parallel programming. He is among the authors and advisers of the ABINIT code distributed freely under the GNU Public License. In particular, he is in charge of the development of the ABINIT-GW branch.

Since 1992, he has been the teaching assistant of several courses for engineering students at UCL (algebra, physical chemistry, thermodynamics, physics). In 2002-2003, he was the teacher of the quantum chemistry course for second-year chemistry students at the Université de Liège (Belgium). In 2005-2006, he taught the materials physics course for third-year engineering students at UCL.

Since 2002, he has been involved in the organisation of four meetings either as the local organiser (ABINIT'02, EXCITING'03, NANOQUANTA '06) or member of the program committee (EXCITING'03, ABINIT'04, NANOQUANTA '06). From these events, he gained some experience in various aspects of meetings organisation ranging from financial support to scientific content passing through very practical aspects such as lodging, meal, or website management. He is the local organizer of NANOQUANTA '06.

Scientific output (from <http://wos.isiknowledge.com>):

29 articles in international peer-reviewed journals (leading to 589 citations)

Five most relevant publications in the last 5 years:

- G.-M. Rignanese, F. De Angelis, S. Melchionna, and A. De Vita
Glutathione Transferase: A First-Principles Study of the Active Site
J. Am. Chem. Soc. 122, 11963-11970 (2000)
- G.-M. Rignanese, X. Blase, and S. G. Louie
Quasiparticle effects on tunneling currents: a study of C₂H₄ adsorbed on the Si(001)-2×1 surface

- Phys. Rev. Lett. 86, 2110-2113 (2001)
- G.-M. Rignanese, F. Detraux, X. Gonze, A. Bongiorno, and A. Pasquarello
Dielectric constants of Zr silicates: A first-principles study
Phys. Rev. Lett. 89, 117601:1-4 (2002)
 - G.-M. Rignanese, X. Gonze, G. Jun, K. Cho, and A. Pasquarello,
First-principles investigation of high- ϵ dielectrics: Comparison between the silicates and oxides of hafnium and zirconium
Phys. Rev. B 69, 184301:1-10 (2004)
 - D. Connétable, G.-M. Rignanese, J.-C. Charlier, and X. Blase
Room temperature Peierls distortion in small diameter nanotubes
Phys. Rev. Lett. 94, 015503:1-4 (2005)

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Patrick Rinke (PR) completed his undergraduate studies in Physics at the Universität Heidelberg in Germany. With a DAAD scholarship he then started his Master of Science (MSc) in physics supervised by Prof. Rex Godby at the University of York in England. In 2000 he obtained his MSc and continued as a PhD student in Prof. Godby's group. His project involved the development of a GW program suitable for calculating quasiparticle excitations in atoms and small clusters. In 2003 he defended his PhD thesis entitled "Exchange and Correlation in Small Spherical Clusters", which was awarded a prize from the Computational Physics group of the Institute of Physics in England. He then joined Prof. Matthias Scheffler's group at the Fritz-Haber-Institut (FHI) der Max-Planck Gesellschaft in Berlin as a post-doctoral researcher. At the FHI he continues his work on the simulation of quasiparticle spectra, applying the GW method to II-VI compounds and group-III-nitrides as well as semiconductor films and surfaces.

During his PhD, he gained considerable programming experience when developing a new GW program. At the FHI he became a developer of the GW space-time code (GWST) - one of the excited states codes used in NANOQUANTA.

He has been a member of the European Research Training Network NANOPHASE since its beginning in 1999 and has greatly benefited from the network events and the scientific community that forms the network. In 2003, he became a joined leader of the NANOPHASE node - and then later of the NANOQUANTA node - at the Fritz-Haber-Institut. As a NANOQUANTA node leader, he is also a member of the NANOQUANTA steering committee. At the FHI, he has also gained experience in supervising PhD-students and Post-Docs.

He has been a co-organiser of the second NANOQUANTA Young Researcher Meeting, which took place at the FHI in May 2004 in Berlin. The meeting was attended by approx. 40 young researchers. In the same year he was also the chief organiser of the FHI's annual garden party - an event with approx. 400 guests. This year he organizes NANOQUANTA '06.

Scientific output (from <http://wos.isiknowledge.com>):

4 articles in international peer-reviewed journals (leading to 14 citations)

Five most relevant publications in the last 5 years:

- P. Rinke, P., A. Qteish, M. Winkelnkemper, D. Bimberg, J. Neugebauer, and M. Scheffler: Band gap and band parameters of InN and GaN from quasiparticle energy calculations based on exact-exchange density-functional theory. Appl. Phys. Lett. 2006 accepted
- C. Freysoldt, P. Eggert, P. Rinke, A. Schindlmayr, R.W. Godby, and M. Scheffler: Dielectric anisotropy in the GW space-time method. Comp. Phys. Comm. 2006 accepted
- P. Rinke, A. Qteish, J. Neugebauer, C. Freysoldt, M. Scheffler: Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. New J. Phys. 2005, 7, 126.
- K. Delaney, P. García-González, A. Rubio, P. Rinke, and R.W. Godby, Comment on "Band-gap problem in semiconductors revisited: Effects of core states and many-body self-consistency". Phys. Rev. Lett. 2004, 93, 249701
- P. Rinke, K. Delaney, P. García-González, and R.W. Godby, Image states in metal clusters. Phys. Rev. A 2004, 70, 063201.

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Francesco Sottile (FS) obtained his degree in Physics in 1999 at the University of Messina (Italy), defending the "laurea" thesis on Electron correlation in jellium spheres: a computational study using Density Functional Theory and Quantum Monte Carlo. In 2003, he completed a PhD at the Ecole Polytechnique (France). His thesis, awarded as best thesis from the Ecole Polytechnique, was dedicated to the "Response function of semiconductors and insulators: from the Bethe-Salpeter equation to time-dependent density functional theory". It presented the basis of a new approach ("Mapping Theory") for an efficient determination of the response functions. In 2004, he moved to Spain in the group of Prof. A. Rubio, his research activity being devoted to the theoretical and methodological (algorithms, computer simulations codes) developments for the electronic and optical properties of systems of biological interest (e.g. hemoglobin, chlorophyll). He recently returned at the Ecole Polytechnique in the group of Dr. L. Reining. Since 2006, he is responsible for and coordinator of "code and theory development" at the Palaiseau node of the ETSF.

He has expertise in programming languages (fortran, c), scripting and web oriented (perl, html, php) languages. He is also a computer simulation code developer, being among the authors of the EXC code and the DP code, as well as the dictator for the open source project EXC.

In 2004, he was in charge of the numerical physics course at the University of Paris VI (third year), and gave lectures on electronic excitations for the computer simulation course at the University of Paris VI (PhD level).

He was one of the organisers of the NANOPHASE Young Researchers' Meeting held in May 2004 in Palaiseau (France). From 2003 to 2006, he was part of the organizing committee of four hands-on

devoted to excited states computer simulation codes in Palaiseau. He also helped (practical and logistic aspects) in organizing the XII International Workshop on Computational Physics and Material Science, held in Gif sur Yvette (France) in January 2004. He takes part of the NANOQUANTA '06 organizing team.

Scientific output (from <http://wos.isiknowledge.com>):

9 articles in international peer-reviewed journals (leading to 48 citations)

Five most relevant publications in the last 5 years:

- F. Sottile, K. Karlsson, L. Reining, and F. Aryasetiawan: Macroscopic and microscopic components of exchange-correlation interactions Phys. Rev. B 68, 205112 (2003).
- F. Sottile and P. Ballone: Fixed-node diffusion Monte Carlo computations for closed-shell jellium spheres, Phys. Rev. B 64, 045105 (2001).
- Fabien Bruneva, Francesco Sottit, Valerio Olevan, Rodolfo Del Sole, and Lucia Reining: Many-Body Perturbation Theory Using the Density-Functional Concept: Beyond the GW Approximation, Phys. Rev. Lett. 94, 186402 (2005).
- Silvana Botti, Francesco Sottile, Nathalie Vast, Valerio Olevano, Lucia Reining, Hans-Christian Weissker, Angel Rubio, Giovanni Onida, Rodolfo Del Sole, and R. W. Godby: Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory, Phys. Rev. B 69, 155112 (2004).
- Francesco Sottile, Valerio Olevano, and Lucia Reining, Parameter-Free Calculation of Response Functions in Time-Dependent Density-Functional Theory, Phys. Rev. Lett. 91, 056402 (2003).

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Ludger Wirtz (LW) studied Physics at the Bonn University (Germany) and the University of Tennessee in Knoxville (USA). He obtained his Master's degree ("Diplom") from Bonn university in 1997. In October 2001, he obtained his PhD from the Vienna University of Technology with a thesis on the theory of ion-surface interaction. After a 4 months research stay at the Oak Ridge National Laboratory (USA), he joined the group of Prof. Angel Rubio at the University of the Basque Country in San Sebastian (Spain) as a post-doctoral researcher. He worked there on the calculation of Raman, infrared, optical absorption, and electron-energy loss spectra of boron-nitride and carbon nanotubes. His position was funded through the European research and training networks COMELCAN and NANOPHASE. In October 2004, he joined the IEMN (Institute for electronics, microelectronics, and nanotechnology) at Villeneuve d'Ascq as a permanent researcher, employed by the CNRS (French national research centre). There, he is continuing his work on excitations in nanotubes and started a project on electronic transport through molecules described by time-dependent density-functional

theory.

In 2005, he joined the organizing team of NANOQUANTA workshops that is in charge for NANOQUANTA'06.

Scientific output (from <http://wos.isiknowledge.com>):

32 articles in international peer-reviewed journals (leading to 227 citations)

Five most relevant publications in the last 5 years:

- Kinetically Assisted Potential Sputtering of Insulators by Highly Charged Ions
G. Hayderer et al.
Phys. Rev. Lett. 86, 3530 (2001)
- Excitons in Boron Nitride Nanotubes: Dimensionality Effects
Ludger Wirtz, Andrea Marini, and Angel Rubio
Phys. Rev. Lett. 96, 126104 (2006)
- Raman spectra of BN nanotubes: Ab initio and bond-polarizability model calculations
Ludger Wirtz, Michele Lazzeri, Francesco Mauri, and Angel Rubio
Phys. Rev. B 71, 241402 (2005)
- Phonon and plasmon excitation in inelastic electron tunneling spectroscopy of graphite
L. Vitali, M. A. Schneider, K. Kern, L. Wirtz, and A. Rubio
Phys. Rev. B 69, 121414 (2004)
- Ab initio calculations of the lattice dynamics of boron nitride nanotubes
Ludger Wirtz, Angel Rubio, Raul Arenal de la Concha, and Annick Loiseau
Phys. Rev. B 68, 045425 (2003)

Co-organizer:

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4. PROVISIONAL LIST OF PROPOSED SPEAKERS AND PARTICIPANTS

We primarily intend to invite scientists representing state of the art research groups in both time-dependent density-functional theory as well as in many-body and BSE theory. In addition we plan to invite speakers who have made a well recognized contribution in related theoretical fields. We further plan to complement the theoretical sessions by invited talks on spectroscopic methods given by distinguished spectroscopists to make closer contact to the experimental characterization of excited-state properties.

Tentative list:

- E.K.U. Gross (Berlin, Germany) (review on TDDFT)
- S.G. Louie (Berkeley, USA) (review on MBPT and quantum transport)
- M. Scheffler (Berlin Germany) (towards exact density functionals)
- A. Rubio (San Sebastian, Spain) (TDDFT as a challenging tool for biophysics).
- U. Von Barth (Lund, Sweden) (conservative approximations to the xc kernel)
- G. Vignale (USA) (density-current and spin TDDFT)

S. Kummel (Bayreuth, Germany) (discontinuities in TDDFT)

K. Burke (Rutgers, US) (measuring the kernel, memory, conductance, excitations in TDDFT)

R. Del Sole (Rome Italy) (many-body approaches to TDDFT)

G. Stefanucci (Berlin, Germany) (TDDFT for Quantum transport)

The call for participation will be mainly directed to scientists specialized in theoretical and computational physics. Contributions ranging from fundamental studies to semi-empirical approaches for complex phenomena are encouraged. The target number of participants is approx. 100. In order to facilitate interaction between scientists belonging to different communities, plenty of question/discussion time will be reserved after each talk and active participation in the round-table discussions will be encouraged

The attendance of graduate students and postdocs will be promoted by including short contributed talks and poster sessions with brief oral introductions. Furthermore, we will encourage Ph.D. students who have presented an outstanding poster to convert it into a short talk. We feel that the inclusion of young researchers is a very important point, because as the "scientists of tomorrow" they are the basis of a strong and healthy scientific community.

5. PREVIOUS EVENTS

The progress in the theoretical treatment of electronic excitations and spectroscopy is reflected in the continuing series of workshops devoted to this topic and in the increasing number of participants (from 50 at the early events to over 100 in 2006). The proposed meeting follows the previous workshops on

'Excited Electrons in Molecules, Solids and Atoms' (Lyon,1997),

'Spectroscopy of Electronic Excitations in Materials' (Valladolid,1998),

'Calculation of Electronic Excitations in Finite and Infinite Systems' (Lyon, 1999)

'Excited States and Electronic Spectra' (Lyon,2000),

'Ab-initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials' (Lyon, 2002),

'Ab-Initio Electron-Excitations Theory: Towards Systems of Biological Interest' (San Sebastian 2003),

'Theory and Modelling of Electronic Excitations in Nanoscience', (Maratea 2004),

'40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges', (Bad Honnef 2005), and

'11th Nanoquanta workshop on Electronic Excitations: a decade of applications of the Bethe-Salpeter Equation', (Houffalize 2006).

These workshops have had an acknowledged contribution to the establishment of a strong community of scientists applying the concepts of MBPT and/or TDDFT in condensed-matter physics. We hence propose to continue this series with the present workshop in Aussois (Rhone-Alpes, France). As described, the meeting in 2007 will have a broader scope, but we would like to keep the overall format of preceding conferences: an informal, general style, ample time devoted to discussions and round-tables, and preference given to contributions by young scientists. Since the main goal of this workshop is to explore future applications and prospects for ab-initio techniques, we are confident that a friendly atmosphere will be more conducive to the achievement of this objective.

6. TUTORIAL ELEMENTS AND ATTRACTION OF NEW RESEARCHERS

To further emphasize the training aspect of the workshop in particular for newcomers to the field two experienced scientists (in principle E.K.U. Gross and S.G. Louie) will be invited to give a review seminar on the state of the art of TDDFT and Many-Body perturbation theory -based applications. These review seminars are intended to be tutorials for those interested in MBPT or TDDFT, but without previous experience in either of the two methods or with ab-initio calculations in general. Poster sessions, chaired by an invited speaker, will be preceded by short oral introductions. The sessions will provide more time for scientific discussions and will give young researchers in particular the opportunity to present their work and to get in contact with fellow scientists and senior researchers. Since the objective of the proposed workshop is to stimulate scientific discourse through oral presentations and poster sessions, we do not plan to hold specific tutorials on excited-state calculations. Nonetheless, ample break time between sessions will help all students and postdocs to share their current research with senior scientists. Finally, the research group leaders will be invited to advertise job and fellowship opportunities as well as other relevant conferences on their respective fields of interest.

7. FINANCIAL INFORMATION

We estimate a total cost of 50.000 Euros. This includes all the expenses for invited speakers, scholarships for selected young scientist, and additional costs for e.g stationery, publicity, coffee breaks, or abstract books. We aim to encourage the participation of young researchers. For this reason we expect that the large part of the funding from the Psi_k Network will be used to provide financial support for European PhD students or postdocs. As a minimal condition to receive a scholarship we will require their active contribution in the form of a talk or a poster presentation. We hope to offer grants of 600 Euros: 300 Euros for living allowance plus 300 Euros for travel expenses. We also rely on a part of the Psi_k funding to invite 2 or 3 keynote European speakers. **Therefore we apply for a total amount of 15.000 Euros.**

8. CO-SPONSORSHIP

We will also apply to local institutions (CNRS, CEA, Universite de Grenoble J. Fourier, Rhone-Alpes region) for further funding (e.g. for invited speakers). As in previous years an American scientist (Prof. John Rehr) has agreed to co-organize the proposed event and to apply for additional funding from American grant agencies (DOE, NSF, etc.) to sponsor the participation of American researchers.

9. LOCATION

The workshop will take place on 18-22 September 2007 at the CNRS Paul Langevin center in Aussois (Rhone-Alpes region, France). This place has a longstanding experience in hosting conferences and scientific meetings and the facilities are suitable for a workshop of the proposed size. The Paul

Langevin centre provides the ideal environment for a stimulating meeting in an informal atmosphere.

10. PARTICIPATIONS FROM AMERICA

Prof. J. R. Rehr at the University of Washington, coordinator of the FEFF Project (<http://leonardo.phys.washington.edu/feff>) and the CSMN Project (<http://www.phys.washington.edu/~cmsn/CRTs/ESESRF>) has accepted to be co-organizer of the proposed events. We believe that this initiative will boost also the collaboration with researchers in the US, who work at the forefront of nanoscience, and will increase the exchange of expertise and knowledge between Europe and the US.

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