Research Networking Programmes

Science Meeting – Scientific Report

***Proposal Title**: Excitations in realistic materials using Yambo on massively parallel architectures*

Application Reference N°: 5745
ESF Activity
Unit: PESC
Activity Title: Advanced Concepts in Ab Initio Simulations of Materials
Activity Acronym: Psi-K2
Science Meeting: School
Location: Lausanne, CECAM Headquarter (Switzerland)
Date of Science Meeting: 13/4/2015 – 17/4/2015
Convenors' Names: Dr. Andrea Marini, CNR Institute for Structure of Matter (ISM), Rome

1. Summary (up to one page)

Characterization and engineering of complex systems in material science often requires an accurate description of their excited-state properties. This school, attended by 33 students (see list below) has provided training in the theory and practice of computing electronic and optical excitations within density functional theory (DFT) and Green's function approaches, and in the application of these techniques to the study of realistic and challenging systems using the Yambo code. A key topic of the school was the use of a massively-parallel environment of the code, suitable for the forefront machines today available in the High Performance Computing centers.

The school has been organized in theoretical lessons on many-body perturbation theory (MBPT) during the mornings, and in practical tutorials on the YAMBO code during the afternoons. Our goal has been to equip students with the fundamental knowledge, practical skills, and computational tools needed to tackle today's challenging problems in materials science involving a good description of electronic excitations beyond the mean-field DFT Kohn-Sham (KS) scheme.

Beside the theoretical lectures and the practical hands-on, a lecture by an experimentalist expert on angle-resolved photoemission (ARPES) and other spectroscopic techniques, has been given. This provided a link between experimentally measured and theoretically computed quantities, thereby highlighting the importance of ab initio MBPT calculations for the interpretation of the experimental results.

Moreover a dedicated lesson on new trends in high-performance parallel computing was given by an expert of the Italian HPC center Cineca to highlight the directions of the next future hardware architectures and capabilities, and hence the challenges and possibilities of scientific computing.

The school has been characterized by a wealth of social activities (social dinner, get together, poster session, closing lunch buffet) and healthy and exciting discussions. All of the organizers talked to the students in order to identify potential problems and critical aspects of their current research.

2. Description of the scientific content of and discussions at the event (up to four pages)

The School focussed on the theoretical background and on the practical use of the MBPT code Yambo, with a view to applying the methods to large or complex systems that require the use of massively parallel computational architectures. Covered topics included the calculation of quasiparticle energies and lifetimes using the GW approximation starting from DFT calculations and the simulation of optical spectra solving the Bethe-Salpeter equation (BSE).

Three of the lectures were keynote talks by invited speakers on advanced computational material science methods, trends in high performance computing, and experimental techniques in photoemission spectroscopy.

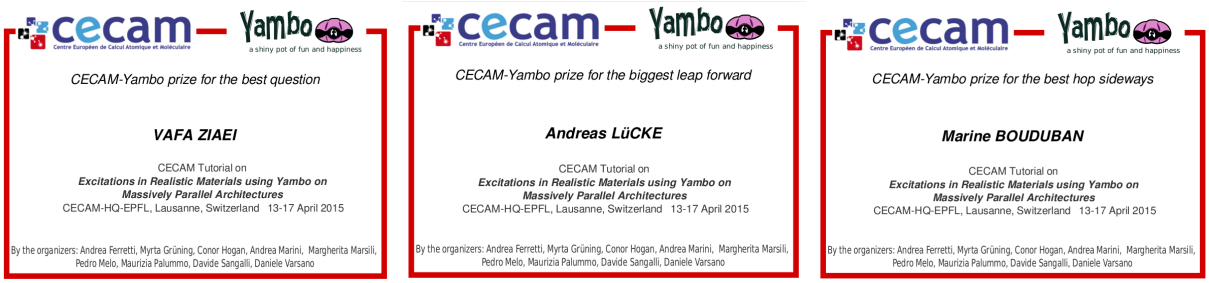
The remainder of the theory and technical lectures have been given by the tutorial organisers. The hands-on sessions have been introduced by one of the developers and supervised by all of the other organisers. A poster session was organized the first day where the students presented their current research.

The school was attended by 33 students, mostly PhD students, from 16 different countries, with backgrounds in physics, chemistry, and materials science. Concerning the lecturers, 11 scientists, one of which is an experimentalist, gave lectures over 5 days. The lecture, tutorials and poster session rooms were provided by Cecam. The lecture room was equipped with a projector.

The tutorial room was equipped with 17 workstations (approximately one per 2 students) and the tutorials were run on some dedicated nodes of the local cluster where the code and the tutorial material had been previously installed by the organizers.

Electronic copies of the lecture notes and tutorials material were made available to the attendees on the yambo website:
http://www.yambo-code.org/events/lausanne2015/index.php

The last day of the school Cecam prizes consisting of MBPT books were awarded to three students for their participation and active contribution to the discussions. The prizes were awarded to Andreas Lücke , Vafa Ziaei, and Marine Bouduban.



Day 1

The inaugural lecture was given by Prof. Nicola Marzari from EPFL, who gave an overview of the successes and challenges of electronic structure calculations, since the birth of DFT focusing on the growing success and still open challenges. Part of the lecture was dedicated to illustrate modern algorithms and strategies to tackle material sciences from a high throughput perspective.

The second lesson by Dr Myrta Grüning (Queen's University Belfast, UK) reviewed the fundamentals of DFT. The lecture highlighted both the strengths and limits of the theory showing why DFT is the basis of almost any ab-initio MBPT calculation, and why DFT, within the KS formalism, cannot be used to predict fundamental gaps and optical excitations. As well, the details of the practical implementation of DFT (ranging from spin unpolarized to non-collinear spin formulations) in a plane-waves basis were presented.

The last theoretical lecture of the first day was given by Dr. Davide Sangalli (CNR-ISM, Rome), who introduced theoretical absorption spectroscopy starting from Maxwell's equations and describing the linear response theory. From the linear response equations he discussed the local field effects and the inclusion of the correlation according to TDDFT. Finally, the extensions of the theory to spin dependent phenomena, surface-related effects, and the possibility to access other spectroscopies like circular dichroism were mentioned.

During the afternoon session, Dr. Conor Hogan (CNR-ISM, Rome) gave the first presentation and hands-on overview of the structure of the Yambo code, its command line options, practical tips to use it on HPC machines, and the structure of the databases and output files produced during a standard run. A step-by-step description of the configuration and installation procedure of the code was also given to help the students running on their local machines once back. An overall view of the different runlevels of Yambo was provided.

Following the tutorial a poster session was held in which students were invited to illustrate their own research and in particular motivate their interest towards MBPT, and the YAMBO code. In the evening, a social get-together was organised in a pub in the center of Lausanne. These two scientific and social events, held on the first day, aimed at encouraging a more informal interaction between lecturers and students, helping to create a lively atmosphere as evidenced by the many questions posed during the rest of the school.

Day 2

The first morning lecture was given by Dr. Simon Moser (invited speaker from EPFL) who discussed the experimental state-of-the-art of ARPES. He first discussed the apparatus and the basic theory underlying the interpretation of photoemission spectra. Standard language and jargon were also introduced. Case studies were then presented and critically discussed with particular emphasis on the experimental limitations and data interpretation.

After the coffee break, Dr. Andrea Ferretti (CNR-NANO, Modena) went back to the theory side by discussing the formal theory of ARPES, starting from the general framework and introducing the most standard approximations (such as the sudden approximation and the three-steps model) adopted in the interpretation of experimental data. The many body spectral function was then introduced as the main quantity to be computed in order to

simulate ARPES and connected to the Green's function theory. Finally, moving from the Hedin's equations, the standard GW approximation to the self-energy was introduced and motivated at different levels of description.

In the afternoon section, Dr. Daniele Varsano (CNR-NANO, Modena) gave a lecture on the GW method, starting from its theoretical foundations and introducing one by one the fundamental (eg the neglection of diagrams) as well as the practical (such as the use of plasmon pole models in the definition of the screened Coulomb interaction, the use of a finite number of terms in the sums over empty states, and the non-self consistency) approximations that make the calculations feasible. The critical variables to be controlled and converged in order to have meaningful results were also illustrated. All these issues were connected to the related variables in the Yambo input file.

In the afternoon Dr. Andrea Marini introduced the practical tutorial illustrating how to use the Yambo code for GW calculations in extended systems and for the determination of quasiparticle energies and lifetimes, discussing also plasmon-pole versus real-axis integration.

Day 3

In the first morning lesson, Pedro Melo (CNR-ISM, Rome) gave a deep and wide introduction to the fundamentals of diagrammatic MBPT. The basic theorems of the many-body theory were introduced in a concise but clear manner by creating clear links with the elemental definitions of the theory, thereby setting a common background for the lectures on Day 4.

Following, Dr. Carlo Cavazzoni, invited speaker from CINECA, gave a lecture on "Trends in parallel computing". He introduced the empirical laws that so far drove the progresses in high performance computing (HPC). He then explained how, due to physical limits those laws no longer hold and as a consequence completely new architectures in HPC will be introduced to allow for further improvements in performance. He stressed how those changes heavily affect codes, and the algorithms behind them, as they need to adapt to those new architectures.

Dr. A Marini then explained how Yambo was changed in order to take advantage of these new trends in HPC architecture and how those changes reflect on the way the user has to prepare a calculation.

The hands-on of the afternoon session was dedicated to the setting of the variables controlling the parallelization of the code. A test case based on the GW calculation on a polyacetylene chain was considered as a demonstrator. Different possibilities in using the multiple parallelization levels of yambo were illustrated focusing on cpu-time and memory usage as well as on the scalability of the code. The final aim of the exercise was to guide the students to an optimal usage of the parallelization levels according to the features of the system studied (k point sampling, number of required bands, and size of the plane wave basis), highlighting the performance of the MPI and the Open-MP protocols separately and mixed together.

The second part of this hands-on was devoted to GW calculations involving spin-orbit coupling (SOC), implemented in Yambo in a fully spinorial formulation. This feature is rather peculiar of Yambo, and, because of its scientific relevance, a tutorial was dedicated to it. For

bulk GaSb, the GW corrections for some high-symmetry points of the Brillouin zone were computed and the results compared with those of a non spin-resolved calculation.

In the evening of Day 3 a social dinner was organised at the Restaurant du Port de Pully, a short trip from CECAM, for all students, organisers, and invited lecturers. This tranquil and spacious venue (chosen by CECAM) proved to be most conducive to lively scientific and social discussions amongst all participants, and the dinner itself was exquisite and well appreciated by all present.

Day 4

In the first lesson of the morning Dr. Margherita Marsili (CNR-NANO, Modena) gave a lecture on the theory of the Bethe-Salpeter equation (BSE). She introduced it in the field of condensed matter theory showing how it describes the electron-hole coupled propagation in a many-body interacting system. The formal derivation from the integro-differential Hedin equations has also been discussed. The solution of BSE in terms of an excitonic two-particle hamiltonian problem and its relation with the macroscopic dielectric function have been illustrated.

Dr Maurizia Palummo concluded the theoretical lessons. Her lecture was focussed on how the excitonic hamiltonian in the transition space looks like when the spin-degree of freedom both in the collinear and non collinear case is taken into account. Different schemes of solvers, like diagonalization or iterative Haydock Lanczos schemes, implemented in Yambo both for hermitian and quasi-hermitian matrixes have been discussed. Several examples of bulk, surfaces, organic molecules as well as nanostructured materials have been discussed in the final part of her talk. In particular the role of spin-orbit in the excitonic spectra of quasi two-dimensional TMDC has been highlighted.

The Hands-on of the afternoon session was dedicated to calculation of absorption spectra via the solution of the BSE. The main variables, converging parameters, and approximations governing these calculations (such as the number of e-h transitions or the neglection of the coupling terms) were introduced and discussed by specific tutorials. A dedicated time was also spent on the effect of spin-orbit coupling on optical spectra of bulk GaSb.

Day 5

The morning of day 5 was dedicated to a tutorial on developing Yambo supervised by Dr Myrta Gruening and Dr Davide Sangalli. Before starting, a short presentation provided the students with the basics on the code structure and philosophy, and then introduced the particular problem, i.e. the implementation into Yambo of the momentum distribution within the independent particle approximation. The tutorial guided the students step by step in the implementation of this new functionality into Yambo. As an outcome the students got familiar with the Yambo code and with the routines and lines in the code that need to be modified when a new functionality is introduced. For students not interested in code development, lecturers were available for theoretical as well as technical questions, and assistance was provided during this session to students who wanted to install Yambo on their local computers or clusters.

3. Assessment of the results and impact of the event on the future directions of the field (up to two pages)

The School was widely advertised as a CECAM - Psik-School through the Psik-mailing list and on other lists such as those of the ETSF and Quantum Espresso, through social media pages, and through personal contacts. A full announcement was also made on the Yambo website. As a result, the school attracted a broad range of students and researchers of different nationalities: the final list included participants of 19 different nationalities coming from 16 different countries, ensuring a global advertisement of the scientific methodology and code as well as the high quality of CECAM-organised events. The financial contribution of the ESF “Advanced Concepts in Ab Initio Simulations of Materials” programme was acknowledged during the School and in the advertising material.

In total, 59 applications were received, although only 33 attendants could be accepted due to the capability of the hands-on lecture room. A number of non-European students (from the US, Korea, China, Morocco) were accepted in advance of the deadline in order to circumvent likely visa issues and guarantee a balanced demographic. We tried to strike a balance between different levels of experience while ensuring that all participants could benefit from the school’s activities. Although we received a number of last minute cancellations, we managed to replace them by European and local (EPFL) researchers. These numbers demonstrate the clear interest in the School.

We strove hard to foster an informal atmosphere in the School that would be conducive to open discussions by hosting a poster session and a social get-together on the first day. Indeed we noticed a marked improvement in communication between lecturers and participants with respect to previous training events we have organised. As a result we were able to deal more effectively with the different experience levels of the students, and devote more time to the few participants who struggled at the beginning with the code. In addition we announced a prize for “Best Question” which also encouraged interesting discussions during the lectures.

We intended that participants at the school would leave not only with an overview of fundamental theory in the field but also with a firm grasp of practical issues in order to apply the Yambo code to realistic problems in their own research. To this end, we dedicated almost a full day (Day 3) to explaining the strategies for using the code effectively on large-scale parallel architectures, exploring these methods in a hands-on session, and offered assistance on Day 5 to those students wishing to install Yambo on their own machines or clusters.

The School marked the first general release of version 4 of Yambo, which offers the capability to tackle large or complex systems through use of massively-parallel machines. Being a rather difficult technical issue to master, the School thus offered direct, selected training in these techniques to the participants.

Having the full team of Yambo developers present and active at the school made it easy for us to dedicate time and assistance to all the participants as necessary. As a result of this, we were able to follow their individual progress, as recognised by the award of two more prizes for the student we felt had made the most progress (“Biggest leap forward”) and to the student

who adapted best to learning techniques outside their own field of knowledge (“Best hop sideways”).
Finally, in order to judge the overall success of the school, we circulated an anonymous online questionnaire (independent of the CECAM survey) about the school's scientific activities and organization (see annex), which was filled in by 25 participants. In the survey participants were asked to rate the different kinds of activities (formal theory, practical lectures, hands-on classes), and invited to submit explicit suggestions and comments on how to improve the various activities.

Feedback from the survey was quite uniform across all levels of experience (16 PhD students, 9 postdoc or higher). Overall, the hands-on sessions and the quality of the lectures were rated very highly, and participants were more than happy with all aspects of the organization. On the negative side, some students found the lectures too advanced. We will use this feedback to improve future schools, e.g. by preparing some introductory material to be circulated before the school, by promoting more interaction with the students, and by reordering and refining some of the lectures and hands-on sessions. Nonetheless, most of the comments we received reflected a great overall satisfaction with the school.

Overall the School was very successful and contributed to training the next generation of scientists interested in computational spectroscopy by many-body methods.

Programme of the meeting

Day 1 - April, 13th 2015 - Basic Concepts

08:45 to 09:00 - Welcome
Realistic Simulations of complex materials. Nicola Marzari

09:00 to 10:00 - Presentation
10:00 to 10:30 - Coffee Break
Electronic structure calculations: DFT and beyond. Myrta Gruening

10:30 to 11:30 - Presentation
The linear response theory and TDDFT. Davide Sangalli

11:30 to 12:30 - Presentation
12:30 to 14:00 - Lunch
HANDS-ON (I). Introduction to Yambo. Installation, interfacing with DFT codes and step-by-step Yambo usage. Conor Hogan

14:00 to 15:30 - Exercises
15:30 to 16:00 - Coffee Break

16:00 to 18:00 - Poster Session
19:00 to 21:00 - Get together

Day 2 - April, 14th 2015 - One Particle Excitations

Experimental state-of-the-art of ARPES. Simon Moser
09:00 to 10:00 - Presentation
10:00 to 10:30 - Coffee Break
GW and Angle-resolved photoelectron spectroscopy (ARPES). Andrea Ferretti

10:30 to 11:30 - Presentation
GW common approximations and practical implementations . Daniele Varsano

11:30 to 12:30 - Presentation
12:30 to 14:00 - Lunch
HANDS-ON (II + III) using the Yambo code: GW calculations for extended systems, quasiparticle energies and lifetimes, plasmon-pole versus real-axis integration. Andrea Marini

14:00 to 15:30 - Exercises
15:30 to 16:00 - Coffee Break
16:00 to 18:00 - Exercises

Day 3 - April, 15th 2015 - Large scale computing with Yambo

Introduction to the Many-Body problem (I): the diagrammatic approach. Pedro Melo

09:00 to 10:00 - Presentation
10:00 to 10:30 - Coffee Break
Trends in parallel computing. Carlo Cavazzoni

10:30 to 11:30 - Presentation
Parallel structure of Yambo. Andrea Marini

11:30 to 12:30 - Presentation
12:30 to 14:00 - Lunch
HANDS-ON (III) using the Yambo code: PARALLELISM. Andrea Marini and Andrea Ferretti

14:00 to 15:30 - Exercises
15:30 to 16:00 - Coffee Break
16:00 to 18:00 - Exercises
19:30 to 22:30 - Social Dinner

Day 4 - April, 16th 2015 - Two-particle excitations

Introduction to the Many-Body problem (II): the diagrammatic approach. Andrea Marini

09:00 to 10:00 - Presentation
10:00 to 10:30 - Coffee Break
Introduction to the BSE, Margherita Marsili

10:30 to 11:30 - Presentation
BSE and TDDFT calculations: general implementation and common approximations. Spin orbit coupling. Maurizia Palummo

11:30 to 12:30 - Presentation
12:30 to 14:00 - Lunch
HANDS-ON (IV+V) using the Yambo code: optical properties, from TDDFT to BSE. Spin orbit coupling. Marsili/Palummo

14:00 to 15:30 - Exercises
15:30 to 16:00 - Coffee Break
16:00 to 18:00 - Exercises

Day 5 - April, 17th 2015 - Hacking Yambo

Coding in the Yambo code. Myrta Gruning and Davide Sangalli

09:00 to 10:00 - Exercises
10:00 to 10:30 - Coffee Break
10:30 to 12:00 - Exercises
12:00 to 12:30 - General Discussion and Conclusion

Full list of speakers and participants

Speakers

Cavazzoni, Carlo - CINECA, Italy
Ferretti, Andrea CNR-Institute of Nanoscience, Modena, Italy
Gruning, Myrta Queen's University Belfast, United Kingdom
Hogan, Conor CNR-ISM, Rome and University of Rome Tor Vergata, Italy
Marini, Andrea National Research Council, Rome, Italy
Marsili, Margherita S3, CNR Istituto di Nanoscienze (NANO), Italy
Marzari, Nicola Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Melo, Pedro University of Coimbra, Portugal
Moser Simon Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Palummo, Maurizia University of Rome II 'Tor Vergata', Italy
Sangalli, Davide CNR-ISM, Uos di Montelibretti, Italy
Varsano , Daniele S3, CNR Istituto di Nanoscienze (NANO), Italy

Participants

Pérez Villegas, César Enrique - Institute for Theoretical Physics, Sao Paulo State University (UNESP), Brazil
Banerjee, Amitava - Materials Theory Division, Ångström Laboratory, Uppsala, Sweden
Biele, Robert - Nano-bio Spectroscopy Group, ETSF, San Sebastian, Spain
Bouduban, Marine - Swiss Federal Institute of Technology of Lausanne (EPFL), Switzerland
Cazzaniga, Marco - Istituto di Scienze e Tecnologie Molecolari - CNR-ISTM - sede Milano, Italy
Cepellotti, Andrea - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Faghihnasiri, Mahdi - Department of Physics, Shahrood University, Shahrood, Semnan, Iran, Iran
Frank, Tobias - University of Regensburg, Germany
FRAYRET, Christine - Laboratoire de Réactivité et Chimie des Solides - UMR 7314 - 33 rue saint-Leu 80039 Amiens, France
Gibertini, Marco - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Gracia-Espino, Eduardo - Umeå University, Sweden
Haldar, Soumyajyoti - Uppsala University, Sweden
Hellgren, Maria - University of Luxembourg, Luxembourg
Katukuri, Vamshi Mohan - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Lee, Hyungjun - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Lücke, Andreas - Universität Paderborn, Germany
Melendez, Juan J. - University of Extremadura, Spain
Menichetti, Guido - Department of Physics University of Pisa and NEST (Istituto Nanoscienze-CNR), Italy)
Miroshnichenko, Olga - University of Oulu, Finland
Ouserigha, Ebiyibo Collins - University of Warwick, United Kingdom
Pasquier, Diego - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland
Perez Jigato, Manuel - Luxembourg Institute of Science and Technology, Luxembourg

Posysaev, Sergei - University of Oulu, Finland
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Saglam, Yildiz Gozde - Middle East TEchnical University, Bilkent University, Turkey
Shahrokhi, Masoud - Physics Department, Faculty of Science, Razi University, Kermanshah, Iran, Iran
Shan, Guangcun - CityU of Hong Kong and CPfS, Max-Planck Institute, Hong Kong
Shukla, vivekanand - Uppsala University , Sweden
Wierzbowska, Malgorzata - Polish Academy of Science, Institute of Physics, Poland
Winkler, Blaž - Materials research laboratory, University of Nova Gorica, Slovenia
Zaari, halima - hD Student in laboratory of magnetism and physics of high energy (LMPHE) Faculty of Sciences, Morocco
Zhou, Liujiang - Bremen University, Germany
Ziaei, Vafa - University of Bonn, Germany
Zoppi, Laura - University of Zurich, Switzerland

Yambo 2015 CECAM School - Participant Feedback Survey ANNEX

Thank you for taking part in the 2015 Yambo school at CECAM, Lausanne! We hope you found it useful and interesting. Please take a few minutes to complete the following short survey which will help us to evaluate our performance and improve future Yambo events.

This is an independent survey by the Yambo organisers and is completely separate from the CECAM evaluation you may have already submitted.

The programme of the school can be found here: programme

1. What is your current position?

Masters or PhD student Postdoc Researcher/Professor

2. Rate the quality of the scientific activities

	Excellent	Good	Fair	Poor
Invited Lectures				
Lectures on fundamentals (morning)				
Lectures on theory/practical implementation (morning/afternoon)				
Hands-on classes (after lunch)				

3. Rate the difficulty of the scientific activities

	Far too difficult	Somewhat difficult	Just about right	Not difficult
Invited Lectures				
Lectures on fundamentals (morning)				
Lectures on theory/practical implementation (morning/afternoon)				
Hands-on classes (after lunch)				

4. Do you have any suggestions for improving the lecture programme?

5. Do you have any suggestions for improving the hands-on sessions?

6. Any other comments, suggestions, or criticisms about the school in general?