Report on the 14^{th} ETSF Workshop on Electronic Excitations: Ab-initio tools for the characterization of nanostructures

Evora, Portugal

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Sponsors: Psi-k, CECAM, ESF-SimBioMa, Fundacão para a Ciência e Tecnologia

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http://www.tddft.org/ETSF2009/index.html

Brief Summary

The workshop has focused on the first-principles description of electronic excitations and spectroscopy of condensed matter, nanostructures, and bio-molecules. Characterization of materials involves the interaction with particles or radiation that brings the system into an excited state. While the ground state, even of very large systems, can usually be well described by density-functional theory (DFT), the calculation of excited states is considerably more involved. In particular three methods for excited states calculations were addressed at the workshop:
i) Time-dependent density-functional theory (TDDFT),
ii) Many-body perturbation theory (MBPT), in particular the "GW-approximation" and the "Bethe-Salpeter Equation",
iii) Quantum chemistry methods.
We have discussed recent advances in both conceptual developments as well as their application to real systems. 95 researchers participated in the workshop. 5 keynote lectures, 8 invited talks, 26 contributed talks, and 30 posters were presented. The workshop reflected in part the activites of researchers of the European Theoretical Spectroscopy Facility (ETSF). However, we were happy to attract also many scientists (in particular, the invited plenary speakers) from outside this institution. This turned our annual workhop into the European reference conference on electronic excitations.

Scientific content of and discussions at the event

Tuesday, 15/09:
The first session on optical properties gave an overview over the use of advanced excited states methods (TDDFT, GW-approximation, Bethe-Salpeter Equation) in various systems. The opening keynote lecture by Steven Louie (UC Berkeley) dealt with the optical properties of graphene nanostructures and various possible device applications. Patrick Rinke (UC Santa Barbara) presented calculations of Auger recombination in nitrides, Hannes Hübener (Ecole Polytechnique, Paris) presented calculations of the second harmonic generation in Silicon. The session ended with two talks on novel materials for solar cells: Julien Vidal (Ecole Polytechnique, Paris) exposed how calculations beyond-DFT can help to improve the understanding of solar cells. Nicola Spallanzani (Modena) discussed photo-excitation in large organic molecules.
In the second keynote lecture, Gustavo Scuseria (Rice University) gave an overview over recent developments in hybrid functionals and on the mixing of the Random-Phase-Approximation with DFT.
In the session on bio-physics, different user projects of the ETSF were presented. Steen Nielsen (Aarhus) gave a keynote lecture on how to perform measurements of absorption spectra of molecular ions in a storage ring

experiment. Marius Wanko (San Sebastián) presented calculations in the QM/MM approach that accompany the experiment. Adriano Mosca Conte (Rome) presented results on the photo-excitation of proteins in the retina of the human eye.

Wednesday, 16/09:

The morning session was mainly devoted to strongly correlated systems. In a keynote lecture, Emily Carter (Princeton) introduced an approach to embed quantum-chemical wave-function methods into periodic DFT. One of the applications of this approach was the *ab-initio* description of the Kondo effect for transition metal impurities in nonmagnetic metallic hosts. Federico Iori and Matteo Guzzo (Ecole Polytechnique, Paris) reported on progress in the description of strongly correlated systems like V_2O_3 and NiO with a self-consistent GW-approach. Martin Stankovski (Louvain-la-Neuve) discussed the effects of self-consistency and semi-core states in the GW-approximation for Zn and Sn oxides. Jim Greer (Tyndall National Institute, Cork) presented a configuration-interaction method where the contributing (singly and multiply excited) configurations are chosen by a Monte Carlo approach. The session ended with a talk by Dietrich Foerster and Peter Koval on the extension of the LCAO method to excited states.

Walter Temmermann (Daresbury) presented a keynote lecture on the self-interaction-corrected local-spin-density (SIC-LSD) method for the calculation of rare earth and actinide compounds. In the following discussion it became clear that more work on the comparison of the different approaches for systems with strong localisation and strong correlations would be desirable: self-consistent GW, SIC-LSD, and dynamical mean-field approximation (DMFT) have lead to enormous advances on different systems, but a detailled comparison of their performances is still missing.

The afternoon session was devoted to the random-phase approximation and functionals. Xinguo Ren (Fritz Haber Institute) assessed the potential of the random-phase approximation for CO adsorption and weakly bonded systems. Esa Räsänen (Jyväskylä, Finland) presented functionals in low-dimensional systems. Ulf von Barth (Lund) derived a correlation-energy functional from time-dependent exact-exchange theory.

Thursday, 17/09:

The first morning session dealt with the general theory for the description of quantum transport. Hervé Ness (York) presented a talk on non equilibrium and many-body effects in quantum transport through nanoscale devices. Hector Mera (CEA Grenoble) discussed the accuracy of conductances obtained from Kohn-Sham wave-functions. Valerio Olevano (Institut Néel, Grenoble) introduced a new quantum transport formalism based on a map of a real 3-dimensional system (lead-junction-lead) onto an effective 1-dimensional system and applied this approach to calculate the conductance through graphene nanoribbons. The second morning session was devoted to the transport properties of carbon nanostructures obtained at Louvain-la-Neuve (Belgium): Simon Dubois presented detailled calculations on the transport through graphene nanoribbons. Zeila Zanolli discussed transport properties of carbon atomic wires and Aurelien Lherbier showed the influence of dopants and defects on the transport in 2D graphene.

The afternoon session was devoted to recent developments of the GW-approximation. Juan María García Lastra (San Sebastián) demonstrated how to use the GW-approximation to calculate image potentials at solid-molecule interfaces. Andreas Gierlich (Jülich) presented all-electron GW calculations for perovskite transition-metal oxides. Arjan Berger (Ecole Polytechnique, Paris) presented a scheme to calculate the GW self-energy without the use of unoccupied states. Pina Romaniello (Ecole Polytechnique, Paris) discussed the self-screening error of GW and the atomic limit of strong correlation within a two-site Hubbard model.

The subsequent poster session covered the whole range of electronic excitations from fundamental development of theory to its application to specific nano- and bio-systems.

Friday, 18/09:

Alberto Castro (Freie Universität Berlin) showed how to use TDDFT and optimal control theory to calculate the design of laser pulses that induce specific reactions in molecules (such as dissociation or isomerization). Ilya Tokatly (San Sebastián) discussed the continuum mechanics of quantum many-body systems in the linear response regime.

The following session dealt with optical properties of different materials: Andre Schleife (Jena) presented an application of the BSE-GW approach to the calculation of the optical spectra of MgO and ZnO in the presence of defects and doping. Marco Cazzaniga (Milano) showed RPA calculations of the electron-energy loss function of ferromagnetic iron. Giancarlo Cappellini presented a systematic TDDFT study of the optical spectra of polycyclic aromatic hydrocarbons. The session ended with a talk by Giovanni Onida (Milano) on

the spectroscopy of monoatomic carbon wires.
In the afternoon, Pierluigi Cudazzo (San Sebastán) presented results towards and ab-initio description of high-temperature superconductivity in dense molecular hydrogen. Frank Fuchs (Jena) discussed the geometry, STM images and band structure of atomic gold-wires on a Ge(001) surface. Hans-Christian Weissker presented TDDFT calculations of the optical

Program

		Sunday, September 13
		arrival day
20:30		Dinner (at the Hotel - Buffet)
		Tuesday, September 15
9:00		Welcome address
9:20	*Steven Louie*	Spectroscopic and Transport Properties of Graphene and Graphene Nanostructures
10:20		Coffee break
10:50	*Patrick Rinke*	Auger recombination rates in nitrides from first principles
11:10	*Hannes Huebener*	Second Harmonic Generation in Bulk Silicon
11:30	*Julien Vidal*	How can ab initio calculations help to improve solar cells?
12:10	*Nicola Spallanzani*	Photo-excitation of light-harvesting supra-molecular triad: a TDDFT study
12:30		Lunch (at the Hotel)
14:30	*Gustavo Scuseria*	New models for mixing wavefunctions with density functional theory
15:30		Coffee break
16:00	*Steen Nielsen*	Absorption spectra of chromophore ions obtained from storage ring experiments
17:00	*Adriano Conte*	A theoretical investigation on the first step of the mechanism of vision in living beings
17:20	*Marius Wanko*	Multiscale Approaches for Protein Spectroscopy
17:40		Round Table — Interaction of ETSF with users
20:00		Dinner (at "Jardim do PaÃ§o" restaurant)
		Wednesday, September 16
9:00	*Emily Carter*	Ab Initio Treatment of Excited States and Strongly Correlated Electrons in Crystals
10:00	*Federico Iori*	In strong correlation do we trust? The paradigm of V2O3
10:20		Coffee break
10:50	*Matteo Guzzo*	Exchange and correlation effects in the electronic properties of transition-metal oxides: The example of NiO
11:10	*Martin Stankovski*	Oxidise this: A study of PAW+QPSCGW calculations on Zn and Sn oxides
11:30	*Jim Greer*	Calculation of electron correlations and excitation spectra from a Monte Carlo configuration generation technique
12:10	*Dietrich Foerster**	Extension of the LCAO method to excited states
12:30		Lunch (at the Hotel)
14:30	*W. Temmermann*	Electronic and Magnetic Properties of Rare Earths and Actinide Compounds
15:30		Coffee break
16:00	*Xinguo Ren*	Assessing the random phase approximation: CO adsorption and weakly bonded systems
16:40	*Esa Räsänen*	Functionals in low-dimensional systems
17:00	*Ulf von Barth*	Correlation energy functional and potential from time-dependent exact-exchange theory
18:00		Cheese and wine tasting at "Rota dos Vinhos"
20:00		Dinner (at "Adeguita do Farrobo" restaurant)

* with Peter Koval

Thursday, September 17

9:00	*Hervé Ness*	Non equilibrium and many-body effects in quantum transport through nanoscale devices
9:40	*Hector Mera*	Are Kohn-Shamm conductances accurate?
10:00	*Valerio Olevano*	Effective 1D theory and generalized Fisher-Lee formula for quantum transport at nanocontacts
10:20		Coffee break
10:50	*Simon Dubois*	Quantum Transport in Graphene Nanoribbons
11:30	*Zeila Zanolli*	Transport properties of carbon atomic wires
11:50	*Aurelien Lherbier*	Charge transport in 2D graphene including dopants/defects: ab initio and tight-binding coupled approach
12:30		Lunch (at the Hotel)
14:30	*Juan Garcia-Lastra*	Classical and Many-Body Theory of Image Potentials at Solid-Molecule Interfaces
15:10	*Andreas Gierlich*	All-electron GW Calculations for Perovskite Transition-Metal Oxides
15:30	*J.A. Berger*	GW without empty states
15:50	*Pina Romaniello*	The self-energy beyond GW
16:10		Coffee break
16:40		Poster Session
20:00		Dinner (at "Jardim do PaÃ§o" restaurant)

Friday, September 18

9:00	*Alberto Castro*	Quantum Optimal Control Theory with TDDFT
9:40	*Ilya Tokatly*	Linear Continuum Mechanics for Quantum Many-Body Systems
10:00		Coffee break
10:30	*Andre Schleife*	From Ideal Bulk to Reality - Interplay of Excitonic Effects with Defects and Doping
11:10	*Claudia Roedl*	Absorption Spectra of Magn. Insulators: Antiferromagn. Trans.-Metal Oxides and Ferrogmagn. CrBr3
11:30	*M. Cazzaniga*	Ab-initio long wavelength dielectric properties of bulk iron
11:50	*Giancarlo Cappellini*	Optical absorption ... polycyclic aromatic hydrocarbons
12:10	*Giovanni Onida*	Spectroscopy of Monoatomic Carbon wires connecting sp2 carbon fragments
12:30		Lunch (at the Hotel)
14:30	*Pierluigi Cudazzo*	Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen
14:50	*Frank Fuchs*	Ab-initio study of atomic gold-wires on Ge(001)
15:10	*Hansi Weissker*	Temperature effects on the electronic and optical properties of silicon clusters
15:30		Final remarks
15:40		Coffee break
16:00		ETSF Members' meeting
20:00		Dinner (Banquet at the Hotel)

Saturday, September 19

departure

List of Posters:

Irene Aguilera	First-Principles Design of Complex Intermediate-Band Photovoltaic Materials.
Magdalena Birowska	Ab initio study of functionalized carbon nanotubes
Björn Oetzel	Ab-Initio Studies of Electronic and Transport Properties of Graphene Nanoribbons
Michel Bockstedte	The merits of DFT-LDA and going beyond it towards excited states: a perspective from defects in SiC
Duanjun Cai	Accurate color tuning of firefly chromophore by modulation of local polarization electrostatic fields
Fabiana Da Pieve	Magnetic circular dichroism and spin polarization in resonant photoemission
Louise Dash	Non-equilibrium inelastic electronic transport: beyond the self-consistent Born approximation for the electron-phonon interaction
Luiz Claudio de Carvalho	First-Principles Study of the Structural and Electronic Properties of the (Al,Ga,In)N Compounds
Xavier Declerck	Electronic and transport properties of boron nitride nanoribbons
Christoph Friedrich	EXX within the full-potential augmented-planewave (FLAPW) method
Pablo Garcia Gonzalez	GW calculations in exactly solvable model systems: The problem of the self-interaction errors
Matteo Gatti	Excitonic effects in the absorption spectrum of sodium at high pressure
Paola Gori	Electronic and optical properties of group IV two-dimensional systems
Jim Greer	The ABC's of Many-Electron Correlated Scattering
Ralf Hambach	First-Principles Approach for Spatially-Resolved Electron Energy-Loss Spectroscopy
Yann Pouillon	Structural and optical transitions of biliverdin
Fabrizio Puletti	Large prebiotic molecules in space: photo-physics of acetic acid and its isomers
Yuchen Ma	excited states of the chromophores within many-body perturbation theory
Anna Miglio	Transparent Conducting Oxides (TCO): tin oxides as a case study
Bruce Milne	Time-Dependent DFT for Elucidation of Stereochemistry: Dermacozine E, a Natural Product from the Mariana Trench
Bruce Milne	FMO-TDDFT Studies of Luciferase from the Japanese Firefly Luciola cruciata
Manolo Ramirez López	Many carrier effects in semiconductor nanostructures
Manolo Ramirez López	Photoluminescence spectroscopy of InGaAs/GaAs quantum wells
Tonatiuh RANGEL	Transport properties of molecular junctions from Many-Body Perturbation Theory
Arno Schindlmayr	Do we know the band gap of lithium niobate?
Martin Stankovski	Oxidise this: A study of PAW + QPSC*GW* calculations on Zn and Sn oxides
Z. Szotek	Structural phase transitions and fundamental band gaps of $Mg_xZn_{1-x}O$ alloys from principles
F. Trani	Ab Initio simulation of photovoltaic materials
José Guilherme Vilhena	Density gradients for the exchange energy of electrons in two dimensions
Ludger Wirtz	The phonon dispersion relations of lead chalcogenides (PbS, PbSe, PbTe)

List of participants

1. Steen Broendsted Nielsen
2. Andres R. Botello-Mendez
3. Alejandro Soba
4. Edgar Bea
5. Hector Mera
6. Marc Torrent
7. Davide Sangalli
8. Nicola Spallanzani
9. Fabrizio Puletti
10. Christoph Friedrich
11. Frank Fuchs
12. Luiz Claudio De Carvalho
13. Xinguo Ren
14. Andreas Gierlich
15. Ludger Wirtz
16. Roberto D'Agosta
17. Peter Koval
18. André Schleife

19. Björn Oetzel
20. Valerio Olevano
21. Paola Gori
22. Fabio Trani
23. Micael Oliveira
24. Miguel Marques
25. Arjan Berger
26. Christine Giorgetti
27. Eleonora Luppi
28. Federico Iori
29. Francesco Sottile
30. Gaelle Bruant
31. Hannes Huebener
32. Hans-Christian Weissker
33. Julien Vidal
34. Lucia Reining
35. Matteo Guzzo
36. Pina Romaniello
37. Ralf Hambach
38. Silvana Botti
39. Valerie Veniard
40. Ulf von Barth
41. Anna Miglio
42. Anne Matsuura
43. Aurélien Lherbier
44. Bruno Bertrand
45. Fabiana Da Pieve
46. Gian-Marco Rignanese
47. Jean-Cristophe Charlier
48. Martin Stankovski
49. Simon Dubois
50. Tonatiuh Rangel Gordillo
51. Xavier Declerck
52. Xavier Gonze
53. Zeila Zanolli
54. Emily A. Carter
55. Gustavo Scuseria
56. Dzidka Szotek
57. Walter Temmerman
58. Jim Greer
59. Carolina Roman
60. Ilya Tokatly
61. Juan María García Lastra
62. Marius Wanko
63. Matteo Gatti
64. Pierluigi Cudazzo
65. Xavier Andrade
66. Yann Pouillon
67. Pablo Garcia-Gonzalez
68. Irene Aguilera
69. Giovanni Onida
70. Marco Cazzaniga
71. Alberto Castro

72. Michel Bockstedte
73. Arno Schindlmayr
74. José Albuquerque D'orey
75. Dietrich Foerster
76. Giancarlo Cappellini
77. Patrick Rinke
78. Steven G. Louie
79. Bruce Milne
80. Claudia Cardoso
81. Duan-Jun Cai
82. Fernando Nogueira
83. Myrta Grüning
84. Tiago Cerqueira
85. Esa Räsänen
86. Yuchen Ma
87. Adriano Mosca Conte
88. Olivia Pulci
89. Karolina Milowska
90. Magdalena Birowska
91. Hervé Ness
92. James Ramsden
93. Louise Dash
94. Rex Godby
95. Tony Patman