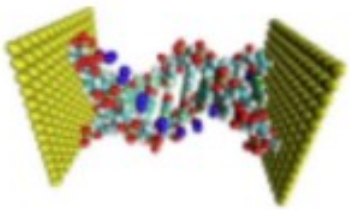
9^{th} ETSF Young Researchers' Meeting

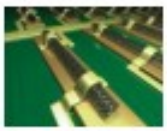
Revolutions in Ab-initio,
closing the circle between theory and experiment

Brussels 21–25 May 2012



ETSF

European Theoretical
Spectroscopy Facility



Website

http://yrm2012.etsf.eu/

Scientific Report

The workshop gathered 56 young researchers from leading international groups and 14 additional participants related to the private sector for the industry day. There were 40 oral presentations (7 keynote speakers, 3 invited speakers from the private sector and 3 invited young researchers for the industry day as well as 27 contributed talks) and 18 posters. The workshop consisted in 8 sessions :

- Industry day
- Ground State
- Electromagnetic Perturbations
- Quantum Transport
- Charged Electronic Excitations
- Neutral Electronic Excitations
- Theoretical Developments
- Algorithms

The first day, dedicated to industry allowed the young researchers to get a better insight into the needs of the private sector. For our industrial participants, it was the opportunity to better understand the possibilities offered by the simulations, in particular ab initio simulations. Three companies already involved in first-principles calculations presented part of their research projects (Mitsubishi Chemical Corp. – Japan, Accelrys – Germany and IMEC – Leuven, Belgium). A round table discussion allowed to tackle the following topics :

- ***Ab initio science:*** What simulations does your industry need?
- ***Ab initio science:*** What can and can't we do at present that is relevant to the private sector and experimentalists?
- ***Ab initio science:*** Is it possible to do fundamental physics in industry?
- ***Ab initio science:*** How does fundamental research in industry differ from academia?
- ***Collaboration:*** How do we make academia and industry work together more efficiently?
- ***Work for YRs:*** What roles can PhD and postdocs have in the private sector?
- ***Work for YRs:*** What skills specific to condensed matter theoretical physicists have you found relevant in industry?
- ***Work for YRs:*** What do companies look for in a CV for industrially relevant ab inito research?
- ***Personal experiences:*** Did you go the academic pathway before applying in that specific company?
- ***Personal experiences:*** Why did you chose your specific company over any other?

This session led to very fruitful discussions about the present and future of the use of first

principles simulations in the private sector.

The other days were mainly devoted to particular topics, methods or techniques in first-principles simulations. The first session about the Ground State consisted in one keynote presentation about the common approximations used in Density Functional Theory (DFT) and 1 contributed talk on van der Waals effects in graphene structures. The keynote talk in the session “Electromagnetic Perturbations” discussed the spin magnetism and spin excitations. The session comprised 3 other contributed presentations : magnetic and optical properties in TiO_2, spin effects in DFT and properties of isomers of silicon slabs. The session on quantum transport started with a general overview of the subject followed by 2 presentations about graphene and 1 presentation about more theoretical aspects of transport. The two sessions about charged and neutral electronic excitations were composed of 1 keynote talk for each of them, presenting the basic aspects about electronic excitations. There were 6 contributed talks in the charged electronic excitations session, mainly devoted to applications of the method : satellites in semiconductors, spectroscopy of TiO_2, Raman spectroscopy of MoS_2, IXS measurements, organic photovoltaics, optical properties of bulk gold. In the neutral electronic excitations session, 6 contributions discussed excitonic effects, shape-depend photoabsorption, photoisoimerization, dynamical effects in optical absorption, color centers and local field effects in Si/CaF_2 interfaces. The next session about theoretical developments started with a keynote talk on new methods in nonequilibrium many-body physics. The session continued with 5 other contributed talks on mainly theoretical aspects in first principles calculations. The keynote talk about the last session (algorithmics) permitted to discuss codes, file formats and libraries. This session comprised 3 contributed presentations about validation of calculations by cross-checking codes, solutions of the GW approximations and Born-Oppenheimer Molecular Dynamics for large systems.

Besides the oral presentations, a poster session was also organized. It gave rise to very interesting discussions. Indeed, wide variety of subjects were presented and the discussions went well beyond these subjects. The meeting provided an informal atmosphere for stimulating discussions between researchers working in this exciting field. The poster session allowed also the young researchers to know each other and get contacts for possible future collaborations. This kind of networking aspect is of tremendous importance in research.

The full booklet of abstracts and program of the workshop by days are available on the website of the conference :

http://yrm2012.etsf.eu/content/Booklet.pdf

The list of participants and contributions is given in the following pages.

Conference program :

21st May 2012 :

Industry Day

9:00	Registration
9:30	Welcome word
9:45	**Masayoshi Mikami** (Mitsubishi Chemical, Japan): "*Theoretical approach for white-LED phosphors*"
10:35	**Geoffroy Hautier** (Massachussets Institute of Technology, USA): "*Using first principles computations to understand, discover and design Li-ion battery cathode materials*"
11:10	Coffee break
11:30	**Martin Stankovski** (Université Catholique de Louvain, Belgium) : "*Present and future of theoretically assisted research*"
12:05	**Johan Carlsson** (Accelrys, Germany) : "*Modelling at Accelrys bridging science and industry*"
12:40	Lunch
14:00	Round table discussion - led by **Martin Stankovski**
15:30	Coffee break
16:00	**Sergiu Clima** (IMEC, Belgium) : "*First principles simulations - Guiding tool for industrial research*"
16:35	**Bruno Bertrand** (Université Catholique de Louvain, Belgium) : "*How to improve the efficiency of thin-film solar cells made of Kesterite? A possible answer from many-body methods*"
17:10	Closing word

List of participants and contributions :

	YRM Meeting				
	First name	Last name	Affiliation	Title of contribution	Contribution type
1	Nicolaev	Adela	LSI, Ecole Polytechnique, Palaiseau	What can we learn from IXS measurements?	Oral presentation
2	Gabriel	Antonius	Université de Montréal	Electron-phonon coupling: including many-body effects with frozen-phonons	Poster
3	Guillermo	Avendano-Franco	Université Catholique de Louvain, IMCN/NAPS	Charge-transfer collisions of H^+ with He using Time- Dependent Density Functional Theory	Poster
4	Matteo	Bertocchi	LSI, Ecole Polytechnique, Palaiseau	Large crystal local-field effects in second-harmonic generation of Si/CaF$_2$ interface: an ab-initio study	Oral presentation
5	Bruno	Bertrand	Université Catholique de Louvain, IMCN/NAPS	How to improve the efficiency of thin-film solar cells made of Kesterite ? A possible answer from many-body methods	Oral presentation (Ind)
6	Bjoern	Bieniek	FHI-MPG, Berlin	Ultra-thin ZnO films on metal substrates from first principle	Poster
7	Andrés Rafael	Botello Méndez	Université Catholique de Louvain, IMCN/NAPS	Quantum Transport in Graphene Nanonetworks	Poster
8	Elena	Cannuccia	Nano-Bio Spectroscopy Group, Universidad del País Vasco UPV/ EHU, San Sebastian	Neutral electronic excitations: a many body approach	Oral presentation (k)
9	Arcesio	Castañeda Medina	MPI, Halle	Excitonic wavefunctions from TDDFT	Oral presentation
10	Alison	Crawford Uranga	Nano-Bio Spectroscopy Group, Universidad del País Vasco UPV/ EHU, San Sebastian	Non-adiabatic transition in the optical spectra of simple molecular systems	Oral presentation
11	Fabiana	Da Pieve	EMAT, University of Antwerp	Visible light absorption and magnetism in doped TiO2 through many body pertubartion theory and spin orbital hamiltonian analysis	Oral presentation
12	Arkady	Davydov	MPI, Halle	Y2O3:Eu phosphor	Poster
13	Xavier	Declerck	Université Catholique de Louvain, IMCN/NAPS	Boron and nitrogen doping of graphene from first principles	Poster
14	John Kay	Dewhurst	MPI, Halle	The Hedin equations and the GW approximation	Oral presentation (k)
15	Marco	Di Gennaro	Université de Liège, Institut de Physique	Ab-initio Spin-Seebeck effect in metal alloys Ab-initio Spin-Seebeck effect in metal alloys	Poster
16	Tanja	Dimitrov	FHI-MPG, Berlin	n/a	n/a
17	Simon	Dubois	University of Cambridge, Canvendish Laboratory	Extending Born-Oppenheimer molecular-dynamics to large-length-scale systems	Oral presentation
18	José María	Escartín	Université Paul Sabatier, Laboratoire de Physique Théorique, Toulouse	Insights into the surface hopping approach from a wavepacket limit	Oral presentation
19	Carina	Faber	Institut Néel, CNRS, Grenoble	Many-body perturbation theory calculations for organic photovoltaics	Oral presentation
20	Johannes	Flick	FHI-MPG, Berlin	Non adiabatic electron-ion dynamics	Poster
21	Matteo	Giantomassi	Université Catholique de Louvain, IMCN/NAPS	Further steps towards a common ground: codes, libraries and file formats within the ETSF simulation software suite	Oral presentation (k)
22	Matteo	Guzzo	LSI, Ecole Polytechnique, Palaiseau	Ab-initio description of satellites in semiconductors	Oral presentation

23	Geoffroy	Hautier	Université Catholique de Louvain, IMCN/NAPS	Using first principles computations to understand, discover and design Li-ion battery cathode materials	Oral presentation (Ind)
24	Linda	Hung	LSI, Ecole Polytechnique, Palaiseau	Spectroscopy of TiO$_2$ valence and semicore states	Oral presentation
25	Jeiran	Jokar	Peter Grünberg Institut and Institute for Advanced Simulation, Jülich	Description of Rabi oscillation in density-functional theory: The effect of spin	Oral presentation
26	Merzuk	Kaltak	University of Vienna, Computational Material Physics	Quasiparticle Spectra from Self-Consistent GW Calculations for Transition-Metal Monoxides	Poster
27	Deniz	Kecik	Paul Scherrer Institut, NUM/ASQ Materials Science and Simulation, Switzerland	Many-body approach compared to Hartree-Fock type and standard-DFT calculations: optical properties of bulk gold	Oral presentation
28	Nicolas	Leconte	Université Catholique de Louvain, IMCN/NAPS	Chemically Tunable Transport Phenomena of Functionalized Graphene	Oral presentation
29	Aurélien	Lherbier	Université Catholique de Louvain, IMCN/NAPS	Simulation of electronic transport in defective graphene. From point defects to amorphous structures	Oral presentation
30	Osman Baris	Malcioglu	Université de Liège, Institut de Physique	Shape managed photo absorption in silicon nanowires	Oral presentation
31	Anna	Miglio	Université Catholique de Louvain, IMCN/NAPS	Electronic and optical properties of tin oxides computed from first principles with different levels of approximation	Poster
32	Seung Kyu	Min	MPI, Halle	Efficient electron dynamics with the planewave-based real-time timedependent density functional theory: Absorption spectra, vibronic electronic spectra, and coupled electron-nucleus dynamics	Poster
33	Alejandro	Molina-Sánchez	University of Luxembourg, Physics and Material Sciences Research Unit	Theoretical Raman spectroscopy of single-layer and few-layer MoS2	Oral presentation
34	Adriano	Mosca Conte	Università di Roma Tor Vergata	Many-Body study of the photoisomerization of the Minimal Model of the Retinal Protonated Schiff Base	Oral presentation
35	Lydia	Nemec	FHI-MPG, Berlin	Graphene on 3C-SiC(111): Ab initio study of structure and stability including van der Waals effects	Oral presentation
36	Micael	Oliveira	Center for Computational Physics, University of Coimbra, Portugal	Common approximations in Density Functional Theory : consequences for ground-state properties	Oral presentation (k)
37	Alessio	Petrone	Dipartimento di Chimica “Paolo Corradini”, Università degli studi di Napoli “Federico II”	A theoretical model for the study of the time-resolved fluorescence	Poster
38	Samuel	Poncé	Université Catholique de Louvain, IMCN/NAPS	Validation of calculations based on electron-phonon matrix elements in Abinit and PWSCF/Yambo/EPW	Oral presentation
39	Tonatiuh	Rangel Gordillo	CEA, DAM, Bruyères-le-Châtel	Modeling of electron transport at the nano-level	Poster
40	Tobias	Sander	University of Vienna, Computational Material Physics	Bethe-Salpeter Equation in the Tamm-Dancoff Approximation (TDA) and beyond	Poster
41	Kiroubanand	Sankaran	Université Catholique de Louvain, IMCN/NAPS, IMEC	Ab initio modeling of defects in high-κ dielectrics for Flash memory applications	Poster
42	Marika	Savarese	Dipartimento di Chimica “Paolo Corradini”, Università degli studi di Napoli “Federico II”	Dyes for fluorescence encoding: a combined experimental and theoretical study	Poster
43	Honghui	Shang	FHI-MPG, Berlin	First principles electron-phonon calculations with numerical atomic orbitals	Poster
44	Sangeeta	Sharma	MPI, Halle	Magnon spectra	Oral presentation (k)
45	Nader	Slama	Université Paul Sabatier, Laboratoire de Physique Théorique, Toulouse	Description of electron correlation by using semiclassical approximations	Poster
46	Lorenzo	Sponza	LSI, Ecole Polytechnique, Palaiseau	Including dynamical effects in optical absorption	Oral presentation

47	Adrian	Stan	LSI, Ecole Polytechnique, Palaiseau	Cutting-edge methods and recent developments in nonequilibrium many-body physics	Oral presentation (k)
48	Martin	Stankovski	Université Catholique de Louvain, IMCN/NAPS	Present and future of theoretically assisted research	Oral presentation (Ind)
49	Nicolas	Tancogne-Dejean	LSI, Ecole Polytechnique, Palaiseau	n/a	n/a
50	Falk	Tandetzky	MPI, Halle	Multiple Solutions of GW-Type approximations	Oral presentation
51	Iris	Theophilou	Peter Grünberg Institut and Institute for Advanced Simulation, Jülich	Spin projected excited states from Unrestricted Hartree Fock	Oral presentation
52	Claudia	Violante	Università di Roma Tor Vergata	Structural, electronic and optical properties of the two isomers of Si(111)2x1	Oral presentation
53	Marton	Voros	Department of Atomic Physics, Budapest University of Technology and Economics	Time-dependent density functional theory calculations on color centers in group four semiconductor nanocrystals	Oral presentation
54	David	Waroquiers	Université Catholique de Louvain, IMCN/NAPS	Assesment of electronic band structure from the Tran-Blaha functional : comparison with Many-Body Theory results	Poster
55	Zeila	Zanolli	Université de Liège, Institut de Physique	Transport in carbon based nanostructures	Oral presentation (k)
56	Jianqiang	Zhou	LSI, Ecole Polytechnique, Palaiseau	Exploring the Performance of the Cumulant Expansion for the Hubbard Molecule	Oral presentation

Industry day

	First name	Last name	Affiliation	Title of contribution	Contribution type
57	Sébastien	Adam	Université Catholique de Louvain, LTTO	n/a	n/a
58	Thomas	Biquet	AGC Glass Europe SA	n/a	n/a
59	Jean-Benoît	Cabo	Institut Supérieur Industriel ECAM	n/a	n/a
60	Johan	Carlsson	Accelrys, Germany	Modelling at Accelrys bridging science and industry	Oral presentation (Ind)
61	Sergiu	Clima	IMEC	First principles simulations – Guiding tool for industrial research	Oral presentation (Ind)
62	Claude	Dierickx	Institut Supérieur Industriel ECAM	n/a	n/a
63	Maurice	Dodémont	AIECAM	n/a	n/a
64	André B.	Mennicken	AIECAM	n/a	n/a
65	Masayoshi	Mikami	Mitsubishi Chemical Corp, Japan	Theoretical approach for white-LED phosphors	Oral presentation (Ind)
66	Jean-François	Theunissen	AIECAM	n/a	n/a
67	Nicky	Thrupp	Université Catholique de Louvain, IMCN/NAPS, ETSF	n/a	n/a
68	Francis	van den Breede	AIECAM	n/a	n/a
69	Guy	Van Geersdaele	Agoria, AIECAM	n/a	n/a
70	Tanguy	Van Regemorter	Université de Mons et Materia Nova	n/a	n/a