ESF final report

10th ETSF Young Researchers' Meeting 2013 in Budapest

Beyond density functional theory – experimental and industrial connections

May 20, 2013 - May 24, 2013

Organizers:

Márton Vörös
Budapest University of Technology and Economics

Matteo Guzzo
École Polytechnique

Adam Gali
Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, Hungarian Academy of Sciences; Budapest University of Technology and Economics

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Budapest University of Technology and Economics

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10th ETSF Young Researchers' Meeting 2013

Beyond density functional theory – experimental and industrial connections

1. Summary

The 10th ETSF Young Researchers' Meeting was held from 20th May till 24th May at the Budapest University of Technology and Economics in Budapest, Hungary. Altogether more than 40 young researchers attended the event, from several different countries, representing many different groups in the field of *ab initio* spectroscopy. The major goals of the event were to give an opportunity for young researchers to present their work with longer talks than usually permitted on other conferences, and to allow for young researchers to network and finally to provide alternative carrier paths by having speakers with industrial background.

The contributions from young researchers were split into several different topics: ground state density functional theory (DFT); electron-phonon coupling and temperature phenomena (ELPH); charged excitations (GW); neutral excitations (Optics); and finally transport calculations (Transport). With the exception of the DFT session, each session started with a long crash-course on the actual topic, which provided the necessary background and up-to-date references to understand more specialized talks. Besides the above sessions and industrial sessions was held with four invited talks. Furthermore, an experimentalist, Fedor Jelezko, from the rapidly growing field of spintronics gave an inspiring cross-disciplinary talk on the nitrogen-vacancy center in diamond. Finally, a poster session and several discussion sessions were also part of the program.

Given the high scientific level of talks and posters and the unanimously positive feedback of both participants and invited speakers, the conference can be considered a huge success.

Description of the scientific content of and discussion at the event

The event started with the ground state density functional theory (DFT) session. Talks covered strategies how to find the ground state geometry of large organic molecules, properties of interfaces, surfaces and point defects in systems of interest to photovoltaic industry. All of these talks underlined how one needs to go beyond the standard treatment, eg. with generally more accurate functionals, to accurately understand or predict ground state properties.

The second session focused on the electron-phonon coupling and temperature phenomena (ELPH). This topic has recently come to the forefront of *ab initio* research as the advance of computational power allows for taking complex interactions into account. Talks covered topics as important as the visible light absorption of silicon (which has not yet been quantitatively characterized theoretically until very recently), which is of crucial importance in the solar cell industry and which is only due to electron-phonon assisted transitions, that is quantum nuclei effects. Other talks concentrated on classical nuclei effects on the optical absorption of nanoparticles and organic molecules which were obtained through molecular dynamics calculations.

Tuesday an industrial session was introduced. This included a talk from György Keserű, the director of the Hungarian Academy of Sciences, Research Centre of Natural Sciences, formerly head of the computational department of Richter Gedeon, a pharmaceutical company in Hungary. He briefly summarized the development procedure of new drugs and how simulations can help through virtual screening strategies. Then, Tibor Höltzl, researcher at Furukawa Electric, showed that how industrial needs result in accurate quantum chemistry calculations on chemical reactions in order to simulate CVD reactors. The third speaker, Johan Carlsson from Accelrys, focused on in silicon development of new composite materials. Finally, although not with an industrial affiliation, Geoffroy Hautier gave a motivating talk on how high-throughput calculations can really help and predict new materials and working principles. These contributions all highlighted that there is a need for *ab initio* computational approaches in industrial research as well, mostly because computations are always cheaper than making experiments and recently we have started entering the era when simulations can have predictive power. We believe that this session was a great help for young researchers to learn about alternative carrier options.

Tuesday, we had a poster session in which eleven posters were presented (only ten appeared in the booklet because we had one late contribution). Several of them originated from the group of Adam Gali, the supervisor of the main local organizer.

Wednesday started with the session on charged excitations (GW). Although the GW method is getting considerable attention as the best tool to understand photoemission measurements concern is attributed to its starting point dependence. This issue was carefully addressed by the invited speaker Fabio Caruso. After that a talk on the fundamentals addressed how usual GW methods converge to the right physical solution, finally a talk was about the comparison on the performance of newly developed functional with many-body approaches.

The largest session was the neutral excitation session (Optics) containing ten talks and spanning two days. There are two approaches that are typically used by the *ab initio* solid state community to understand to optical properties of solids or molecules: the Bethe-Salpeter approach, an equation of motion for the two particle Green's function, and time-dependent density functional theory approach, the time-dependent extension to ground state density functional theory. In principle, both of them should yield the same answer with regards to the polarizability of a system, for example. In practice however, approximations have to be taken which make the Bethe-Salpeter approach generally more accurate but at the same time computationally more expensive as well. Part of the contributions focused on applying these existing methods to understand the optical properties of molecules, nanocrystals. The other part outlined approaches to extend these methodologies to more advanced situations, eg. to understand non-linear properties of surfaces or to include excitonic effects in Raman intensities.

Last, a session on non-equilibrium physics, transport properties (Transport), was held. The transport session had two major branches: talks focused either on purely electronic transport or on thermoelectric transport through the solution of the Boltzmann equation.

Several discussion sessions were held for two major purposes. First, less and less young researchers attend the annual young researchers' meetings. To address this issue, a survey was released before the event took place (it is still available at: http://www.surveymonkey.com/s/BHY97YH). The survey was not only accessible to the participants but to anyone participating on the previous two meetings. Questions addressed issues for the reason of the loss popularity and raised the possibility to change the format of the event. **Second, we have asked the participants to provide one general (not necessarily scientific, but of general interest for young researchers) question at the time of the registration.** We hoped that these would ignite heavy discussions on scientific or less scientific issues related to out field. Typical questions included "Have ab-initio calculations affected our everyday life? In the past decade, have there been first-principles calculations that influenced or gave rase to useful applications?". **These were answered in form of an open discussion where everybody could contribute.**

Assessment of the results and impact of the event on the future direction of the field

In regards of the scientific level, we believe that it reached the level of advanced, more specialized conferences. Almost all talks were followed by several questions and discussions were held also during the poster session. The industrial session provided a sneak-peek into industrially-motivated research. This showed the participants how the skills acquired in academics can be useful in industry as well. This is of crucial importance, since, statistically, not all young researchers will end up working in the academic field.

In regards of the future role of young researchers' meetings. We have received 35 answers for the survey. According to the answers:

(1) The main reason why young researchers do not participate is that supervisors think that students could benefit more from other conferences;

(2) The most important benefit of the YRM is the ability to network with other young researchers with similar backgrounds;

(3) The YRM should not change its current form in future editions;

(4) Anyone could participate on the conference but it should be kept to Master, PhD, PostDoc students with focusing on theoretical research;

(5) The YRM should be publicized in several different ways, including social media.

We concluded that the only way to overcome the barrier of few participants is to urge permanent researchers (specifically the Steering Committee of the ETSF) to encourage their students to participate to the YRM, as without their explicit support, younger students are not likely to choose to come to the YRM independently. This is unfortunate, as they are the ones who can benefit the most from this meeting.

Final program

At the end of this document the final version of the booklet is included as it was printed. The final program contained minor changes with respect to the one in the booklet: one participant did not come and few talks were rescheduled. The below table contains the final version of the schedule of the talks as it appeared on our website: http://etsf.polytechnique.fr/yrm2013/node/12.

20th May **Monday**	**21st May** **Tuesday**	**22nd May** **Wednesday**	**23rd May** **Thursday**	**24rd May** **Friday**
Registration @ hotel	György Keserű			
		GW: Caruso	Optics: Raimbault	
Leave together for uni	Tibor Höltzl		Optics: Gillet	
Welcome words		GW: Tandetzky	Optics: Komarova	
DFT: Supady	CB	GW: Waroquiers	CB	
DFT: Nemec	Johan Carlsson	CB	Optics: Hung	
Coffee break		Optics: Mosca Conte	Transport: Dubois	Discussion
DFT: Pohl	Geoffroy Hautier			CB
DFT: Iacomino		Optics: Stan	Transport: Ibarra	Transport: Leconte
Lunch	Lunch	Lunch	Lunch	Transport: Karlsson
				Closing words
			Fedor Jelezko	
ELPH: Alkauskas	DFT: Bieniek	Optics: Faber		
	ELPH: Forero Martinez	Optics: Baishya	Transport: Gennaro	
ELPH: Poncé	Discussion	Discussion	Transport: Xu	
Discussion		CB	CB	
CB	CB	Optics: Tancogne-Dejean		
ELPH: Antal	Poster session	Optics: Crawford Uranga		
ELPH: Violante				

List of participants

Invited speakers for industrial and experimental sessions:

Fedor Jelezko, Institut für Quantenoptik, Ulm, Germany

Geoffroy Hautier, IMCN, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

György Keserű, Hungarian Academy of Sciences, Research Centre for Natural Sciences

Johan M. Carlsson, Accelrys GmbH, Köln, Germany

Tibor Höltzl, Furukawa Electric

Keynote speakers:

Adriano Mosca Conte; University of Rome Tor Vergata

Audrius Alkauskas; University of California, Santa Barbara

Fabio Caruso; Fritz Haber Institute, Berlin

Simon M.-M. Dubois; University of Cambridge

Other participants:

Adrian Stan; Ecole Polytechnique Palaiseau, France and Univeristy of Jyvaskyla, Department of Physics - Nanoscience Center, France

Adriana Supady; Fritz-Haber-Institut der Max-Planck-Gesellschaft

Alison Crawford Uranga; ETSF Nano Bio Spectroscopy Group, San Sebastian, Spain

Amilcare Iacomino; CSIC and University of the Basque Country UPV/EHU

Andrés Botello-Méndez; UCL-IMCN-NAPS

Aurelien Lherbier; Université catholique de Louvain (UCL/IMCN/NAPS)

Bin Xu; University of Liege

Bjoern Bieniek; Fritz-Haber-Institut der MPG

Carina Faber; Institut Neel, CNRS, Grenoble

Claudia Violante; University of Rome Tor Vergata

Daniel Karlsson; Lund University

David Waroquiers; UCL - IMCN - NAPS

Falk Tandetzky; Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Igor Reshetnyak; LSI, Ecole Polytechnique

Jianqiang ZHOU; ETSFPalaiseau group

Johan Pohl; TU Darmstadt

Kopinjol Baishya; University of Illinois at Chicago

Ksenia Komarova; Photochemistry Center Russian Academy of Sciences

Linda Hung; Ecole Polytechnique

Lydia Nemec; Fritz-Haber-Institut der Max-Planck-Gesellschaft

Marco Di Gennaro; universite de liege

Mehdi Farzanehpour; UPV/EHU, Nano-bio spectroscopy group

Mykhaylo Antal; University of Liege

Nancy Carolina Forero Martinez; LPICM, Ecole Polytechnique, France

Nathaniel Raimbault; LCPQ-LPT (université Paul Sabatier Toulouse)

Nicolas Leconte; UCL/IMCN/NAPS

Nicolas Tancogne-Dejean; LSI, Ecole Polytechnique, Palaiseau, France

Poncé Samuel; Université catholique de Louvain

Wilfredo Ibarra; University of Liege

Yannick Gillet; Université catholique de Louvain - UCL/IMCN/NAPS

Organizers:

Márton Vörös; Budapest University of Technology and Economics

Matteo Guzzo; Ecole Polytechnique, Palaiseau (France) and Humboldt Universitaet, Berlin (Germany)

Tibor Szilvási; Budapest University of Technology and Economics

Tamás Demjén; Eötvös Loránd University & Wigner Research Centre of Physics

Viktor Ivády; Linköping University (Sweden) & Wigner Research Centre of Physics

Bálint Somogyi; Budapest University of Technology and Economics

Krisztián Szász; Eötvös Loránd University & Wigner Research Centre of Physics

Gergő Thiering; Budapest University of Technology and Economics

Supporting organizers (not present on the conference):

Lucia Reining ; LSI - ETSF, Ecole Polytechnique, Palaiseau (France)

Ádám Gali; Budapest University of Technology and Economics & Wigner Researcher Centre of Physics

Péter Richter; Budapest University of Technology and Economics

György Mihály; Budapest University of Technology and Economics

10th ETSF Young Researchers’ Meeting

Budapest University of Technology and Economics
Budapest, Hungary

20-24 May 2013

Sponsors and Partners

We thank the generous financial support from European Science Foundation (ESF).

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ETSF Young Researchers' Meeting

The ETSF Young researchers' Meeting (YRM) is a series of conference held annually under the auspices of the European Theoretical Spectroscopy Facility (ETSF), bringing together young researchers (students and postdocs) working in the field of ab-initio solid-state physics. The main goal of this year's YRM is to give young researchers the opportunity to present their work and to foster interaction between invited speakers (experimentalists, industrial representatives) and young researchers. The peculiarity of YRMs roots in the fact that all young researchers are encouraged to give a 20+5 min talk in an open, friendly environment, where no permanent researchers are present. Talks are then followed by motivating discussions. Each session starts with a longer crash-course on the actual topic, providing younger students the necessary background to understand more specialized talks. The second day of the conference is dedicated to talks given by invited speakers, remaining four days focus on the topics of the ETSF network.

This year's anniversary 10th meeting takes place at Budapest University of Technology and Economics (BUTE), in a conference room provided by the Physics Department. We are deeply indebted for this help. Budapest is a vibrant, lively city and BUTE is located very close to its heart. Besides stimulating talks, discussions, you will have a wonderful time to visit Budapest's most famous sights, including a visit to a thermal bath, and several "ruin pubs". Of course, a football match is also part of the program!

Organizers

Young researchers:

Matteo Guzzo, Humbolt Universitaet, Berlin (Germany)
Márton Vörös, Budapest University of technology and Economics
Tamás Demjén, Eötvös Loránd University & Wigner Research Centre of Physics
Viktor Ivády, Linköping University (Sweden) & Wigner Research Centre of Physics
Bálint Somogyi, Budapest University of Technology and Economics
Krisztián Szász, Eötvös Loránd University & Wigner Research Centre of Physics
Gergő Thiering, Budapest University of Technology and Economics
Tibor Szilvási, Budapest University of Technology and Economics

We would like to thank our supporting organizers who were always there to help and who not only agreed that we spend our time on an event held entirely for students but supported us and encouraged us to do so. We are deeply indebted to them.

Supporting organizers:

Lucia Reining, LSI - ETSF, Ecole Polytechnique, Palaiseau (France)
Adam Gali, Budapest University of Technology and Economics & Wigner Researcher Centre of Physics
Péter Richter, Budapest University of Technology and Economics
György Mihály, Budapest University of Technology and Economics

Schedule

	19th May Sunday	**20th May Monday**	**21st May Tuesday**	**22nd May Wednesday**	**23rd May Thursday**	**24th May Friday**
09:00		Registration at the hotel	**György Keserű**			
09:25				GW **F. Caruso**	Opt. N. Raimbault	
09:50		Leave for uni	**Tibor Höltzl**		Y. Gillet	
10:15		Welcome words		F. Tandetzky	K. Komarova	
10:40		DFT A. Supady	Coffee break	D. Waroquiers	Coffee break	
11:05		L. Nemec	**Johan Carlsson**	Coffee break	Opt. L. Hung	
11:30		Coffee break		Opt. **A. Mosca Conte**	Trans. **S. Dubois**	Discussion
11:55		DFT J. Pohl	**Geoffroy Hautier**			Coffee break
12:20		A. Iacomino		A. Stan	D. Karlsson	Trans. W. Ibarra
12:45		Lunch	Lunch	Lunch	Lunch	M. Gennaro
13:10						Closing words
13:35						
14:00					**Fedor Jelezko**	
14:25		ELPH **A. Alkauskas**	DFT B. Bieniek	Opt. C. Faber		
14:50			ELPH N. C. F.-Martinez	K. Baisya	Trans. N. Leconte	
15:15		S. Poncé	Discussion	Discussion	B. Xu	
15:40		Discussion		Coffee break	Coffee break	
16:05	Registration at the hotel	Coffee break	Coffee break	Opt. N. T.-Dejean	Football match	
16:30		ELPH M. Antal	Poster session	T. Sanders		
16:55		C.Violante		A. C. Uranga		
17:20						
17:45						
18:10	Belgian pub				Szécsényi thermal bath	
evening		City site seeing	Ruin pubs	19:00 dinner		

Monday

	20th May Monday	
09:00 - 09:25	Registration at the hotel	
09:25 - 09:50		
09:50 - 10:15	Leave together for university	
10:15 - 10:40	Welcome words	
10:40 - 11:05	DFT	Adriana Supady: *Conformational search strategies for organic molecules*
11:05 - 11:30		Lydia Nemec: *Electronic structure of epitaxial graphene on 3C-SiC(111)*
11:30 - 11:55	Coffee break	
11:55 - 12:20	DFT	Johan Pohl: *Properties of point defects in* $CuInSe_2$ *and* $CuGaSe_2$ *from screened-exchange hybrids*
12:20 - 12:45		Amilcare Iacomino: *Properties of photoinduced states in water covered Alkali atoms on a Cu(111) surface*
12:45 - 13:10	Lunch	
13:10 - 13:35		
13:35 - 14:00		
14:00 - 14:25		
14:25 - 14:50	ELPH	**Audrius Alkauskas:** *Electron-phonon interactions in wide band-gap semiconductors: implications for photoelectronic devices and materials characterization*
14:50 - 15:15		
15:15 - 15:40		Samuel Poncé: *Validation of calculations based on electron-phonon matrix elements in Abinit and PWSCF/Yambo*
15:40 - 16:05	Discussion	
16:05 - 16:30	Coffee break	
16:30 - 16:55	ELPH	Mykhaylo Antal: *Electron-phonon coupling in heavier elements: from superconductors to thermoelectrics*
16:55 - 17:20		Claudia Violante: *Temperature effects on optical properties of cellulose-based degraded materials*
17:20 - 17:45		
17:45 - 18:10		
18:10 - 18:30		
evening	City site seeing	

Tuesday

	21st May **Tuesday**	
09:00 - 09:25	**György Keserű:** Virtual screening strategies in drug design	
09:25 - 09:50		
09:50 - 10:15	**Tibor Höltzl:** Quantum chemistry for MOCVD simulation	
10:15 - 10:40		
10:40 - 11:05	Coffee break	
11:05 - 11:30	**Johan Carlsson:** Developing new composite materials in-silico	
11:30 - 11:55		
11:55 - 12:20	**Geoffroy Hautier:** Accelerating materials discovery for industrial applications using high-throughput ab initio computing	
12:20 - 12:45		
12:45 - 13:10	Lunch	
13:10 - 13:35		
13:35 - 14:00		
14:00 - 14:25		
14:25 - 14:50	DFT	Bjoern Bieniek: *Ultra-thin ZnO films on metal substrates from first principle*
14:50 - 15:15	ELPH	Nancy Carolina Forero-Martinez: *Computational Study on the Effect of Temperature on the Optical and Electronic Properties of Hydrogenated Silicon Nano-Crystals*
15:15 - 15:40	Discussion	
15:40 - 16:05		
16:05 - 16:30	Coffee break	
16:30 - 16:55	Poster session	
16:55 - 17:20		
17:20 - 17:45		
17:45 - 18:10		
18:10 - 18:30		
evening	Ruin pubs	

Wednesday

	22nd May Wednesday	
09:00 - 09:25		
09:25 - 09:50	GW	**Fabio Caruso:** *The GW approximation to the many-body problem: an approach to theoretical spectroscopy*
09:50 - 10:15		
10:15 - 10:40		Falk Tandetzky: *The physical solution to the GW approximation*
10:40 - 11:05		David Waroquiers: *Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory*
11:05 - 11:30	Coffee break	
11:30 - 11:55	Opt.	**Adriano Mosca Conte:** *Keynote on TDDFT and BSE for neutral excitations*
11:55 - 12:20		
12:20 - 12:45		Adrian Stan: *Demystifying the T-matrix and its relations with other many-body approximations*
12:45 - 13:10	Lunch	
13:10 - 13:35		
13:35 - 14:00		
14:00 - 14:25		
14:25 - 14:50	Opt.	Carina Faber: *Organic photovoltaics: a Bethe-Salpeter/GW study of charge-transfer excitations in coumarins*
14:50 - 15:15		Kopinjol Baisya: *Size and shape dependence of electronic and optical excitations in TiO2 nanocrystals*
15:15 - 15:40	Discussion	
15:40 - 16:05	Coffee break	
16:05 - 16:30	Opt.	Nicolas Tancogne-Dejean: *Nonlinear optical properties of surfaces: Extraction of surface signal*
16:30 - 16:55		Tobias Sanders:*Optical Absorption spectra - The Bethe-Salpeter Equation versus the Time-Evolution Method*
16:55 - 17:20		Alison Crawford Uranga: *Exact vs TDDFT study of the ionization phenomena of a 3D Neon atom*
17:20 - 17:45		
17:45 - 18:10		
18:10 - 18:30		
evening	19:00 dinner	

Thursday

	23rd May Thursday	
09:00 - 09:25		
09:25 - 09:50	Opt.	Nathaniel Raimbault: *Magnetization in extended systems within TDCDFT*
09:50 - 10:15		Yannick Gillet: *Excitonic effects in Raman intensities: an ab initio study*
10:15 - 10:40		Ksenia Komarova: *On ranges of coulomb interactions within density functional theory*
10:40 - 11:05	Coffee break	
11:05 - 11:30	Opt.	Linda Hung: *Valence electron energy loss spectra of* HfO_2
11:30 - 11:55	Trans.	**Simon M.-M. Dubois:** *Efficient quantum transport calculations with optimized support functions*
11:55 - 12:20		
12:20 - 12:45		Daniel Karlsson:*Dynamical competition between disorder and interactions in quantum transport*
12:45 - 13:10	Lunch	
13:10 - 13:35		
13:35 - 14:00		
14:00 - 14:25	**Fedor Jelezko:**	
14:25 - 14:50		
14:50 - 15:15	Trans.	Nicolas Leconte: *Quantum Hall Effect Fingerprints of Chemically Functionalized Graphene*
15:15 - 15:40		Bin Xu: *Calculation of thermoelectric properties from first-principles*
15:40 - 16:05	Coffee break	
16:05 - 16:30	Football match	
16:30 - 16:55		
16:55 - 17:20		
17:20 - 17:45		
17:45 - 18:10		
18:10 - 18:30	Szécsényi thermal bath	
evening		

Friday

	24th May Friday	
09:00 - 09:25		
09:25 - 09:50		
09:50 - 10:15		
10:15 - 10:40		
10:40 - 11:05		
11:05 - 11:30		
11:30 - 11:55	Discussion	
11:55 - 12:20	Coffee break	
12:20 - 12:45	Trans.	Wilfredo Ibarra Hernández: *Effect of pressure on the thermoelectric properties of* Bi_2Te_3
12:45 - 13:10		Marco di Gennaro: *Ab initio study of the Spin Seebeck effect in metallic alloys*
13:10 - 13:35	Closing words	

Part I

Oral contributions

Conformational search strategies for organic molecules

Adriana Supady*, Carsten Baldauf, Volker Blum and Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Methods of theoretical spectroscopy that enable the investigation of optical and vibrational properties of a molecule assume that its structure and the conformational ensemble is known in detail. Unfortunately, this is rarely the case and a conformational search problem must be solved beforehand. For organic molecules the conformational space is mainly defined by the torsional degrees of freedom, i.e. the rotations around single bonds between nonterminal atoms. The size of the resulting space is increasing with the size of the molecule as the number of rotatable bond increases. An exhaustive evaluation of the conformations by discretizing the torsional degrees of freedom quickly becomes infeasible already for a small number of rotatable bonds. Thus we investigate different alternative approaches. In a substructure search, the molecules are divided into smaller subunits of a size that allows for a fast systematic search. The resulting conformations are then combined back into the original molecule. Another technique that we apply for sampling of the conformational space is a genetic algorithm that is an adaptive stochastic optimization method inspired by natural evolution. In this algorithm, a population of random conformations is initialized and stepwise optimized by genetic operations. In order to evaluate the performance of the tested methods, we generate and evaluate a set of conformations where we assign random values to the torsion angles. A good search method should be able to produce significantly better results than such random approach. We present the results of the performance of the different methods on the example of azobenzene-based molecules. The substructure search turns out to be insufficient, mainly because the interreaction between the subunits is neglected. The performance of genetic algorithms is critically dependent on the choice of the recombination parameters and their performance on a particular search landscape. Needed is a robust and well-performing set of such parameters. We systematically address this question in our contribution.

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Electronic structure of epitaxial graphene on 3C-SiC(111)

Lydia Nemec[*]

Fritz-Haber-Institut der Max-Planck-Gesellschaft

SiC is a widely used substrate for the growth of mono- and few-layer graphene. By Si sublimation, large ordered areas of graphene form on the Si side as $(6\sqrt{3} \times 6\sqrt{3})$-R30° commensurate periodic films [1]. Characteristic for the epitaxial growth, is the interface structure, the so called zero-layer graphene (ZLG). This layer consists of a hexagonal carbon mesh which is partially sigma-bonded to the substrate, leaving some silicon atoms unbonded – the ”silicon dangling bonds”. However, the role of these dangling bonds on the electronic structure remains largely unexplored. We present a study of the electronic structure of the carbon-rich surface phases on 3C-SiC(111). Our approach is based on density-functional theory (DFT), using the PBE+vdW functional [2]. At the predicted geometries, hybrid functionals (HSE06) are used to assess the electronic structure of: (1) the partially sigma-bonded "ZLG" phase, (2) mono- and bilayer graphene, and (3) hydrogen- and oxygen intercalated graphene phases. For the oxygen intercalated bilayer graphene, we consider an oxygen-rich interface passivating the Si dangling bonds [3]. For the different phases, we discuss the changes of the electronic structure, addressing the influence of the silicon dangling bonds on the electronic structure of the graphene layer and the effects of saturating these bonds by intercalation. In addition, we investigate how intercalation changes the doping of graphene and the charge transfer from the substrate to the graphene layer. We observe that in the intercalated phases graphene is decoupled from the substrate, making intercalation a promising approach for further studies. Finally, we raise the question if the substructures seen in recent STM measurements [4] are really due to defects or a visualisation of the silicon dangling bonds.

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References

[1] K. V. Emtsev *et al.*, Nature Materials **8**, 203 (2009).
[2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).
[3] M.H. Oliveira *et al.*; Carbon **52**, 83-89 (2013).
[4] Y. Qi *et al.*, PRL **105**, 085502 (2010).

Properties of point defects in $CuInSe_2$ and $CuGaSe_2$ from screened-exchange hybrids

Johan Pohl*

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We have investigated the thermodynamic and electronic properties of intrinsic point defects by screened-exchange hybrid density functional theory. The most important findings are summarized and special emphasis is put on the differences to results from local density functional theory. The signatures of some efficiency-limiting point defects with importance for $Cu(In,Ga)Se_2$ solar cell thin-film devices are discussed and compared to photoluminescence measurements.

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Properties of photoinduced states in water covered Alkali atoms on a Cu(111) surface

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Time programmed desorption and work function measurements reveal that alkali atoms directly adsorbed on the metal Cu(111) substrate can be hydrated by surrounding waters molecules. In addition, the electronic structure as a function of water coverage shows pronounced changes as the water coverage increases. The most striking effect is the appearance of a new state which can be attributed to excess electrons at the alkali-water-cluster, which are stabilized by response of the polar environment. The ability to bind such an electron depends on the type of alkali and increases with increasing dipole moment of the adsorbed alkali along the sequence Na, K, Cs. By means of first-principles DFT modeling we will answer to the questions arising from the experimental observations on: (i) how the water molecules adsorb on the surface in presence of alkali atoms; (ii) how to probe the formation of a solvation shell of water molecules around the alkali ion as suggested by 2PPE measurements; (iii) how the water molecules affect the unoccupied alkali resonances. We will show that the main experimental data can be accurately reproduced by combining configurational averages over the alkali-water clusters distribution at fixed overall water density and the structural averages at fixed number of water molecules within the cluster.

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Electron-phonon interactions in wide band-gap semiconductors: implications for photoelectronic devices and materials characterization

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Electron-phonon interactions are ubiquitous in nature. They are responsible for phenomena as varied as the lush green colour of trees, light-absorption in silicon solar cells, heating of computer chips, and superconductivity. In the last two decades or so there has been a substantial progress in studying these interactions from first principles calculations in a variety of physical systems. In the first part of the talk the general theory of “electrons”, “phonons”, and their mutual interaction will be reviewed. Conditions when the concept of “electron-phonon interactions” is useful will be discussed. In the second part of the talk general methods to calculate these interactions in bulk solids and at defects will be presented. In the third part of the talk specific examples related to wide-band gap semiconductors and their application in energy devices will be discussed: (i) phonon-assisted Auger recombination; (ii) free-carrier absorption; (iii) vibronic broadening of defect luminescence bands; and (iv) nonradiative transitions at defects.

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Validation of calculations based on electron-phonon matrix elements in Abinit and PWSCF/Yambo

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First-principles electronic-structure codes are in constant development. New codes are created, and computational capabilities increase with time. The verification and validation of those codes as well as theoretical methods are of utmost importance if one wants to provide reliable results. In this work we present first a comparative study of calculations based on electron-phonon matrix elements in Abinit and PWSCF+Yambo, with the aim to resolve a discrepancy, observed at the time of writing, between the zero-point motion (ZPM) renormalization of the band gap of diamond as implemented in Abinit with the one found with PWSCF+EPW [1] and PWSCF+Yambo [2]. We first present internal checks in Abinit using finite difference methods versus perturbative approaches (i.e. density functional perturbation theory) as implemented in Abinit. This gives good agreement for the zero point motion for an underconverged (in k and q points) calculation. We then make internal checks for the electron-phonon matrix elements by comparing DFPT with finite difference, which also gives satisfactory results. Afterwards, we compare ground states properties as well as electron-phonon matrix elements from Abinit and from PWSCF. Excellent agreement is observed. We then move forward and analyse the different quantities that make the zero-point motion correction as formulated by Allen, Heine and Cardona [3] both in Abinit and PWSCF+Yambo. The Fan, diagonal Debye-Waller and non-diagonal Debye-Waller are analysed separately. At the time of writing, discrepancies for those terms are still present.

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Electron-phonon coupling in heavier elements: from superconductors to thermoelectrics

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Electon-phonon coupling: The coupling between electrons and phonons (EPC) is at the heart of many technological important phenomena (resistivity, superconductivity, thermoelectricity, etc.) In the past decade impressive progress in modeling has been achived, and this must be extended to important heavy elements which are incrisingly present in the high-tech devices (rare erths, transition elements…). That is why precise estimations of EPC are necessary for a general understanding of all these effects. Molybdenum disulfide (MoS2): transition-metal dichalcogenide has many technological applications as it can be used in flexible electronic devices. This material can be cleaved in layers only one atom thick giving the possibility to build high-mobility chips. It is a potential candidate to replace Silicon in nanoelectronics. It is used to manufacture computers that can be rolled up, or devices that can be affixed on the skin. MoS2 is also superconducting upon K intercalation (KxMoS2) with Tc=6.9 (oK). We study superconductivity in KxMoS2 (x=0.4). Metallic potassium (K) are incrementally loaded in the hexagonal sites of the interstitial spaces between MoS2 layers of the 2H-MoS2 bulk structure generating KxMoS2 (x=0.4) structure. We determine the optimized crystal structure for K0.4MoS2 in a 2x2x1 supercell.

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Temperature effects on optical properties of cellulose-based degraded materials

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Cellulose-based materials (mainly paper and linen) are among the most ancient examples of materials produced by human technology and they still recover a strategic role in our society. Despite their importance, their oxidative degradation process is still not fully understood. A recent work, by Mosca Conte et al. [1], has started to shed light on this topic, finding a strong relation between oxidative chemical changes induced by ageing in cellulose and its yellowing, responsible of optical damages in ancient paper artifacts. In [1] it has been observed that small changes of geometrical configurations of oxidized groups located in cellulose-based supports sensitively affect their optical properties. This suggests that temperature could have an important role in the determination of optical properties of degraded cellulose-based materials. Furthermore, experiments performed on linen samples, have demonstrated that the combination of laser irradiation and high temperature can induce dramatic changes in oxidized groups inside cellulose, and produce unusual phenomena, such as "latent oxidation". To explain these observations, and to improve the theoretical model of Ref. [1], we introduced the temperature effect by combining Car-Parrinello dynamics with TDDFT calculations, and show here our preliminary results.

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Ultra-thin ZnO films on metal substrates from first principle

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In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO films can be used to model catalysts or ZnO surfaces. By means of density-functional theory (DFT - PBE and the hybrid functional HSE) we investigate the structure of ultra-thin ZnO on the (111) surfaces of Ag, Cu, Pd and Pt. In contrast to the bulk, the free-standing ZnO mono-layer adopts a graphene-like structure [1]. We find that this flat structure prevails on the metal substrates and obtain coincidence structures in good agreement with experiment [2, 3]. The influence of O2 and H2 environments is investigated with abinitio thermo-dynamics [4] and surface phase diagrams are presented. Zn- and O-point defects are stabilized in the mono-layer by the substrates that would not be present in the freestanding ZnO mono-layer. With decreasing nobility of the metal substrate, the stability of defects, in particular inter-facial O, increases and the corrugation of the film becomes more pronounced. With increasing H2 partial pressure sparse ring structures occur in Zn poor conditions. Metal supported ultrathin ZnO films therefore do not resemble conventional ZnO surfaces and should be regarded as distinct nano-systems in their own right.

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Computational Study on the Effect of Temperature on the Optical and Electronic Properties of Hydrogenated Silicon Nano-Crystals

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Silicon nano-crystals (Si-NC) have been extensively investigated in view of their electronic and optical properties. However, it is not completely understood how these properties change under realistic experimental conditions. In this study , we address this issue by investigating the thermal dependence of the electronic and optical properties of hydrogenated Si-NC. A combination of density functional theory with Born-Oppenheimer molecular dynamics simulations is used to compute HOMO-LUMO gap values, radiative lifetimes and absorption spectra for Si-NC of different sizes at different temperatures. Spectra are calculated within the independent-particle approximation. This approximation is robust enough to provide and discuss trends with size of the Si-NC and temperature. Two different types of NC structures are considered: surface reconstructed NCs corresponding to spherical sections of the bulk material, where one-fold coordinated Silicon atoms are removed and two-fold coordinated Silicon atoms are bonded to form dimers; and non-reconstructed structures, where the NC is built shell-wise, starting with one atom and adding successively the next shell of neighbours. In both cases, the NC surface is passivated with Hydrogen atoms. For all the structures considered in the present study, HOMO-LUMO gaps decrease linearly with temperature. In general, NCs with non-reconstructed surfaces exhibit larger band gaps than the ones with reconstructed surfaces. Furthermore, even at room temperature, independent-particle spectra show an important broadening which is shifted to lower photon energies as temperature increases. The thermal dependence of the radiative lifetimes is explained in terms of the NC size and reconstruction method.

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The *GW* approximation to the many-body problem: an approach to theoretical spectroscopy

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Many-body perturbation theory (MBPT) provides an optimal framework for treating correlation in interacting many-body systems beyond the single-particle picture. The central object in MBPT is the single-particle Green function G which, under certain assumptions, can be related to measurements in direct and inverse photoemission experiments. For the *ab initio* description of electronic excitations, MBPT is mostly employed within the GW approximation for the self-energy. The GW approximation in its non-self-consistent – i.e., perturbative – formulation (G_0W_0) is the method of choice for the computation band structures and band gaps in semiconductors, and recently an assessment of its performance for finite systems is emerging. This talk will give an introduction into the basic concepts of MBPT and Green functions, with special focus on the GW approximation and its application to the computation of ground- and excited-state properties. Moreover, I will discuss some shortcomings and limitations of perturbative G_0W_0 calculations – as, e.g., the dependence on the starting point – and improvements of the theory based on self-consistent approaches. [1] L. Hedin, Phys. Rev. **139**, A796 (1965).

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The physical solution to the GW approximation

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We show that the equations underlying the GW approximation have a large number of solutions. To the best of our knowledge no such extra solutions have been reported in the literature yet. This raises the questions: Which is the physical solution? And why do numerical methods converge to it, rather than to one of the spurious solutions? We provide theorems which answer both of these questions. These theorems are general enough to cover a large class of similar algorithms. This fact is important for understanding how vertex corrections can be treated without running into unphysical solutions.

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Reference

F. Tandetzky, J. K. Dewhurst, S. Sharma, E. K. U. Gross: arXiv:1205.4274

Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory

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For a set of ten crystalline materials (oxides and semiconductors), we compute the electronic band structures using the Tran-Blaha [Phys. Rev. Lett. 102, 226401 (2009)] (TB09) functional. The band widths and gaps are compared with those from the local-density approximation (LDA) functional, many-body perturbation theory (MBPT), and experiments. At the density-functional theory (DFT) level, TB09 leads to band gaps in much better agreement with experiments than LDA. However, we observe that it globally underestimates, often strongly, the valence (and conduction) band widths (more than LDA). MBPT corrections are calculated starting from both LDA and TB09 eigenenergies and wave functions. They lead to a much better agreement with experimental data for band widths. The band gaps obtained starting from TB09 are close to those from quasiparticle self-consistent GW calculations, at a much reduced cost. Finally, we explore the possibility to tune one of the semiempirical parameters of the TB09 functional in order to obtain simultaneously better band gaps and widths. We find that these requirements are conflicting.

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Keynote on TDDFT and BSE for neutral excitations

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The calculation of optical properties by ab-initio techniques is one of the most difficult goals in condensed matter theory. While the community of chemists usually prefers to use post-Hartree Fock methods, beside Monte Carlo techniques that will not be treated in this talk, physicians make use of methods based on the time-dependent density functional theory (TDDFT) or on many-body perturbation theory (MBPT) mainly by solving the Bethe-Salpeter equation (BSE). Here these two strategies will be reviewed, remembering the most relevant parts of the theory, giving examples, and underlining their limits and the practical differences between the two approaches.

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Demystifying the T-matrix and its relations with other many-body approximations

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The description of optical excitations in strongly correlated systems is a challenging topic. The usual scheme that works for semiconductors and is based on many-body perturbation theory fails for these systems. In this talk I will explore the applicability of the T-matrix approximation to describe electronic excitations in a small Hubbard clusters, at a higher level than the usual Bethe-Salpeter + GW scheme. The aim is to determine the cancellations of different contributions that are dominant in the limit of strong correlations.

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Organic photovoltaics: a Bethe-Salpeter/GW study of charge-transfer excitations in coumarins

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We study within the many-body Green's function GW and Bethe-Salpeter formalisms the excitation energies of several coumarin dyes proposed as an efficient alternative to ruthenium complexes for dye-sensitized solar cells [1]. Due to their internal donor-acceptor structure, these molecules present low-lying excitations which have a strong intramolecular charge-transfer character. We show that combining GW and Bethe-Salpeter calculations leads to charge-transfer excitation energies and oscillator strengths in excellent agreement with reference range-separated functional TD-DFT studies and quantum-chemistry coupled-cluster calculations. This confirms the ability of our approach [2,3] to describe accurately Frenkel and charge-transfer photo-excitations in both extended and finite size systems without any system-dependent adjustable parameter, paving the way to the study of dye-sensitized semiconducting surfaces.

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Size and shape dependence of electronic and optical excitations in TiO2 nanocrystals

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We present results for the electronic structures, quasi-particle gaps, and the absorption spectra of TiO2 nanocrystals of both rutile and anatase phases with various shapes, sizes, and surfaces exposed. We study the size and shape dependences of these electronic and optical properties, computed both within time dependent density functional theory and many-body perturbation methods such as the GW-BSE, using appropriately passivated nanocrystals to mimic bulk termination. Surface e?ects are examined by using nanocrystals of various sizes with particular surfaces, such as (110) in rutile and (101) in anatase phases, exposed. We interpret the resulting optical absorption spectra of these nano crystals in terms of the bulk spectra and compare them with predictions from classical Mie-Gans theory.

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Nonlinear optical properties of surfaces: Extraction of surface signal

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Surface studies play an important role in many fields and a lot of tools using linear optics have been developed, when it is possible to suppress the contribution of the bulk material, like Reflectance Anisotropy Spectroscopy [1]. Another possibility for studying surfaces is to use nonlinear optics and more precisely Second Harmonic Generation. Second Harmonic Generation (SHG) is an extremely versatile tool and is used for decades by experimentalist.

In the case of centro-symmetric materials like silicon, the SHG signal is zero in the bulk and only surfaces and interfaces contribute to the signal. This makes SHG a very exciting tool for analysing surfaces. However, even if SHG for bulk material is well understood from the theoretical point of view [2], there is still a problem for computing second-harmonic surface spectra including local-fields and exitonic effects. From our knowledge, only microscopic calculations (see for example Ref. [3]) of SHG spectra are reported in the literature. The main problem when dealing with SHG from surfaces, using super-cell calculations, is that the system is composed of two surfaces that interfere destructively. We present in this work a way to extract the signal arising from only one surface.

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Optical Absorption spectra - The Bethe-Salpeter Equation versus the Time-Evolution Method

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The Green function formalism is a powerful tool to calculate not only electronic structure within the quasi-particle (QP) picture, but also gives access to optical absorption spectra. The accurate calculation of neutral excitation spectra needs to include important many-particle effects, specifically, the electrostatic attraction between electrons and holes. As a central quantity, the polarizability is calculated from a Bethe-Salpeter like equation (BSE) [1]. It is commonly solved assuming that optically excited states can be represented as a linear combination of produts of N_{occ} occupied and N_{virt} hole states. To calculate the absorption spectrum from the dielectric function one has to diagonalize a matrix of dimension $N_{\mathrm{occ}} \times N_{\mathrm{virt}}$. Even though off-diagonal elements can be neglected for semiconducting materials, as done within the Tamm-Dancoff Approximation, the computational effort and the storage requirement still grow like the fourth order of system size N. In order to treat also structures with several hundred atoms, we employ the Time-Evolution ansatz [2], which avoids diagonalizing the BSE matrix. Since this method requires only a matrix-vector multiplication, we are implementing this method to finally not saving the entire matrix at all. The scaling will reduce to N^3, whereas the total complexity is comparable to a ground state calculation.

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Exact vs TDDFT study of the ionization phenomena of a 3D Neon atom

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In this talk, we analyse the differences between exact [1] and TDDFT ionization phenomena of a 3D Neon atom using the Octopus code [2]. We show the dependence of the total charge of the atom with respect to the intensity of a 93 eV pulse for two different pulse durations of 5 and 30 fs, whose length is given by the temporal FWHM of a Gaussian. The deviations seen between the two methods are interpreted and a few functionals (LDA, GGA(PBE) and the corrected long range potential methods GGA(LB94) [3] and CXD-LDA [4]) are tested. This analysis will be extended to other atoms.

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Magnetization in extended systems within TDCDFT

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The usual definitions of magnetization and polarization become ill-defined when using periodic boundary conditions (PBC). Moreover, with PBC surface effects are artificially removed. To circumvent this, one has to find definitions of magnetization and polarization in terms of bulk quantities. For example, the problem has been solved for the polarisation, which can be expressed in terms of the bulk current density, thanks to the continuity equation. The polarization can then be calculated via time-dependent current-density-functional theory [1,2]. The aim of this work is to show that also the magnetization can be described in a similar way.

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Excitonic effects in Raman intensities: an ab initio study

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Raman spectroscopy is a widely used technique for materials characterization. The dependence of the Raman intensity on the frequency of the incident light is well known: e.g., it is used to amplify the Raman response. Indeed, a resonance phenomenon appears when the exciting light has frequency close to electronic transitions. Unlike for molecules and for graphene, the theoretical prediction of the frequency-dependent Raman response of crystalline systems has received little attention. Indeed, many Raman calculations are nowadays done in the static limit (vanishing light frequency), using Density-Functional Theory [1] and Density-Functional Perturbation Theory [2], thus neglecting excitonic effects. In this work, a finite difference method is used to obtain the frequency-dependent Raman intensity of silicon within the Many-Body Perturbation Theory [3] (ex- citonic effects are included by solving the Bethe-Salpeter equation (BSE) [4]). Since the convergence with the sampling of the Brillouin Zone is extremely slow, a double-grid technique needs to be used. Two main conclusions can be drawn from our analysis. First, the double-grid technique permits to obtain well converged results without requiring huge mem- ory and time requirements. Then, excitonic effects are of crucial importance in the resonance part of the Raman spectrum. The inclusion of these excitonic effects in the computa- tions improves the agreement with the experimental data of Renucci, Tyte and Cardona [5], with respect to analogous results obtained within the independent- particle approach (RPA approximation).

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On ranges of coulomb interactions within density functional theory

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A way of analysing whether the long-range correction approach in density functional theory is adequate for the calculations of the ground and excited state properties is presented. A flexible set of attenuation functions based on a linear combination of error functions is proposed. The particular attention is devoted to the effect of the r_{12} behaviour on the excitation energies of local, Rydberg and charge transfer excitations. Both singlet and triplet transitions of a number of representative molecules (including small molecules, polyenes, acenes, heterocyclic systems with low-lying n-π*-transitions) are analyzed. It was found that the optimal functionals differs for different transitions, but the dependence remains the same for the transitions of the same nature, for example, the dependence for π-π* transitions in polyenes and acenes.

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Valence electron energy loss spectra of HfO_2

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HfO_2 is a high dielectric constant (high-κ) material, and can have cubic, tetragonal, orthorhombic, or monoclinic crystal structure. With potentially widespread applications in metal-oxide semiconductor devices, HfO_2 has been characterized experimentally using electron energy loss spectroscopy (EELS) in various energy regimes. We show how theoretical spectroscopy can validate and complement experimental valence EELS results. Time-dependent density functional theory (TDDFT) is used to simulate spectra for various polymorphs of HfO_2. We discuss how inaccuracies in the band structure can affect the resulting spectra. We also examine plasmon dispersion with increasing momentum transfer.

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Efficient quantum transport calculations with optimized support functions

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The study of electronic transport through nanoscale devices has stirred up a important research effort over the last few years. The demonstration of molecular and nanowire-based sensors, molecular logic gates, graphene transistors suggests a possible transition to a post-silicon era. At the same time, a leap forward has been made in the development of computational tools for evaluating the transport characteristics of nanoscale devices. Among the theoretical scheme for calculating transport at the atomic scale, the non-equilibrium Green's function method occupies a place of choice. In this presentation, an efficient implementation of Green's function based scattering theory is described. Owing to the in-situ optimization of the support functions used for the description of the valence and conduction manifolds, accurate transport calculations can be performed even with minimal basis sets. Test calculations are provided in order to assess the accuracy and efficiency of the method.

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Dynamical competition between disorder and interactions in quantum transport

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We investigate the static and dynamical behavior of interacting fermions in one-dimensional disordered Hubbard chains, contacted to semi-infinite leads [1]. The chains are described via the repulsive Anderson-Hubbard Hamiltonian, using static and time-dependent lattice density-functional theory. To quantify the degree of localization due to disorder and interactions, we adapt the definition of the inverse participation ratio to obtain an indicator which is suitable for quantum transport geometries and can be obtained exactly within density-functional theory. Our approach appears to be able to capture complex features due to the competition between disorder and interactions. Specifically, we find a dynamical enhancement of delocalization in presence of a finite bias, and an increase of the steady-state current induced by inter-particle interactions. This behavior is corroborated by results for the time-dependent densities and for the inverse participation ratio. Recent progress will be presented, where we show that the same phenomena can be seen using Non-Equilibrium Green function techniques.

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Quantum Hall Effect Fingerprints of Chemically Functionalized Graphene

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We theoretically predict unconventional transport fingerprints in the Quantum Hall regime for chemically-functionalized graphene. Upon adsorption of weak densities of monoatomic oxygen (from 0.5 to few percents), and varying the external magnetic field within the experimental reach (from 1 Tesla to several tens of Tesla), two unprecedented magnetotransport features are unraveled. First the formation of Landau levels is found to strongly depend on the nature of charge carriers (electron versus hole), whereas a new zero-energy quantum Hall plateau develops as a result of a localization/delocalization transition driven by impurity-pinned bound states. This suggests the possibility for tailoring QHE characteristics in chemically complex forms of two-dimensional materials, a perspective for metrology calling for further experimental inspection.

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Calculation of thermoelectric properties from first-principles

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The development of new types of thermoelectric materials with a large figure of merit is mainly driven by the needs for sustainable and clean energy. In this respect first-principles study of thermoelectric properties can help to achieve a better understanding of microscopic mechanisms in transport, which provides insight for discovering new materials. To study the thermoelectrical properties, we combine the well known Boltzmann transport theory with the predictive power of density functional calculations. With the exception of the lattice thermal conductivity, all of the required transport coefficients can be obtained using the BoltzTrap code [1], based simply on the electronic band energies. However, this approach is limited by the hypothesis of a constant relaxation time. To go beyond the relaxation time approximation, we have implemented a first-principles algorithm within the ABINIT package [2] to calculate transport coefficients in solids limited by electron-phonon interaction. As a first step, we study metals and heavily-doped semiconductors, where a solution to the Boltzmann equations based on a variational method is adopted [3]. The calculated electrical conductivity is in excellent agreement with measured data, whereas the Seebeck coefficient is less satisfactory. Besides the missing contribution from phonon drag, which is only important at low temperature, an accurate description of density of states around Fermi energy is vitally important.

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Effect of pressure on the thermoelectric properties of $\mathrm{Bi_2Te_3}$

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We present first-principles calculation for Bi_2Te_3 using Local Density Approximation and spin orbit interactions, within the relaxation time approximation. We explore the behavior of thermoelectric properties such as Seebeck coefficient (S), Electronic conductivity (σ) and the related power factor ($S^2\sigma$) under hydrostatic pressure up to $4\,GPa$. Different levels of doping for electrons and holes were taking into account to reproduce the experimental data close to zero pressure. The thermoelectric properties were derived from Boltzmann theory including the transport coefficients. Our computed electronic band structure and thermoelectric properties are in good agreement with experimental and theoretical results at zero pressure.

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Ab initio study of the Spin Seebeck effect in metallic alloys

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Spin-Seebeck effect was discovered in 2008 by Uchida et al. [1] and allows the generation of an spin voltage at the extremities of a ferromagnetic sample subject to a temperature gradient and to a constant magnetic field, even for insulating materials. So far, the effect has raised many conceptual question about the behavior of spin currents in materials. Together with other related phenomena (Spin-Hall Effects [2]), the Spin-Seebeck effect can be potentially revolutionary for spintronics application Initially it was identified as the spin analogous of the Seebeck effect, which is due to an asymmetry in the density of states for carriers. Over the past few years it has become apparent that the two effects are different both in macroscopic characteristics and microscopic origin. The current understanding of the Spin-Seebeck effect relies on a mechanism where a heat current induces a spin wave driven spin current in the materials. Localized magnetic excitations, or magnons, interact with other excitations and allow the propagation of the spin currents, which are then transformed into electrical current by means of Inverse spin-Hall effect [3]. Several models [5] have been proposed in the last year to explain this puzzling behavior, but an exhaustive theoretical explanation is still missing; new experimental results [8, 9] clarify the role of phonons in the substrate and the magnon-phonon interaction in materials, and seem to exclude phonon-magnon drag as a motor for certain systems. In my project, ab-initio calculations are carried out on a Ni-Fe reference system and the magnon- phonon interaction is analyzed by means of Perturbative Density Functional Theory within the Korringa Kohn Rostoker approximation for the magnons.

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Part II

Posters

Simulation of electronic transport in quasi-amorphous graphene

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Graphene, a one atom-thick layer of carbon arranged in a honeycomb lattice, has sparked out intense research activities from both experimental and theoretical sides since almost a decade now. The striking properties of graphene in various fields, such as mechanical, thermal, or electronic transport properties, are intrinsically related to its two-dimensional aspect and to its bipartite honeycomb lattice structure yielding both to the peculiar electronics of Dirac Fermions and pseudo-spin symmetry. From the electronic transport point of view, clean graphene samples exhibit particularly long coherence length and high electronic mobility both interesting for devices applications in nanoelecronics. Graphene provide simultaneously a genuine playground for fundamental researches such as exploration of Anderson (anti-)localization phenomena in two-dimensional systems. In this presentation, simulations of electronic transport in quasi-amorphous graphene structures will be exposed. Employing tight-binding models, and using a real-space order-N Kubo-Greenwood method [1-2], the transport properties of quasi-amorphous graphene structures are computed. The impact of a huge amount of various structural defects disrupting the ideal honeycomb lattice is thus investigated. Starting from a randomized graphene plane, molecular dynamics simulations are conducted to obtain highly defective graphene structures exhibiting both domains of amorphous graphene [3-5] and reconstructed pristine graphene areas. A careful analysis of the transport properties is performed through the Kubo-Greenwood formalism. Structural defects are found to induce strong resonant scattering states at different energies depending on their nature [6-8], inducing extremely short mean free paths and low mobilities. At low temperatures and in the coherent transport regime, large contributions of quantum interferences driving to localization phenomena are predicted. Actually, in regards to the results obtained, such quasi-amorphous graphene structures are predicted to behave as a strong two-dimensional Anderson insulator material [9], which could be experimentally confirmed by the magneto transport measurements at low temperatures for instance.

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A reformulation of the Bethe-Salpeter equation

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One of the approaches to ab-initio spectra calculation is through the Bethe-Salpeter equation, a self-consistent equation for the 4-point connected Green's function. The current state-of-art numerical approach to its solution boils down to first finding the Self-Energy corrections to DFT Green's functions and then solving the BS equation with an approximated kernel using them. Yet it often turns out that parts of these corrections cancel each-other, which means that there is at least in some situations a big computational overhead. The idea of this work is to reformulate the BS equation in such a way that they will no longer contain the interacting Green's function, and yet still remain exact. This will have not only a numerical, but also a physical advantage, as the approximations will be more transparent and therefore more controllable.

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Electrical conductivity in chains of carbon atoms: simulation and experiment

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Chains of sp^2-hybridized carbon atoms constitute the logical one-dimensional phase of carbon with monoatomic thickness. They have been proposed theoretically since a long time, and had been considered hypothetical until they were observed in electron microscopy studies. However, electrical measurements on these monoatomic thick chains had not been feasible until recently. In this work, we present a comparison of the experimental results with DFT and many-body perturbation theory showing that both the contact resistivity and strain in the chain determine their conductivity. Strain transforms the chain from cumulene, with double bonds throughout the chain, to polyyne with alternating single-triple bonds. Furthermore, the strain has a decisive influence on the bandgap of the chain. This is correlated with different experimental I/V-curves resulting from measurements on different chains. A unique cumulene or polyyne configuration is unlikely to exist due to varying strain and the stabilization of dimerization under stress.

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Progress in the theoretical description of photoemission in small syatems: a model study

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The electronic structure of solids can be probed by different types of spectroscopies. Here we focus our discussion on photoemission spectroscopy and how it can be understood theoretically. Direct or inverse photoemission, which removes or adds one electron to the system, respectively, can be described by the one-particle Green's function. Thereby, we avoid the full solution of the many-electron problem. Approximate methods for the calculation of the Green's function have been studied for many years, and many different theoretical approaches have been proposed. The GW approximation, developed by L. Hedin in 1965, is a well established approach for describing the quasiparticle peaks in the spectral function. The cumulant expansion, derived from model systems, is a promising approach for describing the photoemission satellites. However, approximations for describing the satellite structure are still under investigation. Other researchers in our group have already combined the cumulant expansion with the GW quasiparticle correction when modeling bulk silicon. They obtained very good agreement with experimental results for both the quasiparticle peaks and the satellite structure. However, the derivation of this approach uses some rough approximations whose validity has to be investigated. As a test bed, we study the Hubbard model, which is widely used to deal with the physics of strongly correlated materials. Specifically, we choose the Hubbard molecule (the one-electron, two-site Hubbard model) to investigate the performance of this approach in a finite system. This model is very useful for evaluating the validity of different flavors of the cumulant expansion and the GW approximation, since the exact Green's function, and therefore also the spectral function, for this model molecule is known.

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The role of the screening in the density functional applied on transition metal defects in semiconductors

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First principles characterization of structural, electrical and optical properties of point defects in semiconductors is one of the most challenging tasks in computational physics. The underestimation of the band gap of the host semiconductor, the spurious self interaction of the free electrons occupying localized defect states and the image charge interaction of charged defects are just some of the difficulties that arise in the commonly used supercell density functional theory (DFT). Due to the complexity of the problem, simultaneously accurate and practical solution is still under intense research.

In our investigation we show that the promising and nowadays rapidly spreading approach, the HSE06 hybrid functional cannot describe properly the complex system of strongly correlated transition metal (TM) impurities in semiconductors. Our study also reveals that the source of the discrepancies is the homogeneous screening of the bare Coulomb interaction. By introducing the point defect to the host semiconductor, this approximation becomes invalid and causes significant errors for TM impurities. In our study we show that base on the generalized Koopmann's theorem (gKT) one can measure the accuracy of the applied functional in such complex systems. Furthermore, by invoking gKT we developed a correction scheme which can correct the HSE06 functional by introducing an inhomogeneous screening. The corrected charge transition levels and optical excitation energies are remarkably close to the results of experimental measurements and many-body perturbation theory calculations.

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Calculation of the hyperfine tensor related to point defects in silicon carbide: method for defect identification

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The defects are important in semiconductors because they introduce deep levels in the band gap that changes the electronic, optical and magnetic properties. First, they can serve as traps for the majority carriers and often have negative influence on device performance. Second, they often possess a high spin ground state, and produce efficient luminescence upon excitation by light. This may provide a mechanism where the electron spin of the high spin defects can be manipulated by light, and opens a door to manipulating and reading the state of the electron spins. To calculate the hyperfine tensor we use advanced DFT-based technique (semi-local functional and hybrid functional) with projector augmented wave (PAW) methodology. In order to identify the defects in real materials, we compare the calculated hyperfine constants with electron paramagnetic resonance measurements.

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Fluorinated diamondoids to stabilize the negatively charged nitrogen-vacancy center in diamond nanoparticles

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Diamondoids, nanometre sized diamond cages, are of centre of interest in several fields. E. g. nanometre sized diamond particles play important role in quantum information science where nitrogen-vacancy centre of diamonds has been shown as an excellent candidate for solid-state spin qubit. However, the charge of the nitrogen-vacancy center, which takes part in the evaluation of the spin qubit by periodic excitations, strongly depends on the surface properties. The aim of this poster is to show, using time-dependent density functional theory, that systematic fluorination of the smallest diamondoids, adamantane, diamantane and triamantane, increases the stability of the HOMO and the LUMO states gradually. Therefore fluorine modification of the surface of diamondoids can be a solution for the stabilization of negatively charged nitrogen-vacancy centers in diamondoids.

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First principles study of point defects in silicon carbide nanocrystals for in vivo biomarker applications

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Ultrasmall, biocompatible and water-soluble fluorescent nanocrystals are much sought-after to probe biomolecules in living cells. Silicon carbide nanocrystals are promising for bioimaging applications, as they are water-soluble, biologically inert and experimentally achievable with diameter less than 3 nm. However their optical properties are non-ideal for in vivo applications as they emit light in the visible-UV range. We demonstrate here by time-dependent density functional calculations that 1-2 nm sized silicon carbide nanocrystals can emit light in the near-infrared region after introducing appropriate color centers in them, such as tungsten, molybdenum and vanadium related point defects, Si-vacancy and divacancy. According to our results, donor-acceptor pairs such as boron-nitrogen and aluminium-nitrogen can also lower the absorption energies of nanocrystals. The surface of the nanocrystals plays a significant role in the optical properties, and these effects should also be taken into consideration in the calculations.

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Nickel related defects in diamond nanocrystals

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The motivation of my study is the search of color centers in nanoparticles. These may act as biomarkers that can be detected optically (eg. photoluminescence) when introduced to organisms. The carbon-based nano-diamond crystals appear to be biologically compatible and are suitable for in vivo studies. If color centers are introduced to them, which are optically active in the visible or near-infrared range, then they form fluorescent in vivo biomarkers [1]. Nitrogen-vacancy color centers in nanodiamond have being used for this purpose, which gives a very broad luminescence spectrum in the wavelength range 650-750 nm at room temperature. I seeked for alternative fluorescent color centers in nanodiamonds, particularly I focused on nickel related defects. Pristine diamond nanocrystals are already commercially available, a diameter of 5 nm diamond nanocrystals can be created with the blasting method [2]. However, they do not have luminescence in the required energy range. Nickel related optically active defects have been already detected experimentally in bulk diamond [3] showing magnetic properties [4]. Also nickel-nitrogen complexes also has been found in bulk diamond [5]. If these nickel related defects could be injected into the diamond nanoparticles then we could produce biomarkers similar to the nitrogen-vacancy based nanodiamonds. In my study I investigated the optical properties of nickel containing nanodiamonds, in which the quantum confinement and the surface effects on the optical properties can be studied. I have determined the excitation with time-dependent density functional method. I have studied nanocrystals between sizes 0.9-2.0nm, consisting of 69-630 carbon atoms. The surface of the particles have been terminated with hydrogen atoms. I have obtained the excitation energies with TDDFT method. I investigated the states are involved in the excitations. I found that nickel contained nanoparticles are optically active in the wavelength of 400-700 nm, thus with nickel based nanodiamonds serve as alternative fluorescent bioimaging agents.

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The role of anharmonicity in the ab-initio phase diagram of calcium

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In the 32-119 GPa pressure range and at room temperature, a simple cubic phase was reported for calcium in many different experiments. Standard linear response theory, both within density functional perturbation theory and frozen phonon calculations, presents dynamical instabilities for the simple cubic structure in the whole pressure range. Many other possible candidate phases, as well as several possible stabilization mechanisms for the simple cubic phase, have been proposed as the result of ab-initio predictions but the role of temperature on the relative stability of the different phases has not been systematically investigated. We revisit the stability of the three most important candidate phases of calcium for the intermediate pressure range and for various temperatures, taking explicitly into account thermal corrections relative to electronic as well as phononic entropy and anharmonic contributions. This corrects the discrepancies among previous theoretical results and experiments, and presents a different picture of the temperature driven phase transition, which results from dynamical anharmonic stabilization of simple cubic and de- stabilization of the tetragonal phase.

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