2 Psi-k2010 Conference

http://www.fhi-berlin.mpg.de/th/Meetings/psik_2010/

13-16 September

Henry Ford Building (HFB), Berlin, Germany

Since this is the first newsletter after the recent Psi-k2010 Conference, it seems almost natural to dedicate a prominent part of it, specifically the three following subsections, to reminiscing on this event.

In the first subsection we provide only a brief, likely subjective, editorial documentation and selected photographs of the event. In the next subsection we present views, comments and impressions of other participants, because, as Volker Heine said in his closing remarks, “... these are the participants that make the conference”. The ones who have contributed their comments to the newsletter represent different ages, sexes, countries/continents, etc., and their brief reports make a very interesting reading. We are truly grateful to them for taking the time to record their thoughts, comments and impressions for the newsletter.

The final subsection is by Peter Dederichs and is dedicated to the Volker Heine Young Investigator Award and the associated session at the Psi-k2010 Conference.

2.1 Brief editorial documentation of the event

The Conference was organized by Matthias Scheffler (chair), Hardy Gross (co-chair), and Volker Heine (honorary chair), with the help of the whole group of Matthias at the FHI Berlin. The organization seemed perfect from start to finish. The whole team, in black T-shirts with the Psi-k2010 Conference yellow logo, was on stand-by from the registration on the Sunday early evening, 12th of September. Soon the whole foyer of HFB and the outside filled with participants carrying the characteristic black bags with the yellow logo, containing a very imaginative set of useful
conference stuff, and in particular black umbrellas, again marked by the yellow Conference logo. Congratulations to the organizing team for being so insightful and predictive regarding the weather in Berlin.

The Conference was officially opened by Matthias on the Monday morning, who extended a heartfelt welcome to everybody, expressed vividly through the little jelly teddy bears carrying a big red heart, seen in the photo below, welcoming all to Berlin.

Based on the facts, this was the largest of the four Psi-k conferences, with over 1000 participants, five parallel sessions and the same number of plenary talks, about 120 invited talks, 22 symposia and about 700 poster presentations. The latter were distributed over two poster sessions: about 350 posters on a day, with even and odd numbers receiving 1.5 hours slots in succession. This was a very good idea, allowing an easier access to the posters, as well as, giving everyone a chance to see the posters. Of course, a longer time for discussions at any poster would have been useful, although likely difficult to realize, given a very tight programme, and the constantly full and buzzing foyer (see photos below).

It definitely felt very dynamic and full of energy.

Plenary sessions were usually very well attended with the largest, Audimax, hall rather full on all the occasions. The five talks covered a broad range of topics, starting from computational spectroscopy, involving a number of theoretical methods and implemented in Quantum ESPRESSO code (S. Baroni), through fuels from sunlight (J. Nørskov), Berry phase/potential and curvature, and how they impact on the theories of orbital magnetization and electric polarization (D. Vanderbilt), materials genome project (G. Ceder) and finishing with molecular transport junctions (M. Ratner).
Of course, with five symposia running in parallel it was impossible for an individual to visit a substantial number of invited and contributed talks or to get an idea which symposia were most popular. However, it seemed that talks presenting new methodological and computational developments were, as usual, most highly appreciated.

The oral and poster presentations and scientific discussions in the foyer were providing plenty of food for thought, but access to real food was also easy and well managed. The whole food distribution process ran very smoothly. Fruits, snacks and drinks were nearly always available in the foyer, while the lunches and evening meals were served in another building, in close proximity to HFB. The efficient access to food and sitting areas is another thing for which the organizers deserve full marks (see photos below).

The conference dinner was quite unusual and happened on the Wednesday evening/night under the banner “The Conference outing” in an interesting “Rodeo” museum and club (see photos below).

It was certainly a conference dinner with the difference and probably highly regarded by young
participants. The waiting for food was a bit long and tiring, but that was presumably to be considered as an integral part of the unusual set. All in all, with three bands, two DJs and at 1 am several hundred theoreticians still in motion, it was an interesting experience even for the older folks. As a result, the fifth plenary talk was perhaps less attended than the other four, but the numbers were still quite impressive.

A new element of this Psi-k Conference was a Young Investigator Award, set up in the name of Volker Heine, the grand father of the Psi-k family. It was associated with an interesting and well attended session, in which the five finalists gave 30 minutes’ presentations. In one of the following sections Peter Dederichs, the Psi-k Network chairman, reports on this event and the award itself in more detail.

At the closing words, both Volker Heine and Peter Dederichs praised very highly Matthias, Hardy and the rest of the organizing team for a fantastic and smoothly run conference. Not only Volker, seen in the photo below, was applauding them very warmly, but all the remaining participants joined in a long and loud clapping. Below we see Matthias and Hardy, sitting behind each other, having very solemn and concerned faces. Surely, they must have been pleased with the outcome and really happy for being so highly appreciated by everybody. Nevertheless, they must have also been relieved that it was finally over.

The Conference was being very accurately documented in photographs and the album can be accessed from the webpage


In the above write-up we have only selected a very few of them to give it a bit of an ‘archive document’-like feel.

To finish this documentation of the event it seems interesting to look at the distribution of the participants over countries and then continents. In the graphs below, one can see that Europe leads the field, with Germany well ahead with impressive 299 participants, followed by UK (96), France (55), Italy (54), Spain (48), Austria (46), and so on. North America falls behind Asia+Oceania, where Japan leads with 80 participants out of the total of 118. It is perhaps surprising that there were only two participants from the whole continent of Africa, despite the fact that there are a few groups there, in particular in the North African countries, that are active in the field. Maybe even more surprising is the fact that there were only 9 participants representing China, whilst a
small country like Czech Republic had 18 participants.

2.2 Brief Reports on the Psi-k2010 Conference by a Sample of Participants

Comment by John Dobson (Brisbane, Australia)

This was the biggest physics conference I have attended, except for the APS March meeting, which is of course much less focussed. The size of the meeting reflects the very pleasing success of the Psi-k network, and is a tribute to the hard work of many people from Volker Heine onwards. Despite its size and complexity, the meeting ran amazingly smoothly. The programming, the building, rooms and food service were all first-class, and at any sign of a problem the army of helpers in black T-shirts would be there to sort things out. Many thanks to Matthias Scheffler, Hardy Gross, Peter Dederichs, Walter Temmerman and their T-shirt brigade. As a non-EU attendee, I was also impressed by the welcoming and inclusive treatment that I received. In general, the Psi-k network seems to have succeeded in fostering cooperation rather than the competitive approach that is often evident elsewhere in the physics community.

The scientific content and presentation were both of a very high standard, and the subject matter was quite diverse, given the focus area of Psi-k. I will comment on the technical content from my personal viewpoint as a theorist interested in van der Waals physics and related many-body formalisms. For me the highlights from the talks and posters were the following.

(i) The emerging ability to model periodic systems in detail via microscopic many body methods, starting from the RPA/TDDFT correlation energy. Microscopic beyond-RPA corrections (e.g. SOSEX) are also now becoming available, and they seem to improve the theory where tested to date. One of the important achievements of this class of microscopic approach is the reliable ab initio description of dispersion forces in "difficult" systems such as graphitics. There is still a need for much work here, however, since the computational effort of RPA-class theory still precludes
full description of nanostructures with "interesting" geometries and correspondingly large repeat
cells. At least two groups also reported good progress with the tricky "CEP" problem of providing
selfconsistent orbitals for the RPA class of theory. It seems that this can make major improvements
in the description of small systems where "direct" RPA has some serious diseases.

(ii) The progress evident in the modelling of more complex dispersion-bound systems via more
approximate and/or empirical theories. One example was an efficient transcription procedure to
obtain polarisabilities of "compressed" atoms in molecules and solids starting from accurate free-
atom polarisabilities. There was also the discovery (surprising to me at least) that dispersion forces
are important in the stability of beta helices in biomolecules, i.e. in determining secondary structures
rather than just tertiary structure where such effects were already considered to be important.

(iii) The successful application of GW and Bethe-Salpeter equation technologies to predict quasi-
particle and excitonic properties in a variety of solids.

John Dobson
Griffith University
Australia

Comment by Mojmir Šob (Brno, Czech Republic)

Impressions from the 4th Psi-k Conference

I have been lucky enough to have a chance to attend all Psi-k Conferences, starting from the first
one in 1996 to the fourth one, taking place in Berlin in the middle of September 2010. From the
very beginning, these conferences have constituted topical and highly specialized meetings devoted
exclusively to ab initio electronic structure calculations (AIESC) and their applications in solid-state
physics and chemistry, and in materials science.

I have been working in the field since 1974 and, obviously, have greatly welcomed the first Psi-k
meeting in 1996. With the exception of the first Psi-k Conference, I have always taken my whole
group with me. At this Conference, we’ve had a chance to assess the present status of our beloved
ab initio approach and have observed a continually extending range of its applications. It has been
a fantastic achievement of the Psi-k Network and the efforts of the Conference organizers that the
4th Psi-k Conference, now over 3 times larger than the first one (!), has happened.

That large increase in the number of participants indicates unambiguously a steadily increasing
interest in AIESC and their applications. I can also confirm this trend from the field of calculating
phase diagrams, associated with the CALPHAD Journal. When I attended my first CALPHAD
Conference in 2005 in Maastricht (it was the XXXIVth CALPHAD Conference), and had a talk on
application of AIESC, the CALPHAD community was largely reluctant to adopt ab initio results in
their simulations, the CALPHAD scientists were rather sceptical. Five years later, at the XXXIXth
CALPHAD Conference at the Jeju Island in Korea in 2010, about 1/3 of contributions included or
touched upon ab initio input.
Of course, such scepticism is not our problem; we do know that AIESC have their great value and provide results at the most fundamental level. Rapid increase of numbers of scientists adopting our belief is a proof that applications of AIESC constitute a correct and promising direction, although one could perhaps do more. As Gerbrand Ceder said in his talk, "$100\text{Ms are poured into materials research and innovation}, without fully using the benefits that large-scale computational modelling could offer". Maybe we should intensify our propaganda?

The 4th Psi-k Conference brought together more than 1000 scientists of our ab initio belief. The presentations were distributed among 22 symposia which were running in 5 parallel sessions. Plenary and invited speakers were carefully selected to provide topical reviews of most interesting developments in the field and/or their own results illustrating that development. I really enjoyed all plenary talks which had a very high level indeed. Many oral contributed talks also presented very interesting results. Regrettably, it was not possible for one person to attend all five parallel sessions; all of us had to make our choices.

It was a very good initiative to establish the Volker Heine Award for young investigators. The level of the finalists was high indeed and it was a pleasure to meet them at the closing ceremony, as they were awarded their prizes from Peter Dederichs and Volker Heine himself.

Due to limited time at the conference, most of the contributions had to be presented in poster sessions. At this conference we had two evenings to see in total about 750 posters, and that was really impossible. I wish I had more time for posters. Of course, I do realize that it was technically quite hard to organize poster sessions with such a large amount of contributions. Nevertheless, it was a pity, in my opinion, that the posters could not have been exhibited at least during the first three days of the conference in order to give one more time to inspect them in more detail.

Conference dinner was in a very interesting place, however, we experienced somewhat close-packed arrangement (I was not able to establish whether it was the hcp or fcc or some other type of packing).

This, however, does not diminish the huge amount of work exerted by the Organizing Committee chaired by Matthias Scheffler. They have made a very good job indeed and deserve big applauds from all participants of the 4th Psi-k Conference!

Now, that ESF has endorsed the Psi-k Network as one of its possible programmes for the next five years, subject to securing funding from the National Research Councils of the ESF member countries, we can only wish that this financial support will be granted to fund our future activities, including the next big conference. Let us hope that in 5 years, we shall meet again at the 5th Psi-k Conference. Well, extrapolating from the observed trends, it seems that more than 2000 participants can be expected. It will definitely be a challenge for the future Organizing Committee, and we should wish them good luck!

However, such a large number of participants would bring us to the format comparable with the DFG, APS, MRS or TMS Meetings. Thus, maybe we should also think about establishing an organization like APS, MRS or TMS, called e. g. the Psi-k Society, to bring all the scientists from our community closer together, shouldn’t we?

I look forward to attending the 5th Psi-k Conference in 2015!
Sincerely,

Mojmir (Mirek) Šob
Masaryk University
Brno, Czech Republic

Comment by Anton Kozhevnikov (Zürich, Switzerland)

More than a hundred invited talks, hundreds of posters, over a thousand of participants and very intensive personal communication - now we know how the largest conference on electronic structure calculations looks like. Organized by the Psi-k network, the conference took place in Henry Ford Building of the Free University of Berlin during September 12-16. With the absolute certainty we can say that the Psi-k 2010 conference was excellently arranged and conducted. Indeed, five conference halls seated all the interested listeners, there was enough space for the poster session, it was always possible to find a free seat or a table down at the ground floor, internet connection was fast and stable, snacks and drinks were always available and the lunch and dinner meals were really good. The conference brought together many scientists from the electronic structure community, giving everybody a chance to meet new people and charge oneself with new ideas. What else do you need for the productive discussions and intense work? Special thanks must go to the authors of the "participant’s bag" with an abstract book, notepad, pen, city map of Berlin and umbrella, which proved to be the most useful item during this four days. The only thing that I would like to wish to the Psi-k network is "Continue in the same spirit!"

With best regards,
Dr. Anton Kozhevnikov
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SWITZERLAND

Comment by Paweł Buczek (Halle, Germany)

A short account of Psi-k 2010 Conference, Berlin

Paweł Buczek
Max Planck Institute of Microstructure Physics, Weinberg 2, Halle/S., Germany

I must admit that my expectations regarding Psi-k 2010, the first conference of the series I attended, were completely different from reality. I had naively imagined Psi-k as a platform for computational physics craftsmen trying to figure out together the best possible coherent directions for the future
numerical electronic theory. Instead I found myself amidst enormous particulate field with everyone following firmly his/her own path. But not-met expectations do not mean disappointment and let me state I enjoyed Psi-k 2010 enormously.

Not one single plenary or semi-plenary presentation disappointed me. The speakers were fully aware they do not have solely specialists in the audience and often managed to throw bridges between sub-fields or even way beyond the computational condensed matter. I have more mixed feelings about the idea of 12 minute long scientific talks, earlier safely constrained to events like German Physical Society spring meetings and recently gloriously making its way to the most of the modern conferences. While I am strongly convinced that it is not the best practice, I admit that most of these short talks were very well prepared and presented. This kind of presentations offers an excellent overview and often gives a rare chance to meet the speaker in the real life.

And this is exactly what Psi-k 2010 was all about for me. On one hand an opportunity for deepening knowledge and polishing numerical approaches, on the other a chance for seeing what and how it is done and how it is sold and presented; a possibility to exchange gossips, to network and to look for collaborators and allies.

I would like to add only few comments to this general praise. The conference could have easily taken one or two more days and ended up with a reduced number of sessions. It was almost impossible to construct any personal program including even most of the relevant presentations. This severe compression was one of the reasons for the low impact of the poster sessions. Many of the posters were of low quality and even more apparently completely unmanned. The lenght of the meeting might be the only serious flaw (together with the drinks one had to pay for after 6pm) in the well organized event. I loved the night in ”Rodeo” - it is a great idea to give up official and stiff social dinners; I was relieved to hear there would be no ’fun-scientific’ talks that right.

I am sure I will not miss the next Psi-k meeting if I am still in the business.

Comment by Marília J. Caldas (Sao Paulo, Brazil)

Dear Matthias,

I imagine you have already received several messages in the same spirit, so ... one more.

We have all participated in far too many conferences at this time of life, and some of them were really good. I must say yours was the best organized I have ever been to. It made life easy for the students, for which I thank you all very, very much.

Apart from the organization per se, and counting also the quality of the talks and the opportunities for interaction, this last Psi-K was really, for me, one of the best conferences I had the pleasure to attend.

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Marília J. Caldas
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Comment by Julie B. Staunton (Warwick, UK)

Ψκ Conference 2010
September 12 - 16, 2010, Berlin
Julie Staunton, Department of Physics, University of Warwick

Diary of a Conferee.

Monday September 13:
Departmental commitments meant I had to miss first day of conference which is a pity because the programme looks excellent. Eventually arrived in Berlin in the evening - really impressed by Berlin’s public transport. Raining...uh oh, travelling light with no waterproofs. Fortunately Hotel Ravenna close to U-Bahn.

Tuesday September 14:
Up bright and early -bumped into several familiar faces in Hotel before catching bus and train to Henry Ford Building. Still raining...Registered and obtained impressively thick abstracts book and programme. (Also acquired large T-shirt and .. fantastic, an umbrella... now that’s what I call good organisation). It is striking how big the Conference has grown since its 2000 and 2005 predecessors. There are now over 1000 participants. Must be largest international electronic structure conference - the stats demonstrate this. 5 plenary speakers. 22 symposia with 120+ invited talks covering the whole discipline and its impact on condensed matter and materials science.

David Vanderbilt gave an excellent, thought-provoking plenary talk on the role of Berry phase ideas in theories of magnetoelectric effects in multiferroic insulators. There was then a tough choice as to which of the five symposia to attend. I opted for ‘Crystalline, Amorphous and Glassy Alloys’ and enjoyed a series of talks on topics on phase stability and disordered systems. Also gave a talk myself. All talks stimulated good discussion. There was some amusement in a couple of the talks when a disembodied voice floated around the lecture theatre. This turned out to be that of someone in another lecture theatre asking a question which our AV system picked up. After the talks and dinner took the opportunity to discuss some work with colleagues and then looked around the posters.

Wednesday September 15:
Another superb plenary talk by Gerbrand Ceder on hot topical high-throughput ab-initio calculations. Decided then to attend parts of 2 very different symposia to appreciate the scope of our conference. To that end chose the ‘Earth and Planetary Materials and Matter at Extreme Conditions’ on the one hand and ‘Organic Electronics’ on the other. Later attended the V Heine Young Investigator Award session where all the speakers were very impressive. Throughout the day and the day before I found plenty of opportunities for discussions with other conference participants.

Caught the conference bus to Postfuhramt passing by many famous Berlin landmarks. Good evening where I witnessed an interesting experiment on the collective behaviour of condensed
matter physicists at high density where there are competing short- and long-range interactions.

Thursday September 16:
Flight times home meant I had to leave in the morning and miss part of the day. Home in evening - reflecting on a very enjoyable and stimulating conference. Many thanks to all the organizers.

Comment by Warren Pickett (Davis, USA)

Selected Impressions from Psi-k 2010

Warren Pickett
University of California Davis

The brain teeters toward overload when considering how to comment in some useful way on the scientific spectacle of Psi-k 2010. Such a condition is just what one should expect from a four-day period in which 1000 computational electronic structure theorists ("10^3-CEST") convocate for a bidecadal downhaul, from speaker to audience, of the recent progress of knowing the unknowable. Eighty years ago Dirac pronounced the quantum mechanical study of condensed matter ("chemistry") too demanding to fathom, i.e. unknowable. The community is, arguably, at a point where it can be said that this statement is Dirac's "cosmological constant" - a position not withstanding the test of time. Just what should be expected from a meeting of 10^3-CEST would have been guesswork except to the organizers, since it had never happened before in our current universe. I provide just 2-3 selective observations.

Comment from a subjective viewpoint. I attended Psi-k 2010 partially with the American viewpoint in mind, so it was with interest that I noted that Dzidka mentioned I might address the American viewpoint, after which I might segue into more general comments. My specific "American viewpoint" in this context in fact arose from a recent Psi-k Newsletter in which Peter Dederichs pointed out that, in terms of DFT-based publications in journals followed by the Web of Science, the U.S. is in the process of being left in the dust. The U.S. is behind Europe in terms of publications per year and gap is increasing with time. In addition, the U.S. will be overtaken by Asia within a couple of years. Growth in China is at least quadratic (Europe and U.S. growth is linear), so China may overtake the U.S. in such publications before it overtakes it in economic terms. These trends are the kind of messages that may stimulate action in some of the right places (funding offices) if one can attract their attention.

There is widespread belief, probably in Europe but certainly in the U.S., that the origin lies in some basic sociological differences in the funding, indeed in the activity, in the two geographical and geopolitical areas. A central feature – a very evident distinction – is the development and support of robust, user-friendly, open source, supported DFT codes in Europe. Austria and Germany have contributed several. At the risk of upsetting some by being (necessarily) incomplete, I can mention also as active contributors groups in Italy, Belgium, the U.K., Spain, Sweden. I am not totally unaware of the efforts in Japan, where they have codes as well, though I am much less familiar with them.
The modus operandi in the U.S. has been, for some decades, to distribute a large fraction of research funding in large part through teams: from MRSECS to EFRCs (what these acronyms stand for is not so important here). A given professor or national lab leader typically gets research funding from a few directions and works in a few different (albeit related) areas, for three years at a time. Funding from different sources should basically fund distinguishable projects. In Europe the infrastructure culture is different. There are (to overstate the case, but only mildly I hope) professors or single-institution tightly knit groups with long-term funding who can think and act with the longer timescale in mind. The result has been (many) of the aforementioned DFT codes. The U.S. has some quantum chemistry codes but no DFT codes whose acronym would be identifiable to most Europeans (unlike the other way around).

The availability of these DFT codes, and the scientific environment that surrounds them, seem to many of us in the U.S. to be a substantial part of the stimulus that has propelled Europe into their current leadership role in our area of research. with 10^5-CEST at Psi-k 2010 held in Berlin and not in (say) Baltimore. The U.S. does have its “Electronic Structure Methods” annual conference, more than 20 years in the running now, but it has still the challenge (if it aspires to do so) to attract the wider electronic structure community attendance in the U.S. that Psi-k does in Europe. Commendably, East Asian countries also hold a regular electronic structure conference.

Broad observations. I have digressed. The subject of this comment is Psi-k 2010, and the impression it leaves and, possibly, its impact. The foment (which is ferment, without the alcohol) in our field is palpable; new ideas and the implementation to test them continues at a scary rate. Scary, if you have delicate disposition, but in such a vigorous research environment one should think in terms of boldness. We refer to our approach as ‘first principles’ but principles often give way to practicalities with the justification to be tightened up later, with finding ‘what works’ being a profitable way forward. We are, after all, working to know the unknowable.

Some of our Bloch functions have been concealing their intimate private behavior (phase twists) until recently. The bulk electronic structure of topological insulators hosts an entanglement that must be straightened out at the surface, so such insulators must have surface bands through the gap that disentangle the phase warp. (Is it possible there is an analogous phase twist in some insulating surfaces that may lead to yet richer behavior? Sounds only fair.) The excellent plenary exposition was followed by a number of computational investigations, in this field which is only in its infancy. The entanglement may be more subtle than the proofs of its occurrence and of its consequences. The effect requires both spin-orbit coupling and multiple bands. Band structure practitioners understand that spin-orbit coupling introduces phases (complex numbers) into the treatment, arising rudely due to its order of magnitude increase in computational cost (complex arithmetic versus scalar, doubling of the size of the secular equation, if the Kramers degeneracy is not taken into account to counteract the loss of symmetry [distinct spins]). A more intuitive understanding of the (gauge-invariant) Berry curvature is desirable, and the early investigations to do so that were presented provide confidence that this understanding will proceed forthwith.

Comment on part of the future of "psi-k". Note: I use psi-k here to refer not to the biennial conference which should have 1600 attendees in 2015, not to the organization, but to the computational materials theory community that drives the advances, applies them, and furthers the understanding of materials behavior from the first principles viewpoint. One of the notable ad-
vances that is evident from this conference is the impressive extension in the treatment of dynamic electronic behavior.

The continued progress, and several extensions and new applications, in the description of electron dynamics was discussed several symposia (Electronic Excitations: Dynamical Mean Field Theory; Strong Correlations from First Principles; Solar Energy Conversion and Harvesting: Organic Electronics). In rough historical order, the primary topics were GW, tcdDFT, and DMFT. To one who has not kept up with many of the applications of tcdDFT (me), the progress seems impressive indeed.

The GW approach has been around for some time and continues to advance. At the newer end, dynamical mean field theory is showing increasing promise. The impressive advances at this meeting from my viewpoint were from the very significant inroads that time-dependent DFT (tcdDFT) is achieving. This progress illustrates a crucial aspect of DFT: the ansatz is an energy functional with clear formal foundation. LDA (and its immediate offspring) has been enormously successful in spite of a simplistic approximation (extreme locality, whereas exchange and correlation are not really so). Such success can be possible only because the formulation is correct: a (rigorously justified) density functional (theory) is formulated, which is then approximated (necessarily so), and minimized (via the Kohn-Sham approach) to provide the many results that are obtained. The GW approach follows the (many body) Hamiltonian formalism, with energetics evaluated (via the Galitskii-Migdal expression) only extremely rarely, and not yet approaching any application of linear response methods.

The tcdDFT approach is (from my personal view) unexpectedly successful, apparently due to its formal basis and application in terms of a well-formulated energy functional. A time-dependent Hamiltonian alters the emphasis of the theory (away from non-conserved energetics), but the successes build on the formulation. Extending predictive computational theory to strongly correlated materials will surely require treatment of dynamical processes, with the dynamical mean field theory (DMFT) approach being the most widely used a present. Significant further development of DMFT will, in my view, necessitate focus on the functional (thermodynamic grand potential).

A breakthrough in this area was made around the turn of the 21st century when Andy McMahann, Richard Scaletter, and Karsten Held devised a DMFT energy functional in an all-electron LDA+DMFT implementation to model the volume collapse transition in Ce under pressure. Their Kondo volume collapse result remains the most convincing microscopic explanation of this classic problem in correlated electron physics. Their basic functional form has been used occasionally in the subsequent decade with some success. Further progress, almost certainly, relies on the formulation of the functional, necessarily approximated, then minimized, generating the single particle Green’s function and related results (free energy hence thermodynamics; linear response quantities). Obviously full charge self-consistency is essential: advances in accomplishing this is underway in a few groups. This are of research is well positioned to form one of the more exciting symposia at Psi-k 2015.

This highly successful meeting has been a great reminder of how our community has converted the great promise of the 1970s and 1980s into the tremendous success story that it now is. All signs point toward a continuing bright future as more and more materials properties are understood from a first principles viewpoint.
Comment by Samir Lounis (Irvine, USA)

Report on the $\Psi_k$-2010 Conference

Samir Lounis

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The $\Psi_k$ conference is a traditional meeting that covers theoretical and computational research on electronic structure and properties of matter. It takes place every 5 years. This time it has been organized in Berlin where sufficient space is available to host the huge attending community (more than 1000 participants).

The overall organization of the conference was well handled: from the initial stage including registration and submission of scientific contributions to the final stage of talks and posters. Five plenary talks were given and several symposia were organized covering a large number of topics where certainly every participant, even if not expert, could benefit from. It occurred that sometimes, interesting sessions were scheduled at the same time making difficult my personal choices. As an example, I was personally interested in magnetism and strongly correlated systems on Monday while during the last day there were two interesting sessions on the same topic: Excitations (Quantum Dynamics and Electronic Excitations). There was definitely a plenty of choice for the different audiences.

Most of the talks were invited accompanied by contributed presentations and four poster sessions. The latter ones were organized during the evenings of the first two days, giving exposure to interesting and original works. These evening sessions were, in my opinion, very convivial and allowed me, probably other participants as well, great opportunities to exchange and discuss new and old ideas.

I could not attend all talks and cannot report on all presentations I have seen. Thus, I will mention briefly the plenary talks which were very educational. The first plenary speaker, Stefano Baroni, discussed the basic concepts of density functional perturbation theory, the Liouville-Lanczos approach to time-dependent density functional theory and several applications obtained with the quantum-espresso code. David Vanderbilt reviewed the Berry phase and Berry curvature and their crucial role in the theories of electric polarization, orbital magnetization and anomalous Hall effect. To efficiently synthesize fuels from sunlight, new catalysts are required. Jens Norskov introduced and discussed some of the challenges to catalyst discovery and how first-principles calculations can help in designing them. Gerbrand Ceder presented the Material Genome Project that has the objective to perform large scale ab-initio property prediction of all known inorganic materials. Several examples of new compounds were investigated and different short-comings of the usual approximations in the exchange and correlation functionals were mentioned. Mark Ratner discussed transport in molecular junctions and demonstrated by different examples and limiting cases different approaches to tackle this non-trivial problem.

To conclude, I believe that the $\Psi_k$-2010 conference was a success and I am looking forward to the
next one.

Comment by Manuel dos Santos Dias (Warwick, UK)

Psi–k conference report

My name is Manuel dos Santos Dias, and I’m a PhD student under Prof. Julie Staunton at the University of Warwick, working in collaboration with Prof. László Szunyogh of the Budapest University of Technology and Economics. My research and main interests are on nanoscale magnetism. I present my impressions on the Psi–k 2010 Conference in a few paragraphs below.

The scientific program was outstanding. With often three sessions in parallel drawing my attention, it was hard to decide which talks to attend. Moving from one session to a different one was hindered by a somewhat fluid enforcement of the allotted times for each talk. In the first two days the program was quite long, and the poster sessions took place afterwards, in the evening, taking a toll on the people presenting a poster and on those wanting to discuss the posters with their authors — I was part of both groups. The breadth and depth of the research presented was truly exceptional, and of great interest and relevance. To me this was very fruitful.

I wish to highlight a few talks that I found particularly interesting. Prof. Stefan Blügel’s talk, ‘Topologically protected spin textures at metal surfaces’, was an excellent summary of the physical mechanisms giving rise to complex magnetic states in ultrathin films, as unveiled experimentally and theoretically.

On the topic of strong correlations, Prof Zhong Fang’s talk, ‘LDA+Gutzwiller method for strongly correlated systems’, was an interesting addition to the existing manifold of methods and techniques created to address this problem.

As I’m a computational physicist, Prof. Thomas Schultess talk, ‘Petascale computing in condensed matter physics’, was a very compelling review of the development and usage of large scale simulations, even if peppered with an amusing technical incident.

The Volker Heine session was an insightful addition to the conference program. The talk by Dr. Samir Lounis, ‘Investigations of the intriguing magnetic and electronic behaviour at the nanoscale’, was a vivid illustration of how distinct systems with a finite number of atoms are.

The last talk I will mention was given by Dr. Pawel Buczek, ‘Spin dynamics of complex metallic magnets’. He presented a theory of the transverse magnetic susceptibility which incorporates both local moment and itinerant electron magnetism on the same footing, thus reconciling the Stoner and Heisenberg pictures, with very interesting applications.

The Henry Ford building was an excellent choice for the conference venue. Its ample interior and abundant natural lighting made sharing the same space with 1000 people an almost pleasant experience. The lecture halls are comfortable and well equipped, and it was easy to change from one room to another. The conference staff was very helpful. There was some inevitable strife during
the coffee breaks, and some slices of cake became mythological foodstuffs, as I seldom got hold of them. The main meals were also adequate.

I close by commending all the speakers, participants and organisers on making such a good conference possible.

Comment by Hisazumi Akai (Osaka, Japan)

Short report on the Psi-k 2010 Conference in Berlin

Hisazumi Akai

Osaka University, Japan

The number of submitted papers as well as the number of participants at the Psi-k 2010 conference is clear proof of the tremendous vitality of the field of first principles calculations. The plenary and invited talks were extremely stimulating. Moreover, the contributed oral presentations were also uniformly excellent. Indeed, after attending the poster sessions, I came to the conclusion that the program committee faced an almost impossible task in selecting contributions for oral presentation, such was the high standard.

First-principles calculation now seems to be a field that is dominated by techniques such as NMR, photo-emission, STM, and so on. Many authors reported the results of analyses using a reliable and easy-to-use program package (in many cases, VASP). While there is no question that this is a scientifically sound approach, I hope in the future to see more contributions reporting efforts to further develop the fundamental theories and methodologies that are the foundation of first-principles electronic structure calculations. This, of course, probably reflects a general tendency in the field of first-principles electronic structure calculations.

The Psi-k 2010 conference was a great success and I would like to congratulate the organizers, the contributors and all those who attended, for making it so.

Comment by Peter Kluepfel (Reyjavik, Iceland)

Extraordinary events with global impact are kind of daily business here in Iceland. So when I marked the PsiK2010, the "biggest electronic structure conference in the world" in my calender I thought it was funny appearing right next to volcanic eruptions and the collapse of a nation’s financial system and the superlative "biggest" lost some of its magic in this context. But I was about to be taught differently:

The Organizers:

Everyone knows that Germans are well-organized. Thus I was not expecting anything else than a conference running smoothly from welcome reception to closing session. But I
was impressed by the way the organizers managed to keep things as simple and informal as possible. Already the short waiting time and the relaxed atmosphere at the welcome reception made it easy to find time and space to get connected to old friends and collaborators. Short distances between the lecture halls allowed for getting the most of the contributions without the typical ”I will stay here in room X, just because I anyway won’t make it in time to the talk in room Y”-feeling. I don’t want to forget about expressing my appreciation and thanks to the numerous helpers from the FHI and elsewhere. It felt like there was one of them for each participant.

The Contributions:

PsiK2010 offered one of the finest selections of key-note speakers. This already became clear from the first announcements and the conference program. But the plenary talks even got eclipsed by the numerous invited and contributed presentations. It was impressive to see that there is a new generation of highly motivated, intelligent and charismatic scientists propagating electronic structure theory into the 21st century. One of the few negative aspects of the conference is related to the poster sessions which was in my opinion too short. It was impossible to get through all the interesting presentations or to have deeper discussions with all visitors to ones own poster.

Coffee, Cocktails and Cuisine:

An often underrated descriptor for a good conference is given by the quality of food, the permanent availability of coffee and the amount of free alcoholic beverages at the conference outing. But probably nobody had reason to complain about any of those aspects at the PsiK2010. Enjoying the delicious meals and the excellent catering service on site gave enough energy for the afternoon sessions. I was amazed what seems to be considered as ”finger-food” in Berlin, but still also the food at the outing was very tasty.

I’m personally not a friend of big conferences and usually prefer the atmosphere and efficiency of smaller workshops or summer schools. But in case of the PsiK2010 I honestly have to admit that in spite of its extraordinary dimensions it still maintained the character of a small work meeting with plenty of opportunities for scientific exchange, planning of future projects or just chats about the good old times.

I’m looking forward to the next years’ PsiK workshops and hopefully we will all meet again at PsiK2015.

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Comment by Angela Klaoutau (Belém - PA, Brazil)

The Psi-k Conference 2010 confirmed the well-known general opinion about the importance of *ab initio* calculations for many different fields of natural sciences. The huge number of participants, ranging from Ph.D. students to senior researchers, representing many countries, confirms the increasing importance of electronic structure theory and calculations. The Conference topics ranged from Magnetism and Spintronics to Biological Systems, from Superconductivity to Solar Energy Conversion, from Organic Electronics to Multiferroics and Oxides, etc. In the Conference Symposia we heard and discussed about state of the art computer codes for calculations of different phenomena in different classes of systems, and implementations of new ideas for incorporating correlation effects beyond DFT. In this Conference we had the possibility to attend to seminars and discuss at posters sessions: we listened to senior researchers, who have contributed to the development of the electronic structure area, and learned from groups which have developed and continue working on the improvement of computational methods in this area. It was also an opportunity for listening to very bright young researchers, who contribute to our area in developing and applying computational quantum physics to deepen our understanding of materials. The Conference represented an efficient and unique opportunity to exchange and disseminate information among the computational material science community, giving high visibility to research progresses, as well as to get collaborations started.

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### 2.3 Report on Psi-k Volker Heine Young Investigator Award

The Young Investigator Award of Psi-k was announced at the beginning of this year. All young scientists in our field, who had obtained a Ph. D. within the five years preceding the announcement could apply. In total 23 applications were received before the deadline of 17th April 2010. The award committee consisted of four Psi-k Trustees and three outstanding scientists from USA and Japan:

Volker Heine, Cambridge University
Matthias Scheffler, Fritz Haber Institute
Angel Rubio, University Pais Vasco
Peter Dederichs, Research Center Juelich
Marvin Cohen, UC Berkeley, USA
Gerbrand Ceder, MIT, USA
Ferde Aryasetiawan, Chiba University, Japan

The award committee had to select five finalists from the 23 applications who were to present their work at the Award Session of the Psi-k 2010 Conference. This selection turned out to be difficult, since there were about a dozen excellent proposals, which deserved a careful review. The selected five finalists were:

Claudio Attaccalite, Institute Neel, Grenoble
Christoph Freyssoldt, MPI Iron Research, Duesseldorf
Mateo Gatti, ETSF-UPV, San Sebastian
Samir Lounis, UC Irvine and Research Center Juelich
Alexandre Tkatchenko, Fritz-Haber Institut, Berlin

They presented their work in the special Award Session on Wednesday afternoon of the Psi-k 2010 Conference. The session was very well attended and all candidates gave very good talks.

Thus the award committee, chaired by Marvin Cohen, had again a difficult choice. Special care was taken that the committee members, who had a conflict of interest, did not vote for their candidates. The final vote was close. The winner of the Psi-k Volker Heine Young Investigator Award was

Christoph Freyssoldt, MPI Iron Research, Duesseldorf.

The Psi-k Chairman presented to him the award certificate and Volker Heine the cheque of 2500 Euro. Also the other finalists obtained each an award certificate as “Finalist of the Psi-k Volker Heine Young Investigator Award” and a cheque of 500 Euro. In the photographs below, we see both the winner and the whole group of finalists, respectively, in the company of Peter Dederichs and Volker Heine.

In summary, we consider the new Volker Heine Award as very successful. It was great to see that there were very many talented young researchers in our community. For this reason we intend to issue the prize also in the future.

Peter H. Dederichs, Psi-k Chairman