Research Networking Programmes

Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

Proposal Title:

Workshop on
Methods and Algorithms in Electronic-Structure Theory
Ringberg Castle, June 3 - June 6, 2015

Application Reference N°: 5720

Organizers:

Martin Kaupp (Technische Universität Berlin)
Patrick Rinke (Aalto University)
Matthias Scheffler (Fritz-Haber-Institut der MPG, Berlin)
Peter Saalfrank (Universität Potsdam)

1) Summary

The workshop focussed on the development of methods and algorithms in electronic-structure theory and their implementation in state-of-the-art software packages. The workshop featured a wide range of methods for the unperturbed ground state, such as wave-function theory, density-matrix and density-functional theory and Green's function theory, and for various external time-independent or time-dependent stimuli, as well as open quantum systems. The breadth of methods and the combination of perturbed and unperturbed theories gave the

workshop a wide appeal and made it attractive to internationally acclaimed experts in this field.

The mixture of quantum chemists and solid-state physicist created a stimulating environment. Both fields face similar challenges and have been moving towards each other in recent years. However, the “languages” of the two fields still differ and any opportunity for close interaction fosters the development of a common language. The collegial atmosphere of the workshop, the tutorial-style talks that focussed on open problems more than on results, and the long discussion time after every talk, facilitated an active exchange of ideas that brought the electronic structure community one step closer to this common language.

In addition to the cross-fertilization between quantum chemistry and solid-state physics, synergy was achieved by contrasting excited state and time-dependent methods with ground-state theories. Code developers that presented the latest, cutting-edge implementations of advanced electronic structure methods, complemented the method developers.

2) Description of the scientific content of and discussions at the event

The workshop began with presentations on the development of density-functional theory (DFT) for the unperturbed ground state. In a seminal paper, John Perdew, the opening speaker of the workshop, had classified DFT functionals into five categories, equivalent to the rungs of a ladder that represent increasing functionality and accuracy. Functional development for all five rungs of this ladder was presented at the workshop. John Perdew presented a new third rung meta-generalized-gradient functional that satisfies an unprecedented number of exact criteria and yields accurate results for a wide range of systems, including transition metals. A fourth rung local hybrid approach that adjusts the admixture of exact-exchange in the density functional locally in real-space was presented by Hilke Bahmann. Stephan Kümmel contrasted this approach with another fourth-rung functional that corrects for the self-interaction error in the functional. Igor Ying Zhang, Xinguo Ren, Adrienn Ruzsinszky and Georg Kresse made the step to the fifth rung and introduced their latest developments on a self-consistent wave-function based functional that solves the H_2/H_2^+ conundrum and showed ways to go beyond the random-phase approximation (RPA). Georg Kresse and Mauro Del Ben then presented ways to speed up RPA and MP2 implementations. Earlier Jan Evert Baerends had posed the question if Kohn-Sham DFT could be used also for excited states. The answer is that for certain systems and certain spectroscopies, the Kohn-Sham spectrum, computed with appropriate functionals, can be a good approximation of the excitation spectrum. Stefan Grimme gave an overview over their recent work on benchmark sets for electronic-structure-theories development and presented their recent 2^{nd}, 3^{rd}, 4^{th} and 5^{th} rung functionals. E.K.U. Gross introduced their approximation to the extended spin density-functional theory for superconductors, which gives qualitatively correct results for the temperature *vs* exchange splitting dependence of superconductors.

In the context of single-reference coupled-cluster (CC) ansatz in quantum chemistry, Gustavo Scuseria presented their singlet-paired coupled cluster (CCD0) approach, which substantially removes the failures of the traditional CC methods in the strongly correlated limit without having to resort to multi-reference strategies or higher-body cluster operators. A density matrix embedding theory was then introduced by George H. Booth to extend the capabilities of CC approaches to larger systems. Beate Paulus incremental method follows in a similar spirit, whereas Martin Schütz presented ways to speed up CC calculations by exploiting locality. Silke Biermann and Paola Gori-Giorgi presented a different view of strongly correlated systems: dynamical mean-field theory and strongly-correlated DFT.

E.K.U. Gross and Honghui Shang considered perturbations of the ground state due to atomic displacements. This coupling between electrons and phonons gives rise to superconductivity (Gross) and polarons (Shang). The response of electronic systems to external perturbations was also covered in several other talks: A. Scherrer presented efficient spectral decompositions for the calculation of electronic susceptibilties and related quantities, e.g., polarizabilities and Raman spectra, choosing ensembles of water molecules as an example. T. Körzdörfer reported on tuned DFT- and *GW*-based methods for electron affinities and ionization potentials of molecules, and on determining the vibronic fine-structure of corresponding spectra.

The final step to explicitly time-dependent dynamics beyond perturbative treatments was made by S. Sharma, who presented a real-time DFT (TD-DFT) method with laser interaction and spin-orbit coupling to study the laser-pulse induced demagnetization of solids. J.C. Tremblay modeled laser-driven processes such as electron injection in quantum dots and dye-sensitized semiconductors by solving time-dependent Schrödinger or Liouville-von Neumann equations in the basis of states derived either from configuration interaction (CI) or (linear-response) TD-DFT. Similarly, T. Klamroth adopted the TD-CI method for laser control of electron dynamics in molecules, and presented a pilot implementation of time-dependent coupled cluster (TD-CCSD) theory. R. Santra went beyond valence excitations by considering ionization and multi-photon processes in atoms and molecules after X-ray laser excitation, using their XATOM and XMOLECULE program suites.

Two strongly mathematically oriented talks by J. Eisert and R. Schneider illustrated the current status and future perspectives of tensor networks to efficiently treat interacting many-body systems for model Hamiltonians (Hubbard) and *ab initio* quantum chemistry. Finally, C. Draxl gave an overview over the so-called NoMaD repository, a web-based platform to host, organize and share materials data.

3) Assessment of the results and impact of the event on the future directions of the field

The workshop stimulated an interdisciplinary exchange of ideas and knowledge transfer from chemistry, solid-state physics, and materials science. Despite its

small and intimate scale, the workshop will have a lasting impact on methods development in electronic structure theory, because 1) electronic structure theory is the foundation for many developments in these fields and 2) methods development drives progress. The workshop reviewed the current state-of-the-art in methods development and inspired new avenues for more accurate approaches and computational more efficient implementations that will facilitate future discoveries.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

WEDNESDAY, 3rd		THURSDAY, 4th		FRIDAY, 5th		SATURDAY, 6th
		Session 3		**Session 4 (2)**		*The conference ends after breakfast*
		09:00	G. Scuseria	09:00	X. Ren	
		09:40	S. Kümmel	09:40	P. Gori-Giorgi	
		10:20	*Coffee break*	10:20	*Coffee break*	
		10:50	S. Grimme	10:40	B. Paulus	
		11:30	M. Schütz	11:10	A. Ruzsinszky	
				11:40	T. Körzdörfer	
		12:15 Lunch		*12:15 Lunch*		
		Session 4 (1)		**Session 6**		
		13:20	C. Draxl	13:30	R. Santra	
		13:50	S. Biermann	14:10	H. Shang	
		Excursion		14:40	J.C. Tremblay	
16:15	Opening remarks			15:10	M. Del Ben	
				15:50	*Coffee Break*	
Session 1				**Session 7**		
16:30	J. Perdew			16:20	T. Klamroth	
17:10	H. Bahmann			16:50	J. Eisert	
17:40	E.J. Baerends			17:20	R. Schneider	
18:30 Dinner		*18:30 Dinner*		*19:00 Conference Dinner*		
20:00	H. Gross	**Session 5**				
Session 2		20:00	I. Zhang			
20:40	A. Scherrer	20:30	G. Kresse			
21:10	S. Sharma	21:10	G. Booth			

Slots with blue background: 30 minutes talk + 10 minutes discussion

Slots with yellow background: 20 minutes talk + 10 minutes discussion

Annex 4b: Full list of speakers and participants

Speakers

Evert-Jan	Baerends	Vrije Universiteit Amsterdam
Hilke	Bahmann	Technische Universität Berlin
Silke	Biermann	École Polytechnique, Palaiseau Cedex
George	Booth	University of Cambridge
Mauro	Del Ben	Universität Zürich
Claudia	Draxl	Humboldt Universität zu Berlin
Jens	Eisert	Freie Universität Berlin
Paola	Gori-Giorgi	Vrije Universiteit Amsterdam
Stefan	Grimme	Universität Bonn
Hardy	Gross	Max-Planck-Institut fur Mikrostrukturphysik, Halle
Tillmann	Klamroth	Universität Potsdam
Thomas	Körzdörfer	Universität Postdam
Georg	Kresse	Universität Wien
Stephan	Kümmel	Universität Bayreuth
Beate	Paulus	Freie Universität Berlin
John	Perdew	Temple University
Xinguo	Ren	University of Science and Technology of China
Adrienn	Ruzsinszky	Temple University
Robin	Santra	DESY & University of Hamburg
Arne	Scherrer	Martin-Luther-Universität Halle-Wittenberg
Reinhold	Schneider	Technische Universität Berlin
Martin	Schütz	Universität Regensburg
Gustavo	Scuseria	Rice University, Houston
Honghui	Shang	Fritz-Haber-Institut der MPG, Berlin
Sangeeta	Sharma	Max-Planck-Institut fur Mikrostrukturphysik, Halle
Jean Christophe	Tremblay	Freie Universität Berlin
Igor Ying	Zhang	Fritz-Haber-Institut der MPG, Berlin

Organizers

Martin	Kaupp	Technische Universität Berlin
Patrick	Rinke	Aalto University
Matthias	Scheffler	Fritz-Haber-Institut der MPG, Berlin
Peter	Saalfrank	Universität Potsdam

Participants

Alexey	Arbuznikov	Technische Universität Berlin
Jan Gerit	Brandenburg	Universität Bayreuth
Thiago	Branquinho de Queiroz	Universität Bayreuth
Matthias	Dauth	Universität Bayreuth
John Kay	Dewhurst	Max-Planck-Institut fur Mikrostrukturphysik, Halle

Qiang	Fu	Humboldt-Universität zu Berlin
Andris	Gulans	Humboldt-Universität zu Berlin
Arvid Conrad	Ihrig	Fritz-Haber-Institut der MPG, Berlin
Dominik	Kroener	Universität Potsdam
Xiang-Yue	Liu	Fritz-Haber-Institut der MPG, Berlin
Toni	Maier	Technische Universität Berlin
Lukas	Muechler	Princeton University
Tobias	Schmidt	Universität Bayreuth
Tonghao	Shen	Fritz-Haber-Institut der MPG, Berlin
Christian	Stemmle	Freie Universität Berlin
Ute	Werner	Humbolt-Universität zu Berlin