

## 0.1 Report on Summer School "Bandstructure meets Many Body Theory"

Vienna

September 18-22, 2012

$\Psi_k$ , CECAM, SFB-ViCoM

G. Kresse and K. Held

<http://www.cecam.org/workshop-0-834.html>

### Aim of the school

A particular challenge of computational materials science is the calculation of materials in the presence of strong electronic correlations and exchange. In this case, the local density approximation (LDA) or generalized gradient approximation to the exchange correlation potential often yields unreliable results. In recent years we have seen tremendous progress in this field: The aim of the Summer School has been to educate the next generation of scientists in both, bandstructure and many body theory. To this end, there have been lectures in the morning and tutorials in the afternoon.

### Scope of the school

The first day of the summer school was devoted to density functional theory: E.K.U. Gross gave an introduction to DFT and, in a second lecture, explained time-dependent-DFT, emphasizing the importance of functionals. This was supplemented in the afternoon by a tutorial on DFT by P. Blaha, in which also related approaches such as DFT+U and hybrid functionals were tested for SrVO<sub>3</sub>.

On the second day, A. Toschi gave an introduction to quantum field theory, from Feynman diagrams to Green functions. The quantum Monte Carlo (QMC) method for solving lattice models such as the Hubbard model was introduced by R.T. Scalettar, who also guided the students in the afternoon's tutorial on QMC. G. Sangiovanni briefly explained additional aspects relevant for continuous-time quantum Monte Carlo approaches, employed e.g. for solving the dynamical mean field theory (DMFT) equations.

On the third day, R. Godby explained the GW approximation and the differences to DFT. The students did their own GW calculations in the afternoon, in a tutorial organized by G. Kresse and M. Marsmann. M. Head-Gordon introduced state-of-the-art quantum chemistry approaches from configuration interaction to coupled cluster.

On the fourth day, D. Vollhardt introduced DMFT and presented results of DFT and DFT+DMFT calculations. In a tutorial, J. Kunes guided the students on how to arrive from a DFT calculation

at maximally localized Wannier orbitals. These are needed for a subsequent DMFT calculation, which the student's did for SrVO<sub>3</sub> in the second tutorial of the day under the supervision of G. Sangiovanni.

On the fifth day, S. Biermann explained in her lecture the GW+DMFT approach and how to calculate frequency dependent screened interactions. The second lecture was given by R. Noack, who introduced the density matrix renormalization group approach (DMRG). In the subsequent tutorial the students ran their own DMRG calculations.

The school received a very positive feedback from the students who enjoyed the combination of lectures and tutorials, the pedagogical presentations given by world leading scientists in the field.

## Programme

### Day 1 - September, 18th 2012

09:00 to 09:10	Karsten Held	Welcome
09:10 to 10:30	E.K.U. Gross	Density functional theory (DFT)
11:00 to 12:30	E.K.U. Gross	time-dependent DFT
13:30 to 17:30	Peter Blaha	Tutorial DFT

### Day 2 - September, 19th 2012

09:00 to 10:30	Alessandro Toschi	Quantum Field Theory
11:00 to 12:30	Richard T. Scalettar	Quantum Monte Carlo (QMC)
12:30 to 13:00	Giorgio Sangiovanni	Continuous-time Quantum Monte Carlo
14:30 to 17:30	Richard T. Scalettar	Tutorial Quantum Monte Carlo

### Day 3 - September, 20th 2012

09:00 to 10:30	Martin Head-Gordon	Quantum Chemistry
11:00 to 12:30	Rex Godby	GW Approach
13:30 to 17:30	Georg Kresse	Tutorial GW

### Day 4 - September, 21st 2012

09:00 to 10:30	Dieter Vollhardt	Dynamical Mean Field Theory (DMFT)
11:00 to 13:15	Jan Kunes	Tutorial Wannier Function Projection
14:15 to 18:00	Giorgio Sangiovanni	Tutorial DMFT

### Day 5 - September, 22nd 2012

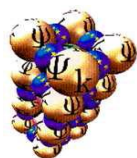
09:00 to 10:15	Silke Biermann	GW+DMFT
10:15 to 11:30	Reinhard Noack	Density Matrix Renormalization Group (DMRG)
12:00 to 14:00	Reinhard Noack	Tutorial DMRG

## List of participants and lecturers

Elias ASSMANN, Silke BIERMANN, Lars BJAALIE, Peter BLAHA, Larisa CHIZHOVA, Andras DEAK, Krzysztof Pawel DYMKOWSKI, Marcus EKHOLM, Gregor FELDBAUER, Qingguo FENG, Anna GALLER, Martin GANAHL, Nirmal GANGULI, Faruk GELES, Rex GODBY,

Luke GORDON, E.K.U. GROSS, Martin HEAD-GORDON, Marcel HIECKEL, Marc HPPNER, Viktor IVDY, Kunes JAN, Alamgir KABIR, Ferenc KARSAI, David KOLLER, Natalia KUROVA, DEBBICHI LAMJED, Stefan LEBERNEGG, Bora LEE, Quifeng LIANG, Jakob LISS, Brajesh Kumar MANI, Martijn MARSMAN, Reinhard NOACK, Martin NUSS, Chris OLSON, Ongun OZCELIK, Tomasz PABISIAK, Nicolaus PARRAGH, Xihong PENG, Andrei Valentin PLAMADA, Stefano PRADA, Kalpataru PRADHAN, Maciej PYLAK, Arthur RIEFER, Malte RSNER, Baisheng SA, Burkhard SACHS, Anta SNCHEZ BOTANA, Giorgio SANGIOVANNI, Richard T. SCALETTAR, Malte SCHLER, Vijay SINGH, Jadwiga Ludmila SLAWINSKA, David TOMPSETT, Alessandro TOSCHI, Dieter VOLLHARDT, Markus WALLERBERGER, Aljoscha WILHELM, Philipp WISSGOTT, Sun YAN, Zhicheng ZHONG,

## Psi-k Network : Towards Atomistic Materials Design



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### **PSI-K WORKSHOP FINANCE REPORT**

<b>Title of the Workshop</b>	Summer School "Bandstructure Meets Many Body"
<b>Workshop Organisers</b>	Prof. Karsten Held & Prof. Georg Kresse
<b>Location of the Workshop</b>	Vienna University of Technology
<b>Dates of the Workshop</b>	18th to 22nd of September 2012
<b>Total Grant from Psi-k</b>	€ 10,000.00

#### **EXPENDITURE**

*(Please complete the tables using numbers ONLY in the amounts fields - the spreadsheet will calculate the totals for you)*

<b>WORKSHOP DELEGATES / SPEAKERS</b>						
Name and Country of Claimant			Travel		Accommodation	Total (€'s)
Bjaalie	Lars	Norwegian	€	11,35	€ 205,00	€ 216,35
Botana	Antia S.	Spanisch	€	15,00		€ 15,00
Deak	Andras	Hungary	€	11,35	€ 205,00	€ 216,35
Debbichi	Lamjed	Tunesian	€	15,00	€ 205,00	€ 220,00
Dymkowski	Krzysztof Pawel	Polish	€	15,00	€ 125,00	€ 140,00
Ekhholm	Marcus	Swedish	€	15,00		€ 15,00
Feng	Qingguo	Chinese	€	15,00	€ 205,00	€ 220,00
Ganahl	Martin	Austrian	€	11,35		€ 11,35
Geles	Faruk	Turkey	€	15,00	€ 205,00	€ 220,00
Gordon	Luke	Irish / U.S.	€	11,35	€ 205,00	€ 216,35
Höppner	Marc	German	€	15,00	€ 145,20	€ 160,20
Ivány	Viktor	Hungary	€	11,35	€ 205,00	€ 216,35
Kabir	Alamgir	Bangladishi	€	15,00	€ 205,00	€ 220,00
Mani	Brajesh Kumar	Indian	€	15,00	€ 205,00	€ 220,00
Kurova	Natalia	Russian	€	11,35	€ 275,00	€ 286,35
Lebernegg	Stefan	Austria	€	15,00	€ 100,00	€ 115,00
Lee	Bora	Korea	€	15,00	€ 125,00	€ 140,00
Liss	Jakob	German	€	15,00		€ 15,00
Nuss	Martin	Austria	€	11,35	€ 205,00	€ 216,35
Olson	Chris	U.S.	€	11,35	€ 125,00	€ 136,35
Ozcelik	Ongun	Turkey	€	335,00	€ 125,00	€ 460,00
Pabisiak	Tomasz	Polish	€	15,00	€ 205,00	€ 220,00
Peng	Xihong	Chinese	€	15,00	€ 205,00	€ 220,00
Parragh	Nicolaus		€	88,00		€ 88,00
Plamada	Andrei Valentin	Romanian	€	11,35	€ 205,00	€ 216,35
Prada	Stefano	Italian	€	11,35	€ 205,00	€ 216,35
Pradhan	Kalpataru	Indian	€	15,00	€ 125,00	€ 140,00
Pylak	Maciej	Polish	€	15,00	€ 125,00	€ 140,00
Qifeng	Liang	Chinese	€	15,00	€ 125,00	€ 140,00
Riefer	Arthur		€	11,35		€ 11,35
Rösner	Malte	German	€	11,35	€ 125,00	€ 136,35
Sa	Baisheng	Chinese	€	184,75	€ 125,00	€ 309,75
Sachs	Burkhard	German	€	15,00	€ 205,00	€ 220,00
Schüler	Malte	German	€	11,35	€ 125,00	€ 136,35
Singh	Vijay Ramdin	Indian	€	15,00	€ 205,00	€ 220,00
Slawinska	Jadwiga Ludmila	Polish	€	11,35	€ 205,00	€ 216,35
Tompsett	David	Australian	€	15,00	€ 125,00	€ 140,00
Wilhelm	Aljoscha	German	€	15,00	€ 205,00	€ 220,00
Gross	Eberhart		€	15,00		€ 15,00
Vollhardt	Dieter		€	15,00		€ 15,00
Scalettar	Richard		€	15,00		€ 15,00
Godby	Rex		€	15,00		€ 15,00
Biermann	Silke		€	15,00		€ 15,00
Head-Gord	Martin		€	15,00		€ 15,00
Kunes	Jan		€	15,00		€ 15,00
Sangiovanni	Giorgio		€	15,00		€ 15,00
Noack	Rainer		€	15,00		€ 15,00
<b>Total Travel &amp; Accommodation</b>						<b>€ 6.801,85</b>

<b>WORKSHOP REFRESHMENTS / CONFERENCE DINNERS</b>			
Date	Tea / Coffee	Lunch / Dinner	Total (€'s)
18th of September 2012	€ 306,58	€ 306,58	€ 613,15
19th of September 2012	€ 306,58	€ 306,58	€ 613,15
20th of September 2012	€ 306,58	€ 306,58	€ 613,15
21st of September 2012	€ 306,58	€ 306,58	€ 613,15
22nd of September 2012	€ 306,58	€ 306,58	€ 613,15
<b>Total Refreshments</b>			<b>€ 3.065,75</b>

<b>MISCELLANEOUS EXPENDITURE</b>		
Details	Total (€'s)	
Conference packages	€ 97,50	
Office supplies	€ 14,90	
Taxi (delivery conference packages)	€ 13,00	
Bank service charge	€ 5,08	
<b>Total Miscellaneous</b>		<b>€ 130,48</b>

<b>Total Travel &amp; Accommodation</b>	€	<b>6.801,85</b>
<b>Total Refreshments</b>	€	<b>3.065,75</b>
<b>Total Miscellaneous</b>	€	<b>130,48</b>
<b>TOTAL EXPENDITURE</b>		<b>€ 9.998,08</b>

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