

0.0.1 Report on the School on "Electronic Structure Calculations and Correlated Materials"

Ecole Prédoctorale, Les Houches, France

August 27th - September 8th, 2006

Sponsors:

European Science Foundation through the Psik Programme

Ministère de la Jeunesse, de l'Éducation Nationale et de la Recherche, France

Centre National de la Recherche Scientifique (CNRS), France

Direction des Sciences de la Matière du Commissariat à l'Énergie Atomique (CEA/DSM), France

Organizers: S. Biermann and B. Amadon

<http://www.cpht.polytechnique.fr/LesHouches.html>

Summary

The School on "Electronic Structure Calculations and Correlated Materials" was held from August 27th to September 8th, 2006, at the Physics School of Les Houches, France, bringing together 45 participants and 12 lecturers. Topics covered ranged from materials properties, electronic structure theory to modern approaches for first principles calculations for materials with strong electronic Coulomb correlations.

General scientific scope of the School

In recent years, electronic structure calculations for materials with strong electronic Coulomb correlations have developed into a new research field at the border between band structure theory and field theoretical techniques for the solution of quantum many-body problems. The most prominent example of a method that has evolved from merging these two elements is the so-called

LDA+DMFT scheme which combines dynamical mean field theory with density functional theory within the local density approximation. Further developments concern incorporating the GW approximation into techniques for strongly correlated systems, or making the whole arsenal of band structure techniques – ranging from muffin-tin to plane-wave implementations – available in the framework of LDA++ theories.

Since this area of research requires knowledge of both, electronic structure and many body techniques, it is not easily accessible for younger students, starting their PhD. On the contrary, most researchers working presently in the field started their research career in either of the two parts and acquired some education in the other part only later on. The Les Houches summer school on “Electronic Structure Calculations and Correlated Materials” tried to fill this gap and to allow even beginning graduate students to acquire simultaneously knowledge and understanding in both parts of the field. The following topics were covered:

- Introduction: Electrons in Solids
- Materials properties, materials classes
- Density Functional Theory
- Different implementations: about plane waves, muffin tins and PAW
- Molecular Dynamics and Car-Parrinello techniques
- Introduction to Green’s functions and fermionic path integrals
- Strongly correlated materials: physical effects and theoretical descriptions
- Lattice models of correlated materials and Dynamical Mean Field Theory
- The Mott transition
- The LDA+DMFT scheme
- Advanced topics: TDDFT, GW, extensions of DMFT
- Overview of experiments and experimental techniques: photoemission, NMR and optics

Participants

The number of applicants (more than 80) exceeded by far the number of available places: only 45 could attend the school. As the school was geared in particular at beginning graduate students, an important percentage of the participants were indeed masters students (the youngest being 20 years old), the majority were PhD students in their first two years; four postdoctoral researchers were admitted. Twenty different nationalities were represented among the participants and lecturers; the distribution is given in Table I.

Table 1: Lecturers

Bernard Amadon	CEA Bruyères-le-Châtel, France	Organizer
Silke Biermann	Ecole Polytechnique, Palaiseau, France	Organizer
Stefano Baroni	SISSA, Trieste, Italy	Lecturer
Julien Bobroff	Université Paris-Sud, Orsay, France	Lecturer
Fabien Bruneval	ETH Zürich, Switzerland	Lecturer
Antoine Georges	Ecole Polytechnique, Palaiseau, France	Lecturer
Alexander Lichtenstein	Universität Hamburg, Germany	Lecturer
Bernd Meyer	Ruhr-Universität Bochum, Germany	Lecturer
Marcelo Rozenberg	Université Paris-Sud, Orsay, France	Lecturer
Andres Santander	Université Paris-Sud, Orsay, France	Lecturer
George Sawatzky	University of Vancouver, Canada	Lecturer
Francesco Sottile	Ecole Polytechnique, Palaiseau, France	Lecturer

Location

The school took place in the “Ecole de Physique des Houches”. Les Houches is a resort village in the Chamonix valley in the French Alps. The school is located in a group of chalets surrounded by meadows and woods, at an altitude of 1150 m facing the Mont-Blanc range – once more it proved true that such a beautiful environment stimulates intellectual activity, and that hiking and mountaineering activities during leisure time promote scientific exchange among participants and lecturers.

Remarks: specific features of the school and impact

The atmosphere of the school was marked by the high motivation of the students (and lecturers!). Informal exchange and discussion took a large place, and several lectures turned into discussion sessions where the students participated actively. Moreover, every effort was made to provide links between the different lectures, in order not to give the participants the impression to attend just a series of independent courses. Special tutorial/question sessions helped to clarify problems, stimulate further discussions and meet particular interests of the students. Several exercise sessions allowed the students to test their understanding of the freshly acquired knowledge.

The students had quite different backgrounds, some of them working more or less in the field or on particular aspects of it, others exploring a new research field. All of them actively used the chance to get a wider view of the field, to get familiar with its physical and technical questions, and there is certainly hope that for some of the students who were not previously working in the field the school has a long-term effect concerning their choices of PhD theses,

Table 2: Nationalities of participants and lecturers

Nationality	Number of Participants	Number of Lecturers	Total
Italian	6	2	8
German	6	2	8
French	3	4	7
US	4	-	4
Russian	3	1	4
Swedish	3	-	3
Chinese	3	-	3
Argentinian	1	1	2
Colombian	1	1	2
Czech	2	-	2
Spanish	2	-	2
Turkish	2	-	2
Austrian	2	-	2
Indian	2	-	2
Dutch	-	1	1
Swiss	1	-	1
Algerian	1	-	1
Korean	1	-	1
UK	1	-	1
Iranian	1	-	1

postdoctoral research or job orientation.

List of Participants and Lecturers

Adams, Donat
Amadon, Bernard
Amaricci, Adriano
Antipov, Andrey
Arhammar, Cecilia
Augustinsky, Pavel
Baroni, Stefano
Bergqvist, Lars
Biermann, Silke
Bourgeois, Antonin
Bobroff, Julien
Bruneval, Fabien
Bultmark, Fredrik
Burnus, Tobias
Chan, Maria
Cossu, Fabrizio
Cricchio, Francesco
Djedai, Saoussen
Dobrindt, Jens
Drosdoff, David
Folgueras, Ana
Georges, Antoine
Gougoussis, Christos
Gurel, Tanju
Ismer, Jan-Peter
Jelinek, Pavel
Kim, Duckyoung
Krivenko, Igor
Lichtenstein, Alexander
Lukoyanov, Alexey
Meyer, Bernd
Muller, Carsten
Paier, Joachim
Pardini, Lorenzo
Poilvert, Nicolas
Rowlands, Derwyn
Rozenberg, Marcelo
Sadatshafaie, Ghazal
Sakiroglu, Serpil
Salguero, Andrea
Sanchez, Kefren
Santander, Andres
Sawatzky, George
Schoellhammer, Gunther

Sordi, Giovanni
Sottile, Francesco
Sun, Sineng
Tarafder, Kartick
Tibbetts, Kevin
Tomczak, Jan
Tubman, Norman
Venturelli, Davide
Vildosola, Veronica
Wadehra, Amita
Walther, Christian
Zhang, Feiwu
Zhou, Fei

List of Posters

- Fe²⁺ impurities in mantle forming minerals
Donat Adams
- Electronic structure calculations and nonlinear optical properties of alpha H-Pd structure in predefined H-concentration and temperature conditions
Andrey Antipov
- Kondo asymptotics in SIAM: Parquet approach
Pavel Augustinsky
- Distorted augmented planewaves
Fredrik Bultmark
- Importance of spin-orbit coupling on the magnetism in the ruthenates
Tobias Burnus
- The magnetic susceptibility of interacting heisenberg q-system
Saoussen Djedai
- Ab initio pressure-dependent vibrational and dielectric properties of CeO₂
Tanju Gurel
- Formation, fractional conductance and enhanced reactivity of Au monoatomic chains with impurities
Pavel Jelinek
- Analytical continuation of QMC data: stochastic regularization approach
Igor Krivenko
- The LDA+DMFT(QMC) method for the transition metal materials
Alexey Lukoyanov
- Modeling catalytical surface reactions on ceria surfaces
Carsten Muller
- Hybrid functionals applied to extended systems
Joachim Paier
- Ab-initio investigation of adsorption of acetone on small gold clusters
Ghazal Sadatshafaie
- Microscopic ab-initio study of the electronic and magnetic properties of triazole-bridged Fe(II) polymers
Andrea Salguero
- Theoretical Modelling of Intermediate Band Solar Cell Materials Based on Metal-Doped Chalcopyrite Compounds
Kefren Sanchez

- Approximative implementation of hybrid functionals for fast and accurate simulations with the PAW method
Sineng Sun
- Effect of short range ordering on the optical properties of disordered systems
Kartick Tarafder
- Quasi-particle band structure of VO₂
Jan M. Tomczak
- First principles calculations on band offsets of semiconductor heterostructures
Amita Wadehra
- LDA+U calculation of CeO₂ and Ce₂O₃ and their intrinsic defects
Christian Walther
- Theory of magnesium silicates with bearing Fe and Al in the lower mantle and the Earth's D'' layer
Feiwu Zhang
- Configurational electronic entropy and phase diagram of Li_xFePO₄
Fei Zhou

Table 3: Program

Monday 28/8		
8:45 - 10:15	Welcome	S. Biermann, B. Amadon
10:30 - 12:00	Density Functional Theory I	S. Baroni
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Density Functional Theory II	S. Baroni
17:15 - 18:45	<i>Poster session</i>	
Tuesday 29/8		
8:45 - 10:15	Density Functional Theory III	S. Baroni
10:30 - 12:00	Implementations I: plane waves	B. Meyer
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Materials I	G. Sawatzky
17:15 - 18:45	Molecular Dynamics	B. Meyer
Wednesday 30/8		
8:45 - 10:15	Materials II	G. Sawatzky
10:30 - 11:15	Implementations II: localized basis sets	A. Lichtenstein
11:15 - 12:00	LDA+U I	A. Lichtenstein
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	-	
17:15 - 18:45	-	
Thursday 31/8		
8:45 - 10:15	Tutorial on Materials	G. Sawatzky
10:30 - 12:00	Many-body techniques	S. Biermann, B. Amadon
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 16:15	Implementations III: PAW	B. Amadon
16:15 - 17:00	Introduction to Models	S. Biermann
17:15 - 18:45	Experimental techniques I: photoemission	A. Santander
Friday 1/9		
8:45 - 10:15	LDA+U II	A. Lichtenstein
10:30 - 12:00	Time-dependent density functional theory	F. Sottile
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Green's functions	A. Georges
17:15 - 18:45	Exercices on Many-Body techniques	S. Biermann, B. Amadon
Saturday 2/9		
8:45 - 10:15	The GW approximation	F. Bruneval
10:30 - 12:00	Questions	B. Amadon, S. Biermann,
12:00 - 15:30	<i>Lunch break</i>	F. Bruneval, A. Lichtenstein,
15:30 - 17:00		A. Santander, F. Sottile
17:15 - 18:45		

Table 4: Program 2nd week

Monday 4/9		
8:45 - 10:15	Introduction 2nd week & Questions	S. Biermann
10:30 - 12:00	Dynamical Mean Field Theory I	A. Georges
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Time-dependent density functional theory II	F. Sottile
17:15 - 18:45	Dynamical Mean Field Theory - Exercices	A. Georges
Tuesday 5/9		
8:45 - 10:15	Dynamical Mean Field Theory II	A. Georges
10:30 - 12:00	LDA+DMFT I	A. Lichtenstein
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Many body algorithms I	M. Rozenberg
17:15 - 18:45	Experimental techniques: Optics	A. Santander
Wednesday 6/9		
8:45 - 10:15	LDA+DMFT II	B. Amadon, S. Biermann
10:30 - 12:00	Many body algorithms II	M. Rozenberg
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00		
17:15 - 18:45		
Thursday 7/9		
8:45 - 10:15	Dynamical Mean Field Theory III	A. Georges
10:30 - 12:00	Many body algorithms III	M. Rozenberg
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Experimental techniques: NMR	J. Bobroff
17:15 - 18:45	Questions	all lecturers
Friday 8/9		
8:45 - 10:15	Summary	B. Amadon, S. Biermann
10:30 - 12:00	Perspectives	S. Biermann
12:00 - 15:30	<i>Lunch break</i>	
15:30 - 17:00	Departure	
17:15 - 18:45		