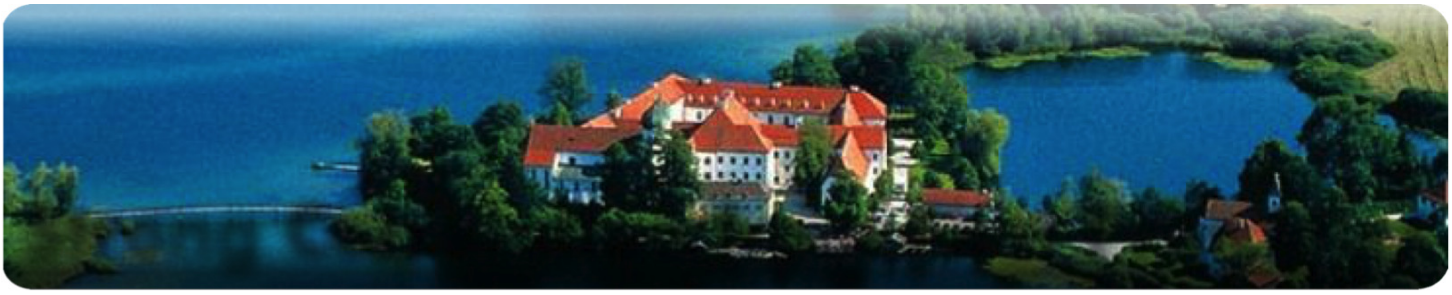

Strong Correlation from First Principles

Monastery Seeon, Bavaria, Germany

August 30 – September 2, 2011

Organizers

Silke Biermann (Ecole Polytechnique, Palaiseau)
Patrick Rinke (Fritz Haber Institute, Berlin)

-Final Report-

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The workshop Strong Correlation from First Principles (SC1p) was held at Kloster Seeon from August 30 to September 2, 2011. The first-principles description of strongly correlated materials (typically materials containing partially filled d- or f-shells) is one of the great challenges in condensed matter physics. Strongly correlated materials such as complex oxides are becoming evermore important for technological applications, while simultaneously offering a plethora of physical phenomena (e.g. high temperature superconductivity) that continue to challenge our current understanding. Many disjointed approaches to tackle the problem are currently being pursued in the electronic structure community, by many-body theorists and quantum chemists. The SC1p workshop brought together 45 scientists from different communities who actively debated the very foundations of the challenges that lie ahead. The momentum generated by SC1p will be carried forward to a symposium with the same name at the March Meeting of the German Physical Society in Berlin in 2012 that has already been approved. The success of the SC1p workshop this year makes us confident that a series of workshops dedicated to the first principles treatment of strong correlations could develop. This series could provide the synergy to shape the future development in this important research area and would provide a unique opportunity to promote this emerging field in the European research landscape.

45 participants from leading international groups attended the workshop and presented 16 oral contributions (11 invited and 5 contributed talks) as well as 24 posters. Two overview talks on the first evening introduced the subject from two different angles. Over the course of the next three days invited experts presented their current results and insights into the topic. We had deliberately limited the time for presentations to 25min and reserved 20min for discussion after each presentation. For contributed talks the partition was 15min and 10min. This turned out to be an excellent idea, because it really encouraged lively discussion after each talk that continued into the coffee, lunch and dinner breaks. It also gave younger researchers the opportunity to participate in the discussions and to ask questions, which is often not the case at large conferences that permit only a limited number of questions that are then taken up by established scientists in the field.

Since two different communities with different philosophies and viewpoints came together in this workshop the discussions were very insightful for all participants. This was also the motivation for the round table discussion that took place Thursday morning. We had realized that many participants had submitted abstracts on the same materials system (transition metal monoxides). To spare the audience from having to hear the same introductory material several times, we decided to pool the presentations into one moderated round table, in which each speaker was given 5min to introduce the most important results or open problems. The ensuing discussion was active and productive (also thanks to the excellent moderation of G. Sawatzky) and makes us confident, that this format might be a viable alternative to the usual presentation style at scientific conferences.

Kloster Seeon in Bavaria provided the perfect venue for the workshop. The local organization at Kloster Seeon was smooth and extremely professional. The technical facilities in the conference room were state-of-the-art and easy to use. Posters were mounted in the coffee area and were on display for the whole duration of the workshop. This facilitated active discussions in front of the posters well beyond the time of the poster session on Wednesday evening. The fact that accommodation and conference facilities share the same premise at Kloster Seeon and that lunch and dinner were also served on site provided an informal atmosphere for stimulating discussions and gave conference attendants ample time to exchange ideas.

Program

Tuesday, 30 Aug.	
19:00 - 20:15	**Dinner**
20:15 - 20:30	Welcome
20:30 - 20:55	Antoine Georges (CPHT-Ecole Polytechnique): *Strong Electronic Correlations: what they are and how to treat them*
20:55 - 21:15	Discussion
21:15 - 21:40	Lucia Reining (LSI, Ecole Polytechnique): *Correlation: coupling of excitations*
21:40 - 22:00	Discussion
Wednesday 31 Aug.	
09:00 - 09:25	Alexander Lichtenstein (University of Hamburg): *Strong Electronic Correlations in real materials*
09:25 - 09:45	Discussion
09:45 - 10:05	Hong Jiang (Peking University): *Electronic band structures of d- and f-electron systems from GW@LDA+U perspective*
10:05 - 10:20	Discussion
10:20 - 10:50	**Coffee Break**
10:50 - 11:10	Jan Kuneš (Institute of Physics, Praha): *Multireference Local States in Solids with Dynamical Mean-Field Theory*
11:10 - 11:25	Discussion
11:25 - 11:40	Bernard Amadon (CEA – Département de Physique): *An LDA+DMFT implementation in the Projector Augmented Wave: Applications to f electrons systems*
11:40 - 11:50	Discussion
12:00	**Lunch**
14:00 - 14:25	Hardy Gross (MPI Halle): *Density-matrix functional theory of strongly correlated solids*
14:25 - 14:45	Discussion
14:45 - 15:10	Xinguo Ren (Fritz-Haber-Institut): *Towards a general-purpose first principles method: a critical assessment of the random phase approximation and beyond*
15:10 - 15:30	Discussion
15:30 - 16:00	**Coffee Break**
16:00 - 16:15	David Jacob (MPI Halle): *COHSEX+OCA and COHSEX+DMFT for nanoscopic conductor*
16:15 - 16:25	Discussion
16:25 - 16:40	Loig Vaugier (CPHT-Ecole Polytechnique): *Hubbard U from the constrained Random Phase Approximation (cRPA) within a full-potential linearized augmented plane wave approach: Trends for 3d and 4d transition metal perovskites*
16:40 - 16:50	Discussion
17:00	Poster session
19:00	**Dinner**

Thursday 01 Sept.	
09:00 - 09:20	Sokrates Pantelides (Vanderbilt University): *Density functional theory for d-electron systems - Are there really strong correlations?*
09:20 - 09:35	Discussion
09:35 - 09:50	Cyril Martins (CPHT-Ecole Polytechnique): *Spin-orbital polarization in paramagnetic transition metal oxides: Sr_2IrO_4 versus Sr_2RhO_4*
09:50 - 10:00	Discussion
10:00 - 10:30	**Coffee Break**
10:30 - 12:00 Chairman: G. Sawatzky	Roundtable discussion: Transition metal monoxides Contributors: Kuneš, Jiang, Gatti, Schroen, Thunstroem, Guzzo, Lichtenstein and whoever wants to say something on transition metal monoxides (please contact S. Biermann) a) Short general introduction -15 min- to MnO, NiO, FeO, CoO by the Chairman b) Every speaker has max. 3 to 4 slides and max. 5 minutes
12:00	**Lunch**
Excursion	
20:00	**Dinner**
Friday 02 Sept.	
09:00 - 09:25	George Sawatzky (UBC – Departement Chemistry): *Effective Coulomb and multiplet interactions in correlated electron systems: Experimental determinations and importance of non uniform polarizability*
09:25 - 09:45	Discussion
09:45 - 10:10	Philipp Werner (ETH Zürich): *Dynamical screening in correlated electron materials*
10:10 - 10:30	Discussion
10:30 - 11:00	**Coffee Break**
11:00 - 11:15	Michele Casula (UPMC Paris): *Satellites and large doping- and temperature dependence of electronic properties in hole-doped $BaFe_2As_2$*
11:15 - 11:25	Discussion
11:25 - 11:50	Giorgio Sangiovanni (Vienna University of Technology): *Dynamical Vertex Approximation for Nanoscopic Systems*
11:50 - 12:10	Discussion
12:15	**Lunch**
13:30	**Departure**

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