cecam Centre Européen de Calcul Atomique et Moléculaire	**Workshop Scientific Report** Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.
Title	What about U? -- Strong correlations from first principles
Dates	June 17, 2014 to June 20, 2014
Location	Lausanne (CECAM HQ)
Organizers	Silke Biermann (Ecole Polytechique, France) Matteo Cococcioni (Swiss Federal Institute of Technology, Switzerland) Stefano de Gironcoli (International School for Advanced Studies, Italy) Patrick Rinke (Fritz Haber Institute, Germany)

Scope of the workshop (maximum 200 words)
Describe the scientific area covered by your workshop (please avoid the use of acronyms where possible)

Correlated materials, such as complex oxides, offer a rich variety of physical phenomena (e.g. high temperature superconductivity, metal-insulator transitions, and phenomena resulting from a complex entanglement of spin-, charge, orbital- and structural degrees of freedom) that continue to challenge our current understanding of many-body quantum systems. Current and future applications are plentiful, ranging from oxide electronics, fuel cells, battery materials, homogeneous and heterogeneous catalysts, high Tc superconductors, spintronics devices to colossal magneto-resistant materials.
The scope of the workshop was to create the occasion and the conditions for developing synergies between scientists working on the development of various methods to improve the treatment of strong electronic correlations in first-principles approaches. We realized this objective by identifying several aspects and manifestations of electronic correlations and focused the presentations and discussions at the workshop on the computational approaches that can treat these aspects. We achieved a comparative overview by bringing together scientists active in density functional theory, wave-function-based (quantum chemistry) and many-body theories (including both, perturbative and non-perturbative techniques). By encouraging the cross-fertilization of these fields we hope to inspire new ideas and to stimulate the conception of more general, flexible and versatile computational tools able to make strongly correlated electrons tractable at reasonable computational cost.

Main **outcomes**

What important questions did you plan to ask and answer during the workshop? Please use a short bullet for each question.

Following the workshop, what do you think the four most important scientific advances are required in your area over the next 3-4 years? List in order of importance.

What levels of computing power will be required to solve these problems? Score each problem: 1) desk top computing, 2) departmental machines, 3) national supercomputers, 4) Current European Supercomputers (PRACE resources) 5) Leading edge peta-flop or exa-flop machines.

The following issues have been discussed in detail at the workshop:

1) In many insulators, spectroscopic data can be captured with broken-symmetry solutions, provided a Hubbard-like or exact-exchange correction is added to the DFT energy functional (and the Hubbard interactions are computed properly, see below). However, the energy scales of the associated ordering being often quite inferior to the value of the gap, methods that do not have to rely on symmetry breaking to open
the gap appear conceptually more convincing. Indeed, the problem can be traced back to the incapacity of static mean field approximations to describe fluctuating local moments. These deficiencies are cured e.g. by techniques explicitly averaging over different configurations ("Disordered local moment"-type approaches) or truly dynamical descriptions such as dynamical mean field theory and its extensions.

2) Studies on model Hamiltonians show that the improvement of approximate DFT exchange-correlation functionals probably requires and explicit dependence on the two-body density and not just the density itself. Electronic correlations can result in very minor changes in the electronic charge density (e.g., in the bond regions), which are difficult to control through functionals of the density only.

3) The exchange-correlation functionals of DFT need to be improved to capture important features of correlated systems (as, for example, the development of barriers and steps in the interstitial regions, or electron localization at large interatomic distances).

4) Quantum chemistry (QC) can provide very useful guidelines to improve density functionals for strongly correlated ground states. At the current stage, integrated DFT-QC approaches, using wave-function based methods locally, on selected (localized) manifolds, or specific parts of the (range separated) interactions provide significant improvements in the description of electronic correlations with respect to
conventional local or semilocal DFT functionals. A more complete theoretical incorporation of QC into DFT is yet to be developed.

5) QC computational approaches (e.g., coupled-cluster theory) that are well suited to capture dynamical correlations can be extended to effectively describe strong (static) correlations through the selection of low-seniority wave functions. The mean-field (N3) cost of this approach holds promises for its extension to larger systems and approximate DFT functionals.

6) Quantum Monte Carlo (QMC) can be used to effectively solve both QC problems and model Hamiltonians. For realistic systems, full configuration interaction QMC has the potential to become a long sought benchmark method for solids (even though these
techniques remain still all too often prohibitively heavy).

7) Corrections to approximate DFT functionals explicitly designed to impose a linear dependence of the total energy on the number of particles or on the occupation of selected states can effectively improve the description of electronic correlations. While the use of Hubbard-based corrective Hamiltonians or scissor operators is well established for this purpose, new approaches based on rewriting the correlation energy in terms of selected density matrix fluctuations are promising.

8) Realistic dynamical mean field (DMFT) methods have taken a strong leap forward recently, with (a) the development of techniques calculating effective Hubbard and Hund's interactions from first principles (within the constrained random phase approximation and related methods), and (b) the possibility of directly addressing dynamical screening effects within the DMFT calculations. Combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") has by now become a well-established (even though still heavy) tool, addressing e.g. corrections to ligand states or incorporating non-local charge fluctuations.

9) While Green's function calculations in the GW approach are applied to an ever increasing number of correlated systems, the description of Mott insulating states requires symmetry breaking to yield spectra in accordance with experiment.

10) The Bethe-Salpeter approach for the 2 particle Green's function captures electron-hole pairs, i.e. the correlated motion of electrons and holes, in a variety of systems and at various length scales. Most important advances needed in the field in the next years:

1) Stronger links between quantum chemistry and solid-state physics. In both fields, the challenge is to treat systems with degenerate states and in both fields the proposed solutions and the favorite techniques differ. Here, even stronger synergies could be expected in the future.

2) To improve the theoretical integration of QC approaches and DFT functionals; design of density functionals able to reproduce selected aspect of the many-body wave function of correlated systems. Preliminarily: clear identification of specific features of the ground state wave function of different types of systems (e.g., metals, band and Mott insulators).

3) Refinement of methods to compute the strength of effective electronic interaction parameters to be used in corrective approaches (e.g., DFT+U and DFT+DMFT).

4) Definition of more precise and reliable energy functionals for correlated systems allowing for the accurate comparison between total energies and for the efficient calculation of energy derivatives.

5) Integration of corrected functionals into methods to compute excitations from the ground state (e.g., GW) in order to capture the effects of strong correlation and improve the comparison with experiments.

Most of the advancements in the field outlined above require significant theoretical work whose implementation and testing can mostly be completed on departmental machines and national computational resources.

Assuming sufficient administrative support to be in place, has the workshop identified research areas that might be funded by the EU 2020 programme? Please list any EU or other collaborative opportunities emerging as bullet points. (maximum 200 words)

Strongly correlated systems are ubiquitous and technologically important, while methodologically still very challenging. Funding opportunities should therefore address two aspects: 1) fundamental research on methodology and computational algorithms and 2) specific materials applications.

In addition to the pure scientific importance of the areas discussed in your workshop, do you believe that progress in this field would be of interest to European Industry? Can you name any companies and contacts, which should be kept informed? (maximum 200 words)

Strongly correlated materials are at the core of ever increasing applications of great technological relevance, ranging from solar cells to magnetic information storage devices, from Li-ion battery materials, to thermo-electrics and multiferroics, to name just a few. The development of better computational techniques able to model and predict their behavior is thus of high potential interest for industries focused on such applications. The interactions between European research groups dedicated to the atomistic modeling of materials properties (as regrouped within the PsiK-network that cofinanced our workshop) and industrial partners have been documented in two recent reports that clearly establish the economic benefits of materials modelling using DFT methods and beyond, as dealt with in our workshop. The references to the reports are given below.
http://www.psi-k.org/reports/Economic_impact_of_modelling.pdf
http://www.psi-k.org/reports/PsiK_industry_interactions_report.pdf