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	Challenges and solutions for GW calculations in complex systems
Organizers	F. Giustino, A. Rubio, P. Umari

Scope of the workshop (one-two paragraphs)

The Workshop "Challenges and solutions in GW calculations for complex systems" was meant to be an opportunity to (1) bring all the major players in the GW method up to date in the most recent developments in the field, (2) review the available software implementations, (3) define standardization criteria to render the comparison between GW calculations from different codes meaningful, and (4) identify future major challenges in the area of quasiparticle calculations.

Main **outcomes** of key presentations (one page)

We had two talks describing quasiparticle calculations of defect energies in semiconductors and oxides (Louie, Bruneval). We had four talks on the use of GW calculations for metal/molecule contacts and for quantum transport calculations: Hybertsen (reporting also on new static approximations to the self-energy), Neaton (interfacial energy-level alignment and effect of off-diagonal matrix elements of the self-energy), Ferretti (off-diagonal corrections to the GW self-energy in quantum transport), Thygesen (fully self-consistent GW calculations for metal/molecule interfaces on localized Wannier basis). Three talks focused on the use of self-consistent GW: Van Schilfegaarde (review of the formalism and application to magnetic systems), Rinke (all-electron self-consistent GW), Thygesen (GW calculations for quantum transport). Two talks focussed specifically on the use of GW techniques for correlated electron system (Miyake, Gatti), and three talks reported on total energy calculations based on the GW method (Godby, Rinke, Ismail-Beigi). We had five talks on GW calculations without empty states (Louie, Galli, Huebener, Umari, Berger). These talks stimulated an intense discussion as described in the following section. All-electron GW calculations were reported by Ambrosch-Draxl, who performed a very systematic comparison between all-electron and pseudopotential calculations. We also had reports on the use of Coulomb truncation techniques (Martin-Samos), the use of GW for spin-dependent transport (Bluegel), X-ray spectroscopy (Rehr), the accuracy limit of GW calculations set by zero-point vibrations of the lattice (Marini), an update on the recent controversy about the electronic structure of ZnO (Rignanese), self-consistent solutions of the Dyson and Kadanoff-Baym equations (Stan), and applications to graphitic systems (Lebegue).

Report on selected discussions (one page)

eg. Were there interesting hints for new research? for new developments? for collaborations?

There has been an ongoing discussion throughout the workshop about the need of removing unoccupied states from the calculations of the screened Coulomb interaction. Several speakers proposed interesting strategies: approximations of the Kohn-Sham states at high energy using symmetrized planewaves and diffuse orbitals (Louie), use of an effective energy technique (Berger), use of a small number of dielectric eigenvalues obtained by iterative diagonalization (Galli), the use of the self-consistent Sternheimer method (Huebener), and the use of the Lanczos recursion method (Umari). There is a consensus on the need of eliminating empty states in order to bring GW calculations on systems with hundreds of atoms. Another interesting discussion took place around the accuracy of localized basis sets for calculating the GW self-energy. Several speakers reported on the use of localized basis sets (Rinke, Thygesen, Umari, Bluegel, Huebener), although no systematic tests on the convergence with basis sets were reported. An important point of the workshop has been to try and establish the accuracy of GW quasiparticle calculations. On the optimistic end we heard of accuracies around 0.2-0.3 eV (most speakers), but for instance in the case of ZnO the results appear rather sensitive to the convergence with empty states and to the method used for carrying out frequency integrations (Rignanese). Also it was pointed out that claiming an accuracy below 0.2-0.3 eV may not be meaningful if we consider that lattice vibrations may lead to zero-point effects which may go up to 0.6 eV (Marini, Giustino).

To what extent were the **objectives** of the workshop achieved (strong points, weak points)? (one paragraph at least)

This workshop has been extremely successful insofar all the main groups active in the area of GW calculations (both development and application) were represented, and also the discussions were lively and motivating. The workshop highlighted a recent trend across all groups to make a substantial effort in order to render their software and calculations reproducible. As anticipated in the workshop proposal, there is a growing need to standardize the technical details of GW calculations and the corresponding software implementations. It is likely that this workshop will lead to define quality control strategies in the near future, and in this sense maybe a follow-up workshop in 2013 focussing entirely on validation and standardization would be in order. We point out that our unusual workshop format, comprising of 25 min talks followed by 20 min discussions, proved very successful. Indeed all participants appreciated the opportunity for in-depth discussions following each talk, and the workshop resembled more of an intense round-table discussion than a showcase for the results of individual groups.
In addition, this workshop has been so successful that the Editors of the European Physical Journal B have offered us the opportunity to edit a Special Issue of their journal reporting on the key advances in the area of GW calculations as presented within this workshop.

Do you have suggestions for new workshops/tutorials/conferences on the topic?

We have just submitted a proposal for a Tutorial on "GW quasiparticle calculations in condensed matter physics and nanoscience" (organizers: Marini, Umari, Giustino, Rubio). We will explore the possibility of a follow-up workshop in 2013 with a more focussed discussion on validation and standardization.