CECAM Workshop Scientific Report

Workshop: Perspectives of many- particle methods: total energy, spectroscopy and time-dependent dynamics

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I. Summary

The field of computational chemistry, physics and material science made recently tremendous steps toward a first-principle description of excited state and correlated electronic systems including solids, nanostructures and macromolecular resp. bio-molecular systems. The impact of the applications strongly depends on the underlying methods and the achieved accuracy by accurately treating non-local interactions, electron correlations and time-dependent processes in electronic ground and excited states. This not only concerns accurate total energies and forces but also a quantitative description of spectroscopic signals and related time-dependent electron and coupled electron-ion dynamics. Despite considerable progress in the field various challenges remain to be solved in the future, addressing

- Many-body interactions – new XC functionals
- Perturbation treatment of quasi-particles beyond DFT
- Strong electron correlations, dynamical mean field theory and beyond
- Time-dependent DFT beyond the adiabatic approximation, two particle excitations

Of prime importance is the development of next-generation realistic many-body computational tools which are fast, reliable and are able to describe non-trivial quantum dynamics of complex systems. In order to address these problems, new integrated software tools for realistic quantum simulations of correlated systems need to be developed for a broad scientific community [1]. One possible direction to open new fields of applications is the combination of approaches developed in different communities, which shall be fostered at this workshop.

The program consisted of 30 invited talks of 40 minutes (35+5) each and one poster session presenting 29 posters. In addition, many social events (reception and conference dinner) to allow for informal exchange were held. The invited talks were given by well-established scientists from the different theoretical communities, which acted as platform for interesting cross-/interdisciplinary discussions. The invited talks were followed by a poster session where the younger participants could show their scientific work and exchange of ideas with a broad knowledge in computational chemistry, solid state physics and computational materials science. The organization was very compact with the scientists accommodated in the same hotel fostering exchange and discussion between the participants also outside the meeting room.

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II. Scientific content, main outcome of key presentations, selected discussions

The workshop succeeded in the following objectives: This workshop brought together people from different correlated electron communities, solid state physics, computational material science and quantum chemistry to discuss a possible synergies and new ideas in quantum many-body methods.

The workshop became a forum to brainstorm ideas about solutions to important correlated-electron problems and identify new directions for many-body method development and challenging applications. The presentations have shown, there is already active ongoing exchange between many-body solid state theoretical physics and wave function based correlated quantum chemistry. Developers of different methods and codes are initiating design of a new generation software tools for many-body quantum modelling of realistic complex systems. The delivery of this technology to a broad community will facilitate future breakthroughs on high-impact materials science problems in magnetic nano-science, transitions-metal biophysics and new energy storage, unconventional high-temperature superconductivity, functional material design.

Computational materials sciences are outstanding growth areas of research. In the future an increasingly larger part of our technological development will depend on computer applications, in particular in materials, nano and bio-nano sciences. Ab-initio calculations based on the density functional theory, wave function based quantum chemistry in combination with dynamical mean-field theory and various quantum embedding schemes can make a considerable progress in the field of nanostructures with d- and f-elements which usually means strong electron correlations. Moreover, wave function-based schemes offering the systematic pathway for approximating the electronic Schrödinger equation will become more and more efficient, so that also highly complex systems will be and are already accessible today. Prospects of method unifications to approach challenging problems such as electron correlations in complex systems, non-local interactions and dynamical correlations, dynamics and non-equilibrium phenomena have been discussed throughout the workshop.

III. Assessment of the results and impact on future direction of the field

The key challenge in constructing highly accurate theoretical descriptions of the most difficult systems in physics, chemistry, biology and materials science is the seamless bridging of different length and time scales. Generally, accurate theories for specific time and length scales exist, but these theories break down in the aforementioned systems because it is no longer possible to treat the different time and length scales independently. For example, highly accurate theories for the electronic structure of small molecules have been developed by chemists, while the solid-state physics community has developed successful descriptions of extended systems. However, the description of localized defects in solids or adsorbed molecules on surfaces or nanostructure requires a joint description of extended and localized aspects.

To overcome this challenge, it is necessary that a dialogue and exchange of ideas between researchers from different communities is established. While such an exchange has been achieved in this conference, the conference has also brought to light that progress in one area of science often remains unknown in closely related areas. To overcome this obstacle, we recommend that further, possible regular interdisciplinary exchanges in the form workshops and conferences are organized.

As described in the previous section, we believe that the scientific exchange of researchers from different disciplines is key to make progress in the most challenging problems of theoretical materials modelling. This exchange can be achieved by interdisciplinary conferences and workshops. Moreover, it would be desirable to enable exchange not only at the level of researchers, but also at the level of PhD and Masters students.

The field of theoretical materials modelling relies strongly on the availability of state-of-the-art computer code and computing resources. Therefore, the continued funding for the development of modelling software is an important infrastructure requirement: Only when codes are freely available, can new ideas be tested and developed by a broad community of researchers.

Since new codes that address the most challenging materials systems will push the limits of current supercomputing resources, it is also commendable that funding of these resources remains significant.

IV. Relevance of the field for EU Horizon 2020 and for Industry

Exchange of ideas should in our view to be substantiated by interdisciplinary training programs. Promoting for instance wave function based quantum chemistry expansions to extended correlated systems based on techniques like dynamical mean field theory requires researchers to have solid understanding in both fields. The same holds for combinations of time-dependent density functional theory and non-equilibrium Green function techniques to tackle photo-excited systems. We believe that a coordinated research training groups or research units supporting PhD students and young researchers doing their work in method developments and offering the necessary broad postgraduate education will be very helpful in this context.

Progress in the field of many body physics and wave function based correlated quantum chemistry is fundamental to many European industries connected to high-tech materials design and device applications. Examples are

- Advanced hybrid photovoltaics
- Photo-catalytic processes in energy storage and pollutant degradation
- Hybrid nano/bio-systems for medical applications
- Single-defect-based quantum optical and spintronic devices

Such directions can be strengthened by focused research projects for the development of new materials and devices in key enabling technologies. The field of nanodevices is currently opening to new materials, especially 2D. The EU flagship on graphene and 2D materials is indeed expected with the aid of computational predictions to produce several new outcomes. However, technological innovation is not limited to these novel materials.

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The Organizers