## EMERGING RESEARCH FRONTS - 2008

### October 2008

**Giovanni Onida, Lucia Reining & Angel Rubio talk with *ScienceWatch.com* and answer a few questions about this month's Emerging Research Front Paper in the field of Physics. The authors have also sent along images of their work.**

**Article: Electronic excitations: density-functional versus many-body Green's-function approaches**
Authors: Onida, G;Reining, L;Rubio, A
Journal: REV MOD PHYS, 74 (2): 601-659 APR 2002
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**SW: Why do you think your paper is highly cited?**

This paper is focused on the description of excited state properties, by further developing and uniting two different previously existing theoretical approaches. Namely, we have established the bridge between Many-Body Perturbation Theory (MBPT) and Time-Dependent Density Functional Theory (TDDFT) to calculate the excited states, and fostered several directions along the way leading to the routine performance of *ab initio* computation of electronic excitations in physics, chemistry, and biophysics, for academic or for industrial research purposes.

**SW: Does it describe a new discovery, methodology, or synthesis of knowledge?**

Definitely, it describes a synthesis of knowledge and a new methodology. It is not a common review compiling results and know-how: it provides new insight and developments in a coherent and complete framework. This is one of the important aspects behind the impact of the work, the novelty in methodology and understanding. In 59 pages, this review spanned the following subjects: after giving strong motivation toward theoretical developments, which are required by new experiments, we introduce the common ingredients to both Green's function theory (GFT) and TDDFT.

*Coauthor*
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The role of the dielectric function, as well as that of local fields is explained; then, 4-points and 2-points equations and kernels are introduced. Green's functions, and their connection to experiments, are briefly reviewed, prior to the introduction of Hedin's equations and the GW method. The latter is compared with Density Functional Theory (DFT), for the calculation of total energy differences. Density Functional Theory,

Then, we come to two-particle excited states and the electron-hole interaction, leading to the Bethe Salpeter Equation (BSE). After that, TDDFT is briefly reviewed, and extensively compared with the BSE scheme, also giving some example in the limit of non-overlapping orbitals.

Finally, applications to infinite and finite systems, a list of FAQ, and three appendices conclude the paper. The last appendix contains, in a nutshell, the idea that it should be possible to derive, from the BSE scheme, an exchange-correlation kernel to be used in TDDFT.

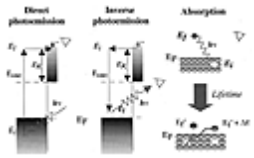
*Coauthor Angel Rubio*

**SW: Would you summarize the significance of your paper in layman's terms?**

The interaction between electromagnetic radiation and matter is of fundamental interest. It creates excitations in the materials leading to phenomena with enormous consequences in completely different domains such as technology, chemistry, materials science, climate science, renewable energies, biology, and medicine.

These consequences can be desired (like photosynthesis) or not (as in the case of radiation damage due to nuclear waste), but are, in most cases, quite complicated to describe and predict. This is not only true for the systems one encounters in "real life," but also holds for the materials that a scientist or engineer may investigate in an academic or industrial laboratory.

Figure 1:



+ View larger image & details.

More and more, spectroscopic techniques probing the electronic response are used in the investigation of rather complex systems, in order to get information about their electronic structure as well as their structural properties or their chemical composition. Defects, impurities, or surface reconstructions induce, in general, changes in the electronic states. These modifications give rise to new structures, modified energetic positions, or intensity changes in the electronic spectra. "Question matter, and the electrons will answer!" so one could say, but, for this, one should understand the electrons' language.

This explains why a large field of research in computational physics is related to the characterization of the electronic, structural, and bonding properties of many-electron systems: nanostructures, surfaces, and extended solids as well as their interactions.

Our *Review of Modern Physics* article has become a key document in the excited-state scientific community, and, with an increasing number of citations, an inspiration for much further research. Moreover, versatile numerical tools for treating electronic excitations, based on this approach, have then been developed in our community. These tools are made available to a wider scientific community through the European Theoretical Spectroscopy Facility (ETSF).

**SW: How did you become involved in this research and were any particular problems encountered along the way?**

We realized that the communities of physicists and chemists, working with two different methods—namely those using the Green's function approach and those based on the time-dependent DFT—would have benefited from a general formulation which could be applied to both.

One of the main problems was the lack of a common language. We found the best way to encompass it by organizing a series of workshops, and inviting people from both communities. Sharing formalism and establishing similarities and differences, has in fact, finally become the key to discovering new synergies from these two approaches.

**SW: Where do you see your research leading in the future?**

The long-term impact of our work is expressed in the concept of the ETSF, a platform offering to the scientific community, in both academia and industry, a remote access to user-friendly spectroscopy computer codes (and the associated expertise) for nanoscale systems and advanced materials.

ETSF has the ambition to become the world-wide reference point for the quantum description of excitations in complex systems on the nanometer scale. Groups that obviously benefit are large national and European infrastructures like synchrotrons, companies working in fields like materials design for opto-electronics, as well as smaller experimental and theoretical groups in the field of nano-, bio-, and materials-science.

**SW: Do you foresee any social or political implications for your research?**

Not in the immediate future, but a potential social impact could stem from applications of the ab initio methods for the prediction of electronic excitations to diverse fields such as nanomedicine, renewable energy (photovoltaic cells), and semiconductor nanostructured devices relevant for electronic appliances.

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**Figure 1:**

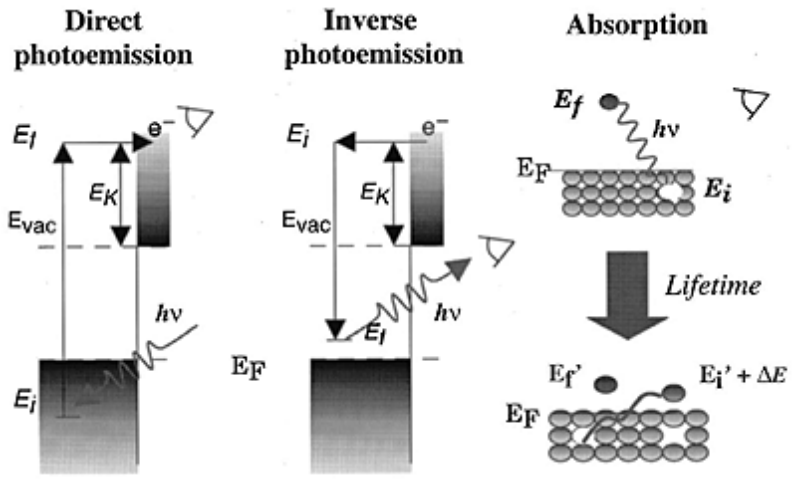


**Figure 1:**

Schematic representation of the excitations involved in spectroscopies such as direct photoemission, inverse photoemission, and absorption. Probing excitations allows one to gain insight on the structural and electronic properties of matter..

Keywords: many-body perturbation theory, time-dependent density functional theory, ab initio computation of electronic excitations, physics, chemistry, biophysics, green's function theory, bethe salpeter equation, electronic excitations, european theoretical spectroscopy facility, nanomedicine, renewable energy (photovoltaic cells), semiconductor nanostructured devices.

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