

	<h2 style="text-align: center;">Tutorial Scientific Report</h2>
	<p>Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.</p>
Title	<h3 style="text-align: center;">Theoretical Spectroscopy Lectures</h3>
Dates	<p style="text-align: center;">May 13-17, 2013</p>
Location	<p style="text-align: center;">CECAM-HQ-EPFL, Lausanne, Switzerland</p>
Organizers	<p>Valerio Olevano (CNRS Institut Néel, Grenoble, France) Francesco Sottile (Ecole Polytechnique, Palaiseau, France) Gian-Marco Rignanese (Université Catholique de Louvain, Belgium)</p>
<p>Aim(s) of the Tutorial (maximum 200 words)</p> <p>The aim of the school was to give an introduction, up to covering also advanced aspects, on the theories, the approximations, the methodology, and finally the numerical and practical approaches to the calculation of electronic excitations and spectra in condensed matter.</p> <p>Electronic excitations are probed by experimental spectroscopies, such as optical absorption, energy-loss (EELS) and photo-emission (direct or inverse) spectroscopy (PES, ARPES).</p> <p>From the theory point of view, excitations, excited state properties and related spectra, are unfortunately out of the reach of the successful density-functional theory (DFT). Indeed, DFT is a ground state theory only. However, in the last twenty years other ab-initio theories and frameworks emerged, able to describe electronic excitations and spectroscopy. Among them, time-dependent density-functional theory (TDDFT) and many-body perturbation theory (MBPT) (also known as Green's function theory) in the GW approximation and in the Bethe-Salpeter equation BSE approach, have become more and more used. Computational solutions and reliable codes have been developed in order to implement these theories and to provide tools to calculate excited state properties. The present school focused on these points, covering theoretical, practical, and also numerical aspects of TDDFT and MBPT, as well as codes implementing them (ABINIT, DP, EXC).</p>	

Outcomes:

What were the most important learning objectives of the tutorial? Were these achieved? What could have been improved? (maximum 200 words)

The learning objectives of the tutorial were to provide to the students very few but basic, important crucial points of the taught theories, and rather pass to see immediately their practical implementation to assimilate them quickly and more deeply. By this way it was possible to stimulate them to go beyond by themselves, and take advantage of the time we left for discussions (and also the practical sessions afternoons) for asking questions on more advanced issues. We believe that once the fundamental pillars of the theories are well clear and in place thank to having manipulated them by the hands-on, they will be able once at home to go beyond by themselves and deepen the arguments they are interested in referring to the literature we indicated them.

Another learning objective was to underline very clearly what are in the analyzed theories the most common errors, wrong beliefs, unproper simplifications that could seriously affect their correct understanding of the theory and so, the correctness of the scientific results they are going to provide in future. We considered this last aspect a real service we were offering not only to the students, but to our whole scientific community that in this way can take full advantage of the work of the future new researchers.

The presentation of the theory and theoretical aspects of codes' implementations took place in the morning sessions, while the afternoon sessions were devoted to practical hands-on in the use of the codes to get realistic theoretical results on prototypical real condensed matter systems.

From the organizers' point of view the school has been a frank success. Thanks also to the cumulated experience of last editions, and to a good team-work among tutors, the lectures have been largely considered appropriate in length, complexity and clarity, by the students. The participation level has always been very high, and we have been glad to notice how, sometimes, the discussion time has been stretched much over the allocated time, in particular for the most sensible lectures (MBPT and TDDFT). Almost none of the students took the Wednesday afternoon free, preferring a discussion with the lecturers or continuing the hands-on in his/her own account. Incidentally none of the tutors used the upstairs room dedicated to them, in order to privilege a continuous availability to the students.

No major problems have been encountered in this school, while the organization and the connection with Marianne, Bogdan, Nathalie and Dominic (thanks for letting us feel most welcome) was flawless.

Report on the feedback from the “students” (one paragraph at least)

During the week all the lecturers received warm appreciations by the students. Of course, the CECAM got the official feedback reports from the students and can evaluate better this aspect. We can say also that the particular shape of the school, organized such that the theoretical morning part was immediately followed by the afternoon practical hands-on illustrating the theory, helped a lot the students to grasp more easily very difficult theoretical concepts, like in the case of many-body theory. In particular on many-body theory, there was consensus among the students about the crucial need of training on such theory and its implementations into codes. We had programmed a free afternoon. But we let the students decide whether to take this free afternoon or stay at the CECAM location for a further afternoon training: we were pleased to see that the large majority of them decided to stay to take advantage of a further hands-on tutorial, and further, with more freedom on the preferred topics to deepen, very often on the research lines they were carrying on at home and for which they considered this school a valuable resource. Unfortunately, we hadn't the possibility for a trip on the boat during that afternoon, but we had pleasant time altogether, tutors and students, during the evenings and at dinner that we had always together (like lunches also): this helped also a lot to very quickly "break the ice" and helped a lot the student to be less shy and even at the second day, they felt much more free to ask any question they had in mind, without caring too much.

Do you have suggestions for new related tutorials?

We think that the spirit of socialisation of our tutorial, which was in place since the first day, could be an important suggestion for all tutorials organized by the CECAM: it is extremely important to reduce very quickly the barrier between tutors and students, so that they can really profit at best and take full advantage of the one week close contact of somebody that can teach them what they will need in their future works.