SEMINAIRE ISMO

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Nonlinear optical spectroscopy
in finite and infinite systems

Nonlinear optics is an exciting field which has many applications in different areas like materials science and chemistry. Its beginning dates back to 1961 when second-harmonic generation (SHG) was observed for the first time by P. Franken *et al*. The nonlinear phenomena were treated in the perturbation regime which made possible to develop techniques for efficiently converting laser light from one wavelength to another. However, the situation completely changed when high-harmonic generation (HHG) was discovered by Mcpherson *et al.* in 1987. In fact, new non-perturbative understanding of nonlinear optics was necessary to explain the nature of HHG. Moreover, recently, the unique physics of HHG was used to produce the first attosecond pulse source which makes possible the real-time observation of atomic-scale electron dynamics.

In this seminar I will present my work on theoretical nonlinear optical spectroscopy on SHG in solids and HHG in atoms and molecules.

A theoretical approach which is based on Time-Dependent Density-Functional Theory (TDDFT) was developed for the calculation of second-order susceptibility. In this formalism it is possible to include straightforwardly many-body effects such as crystal local fields and excitons. I will show SHG spectra for different materials such as semiconductors and interfaces with a particular attention to strained silicon. Beyond the perturbative regime, I will show HHG spectra by directly solving the time-dependent Schrödinger equation, namely the Time-Dependent Configuration-Interaction (TDCI) putting in evidence the role of Rydberg bound-states and continuum levels in the field-induced electronic dynamics.

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