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Some Theoretical Challenges from X-ray Free-Electron Lasers

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X-ray Free-Electron Lasers (FEL's) have started operating a few years ago. The
salient features of these x-ray sources are the very short pulses, down to a few femtoseconds duration; the extremely high peak power, up to the ~ 100 GW range and beyond; the peak brilliance, exceeding that at the best synchrotron sources by many orders of magnitude. Experiments using these revolutionary sources open up new frontiers for x-ray physics, and a few examples shall be given to underline the most important aspects.

Both experimental observations and theoretical considerations show that interaction between FEL pulses and atomic, molecular and condensed matter takes place under conditions that are quite different from the usual. The intensity of the radiation field is in a regime where important non-linearities are expected and indeed observed. Phenomena familiar from laser physics at much longer wavelengths (multi-photon absorption processes, saturated absorption, sum-frequency generation, stimulated Raman scattering) are entering the x-ray domain. Modelling of these effects has been restricted to few-atoms systems or to semi-empirical methods. An ab-initio electronic structure description of these phenomena in the x-ray region for condensed matter systems is challenging; for example, the description of saturated absorption requires an accurate description of the probability of multiple excitation of core levels, of core level shifts, of radiation and Auger recombination rates.

At the same time, the very short duration of the pulses opens up the possibility to explore the dynamics of electronic and structural properties on an unprecedented time scale, well below the picosecond region. The challenges, but also the potential scientific payoff, for theoretical investigations of time-dependent properties are briefly described.

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