

# Real-time TDDFT simulations of laser-driven valence and core electron dynamics in solids

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## Abstract

Developments in ultrafast laser spectroscopies over the last two decades have led to a wide variety of experimental protocols for time-domain investigations of electron dynamics in materials. Laser pulses driving valence- and core-level excitations across both linear and nonlinear light-matter interaction regimes are increasingly utilized to probe and control electron dynamics on femtosecond to attosecond timescales [1]. In this context, nonperturbative theoretical methods are increasingly relevant to guiding experimental efforts and aiding the interpretation of complex time-resolved and/or nonlinear spectroscopies. In solid-state systems, the velocity-gauge formulation of real-time TDDFT (VG-RT-TDDFT)[2] has emerged as an efficient first-principles framework for describing laser-matter interactions and has been utilized within the past decade to model a number of strong-field phenomena [3], [4]. I will describe recent efforts to extend this versatile approach towards a unified description of valence and core electron dynamics in solids with a focus on ultrafast core-level spectroscopies in both the linear and nonlinear X-ray regimes[5], [6]. In particular, recent developments in TDDFT that enable accurate descriptions of important solid-state excitonic effects in the time-domain will be discussed.

## References:

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