

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Real-time TDDFT simulations of time-resolved core-level spectroscopies in solid state systems. SRI CHAITANYA DAS PEMMARAJU, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, THEORY OF NANOSTRUCTURED MATERIALS FACILITY TEAM — The advent of sub-femtosecond time-resolved core-level spectroscopies based on high harmonic generated XUV pulses has enabled the study of electron dynamics on characteristic femtosecond time-scales. Unambiguous interpretation of these powerful yet complex spectroscopies however requires the development of theoretical algorithms capable of modeling light-matter interaction across a wide energy range spanning both valence and core orbitals. In this context we present a recent implementation of the velocity-gauge formalism of real-time TDDFT [1] within a linear combination of atomic orbital (LCAO) framework, which facilitates efficient numerical treatment of localized semi-core orbitals. Dynamics and spectra obtained from LCAO based simulations are compared to those from a real-space grid implementation [1]. Potential applications are also illustrated by applying the method towards interpreting recent atto-second time-resolved IR-pump XUV-probe spectroscopies investigating sub-cycle excitation dynamics in bulk silicon [2].

[1] Yabana et al., Phys. Rev. B 85, 045134 (2012)

[2] Schultze et al., Science, 346, 1348 (2014)

SRI CHAITANYA DAS PEMMARAJU
Lawrence Berkeley National Laboratory

Date submitted: 05 Nov 2015

Electronic form version 1.4