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First-principles interpretation of attosecond time-resolved XUV absorption spectroscopy of laser excited Silicon SRI CHAITANYA DAS PEMMARAJU, Lawrence Berkeley Natl Lab, SHUNSUKE SATO, KAZUHIRO YABANA, University of Tsukuba, KRUPA RAMASESHA, University of California, Berkeley, MARTIN SCHULTZE, Ludwig-Maximilians-Universitat, STEPHEN R. LEONE, University of California, Berkeley, DAVID PRENDERGAST, Lawrence Berkeley Natl Lab — The availability of ultrafast x-ray pulses both from powerful free electron laser light-sources as well as table top high-harmonic generation, has significantly enhanced the utility of core-level spectroscopies as probes for investigating dynamical processes in functional materials. Theoretical approaches to complement these time-domain experiments are therefore actively being developed. In this study we employ a combination of real-time time-dependent density functional theory (TDDFT), occupancy-constrained density functional theory and many-body perturbation theory approaches to help interpret spectral signatures observed in attosecond time-resolved core-level spectroscopic measurements on laser-excited silicon. Using non-equilibrium electron-hole densities obtained from real-time TDDFT simulations of the valence electronic structure we estimate the transient modulation of L-edge absorption in femtosecond infrared pump - attosecond XUV probe experiments. We further estimate the contribution of electron-phonon and electron-electron scattering mechanisms to the lifetime broadening observed in measured L-edge spectra using occupation-constrained density functional theory and GW calculations respectively.

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