Abstract Submitted
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**A new time-dependent ab-initio close-coupling program for atomic ionization**[1] LUCA ARGENTI, Dept. Physics and CREOL, Univ of Central Florida, USA, TOR KJELLSSON LINDBLOM, Stockholm University, Sweden, COLEMAN CARIKER, Univ. Central Florida, USA, THOMAS CARETTE, EVA LINDROTH, Stockholm University, Sweden — We present a time-dependent program to compute the photoionization of polyelectronic atoms by arbitrary light pulses. The program merges the capabilities of the Stock B-spline close-coupling structure code [1] with those of the time-dependent two-active-electron code described in [2]. It builds a close-coupling space in which multi-reference parent ions [3] are augmented with a spherical B-spline basis up to an assigned radius R. The initial state is evolved under the influence of external light pulses by solving the time-dependent Schroedinger equation with a second-order split-exponential propagator. Reflection at the box boundary is prevented by channel-specific complex-absorbers. The channel- and energy-resolved photoelectron spectrum is computed by projecting the wavefunction on a complete set of scattering states, after the external pulses are over. The program predictions are benchmarked against test simulations in helium [2], and applied to selected attosecond pump-probe simulations for the argon atom. [1] T Carette et al., Phys. Rev. A 87, 023420 (2013). [2] L Argenti and E Lindroth, Phys. Rev. Lett. 105, 053002 (2010). [3] C Froese-Fischer et al., Comp. Phys. Commun. 176, 559 (2007). [4] mcs.anl.gov/petsc.

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