Analysis of multi-orbital contributions in HHG spectra through multiple single active electron simulations\(^1\) RAN REIFF, TENNESSE JOYCE, AGNIESZKA JARON-BECKER, ANDREAS BECKER, JILA and Department of Physics, University of Colorado, Boulder — In multielectron atoms, full ab-initio simulation of high harmonic generation (HHG) spectra is not computationally feasible. The single active electron (SAE) approximation considers the dynamics of one electron in a frozen potential from the remaining electrons. Comparisons with multielectron methods (TDDFT, MCTDHF) have shown that SAE simulations (for an electron in the outer valence shell) often accurately reproduce HHG spectra up to the active electron’s cut-off \((I_p + 3.17U_p)\) but fail to reproduce a second or extended plateau attributed to inner-shell electrons. We present inner-shell SAE potentials and simulations which, in conjunction with valence SAE results, display the expected plateau behavior without dynamic multielectron interactions.

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Ran Reiff
JILA and Department of Physics, University of Colorado, Boulder

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