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Soft X-ray ionisation of atoms within TDDFT and nuclear effects on the attosecond TRPES of ethylene

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First, I will demonstrate the capabilities of time-dependent density functional theory (TDDFT) for strong-field, short wavelength (soft X-ray) physics, as compared to a formalism based on rate equations. TDDFT provides a very good description of the total and individual ionization yields for Ne and Ar atoms exposed to strong laser pulses over a wide range of intensities.
Second, using TDDFT we examine the energy, angular and time-resolved photoelectron spectra (TRPES) of ethylene in a pump-probe setup. Studying the photoemission spectra provides us direct access to the dynamic evolution of the molecule's electronic levels. Further, by including the nuclei's motion, we provide direct chemical insight into the chemical reactivity of ethylene.

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