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Real-time TDDFT for non-linear pump-probe processes

I will present fundamental insights on pure electron dynamics captured by pump–probe attosecond transient spectroscopic techniques, within the realms of real–time time-dependent density functional theory [1-4]. The method incorporates both scalar and spin-orbit relativistic effects variationally using modern atomic mean-field eXact two-component (amfX2C) Hamiltonian [4], necessary for X-ray region processes. I will address how this technique records the signature of the transient dynamics triggered by the pump pulse imprinted onto the molecular response to probe pulse, including effects of additional degrees of freedom (pump pulse features and pump–probe time delay) absent in conventional spectroscopy. Furthermore, unique spectroscopic signals triggered by a chiral laser pulse interacting with an achiral molecule will be highlighted [5].
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