# ABSTRACT

## X-ray time resolved spectroscopy of molecules driven by strong IR fields

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A main aim of our work is to understand what kind of experiments can be performed in material and fundamental sciences with the high brilliance, short and coherent X-ray pulses generated by X-ray free-electron laser sources and harmonic generation X-ray lasers. As one example, we overview some basic physics underlying IR-X-ray pump-probe spectroscopy. Particular features of the spectroscopy are highlighted, such as the dependence on phase of the IR pulse, duration and delay time of the X-ray pulse, and molecular orientation. The quantum control of the nuclear wave packet in the ground state and probe of the nuclear motion by femtosecond UV and X-ray pulses gives unique opportunities to study different dynamical processes: For example, the results of our modeling indicate that X-ray pump-probe spectroscopy is a proper tool to study the dynamics of proton transfer in different systems. We observe that the trajectory of the nuclear wave packet, as well as the trajectory of the X-ray spectra, are strongly affected by the absolute phase of the IR pulse. We demonstrate an anomalous enhancement of the electronic recoil effect by strong IR radiation. We discuss different aspects of X-ray pump-spectroscopy for overlapping and time delayed pump and probe pulses. Finally, we outline new modeling tools for coherent multi-X-ray absorption and discuss their possible applications.

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References:

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