

高次高調波によるアト秒 X 線パルスの増幅

Amplification of X-ray attosecond pulses

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研究成果概要

In 2025, our work focused on high-harmonic generation (HHG) simulations aimed at increasing the yield in the 200–250 eV region (water window, ~ 6 nm), motivated by ongoing experimental development at QST (Nara). The central goal was to identify realistic parameter windows for short-wavelength HH emission in ion-based and plasma-assisted schemes, with a particular emphasis on phase matching. We performed systematic 3D propagation simulations (3D SFA propagation model) for Li-based media (Li⁺ and plasma-assisted cases), scanning pressure, propagation length, pulse energy (intensity), and especially free-electron density as a key phase-matching control parameter. A main outcome is that the appearance of an enhancement near ~ 200 eV is governed primarily by propagation and phase matching and is highly sensitive to the free-electron density. Intermediate electron densities can produce a pronounced enhancement around 200 eV, while too low electron density leads to propagation that destroys the high-energy signal and too high electron density introduces strong phase mismatch that suppresses the targeted spectral region. During 2025 we also improved the reliability of the modelling by identifying numerical instabilities that had previously overestimated the influence of an initial plasma contribution. After diagnosing the issue, we reran higher-accuracy (and significantly more expensive) simulations to produce robust spectra suitable for experimental decision-making. A further result in 2025 was the evaluation of neutral dispersion from Li⁺ ions. Using an ab initio estimate of the static polarizability of Li⁺ (Hartree–Fock), we found that, for the parameter ranges explored, neutral dispersion remains negligible compared with plasma dispersion, confirming that free-electron control is the dominant factor for phase matching in our current scenario. Finally, we completed a comparative simulation study of 800 nm versus 400 nm (second-harmonic) pumping. The calculations indicate that 400 nm pumping can provide about two orders of magnitude higher HH signal than 800 nm under comparable conditions, with the optimum pressure shifting to the few-mbar range and with reduced saturation within accessible pulse energies. This result directly influenced planning discussions, with collaborators proposing 400 nm pumping as the main direction for the next fiscal year experiment, targeting phase matching around ~ 250 eV.

Because single high-fidelity propagation runs can require on the order of weeks of wall-clock time, a comprehensive optimization (electron density, pressure, propagation length, and intensity) is only feasible with continued access to large-scale HPC resources. We therefore request supercomputer allocation in 2026 to complete the systematic optimization of the 400 nm-driven scheme and to deliver quantitative predictions of the optimal experimental parameters for robust short-wavelength HH generation.