Theoretical Simulation of Subcycle Reciprocal-Space Images of Electron Density Driven by a Strong Laser Field

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We have investigated the response of insulators to strong light fields using time-dependent density functional theory (TDDFT) [1]. When the field strength becomes comparable to the intrinsic electric field within the material, the system exhibits extremely nonlinear responses that cannot be described by perturbative expansions. To accurately capture these dynamics, it is necessary to solve the time-dependent Kohn-Sham equation directly in real time. The SALMON-TDDFT code [2] provides a platform for solving the Kohn-Sham equation for crystalline solids, molecules, and atoms. In this study, we performed simulations using system B at SCC-ISSP.

We conducted TDDFT simulations to obtain subcycle reciprocal-space images of the electron density in monolayer hexagonal boron nitride (hBN) and graphene under an intense electric field. The corresponding real-space electron densities were derived via spatial Fourier transforms. The applied electric field was linearly polarized, with a full width at half maximum (FWHM) duration of 14 fs, a photon energy of 0.4 eV, and a peak intensity of 1 TW/cm².

Under the influence of the peak electric field, the electron distribution becomes significantly distorted. In monolayer hBN, the low-frequency components of the reciprocal-space electron density exhibit oscillations that vary nearly linearly with the applied field strength. Our simulations suggest that these dynamics correspond to electron hopping between two distinct B–N bonds in response to the field. In contrast, graphene does not show such linear field-dependent oscillations.

References

[1] Erich Runge and E. K. U. Gross, Phys. Rev. Lett. 52, 997 (1984).

[2] https://salmon-tddft.jp/, M. Noda, S.A. Sato, et al., Computer Physics Communications. 235, 356 (2019).