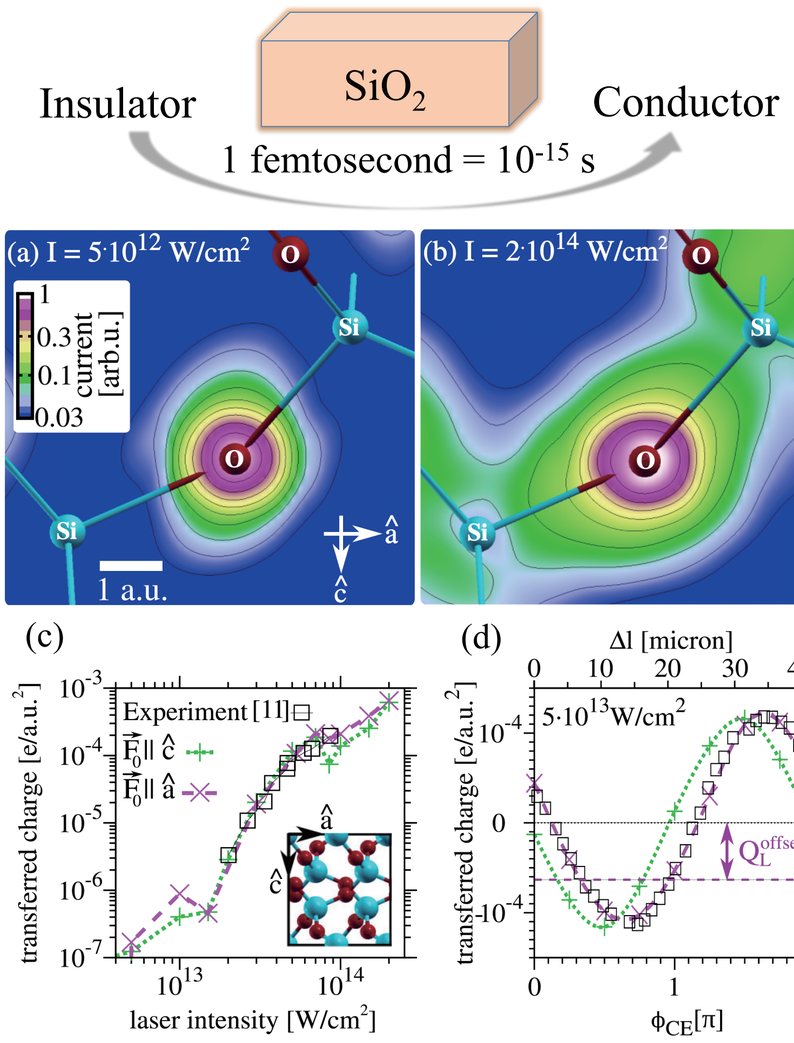
Quantum Condensed Matter Physics

Time-Dependent Density Functional Theory for Ultrafast Dynamics Induced by Laser Pulses

Time-dependent density functional theory (TDDFT) is widely used to describe electron dynamics in atoms, molecules, and solids induced by light fields. We have been developing a real-time and real-space computational code to solve the time-dependent Kohn-Sham equation in crystalline solid, the basic equation in TDDFT. The code is efficiently parallelized in k-points and orbitals in the time evolution calculations. The code may be used to calculate dielectric function, ultrafast electron-phonon dynamics of femto- and attosecond time scales induced by intense ultrashort laser pulses, and coupled dynamics of electrons and electromagnetic fields in the multiscale implementation of the code.

A recent experiment showed that SiO2, an insulator, can behave like metal when it is illuminated by an intense laser within femtoseconds, which is million times fast than a GHz CPU cycle, as shown in the upper-panel of the right figure. We have applied the real-time TDDFT method to investigate the mechanisms of the intense-ultrafast-laser material interaction and found that the electric current is formed around the Oxygen site [Fig. (a)] for a weak field and then spreads to the bulk along the O-Si bound direction [Fig. (b)] for a strong field. The simulated charge transfer per laser pulse [Fig. (c)] and the detail carrier-envelop phase dependence [Fig. (d)] are in good agreements with the measurements. Our studies may help to produce an ultrafast optical switcher on a femtosecond time scale.

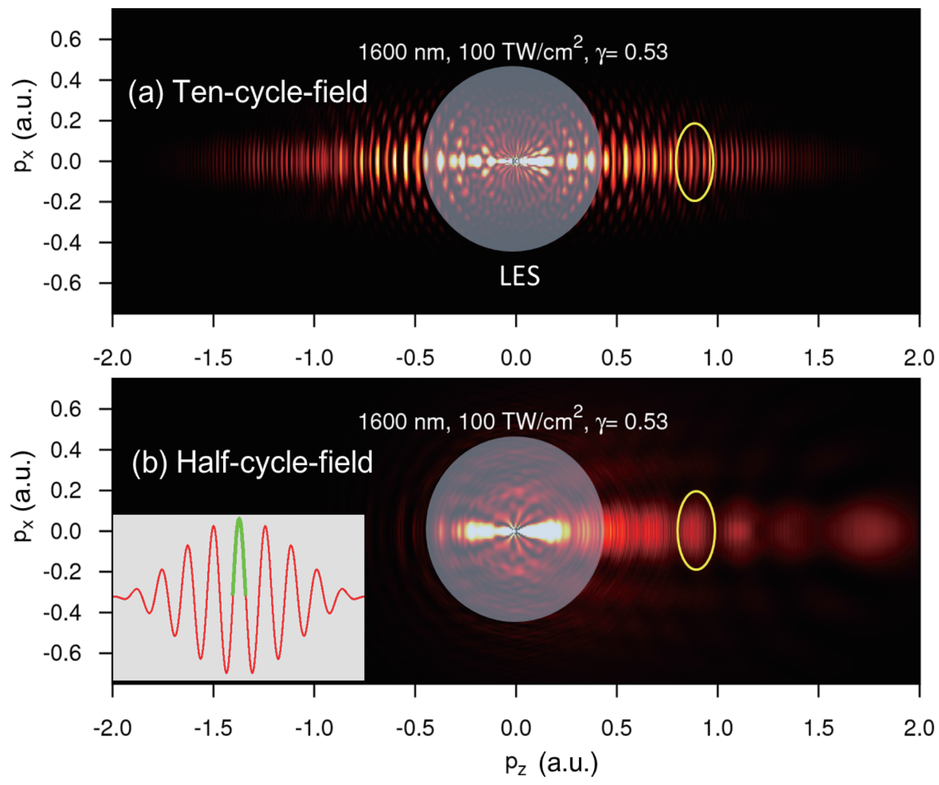


Physical Review Letters **113** (2014) 087401.

Time-Dependent Schrödinger Equation for Atomic Ionization in Intense Laser Fields

We have been developing an effective method to solve the time-dependent Schrödinger equation (TDSE) by using a generalized pseudospectral method in the energy representation. Instead of solving the differential TDSE, we solve the integral TDSE, which allows us not only to simulate the observable quantity, but also to analyze the detailed dynamics by switching on and off certain interactions at a given time. Recently we have refactored the code to our GPU cluster (HA-PACS) and speeded up the simulation greatly.

Rescattering process, as illustrated in the upper-panel of the right figure, is a key step to understand and control the dynamics of atoms in intense laser fields. The process can be used to generate atto-second (10-18 s) pulses or image the molecular structure, and push the femto-chemistry into atto-chemistry. Unfortunately, such a process cannot be observed directly from experiments. By comparing the simulated electron momentum spectra from a full laser pulse [Fig. (a)] and from a half cycle field of the pulse [Fig. (b)], we clearly identified that the multiple scattering is responsible for the low energy structure (LES) of the photoelectron in a middle infrared laser field. Comparing our simulation with measurements, we may obtain the molecular structure and electron wave function information.



Physical Review A **88** (2013) 013410.