Understand and control of quantum dynamics by pulsed lasers in an ultra-short time scale

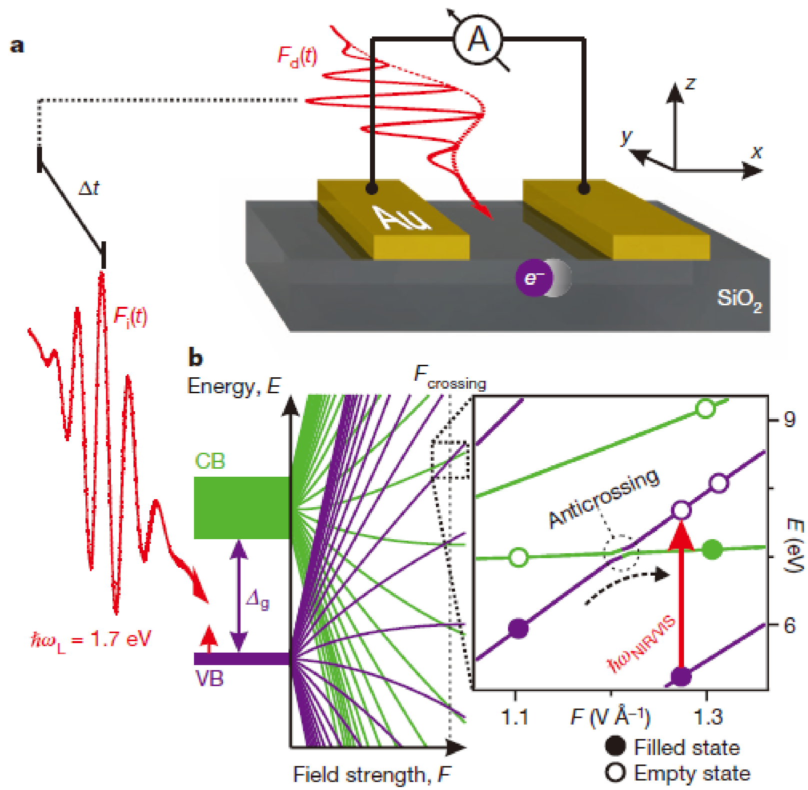
Xiao-Min Tong

Division of Quantum Condensed Matter Physics

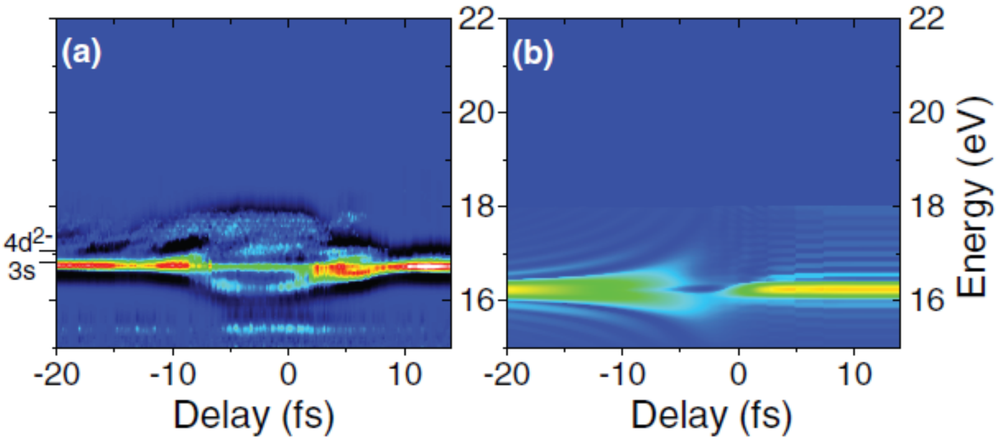
Outline:

- What we are working on laser-material interactions
  - ***Understand*** the mechanism and ***Control*** material properties
  - ***Built*** a tool to “see” what happens in a quantum system
- Computational Methods
  - Working Equations: Time-dependent Schrodinger equation (PDE)
  - Main structure of the simulation code: how to use GPU effectively
- Examples
  - Mechanism of atomic ionization in mid-infrared laser field
  - Control transparency of a material in attosecond domain
- What we expect from HPC
  - Good support: minimize the work on refactoring the code
  - Easy control on the numerical precision

Our Research Goals: Control



HA-PACS



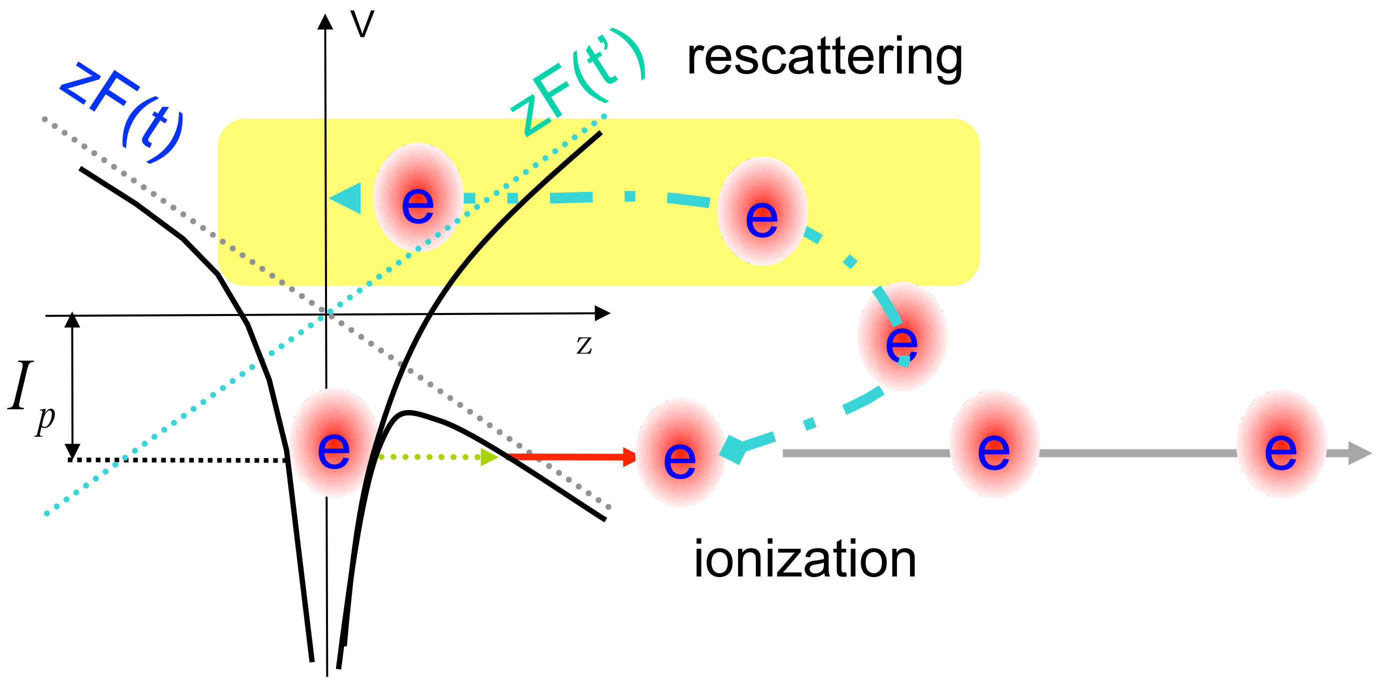
PRA **87** (2013) 063413.

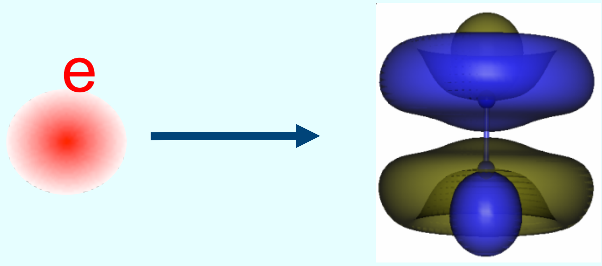
Insulator ➔ conductor (1 fs)

A. Schiffrin, *et. al.,* Nature **493** (2013) 70

1fs: 1,000,000 GHz

Our Research Goals: Mechanism



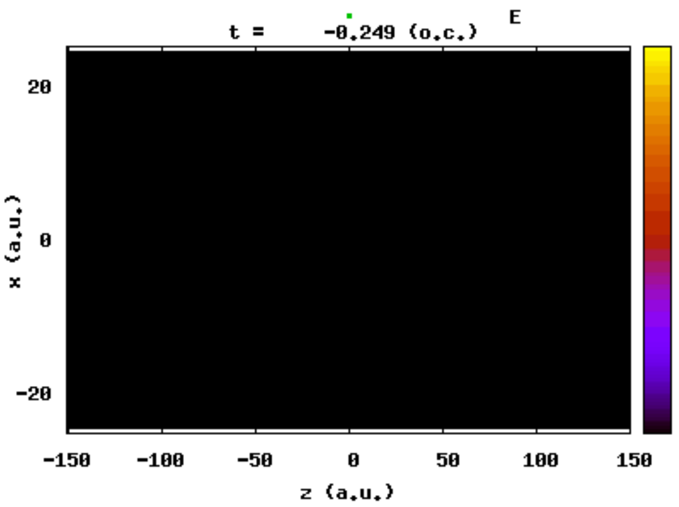


(a) HHG X-ray laser (Water window)

(b) Electron microscope

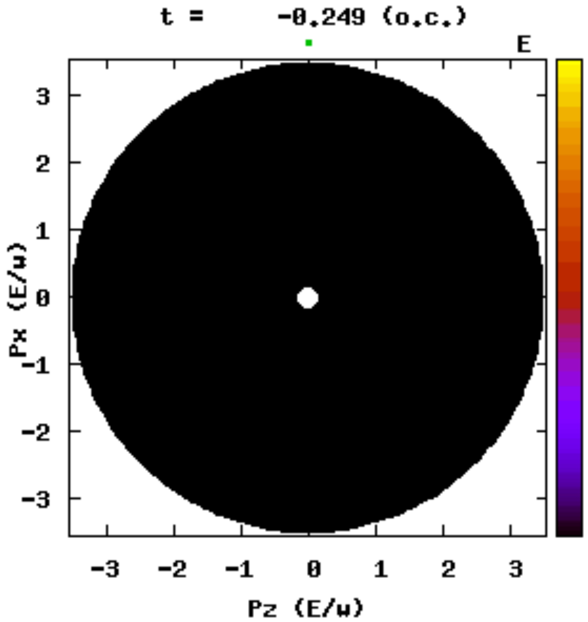
Rescattering wave-packet

Space



$$|\Psi_j(t)|^2$$

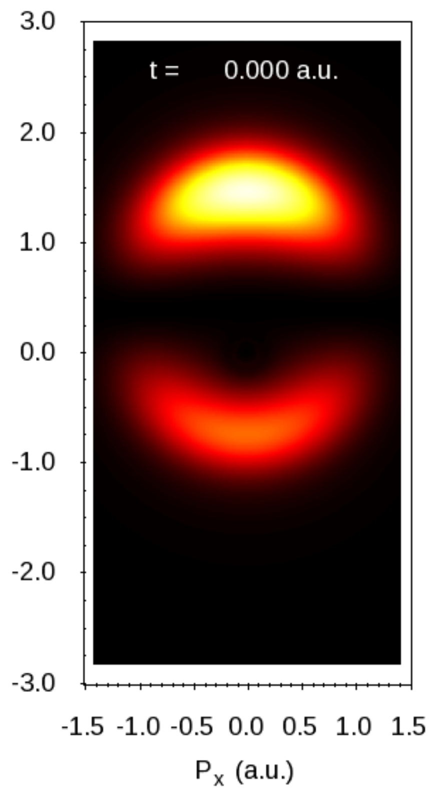
momentum

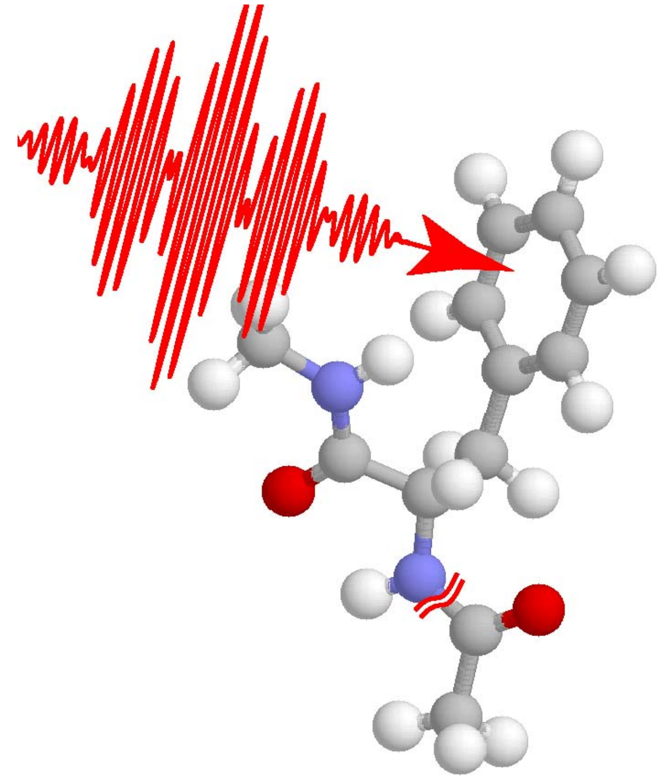


$$\frac{dP(E,\Omega,t)}{dEd\Omega}$$

PRL **99** (2007) 093001.

Our Research Goals: Mechanism





Optic holography

Electron holography

Role of Theoretical Simulation

- Explain the experimental observation:
- understand the mechanism: rescattering
- extract the information from experiment: molecular structure
- Search a way to control quantum processes: photoabsorption
- Many more …

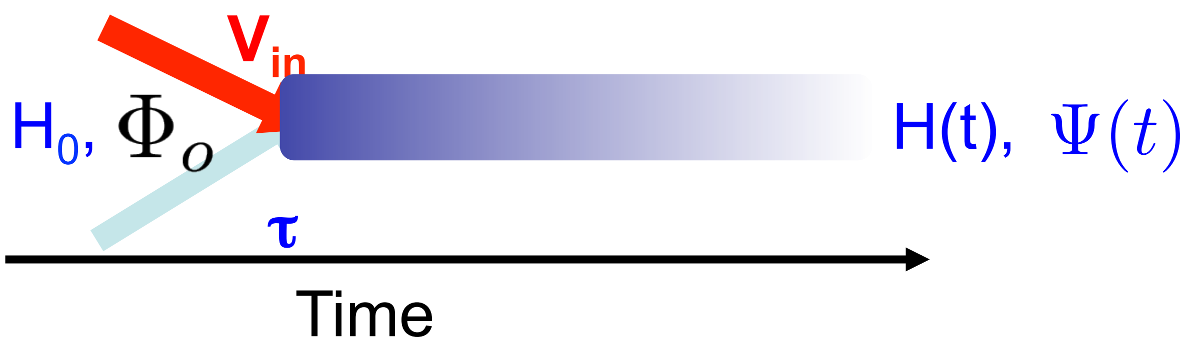
Theoretical Method: Working Equations

TDSE in differential form

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \quad \text{with} \quad \Psi(t=-\infty) = \Phi_0$$

TDSE in integral form

$$\begin{aligned}\Psi(t) &= -i\int_{-\infty}^{t} e^{-i\int_{\tau}^{t} H(t')dt'} V_{in}(\tau) e^{-iH_0\tau}\Phi_0 d\tau + e^{-iH_0 t}\Phi_0 \\ &= -i\int_{-\infty}^{t} U(t,\tau)V_{in}(\tau)U_0(\tau,-\infty)\Phi_0 d\tau + U_0(t,-\infty)\Phi_0\end{aligned}$$



Theoretical Method: Time Propagator I

Second order split-operator-method in the energy representation

$$\Psi(t+\Delta t) = U(t+\Delta t, t)\Psi(t) = e^{-iH\Delta t}\Psi(t)$$
$$\approx e^{-iH_0\Delta t/2} e^{-iV(t)\Delta t} e^{-iH_0\Delta t/2}\Psi(t) + O(\Delta t^3)$$

[Chem. Phys. **217** (1997) 119]

Discretize space in pseudo-spectral grid:

$$H_0 = H^0_{r_i,r_j}(\ell), \quad \Psi(r_i,\theta) = \sum_\ell R_\ell(r_i) Y_{\ell,m}(\hat{\mathbf{r}}), \quad \Psi(r_i,\ell) = R_\ell(r_i)$$

Time-propagation → vector, matrix operations → blas

Easy refactor to modern computers, GPU cublas, MIC ??

C(i) ← F[A(i)]*B(i) ?

Structure of code (machine)

One MPI thread

OpenMP+ mkl

Cublas + CUDA C

HA-PACS

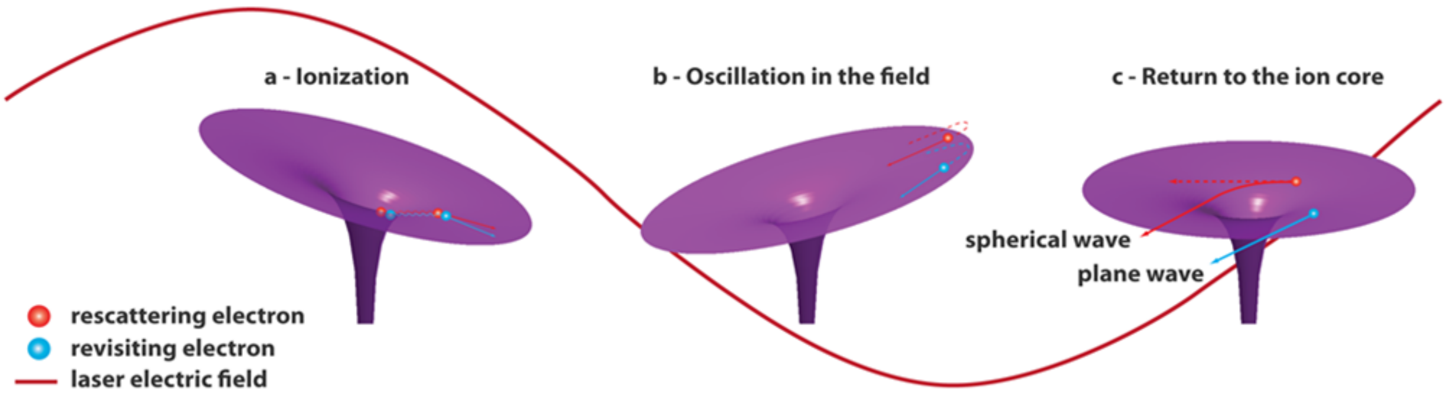
Device = mod(myid,4)

MPI (node 0)	MPI (node 0)	......	
Thread 0 (Device 0)	Thread 4 (Device 0)		
Thread 1 (Device 1)	Thread 5 (Device 1)		
Thread 2 (Device 2)	Thread 6 (Device 2)		
Thread 3 (Device 3)	Thread 7 (Device 3)		

Example 1: Mechanism of ATI in mid-IR Field

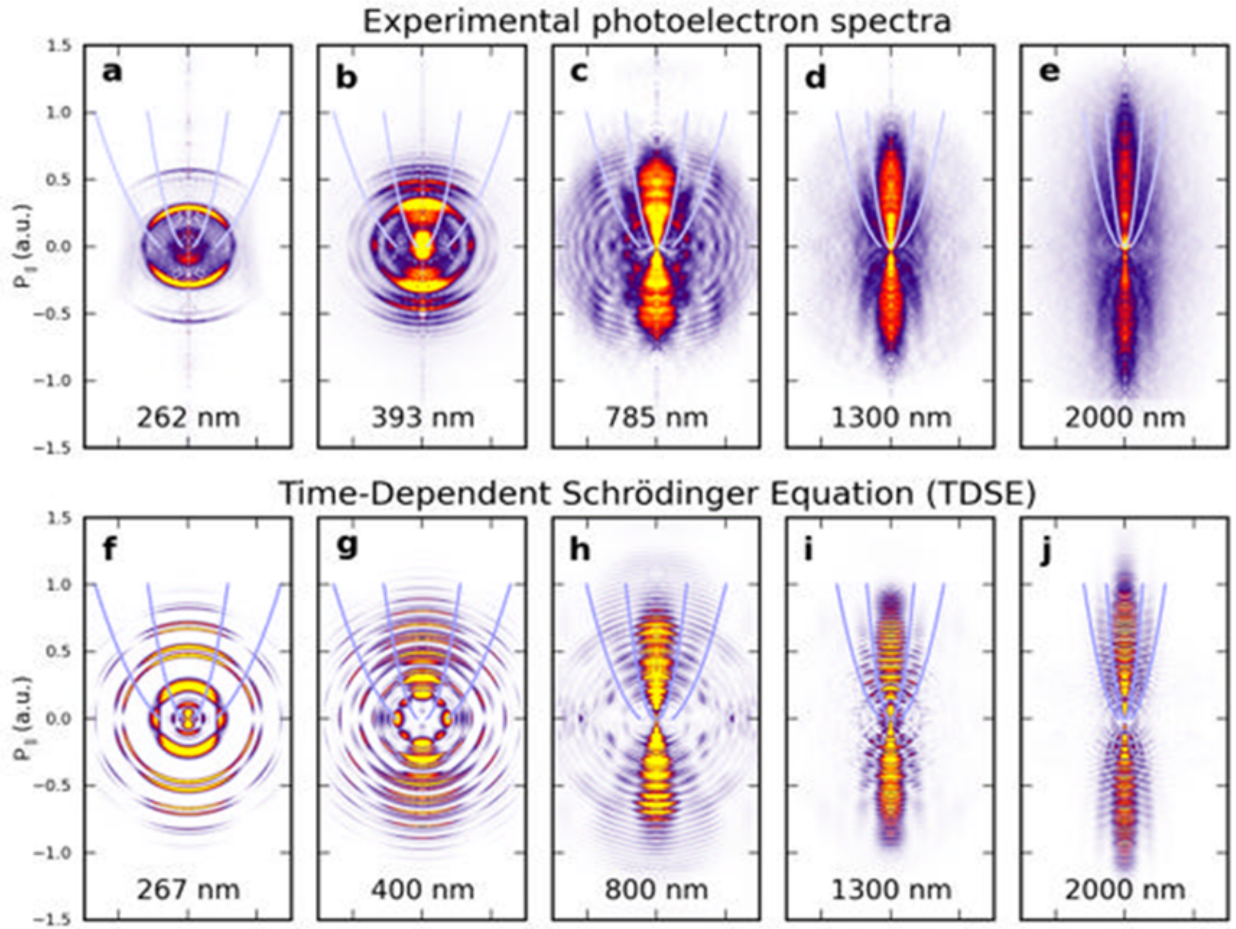
ATI: above-threshold ionization

Physical Process: $$A + n\,h\nu \rightarrow A^{+} + e$$



- understand the structure:
  interference between the returning and rescattering electrons
- Information encoded in the structure:
  inner-work: how the electron interacts with the parent core

Example 1: Mechanism of ATI in mid-IR Field



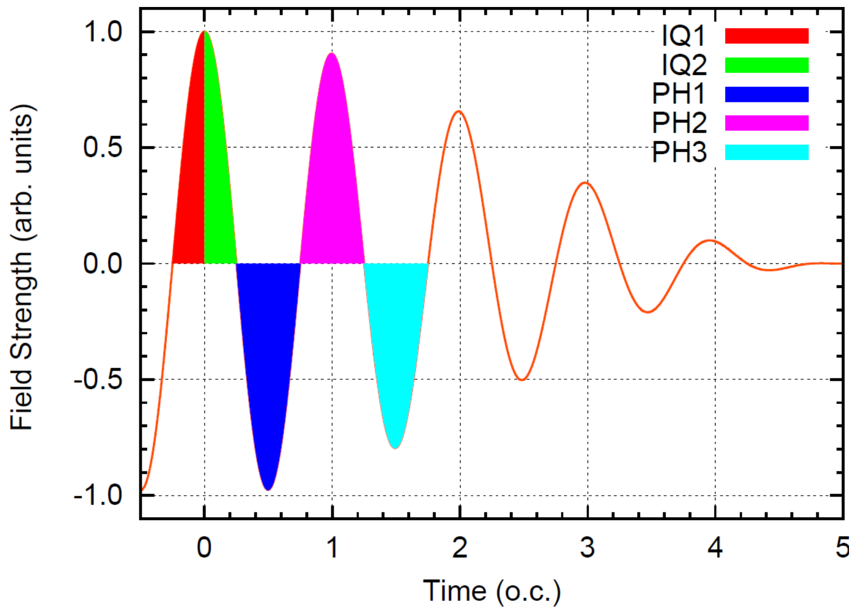
PRL **109** (2012) 073004.

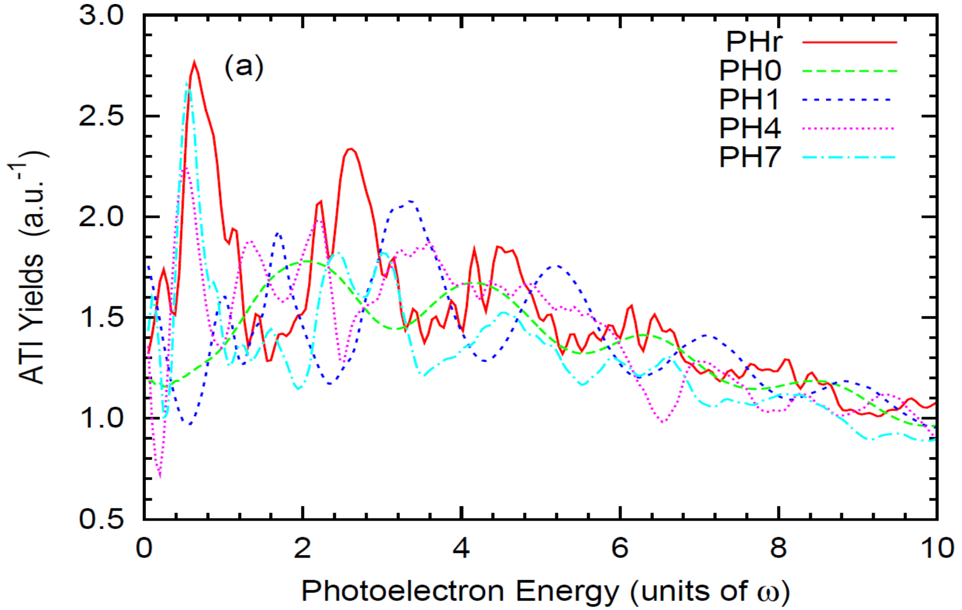
HA-PACS: 5 nodes, 20 hrs

Example 1: Mechanism of ATI in mid-IR Field

Separate the tunnel ionization from propagation:

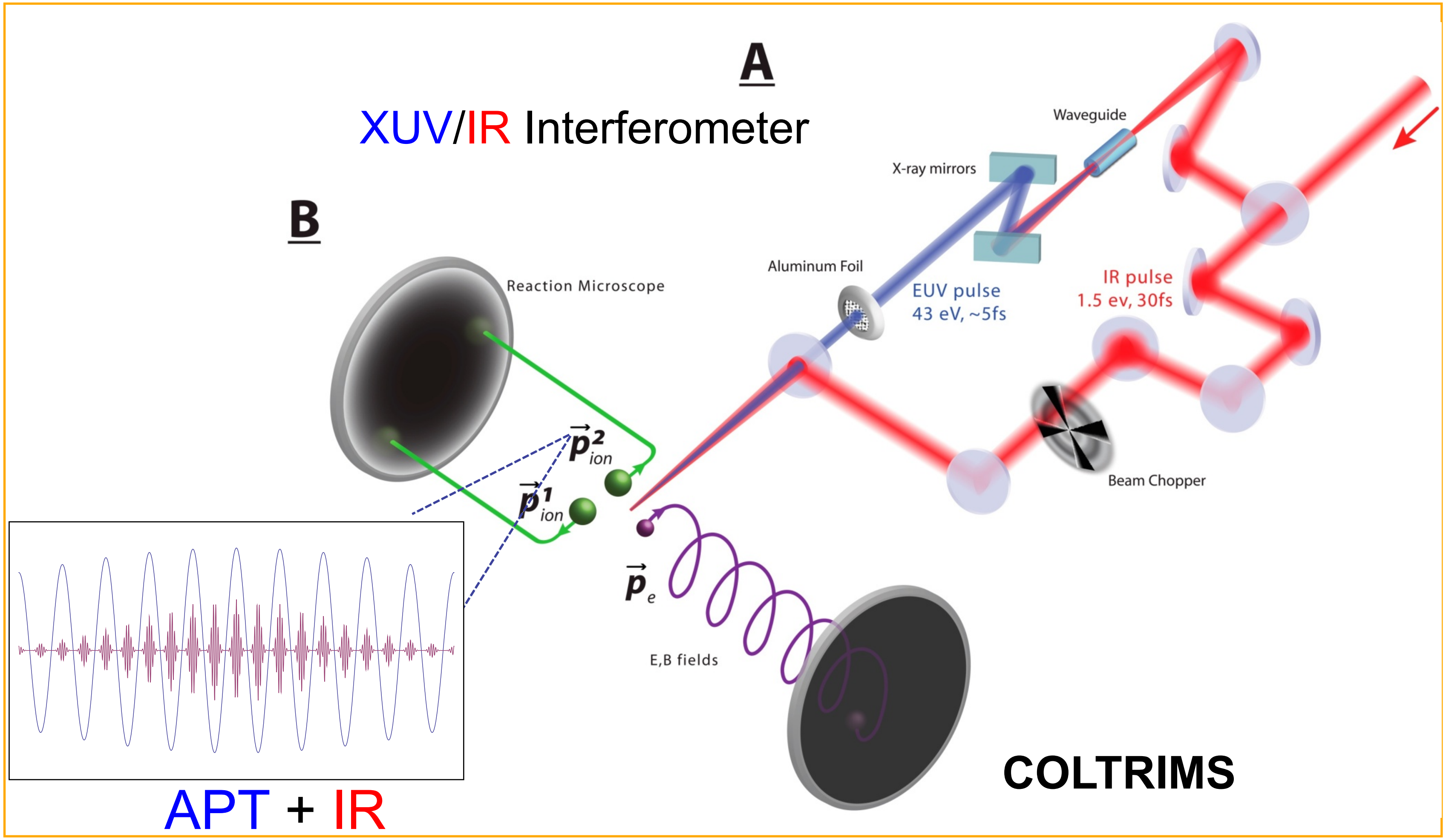
$$\Psi_k = U(\infty, t_{k+1}) \int_{t_k}^{t_{k+1}} U(t_{k+1}, t) V_{ext}(t) e^{-iH_0 t} \Psi_0 dt$$



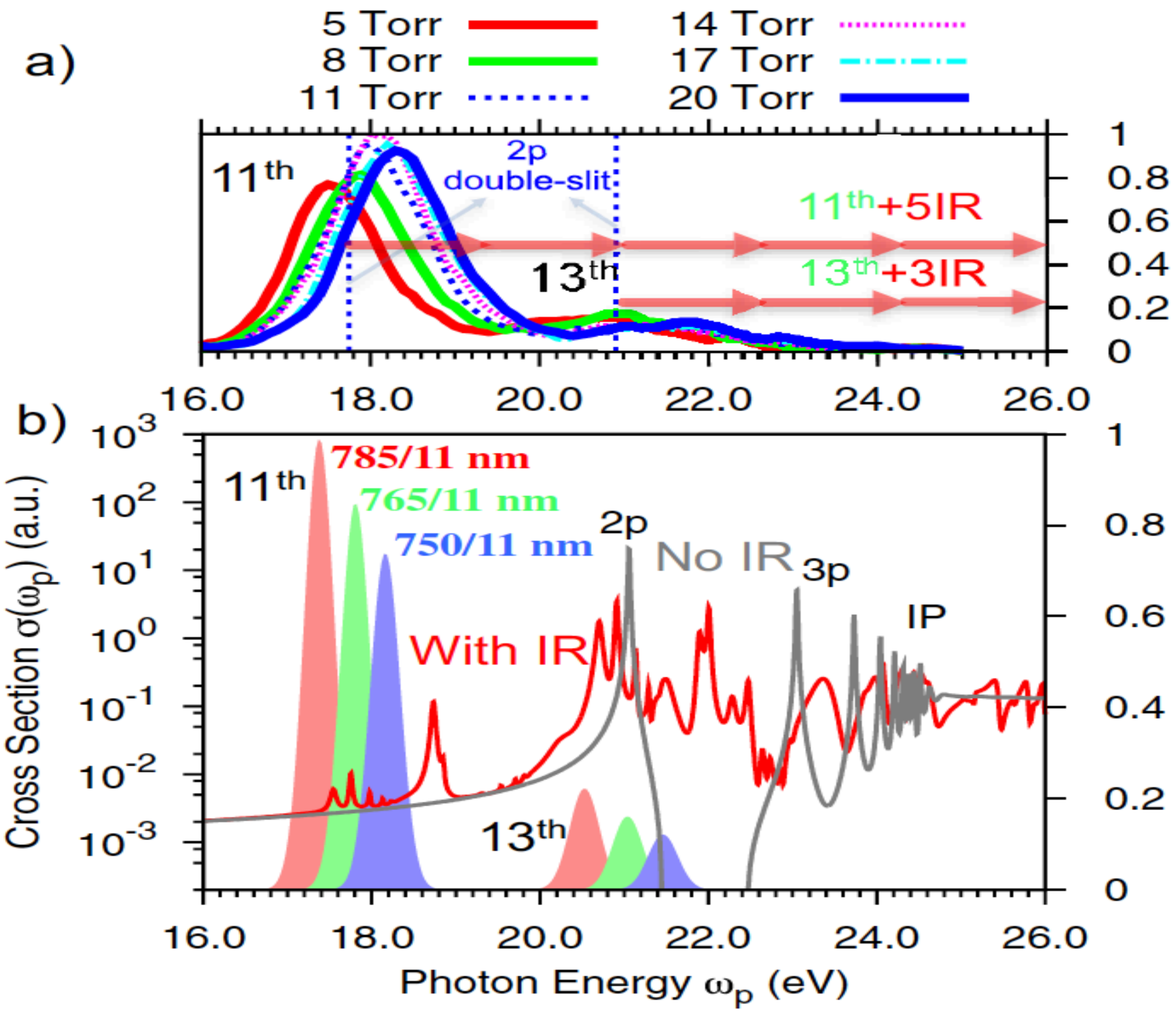


Low Energy Structure comes from multiple re-scattering.

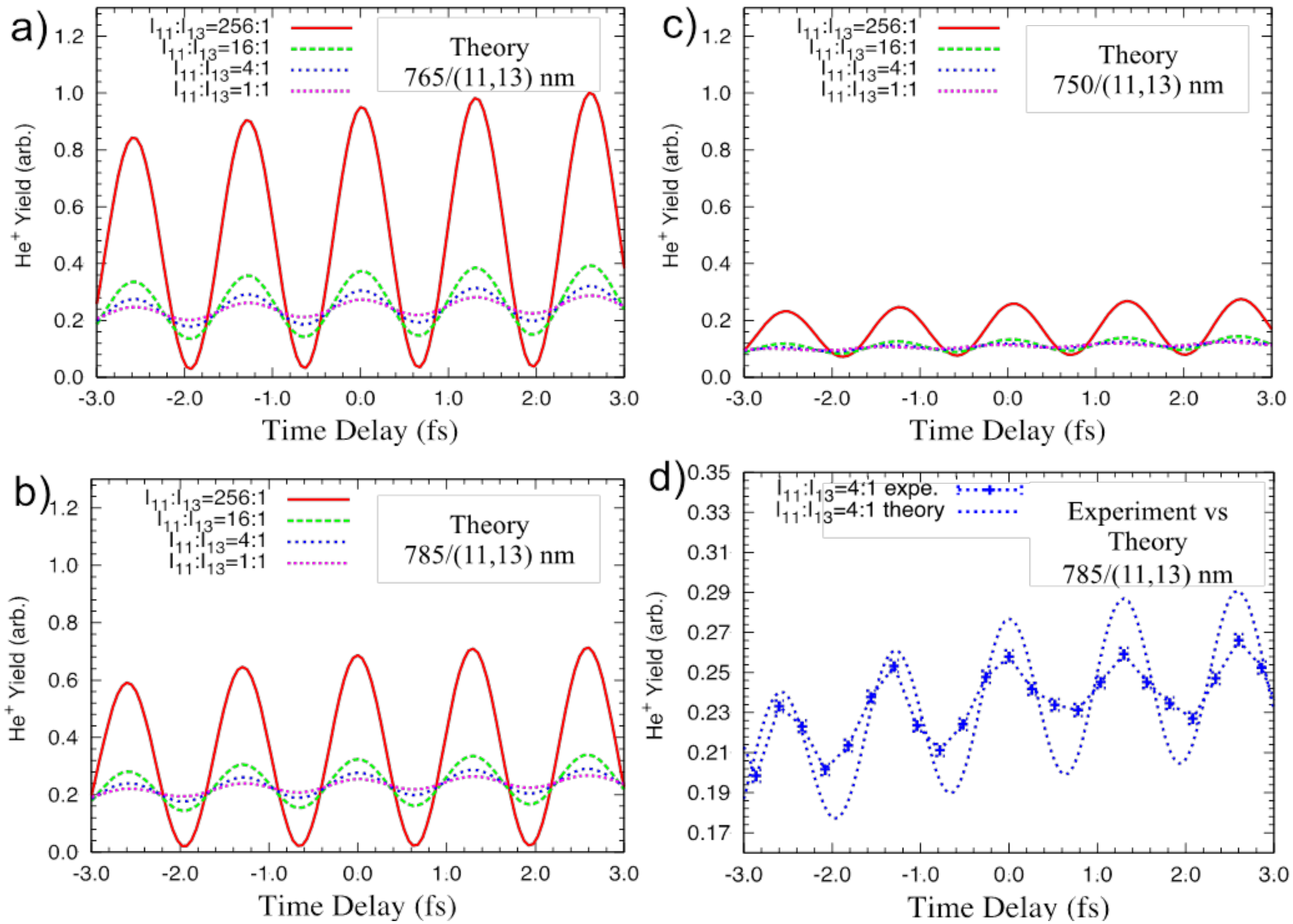
Control transparency in attosecond time scale



IR assistant Photoabsorption cross sections



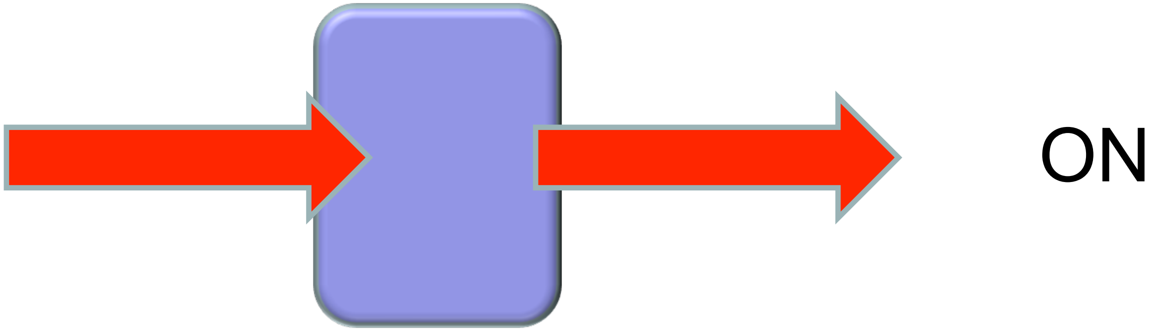
Control transparency



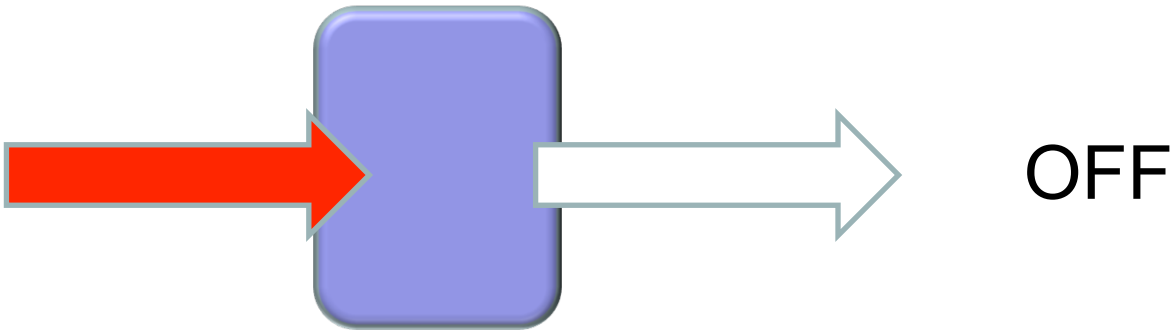
PRL **106** (2011) 193008.

Applications:

Generate a super-fast optical switch



in femto or atto second time domain



What we expect from HPC

✧ A better machine: fast in speed and large in memory

✧ Easy to refactor the code: CPU, GPU, MIC …

$$\bar{\Psi}(x_i, y_j, z_k) = e^{-iV(x_i, y_j, z_k)}\Psi(x_i, y_j, z_k)$$

$$C(i) = A(i) * B(i)$$

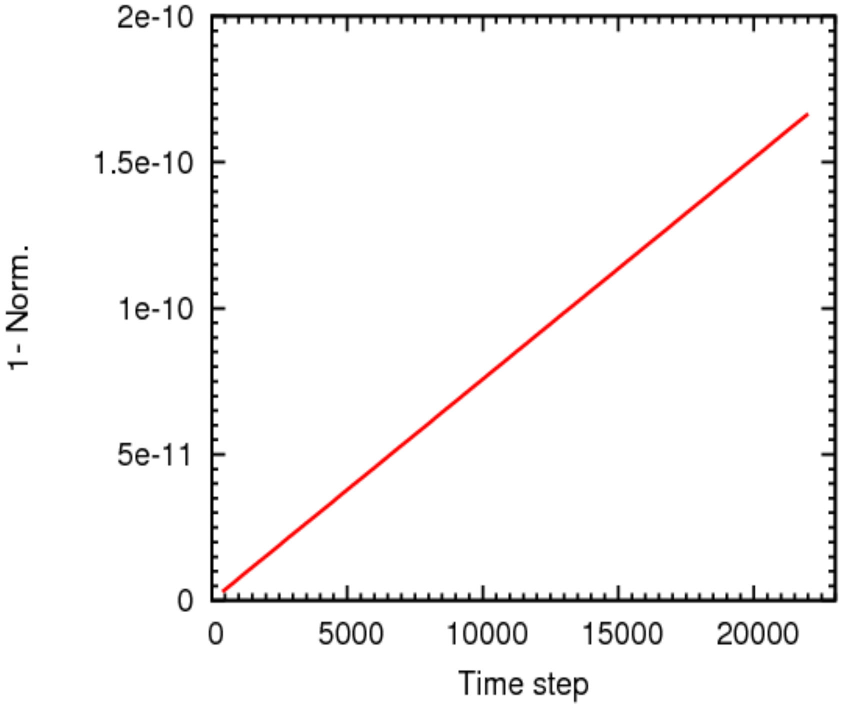
✧ PGI acc, OpenAcc SIMD

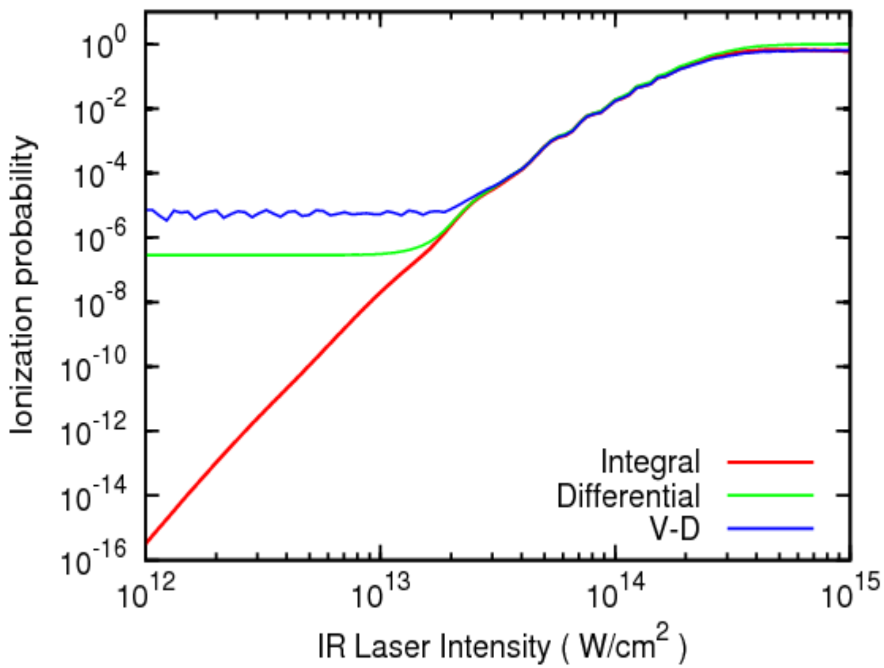
Numerical accuracy:

One time-step: random, round-off, double-complex, 10^{-14} (norm)

Time propagation: systematic error:

✧ Numerical accuracy: real (kind=4, 8, 16), real(kind=12) ??





Acknowledgments

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