Dynamics and Correlations in Exotic Nuclei
Yukawa Institute for Theoretical Physics, Kyoto Univ.
Sept. 23, 2011

Real-time TDDFT for molecules and solids

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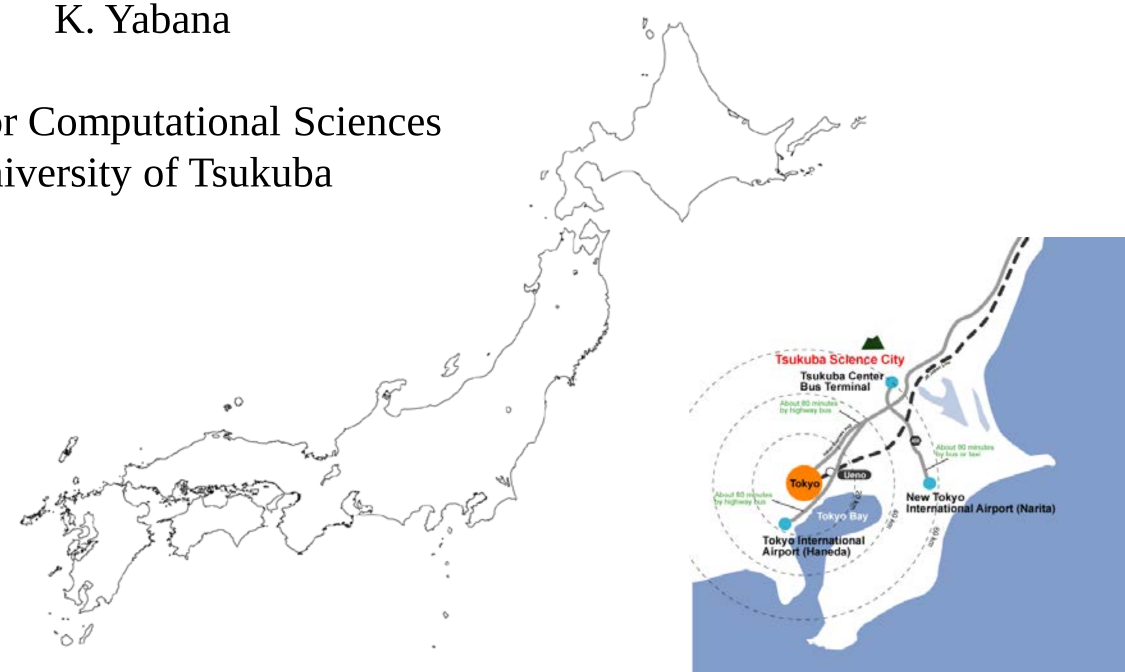
Center for Computational Sciences
University of Tsukuba



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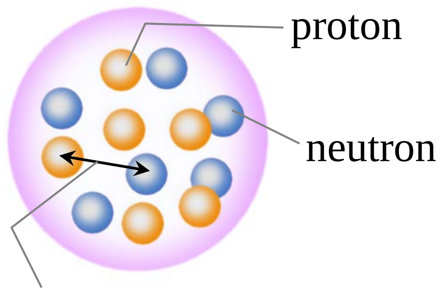
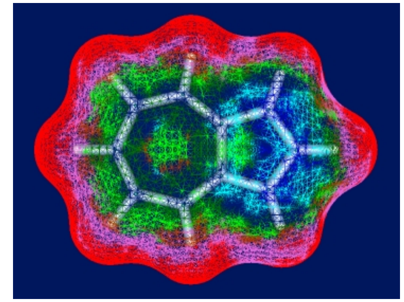
G.F. Bertsch (NP)	U. Washington





	Nuclei Composed of nucleons	Atoms, Molecules, Solids Electron many-body systems
Size	10^{-15}m	10^{-10}m
Energy	1MeV	1eV
Time	10^{-23}s	10^{-17}s
Mass	10^{9}eV	5×10^{5}eV
Interaction	Nuclear force (Strong interaction)	Coulomb force
Statistics	Fermion	Fermion

Time-Dependent Density Functional Theory

Successful for quantitative description of many-fermion dynamics

Nuclei (nucleon dynamics)	Atoms, Molecules, Solids (electron dynamics)

Linear response regime

- Giant resonances ((Q)RPA)	- Low-lying electronic excitaiton in molecules - Optical response of molecules and solids

Nonlinear regime, Initial value problem

- Heavy ion collision	- Laser science (Intense and ultra-short laser pulse)

History: (TD)DFT in nuclear and electronic systems

Nuclear Physics

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Late 1990's ~ Development of
Quantum chemistry method

Continuum RPA

- Linearized TDDFT, spherical system, scattering boundary condition -

$$\delta\rho(\vec{r}) = \int d\vec{r}\,'\Pi_0(\vec{r},\vec{r}\,',\omega)\left\{\int d\vec{r}\,''\frac{\delta h(\vec{r}\,')}{\delta\rho(\vec{r}\,'')}\delta\rho(\vec{r}\,'') + V(\vec{r}\,')\right\}$$

$$\Pi_0(\vec{r},\vec{r}\,',\omega) = \sum_j \phi_j^* G(\hbar\omega + \varepsilon_j)\phi_j + \phi_j G(-\hbar\omega + \varepsilon_j)\phi_j^*$$

$$G(\vec{r},\vec{r}\,',E) = \langle\vec{r}|\frac{1}{E-h_0}|\vec{r}\,'\rangle = \sum_L \frac{u_L(r_<)v_L(r_>)}{rr'}\sum_M Y_{LM}^*(\hat{r})Y_{LM}(\hat{r}')$$

Nuclear Dipole Giant Resonance

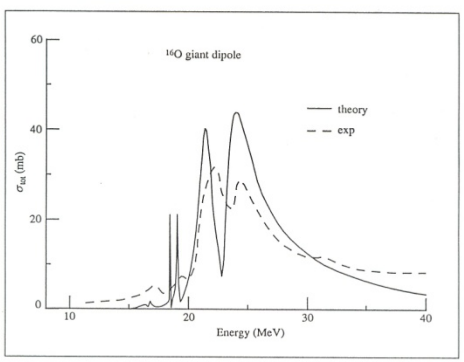
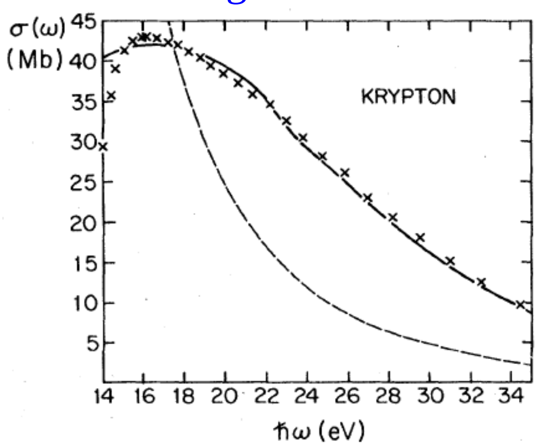


Fig. 9.1. Giant dipole resonance in ^{16}O. Dashed line: experimental; solid line, continuum RPA theory (Shlomo and Bertsch (1975)).

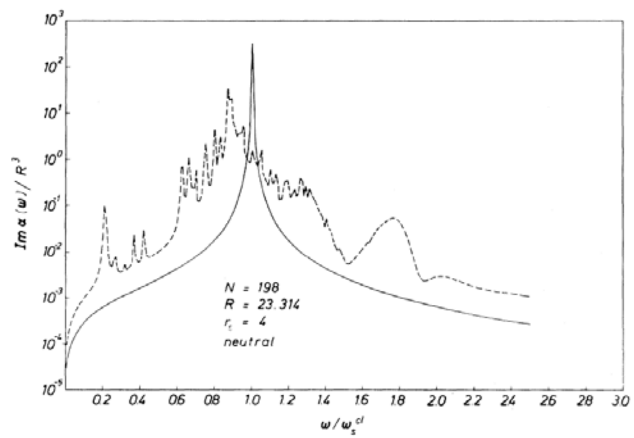
Shlomo, Bertsch 1975

Photoabsorption of Rare gas atom



Zangwill, Soven 1980

Giant Resonance in Metallic clusters (Mie plasmon)



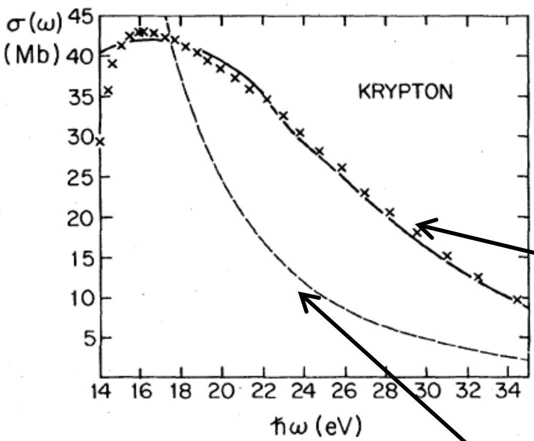
Ekardt 1984

$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2+\sum_a V_{ion}(\vec{r}-\vec{R}_a)+e^2\int d\vec{r}\,'\frac{n(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|}+\mu_{xc}(n(\vec{r},t))+V_{ext}(\vec{r},t)\right\}\psi_i(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)$$

$$n(\vec{r},t)=\sum_i|\psi_i(\vec{r},t)|^2$$

Important residual interaction
- Dynamical Screening Effect

Photoabsorption of
Rare gas atom



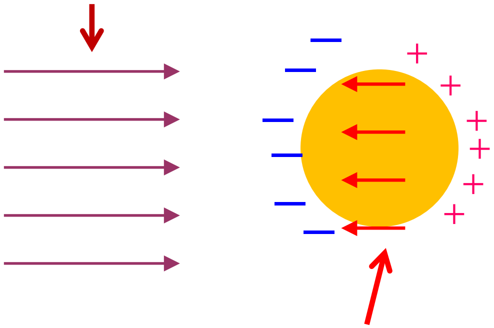
TDDFT accurately reproduces σ(ω).

Zangwill, Soven 1980

Without residual interaction
(without dynamical screening effect)

$$E_{ext}(t)$$

$$V_{ext}(\vec{r},t)=eE_{ext}(t)z$$



$$E_{ind}(t)$$

$$V_{ind}(\vec{r},t)=e^2\int d\vec{r}\,'\frac{\delta n(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|}+\frac{\delta\mu_{xc}}{\delta n}\delta n(\vec{r},t)$$

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Nonlinear regime: Initial value problem

Nuclear fusion reaction of ^{16}O-^{16}O

Spatial grid: 30x28x16 (10^{-15}m), Time-step 4x10^{2} (10^{-22}s)

H. Flocard, S.E. Koonin, M.S. Weiss, Phys. Rev. 17(1978)1682.

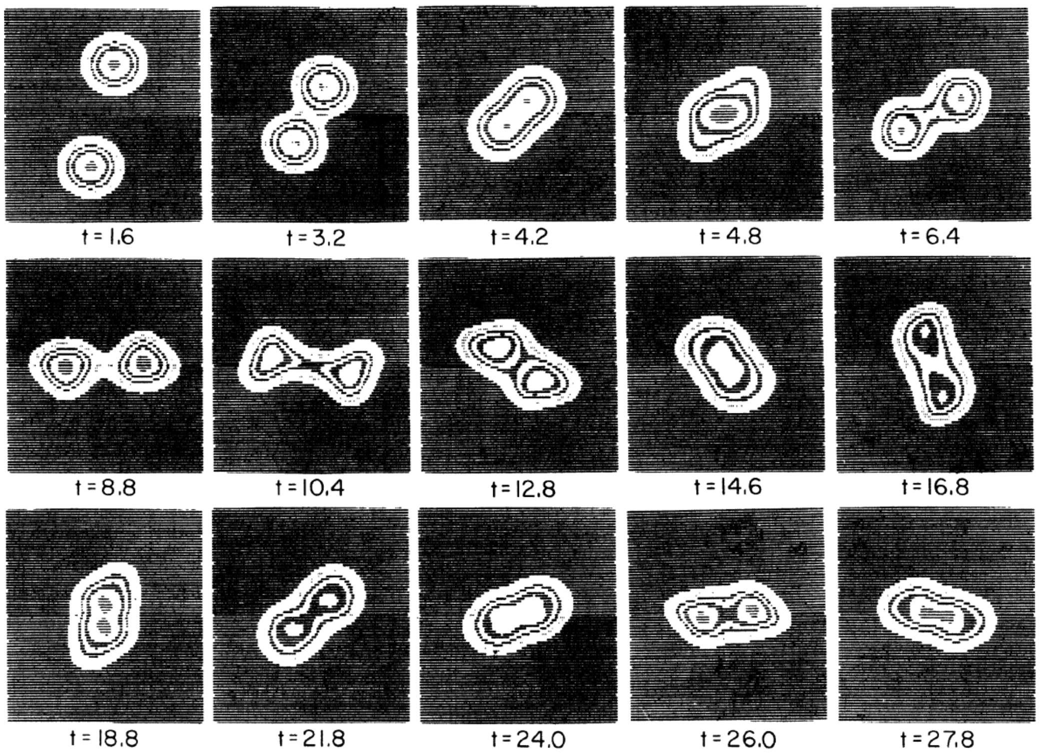

FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{1ab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

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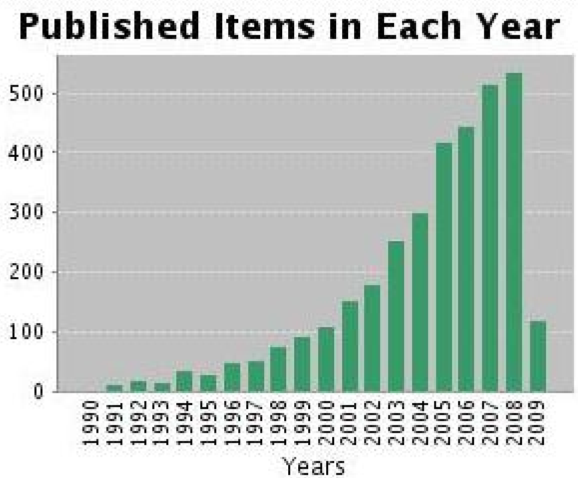
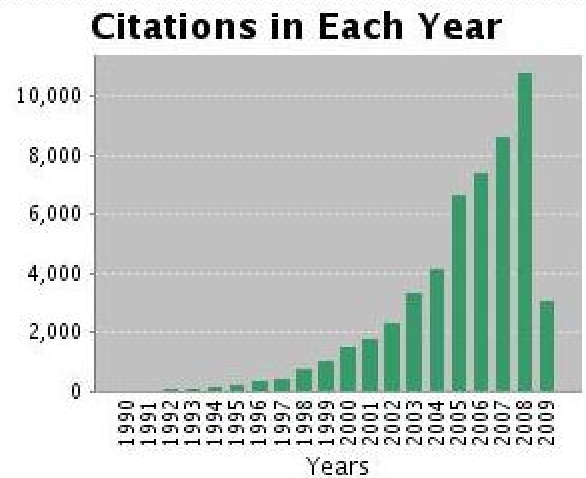
TDDFT in Web of Science

Citation Report Topic=(Time dependent density functional theory or time dependent local density approximation)

Timespan=All Years. Databases=SCI-EXPANDED, SSCI, A&HCI.

This report reflects citations to source items indexed within Web of Science. Perform a Cited Reference Search to include citations to items not indexed with





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	2005	2006	2007	2008	2009	Total	Average Citations per Year
	6719	7443	8659	10809	3112	53,468	1980.30
1. Title: DENSITY-FUNCTIONAL THEORY FOR TIME-DEPENDENT SYSTEMS Author(s): RUNGE E, GROSS EKU Source: **PHYSICAL REVIEW LETTERS** Volume: **52** Issue: **12** Pages: **997-1000** Published: **1984**	173	165	160	202	57	1,292	49.69
2. Title: Treatment of electronic excitations within the adiabatic approximation of time dependent density functional theory Author(s): Bauernschmitt R, Ahlrichs R Source: **CHEMICAL PHYSICS LETTERS** Volume: **256** Issue: **4-5** Pages: **454-464** Published: **JUL 5 1996**	170	179	167	193	56	1,280	91.43
3. Title: Molecular excitation energies to high-lying bound states from time-dependent density-functional response theory: Characterization and correction of the time-dependent local density approximation ionization threshold Author(s): Casida ME, Jamorski C, Casida KC, et al. Source: **JOURNAL OF CHEMICAL PHYSICS** Volume: **108** Issue: **11** Pages: **4439-4449** Published: **MAR 15 1998**	168	171	200	176	52	1,245	103.75
4. Title: An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules Author(s): Stratmann RE, Scuseria GE, Frisch MJ Source: **JOURNAL OF CHEMICAL PHYSICS** Volume: **109** Issue: **19** Pages: **8218-8224** Published: **NOV 15 1998**	146	156	163	184	64	1,135	94.58

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Linear polarizability from real-time TDDFT calculation

$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2+\sum_a V_{ion}(\vec{r}-\vec{R}_a)+e^2\int d\vec{r}'\frac{n(\vec{r}',t)}{|\vec{r}-\vec{r}'|}+\mu_{xc}(n(\vec{r},t))+V_{ext}(\vec{r},t)\right\}\psi_i(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)$$

$$n(\vec{r},t)=\sum_i|\psi_i(\vec{r},t)|^2$$

Basic idea

K. Yabana, G.F. Bertsch, Phys. Rev. B54, 4484 (1996)
K. Yabana et.al, phys.stat.sol.(b)243, 1121 (2006)

Applied electric field: $V_{ext}(\vec{r},t)=eE(t)z$

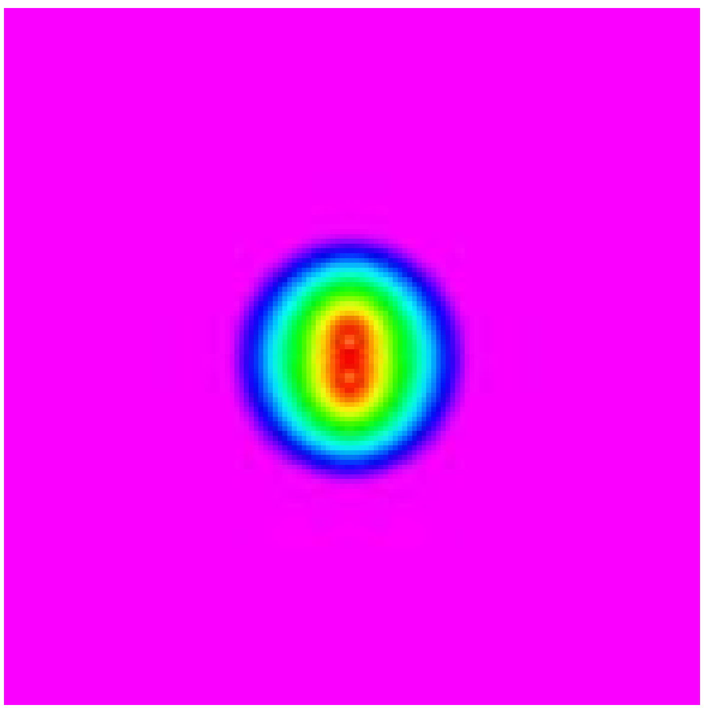
Induced polarization: $p(t)=\int d\vec{r}\, z n(\vec{r},t)=\int dt'\alpha(t-t')E(t')$

Frequency dep. polarizability: $\alpha(\omega)=\int dt\, e^{i\omega t}\alpha(t)=\frac{\int dt e^{i\omega t}p(t)}{\int dt e^{i\omega t}E(t)}$

Simplest choice: $E(t)\propto\delta(t)$ then, $\alpha(\omega)\propto\int dt e^{i\omega t}p(t)$

Linear response in real-time:
Hit the molecule and see response.

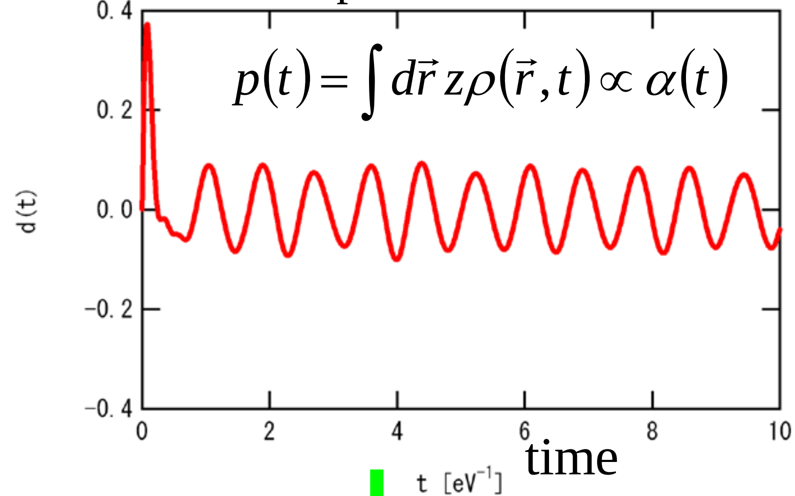
$$V_{ext}(\vec{r},t) \propto \delta(t) z$$



Ethylene (C_2H_4) molecule

Dipole moment

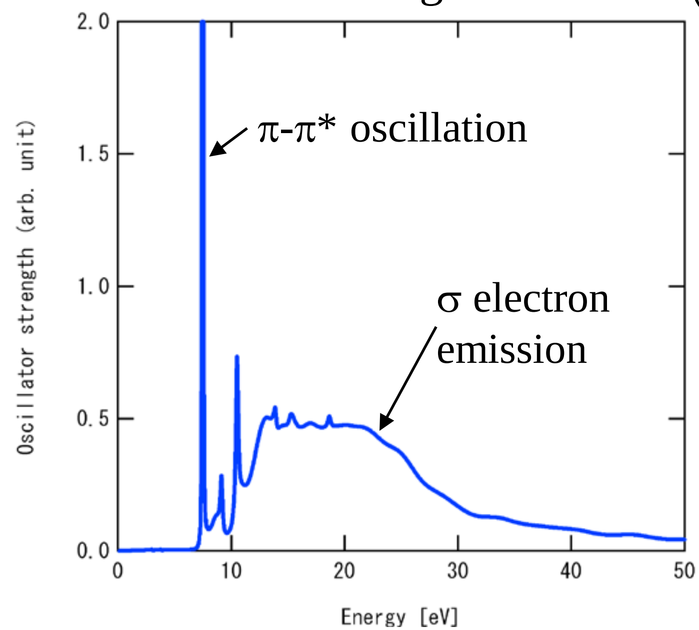
$$p(t) = \int d\vec{r}\, z \rho(\vec{r},t) \propto \alpha(t)$$



time

Fourier transf.

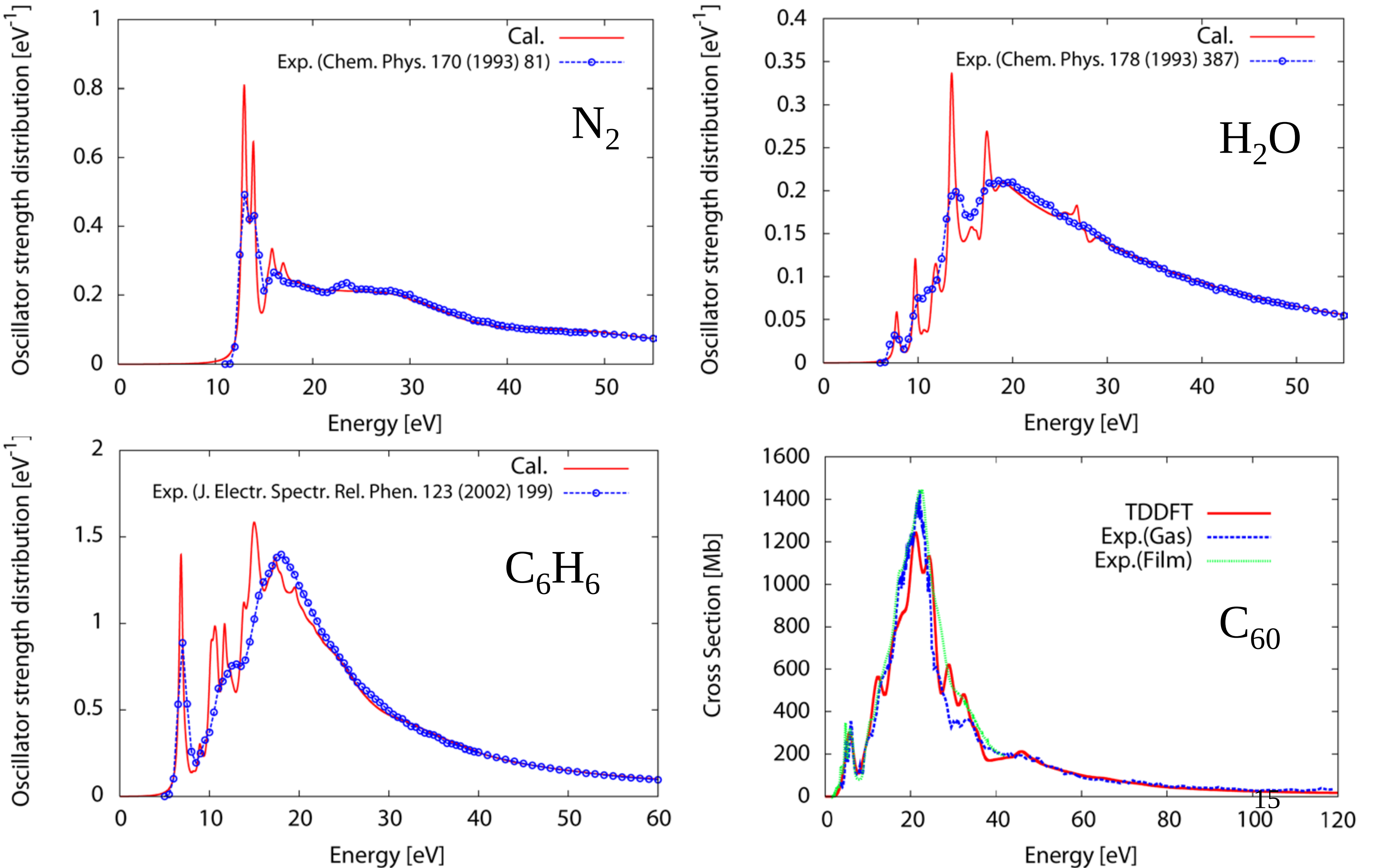
Oscillator strength $\propto \omega \, \mathrm{Im}\, \alpha(\omega)$



Excitation energy

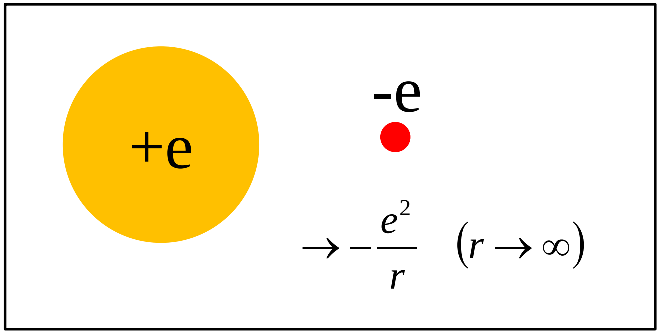
Oscillator strength distribution from real-time TDDFT

K. Yabana, Y. Kawashita, T. Nakatsukasa, J.-I. Iwata, Charged Particle and Photon Interactions with Matter: Recent Advances, Applications, and Interfaces Chapter 4, Taylor & Francis, 2010.



$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2+\sum_a V_{ion}(\vec{r}-\vec{R}_a)+e^2\int d\vec{r}'\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}+\mu_{xc}(n(\vec{r}))\right\}\phi_i(\vec{r})=\varepsilon_i\phi_i(\vec{r})$$

$$\rightarrow 0 \quad (r\rightarrow\infty) \qquad\qquad \rightarrow -\frac{e^2}{r} \quad (r\rightarrow\infty)$$



LDA cannot describe correct asymptotic behavior (self-interaction problem)

Nonlocal Fock potential has correct form

Here we employ van Leeuwen – Baerends potential (LB94)

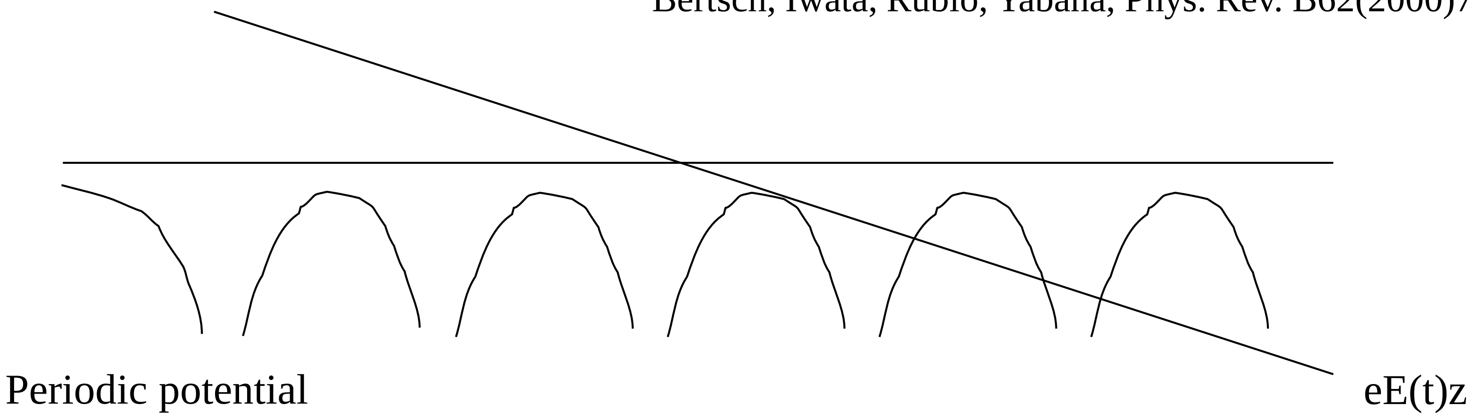
$$v_{xc}^{\sigma}(\vec{r})=-\beta n_{\sigma}^{1/3}(\vec{r})\frac{x_{\sigma}^2}{1+3\beta x_{\sigma}\sinh^{-1}(x_{\sigma})} \quad \rightarrow -\frac{1}{r} \quad (r\rightarrow\infty) \qquad x_{\sigma}=\frac{|\nabla n_{\sigma}|}{n_{\sigma}^{4/3}}$$

Asymptotically correct behavior at large distance.
HOMO energy = - IP

$$\ln e^{-\alpha r} \propto r$$

Linear response in crystalline solid

Bertsch, Iwata, Rubio, Yabana, Phys. Rev. B62(2000)7998.



For periodic Hamiltonian, we may apply Bloch's theorem

$$\psi_{nk}\left(\vec{r}+\vec{R}\right)=e^{i\vec{k}\vec{R}}\psi_{nk}\left(\vec{r}\right), \qquad h\left(\vec{r}+\vec{R}\right)=h\left(\vec{r}\right)$$

Linear potential eE(t)z violates periodicity of the Hamiltonian.

↓

We may recover periodicity by gauge transformation, employing vector potential

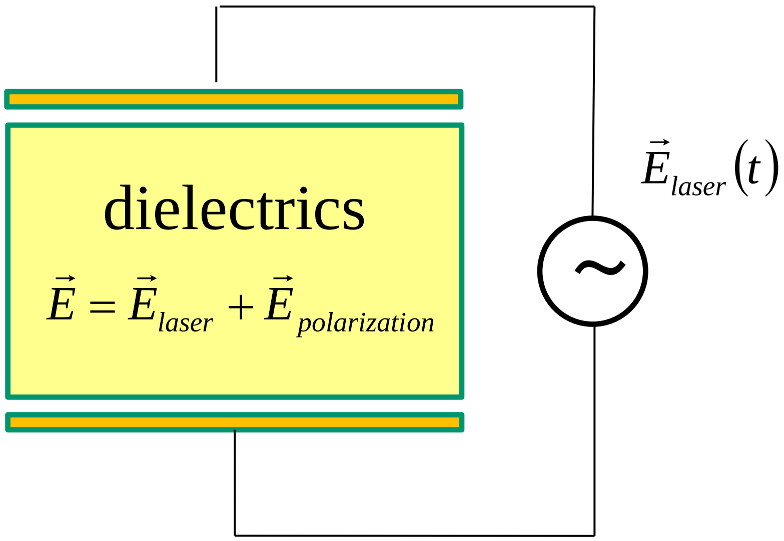
$$\vec{E}=-\vec{\nabla}\phi-\frac{\partial\vec{A}}{\partial t} \qquad \phi=eE(t)z \Leftrightarrow \vec{A}=\hat{z}e\int^{t}dt'\,E(t')$$

$$i\hbar\frac{\partial}{\partial t}\psi(t)=\left[\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}(t)\right)^{2}-e\phi(\vec{r},t)\right]\psi(t)$$

Equation for vector potential: Dynamics of induced polarization

Uniform electric field by
- Applied laser pulse
- Induced polarization

$$\vec{A}(t) = \vec{A}_{laser}(t) + \vec{A}_{polarization}(t)$$



$$\vec{E}(t) = -\frac{\partial \vec{A}(t)}{\partial t}$$

$$\vec{A}(t) = -c\int^{t} \vec{E}(t)dt$$

Equation for polarization

$$\frac{d^2 \vec{A}_{polarization}(t)}{dt^2} = \frac{4\pi}{V}\int_{cell} d\vec{r}\ \vec{j}(\vec{r},t)$$

$\vec{A}(t)$ ↓ ↑ $\vec{j}(\vec{r},t)$

TDKS equation

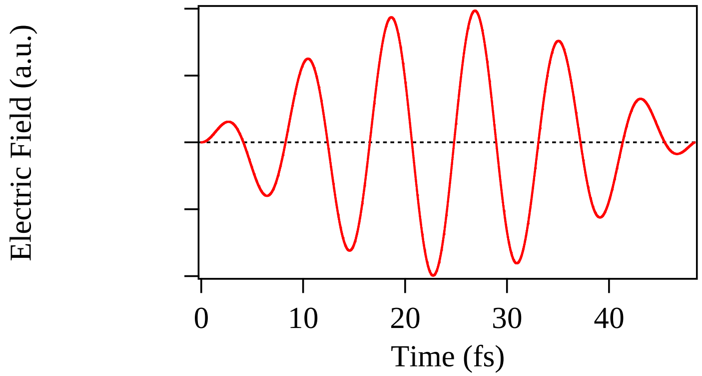
$$i\hbar\frac{\partial}{\partial t}\psi_i = \frac{1}{2m}\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right)^2\psi_i - e\phi\psi_i + \frac{\delta E_{xc}}{\delta n}\psi_i$$

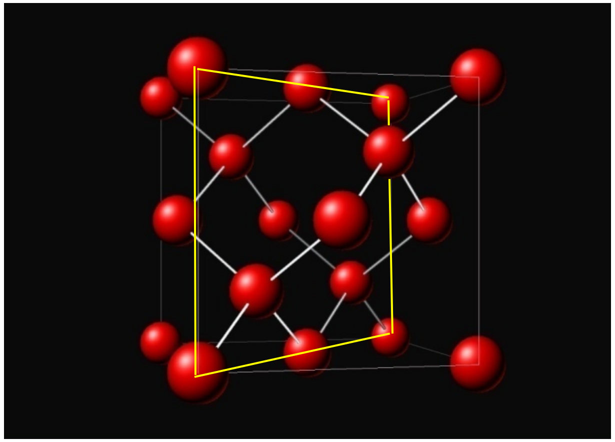
$$n = \sum_i |\psi_i|^2 \qquad \vec{j} = \frac{1}{2m}\sum_i\left(\psi_i^*\left(\vec{p} + \frac{e}{c}\vec{A}\right)\psi_i - c.c.\right)$$

Bertsch, Iwata, Rubio, Yabana, Phys. Rev. B62(2000)7998.

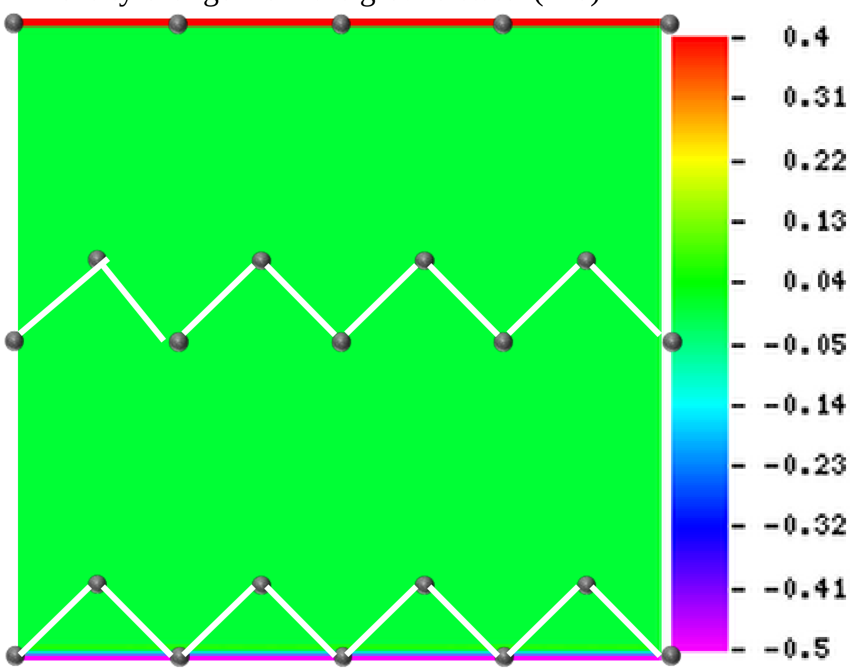
Electron dynamics in bulk silicon under intense laser pulse

$I = 3.5 \times 10^{14}$ W/cm^2, T=50 fs, $\hbar\omega$=0.5 eV

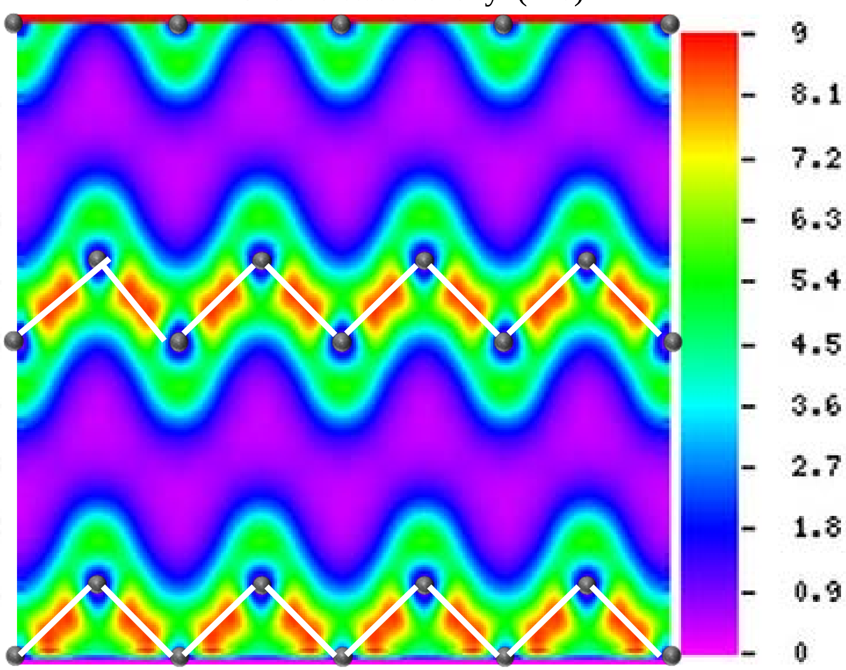




Density change from the ground state (110)

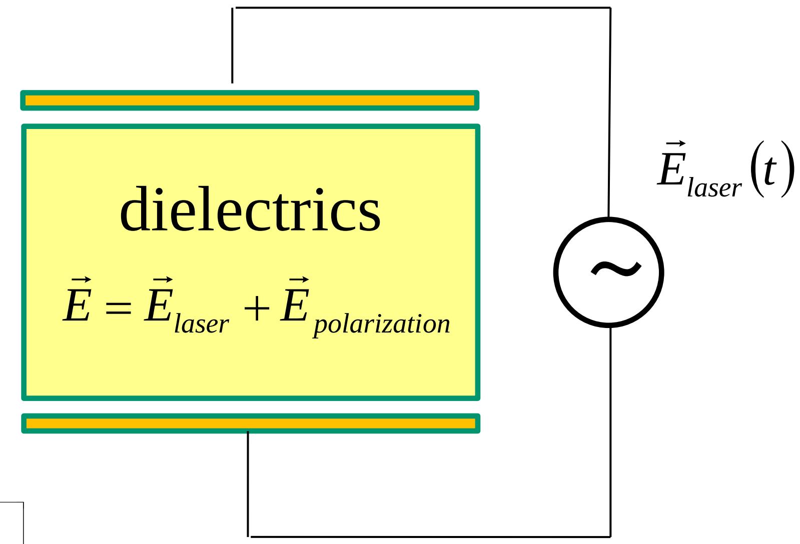


Ground state density (110)

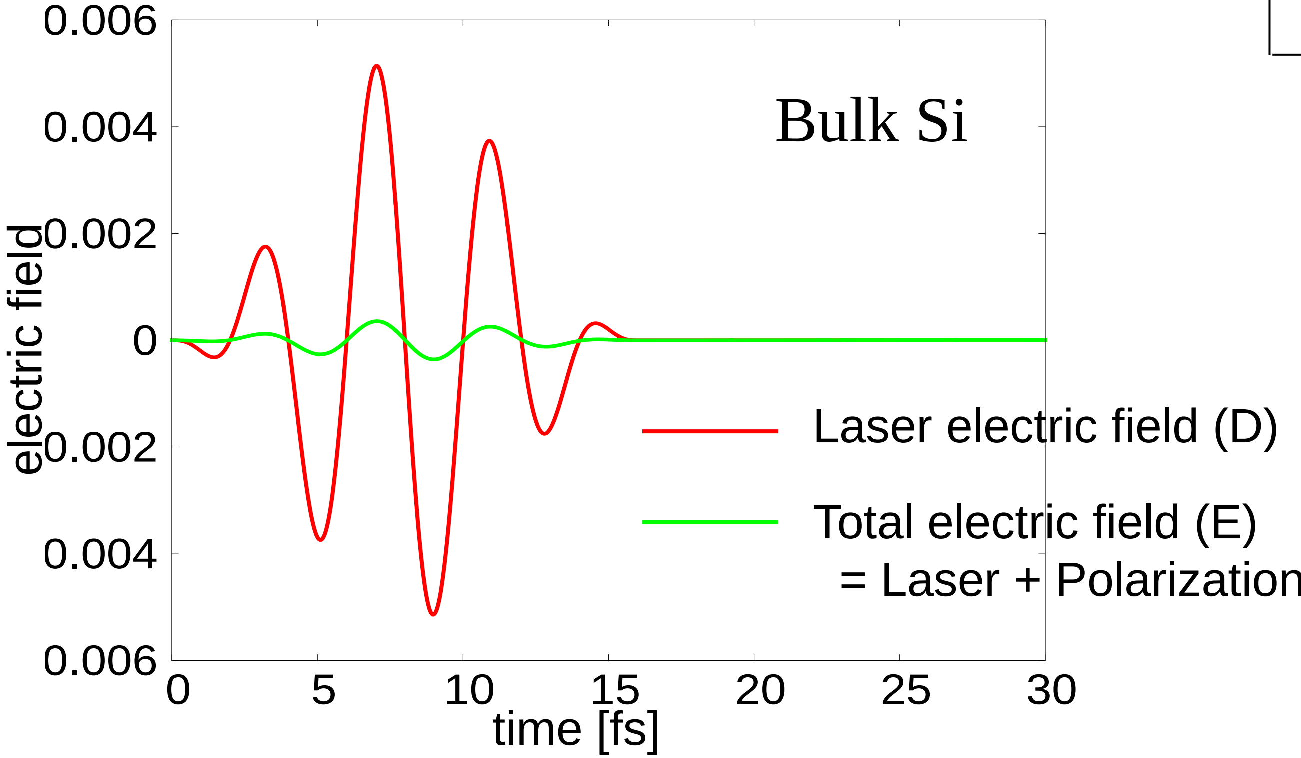


Red +
Green 0
Blue -

E_{total} vs E_{laser} : Dielectric screening



Calculations: I=10^{12}W/cm^2, ħω=1.03eV

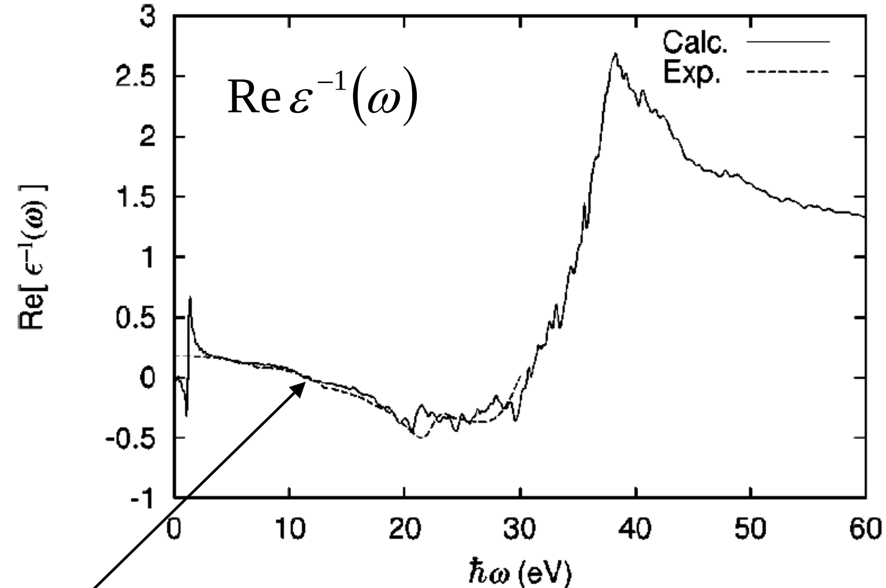


$$D = \varepsilon(\omega)E \qquad \varepsilon \approx 14 \quad (\text{TDDFT})$$

Response to weak-field: dielectric function within TDDFT

Bertsch, Iwata, Rubio, Yabana, Phys. Rev. B62(2000)7998.

$$\frac{1}{\epsilon(\omega)} = \frac{\int dt e^{i\omega t} \frac{dA_{\rm tot}(t)}{dt}}{\int dt e^{i\omega t} \frac{dA_{\rm ext}(t)}{dt}}$$

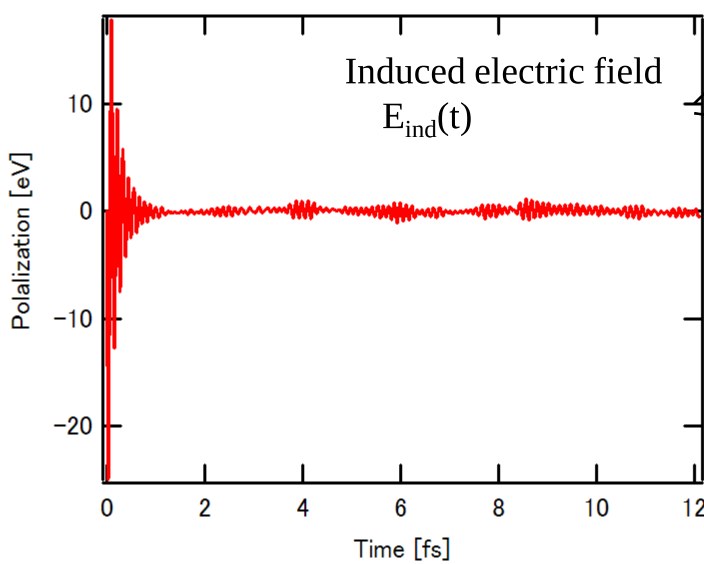


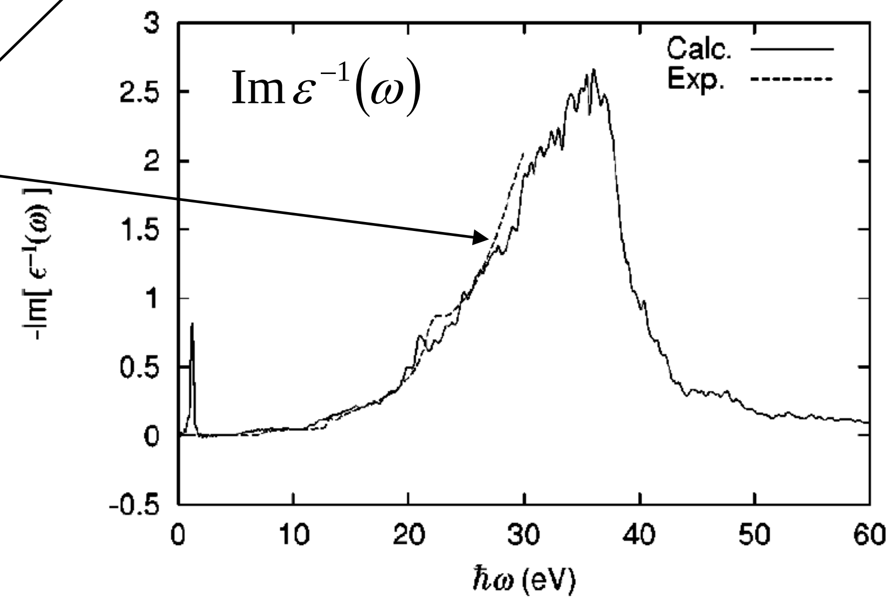
Response to inpulsive field

$$A_{ext}(t) = A_0\,\theta(t)$$

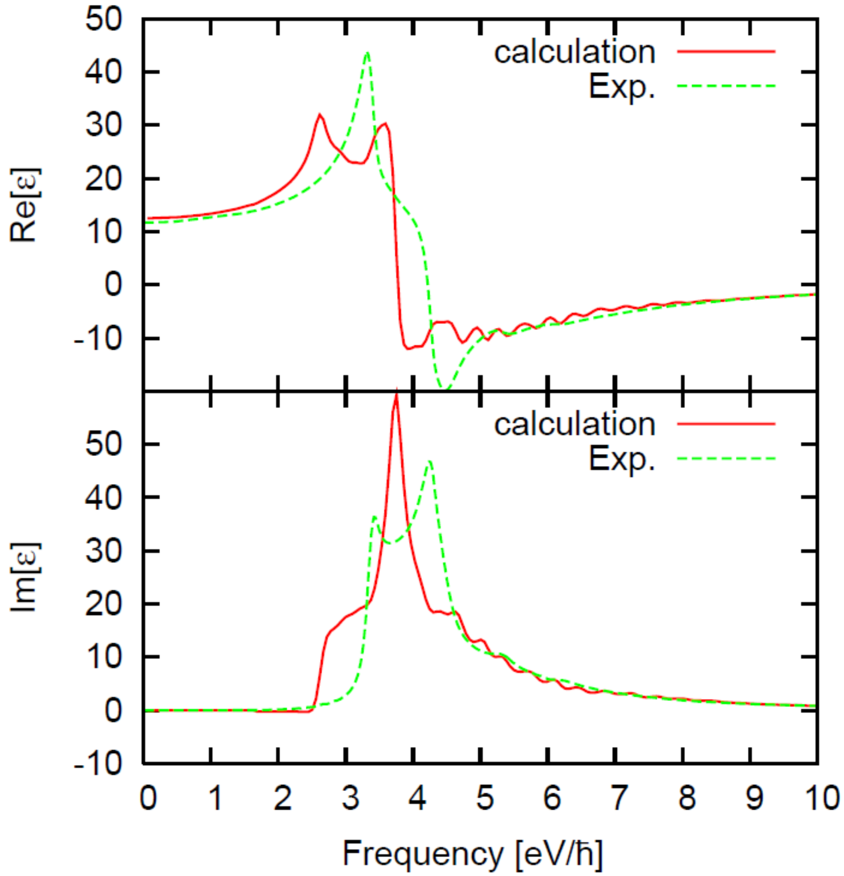
$$E_{ext}(t) \propto \delta(t)$$

Example: diamond





Dielectric function of Si
in TDDFT (Adiabatic LDA)



Quantitatively not sufficient
- Too small direct bandgap
- Lack of excitonic structure

Dots: experiment
Dash-dotted: RPA
Solid: Bethe-Salpeter
(electron-hole interaction considered)

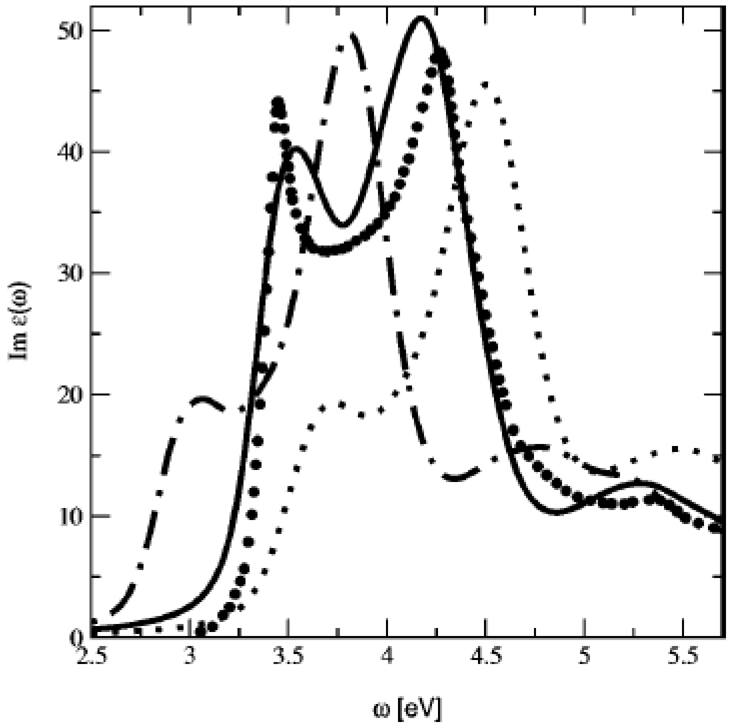
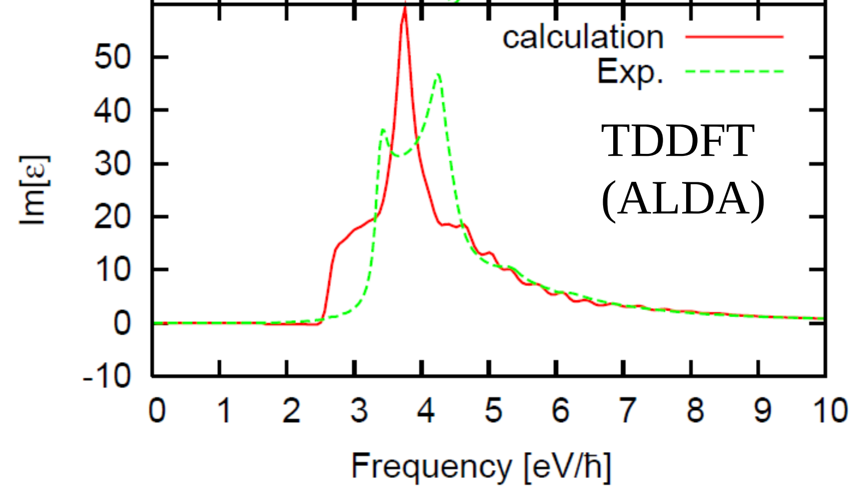
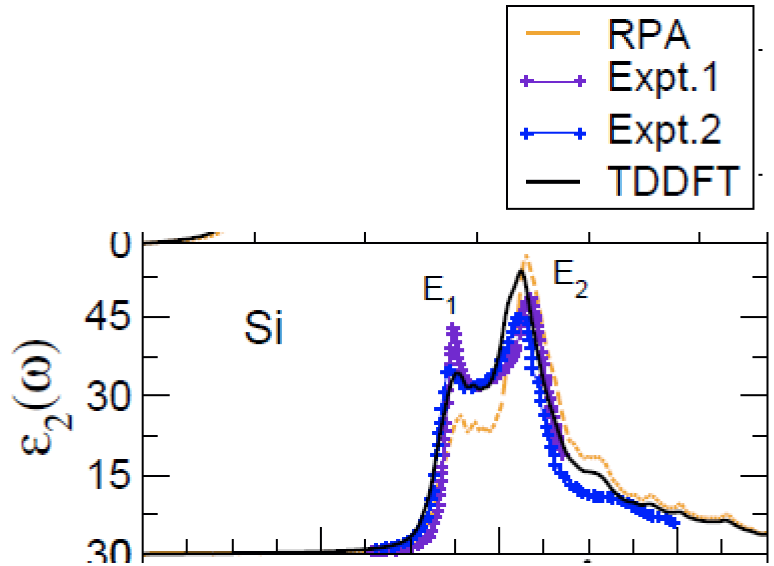


FIG. 5. Silicon absorption spectrum [Im(ε_M)]: ●, experiment (Lautenschlager *et al.*, 1987); dash-dotted curve, RPA, including local field effects; dotted curve, *GW*-RPA; solid curve, Bethe-Salpeter equation.

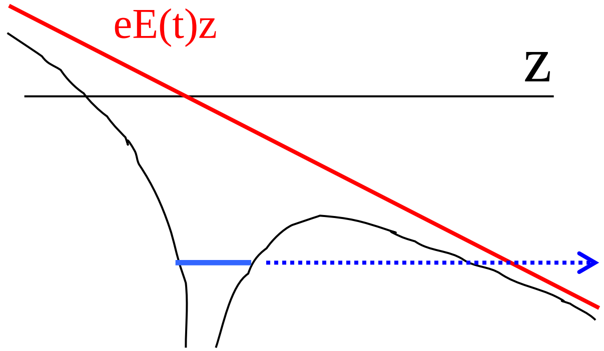
G. Onida, L. Reining, A. Rubio,
Rev. Mod. Phys. 74(2002)601.





arXiv:1107.0199 (July 1, 2011)
S. Sharma, J.K. Dewhurst, A. Sanna, E.K.U. Gross,
Bootstrap approx. for the exchange-correlation kernel of time-dependent density functional theory

TDDFT in nonlinear regime: Intense and Ultrashort Laser Pulse



Electric field of laser pulse
≅ Electric field inside materials

Intense field — 10^{13}-10^{15} W/cm^2

Quantum
Nonlinear
Nonperturbative

Classical
Relativistic

Ultrashort — 10^{-15}s (1 femto sec)

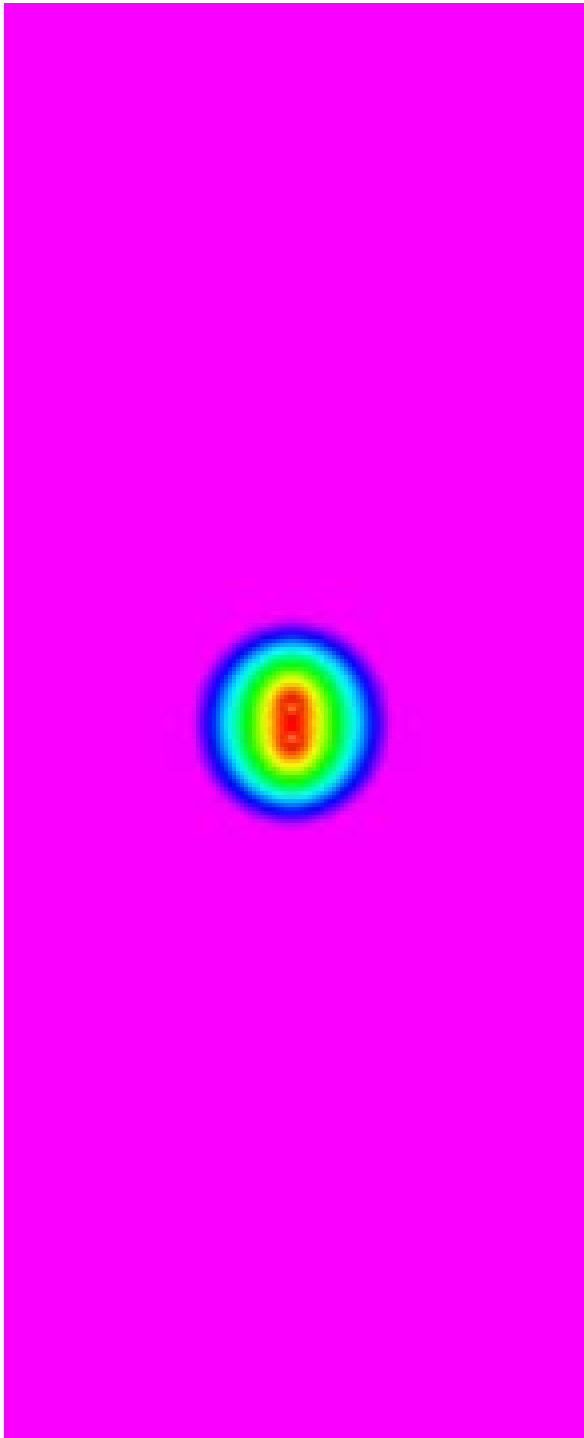
frozen ion

frozen electron

Intense laser pulse on atoms and molecules induces nonlinear electron dynamics

Rescattering phenomena

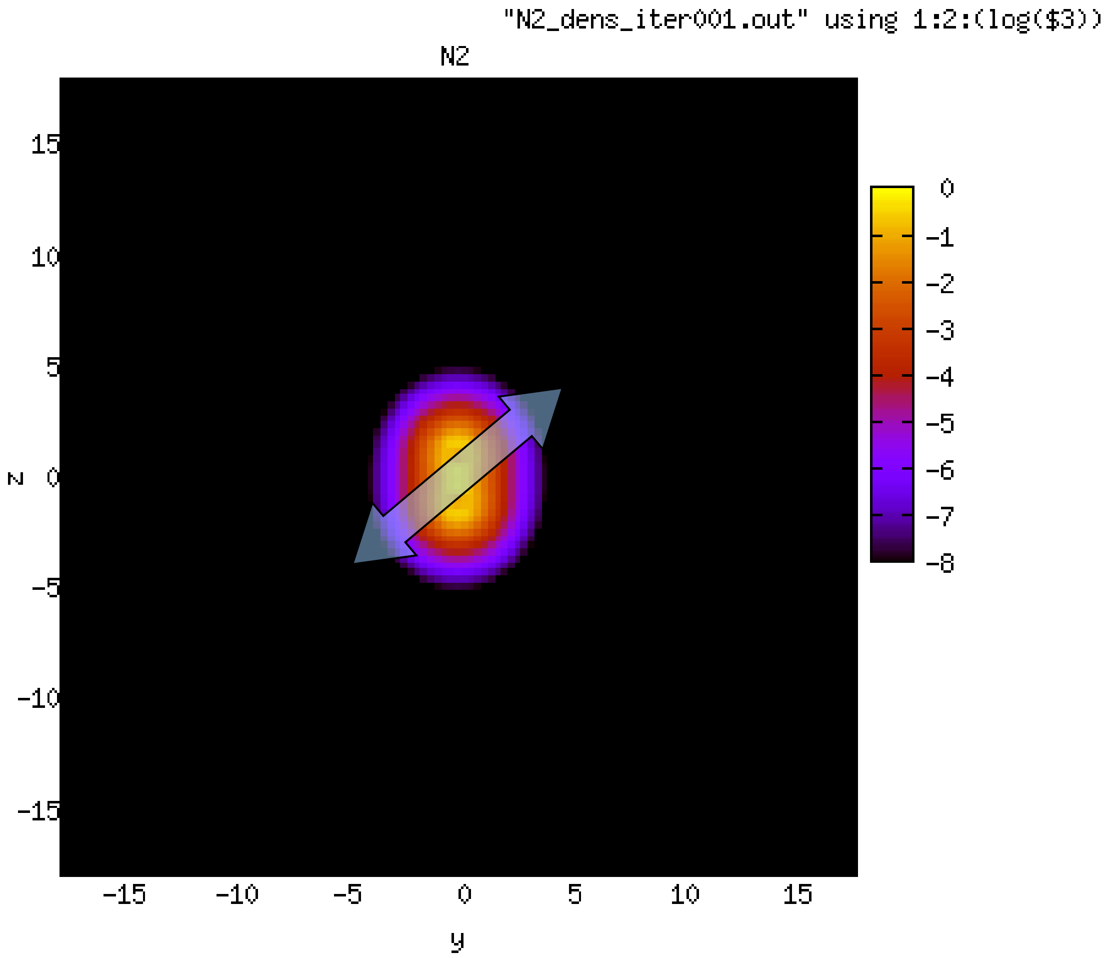
- Ultrashort X-ray
- Atto-second science
- Molecular orbital tomography
- …



Ethylene (C_2H_4) molecule

Coulomb explosion: N_2 molecule under intense laser pulse

$I=3.35\times10^{15}$W/cm^2, 27fs



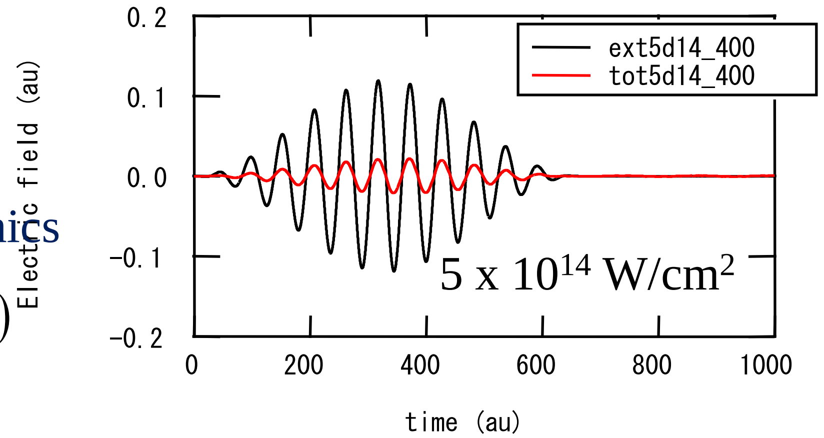
Y. Kawashita, Ph.D thesis

As the laser intensity increases,

$E_{ext}(t)$ vs $E_{tot}(t)$

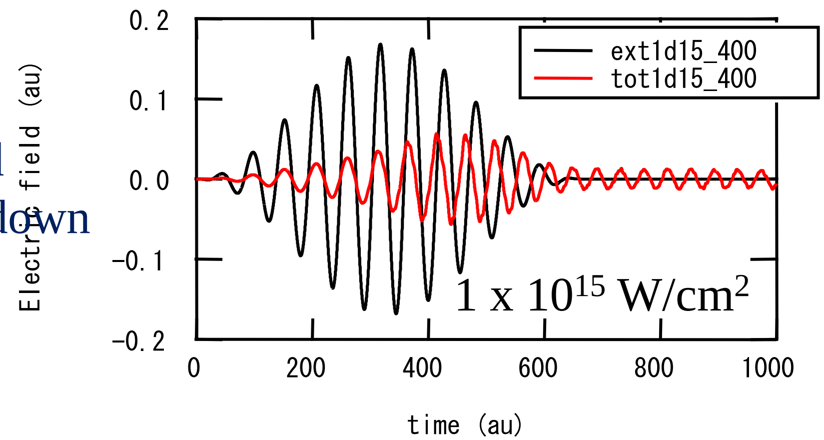
Weak field:
Dielectric dynamics

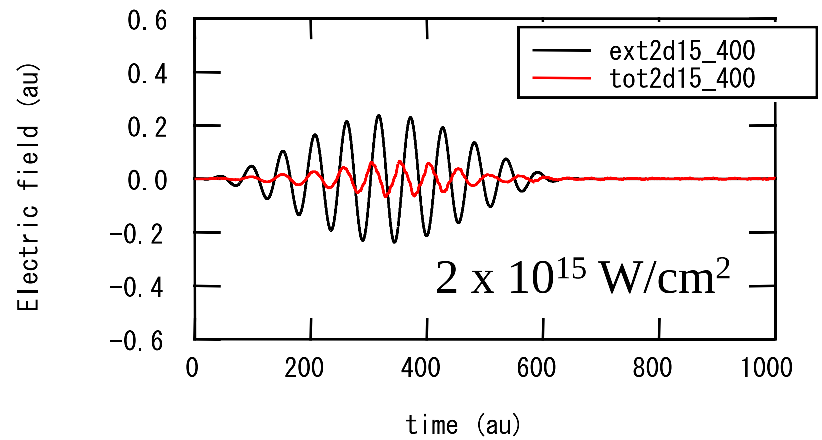
$$E_{tot}(t) \propto \frac{1}{\varepsilon(\omega)} E_{ext}(t)$$



Diamond
frequency: 3.1eV
pulse length: 16fs

Threshold
for breakdown





T. Otobe, M. Yamagiwa, J.-I. Iwata, K.Y. T. Nakatsukasa, G.F. Bertsch, Phys. Rev. B77, 165104 (2008)

Behavior around breakdown
(1×10^{15} W/cm^2, 3.1eV, 40fs)

Initial stage < 15fs, dielectric screening

$$\varepsilon(0) \approx 5.7$$

Substantial excitation, 15-20fs

- phase difference between $E_{ext}(t)$ and $E_{tot}(t)$
- rapid increase of excited electron number and energy transfer
  $\Rightarrow$ Dielectric breakdown

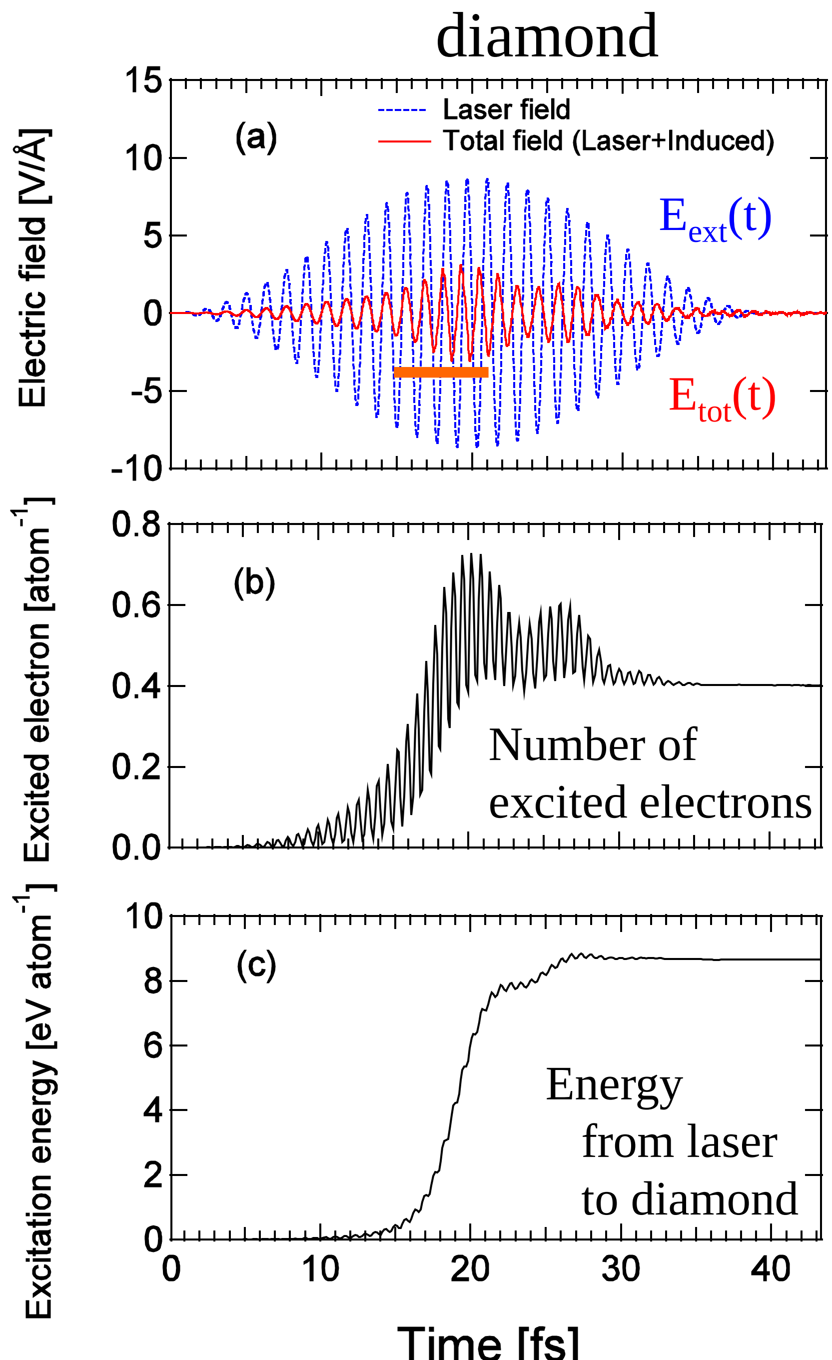
Metallic response, > 25 fs

- no further increase of excited electron number and energy transfer

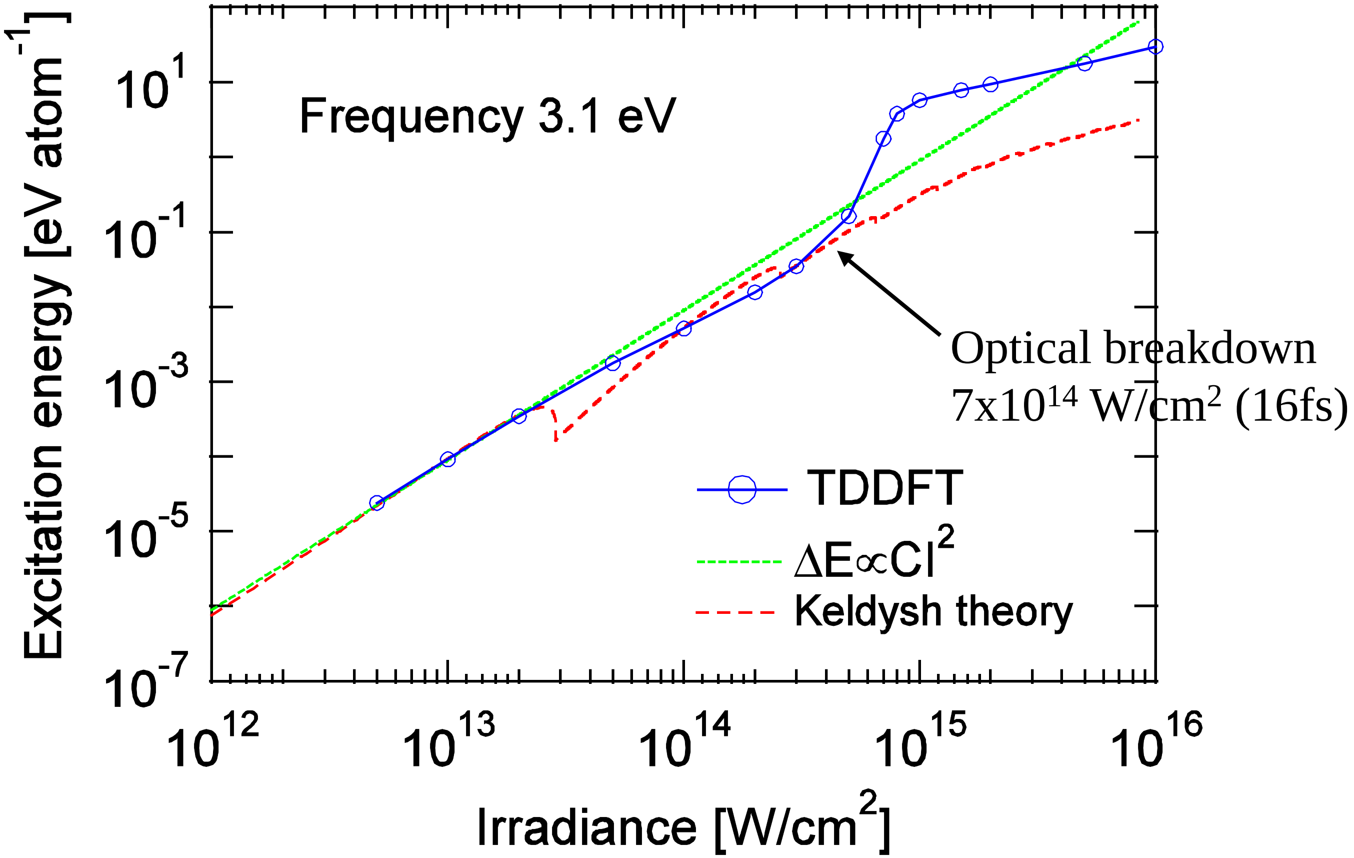
Note: plasma frequency for 0.4/atom

$$\omega_p = \left(\frac{4\pi n_{ex}}{m\varepsilon(0)}\right) \approx 4\text{eV}$$

close to frequency of laser pulse, 3.1eV



Energy transfer from laser pulse to diamond



Two photon curve (green)
Analytic theory by Keldysh (1965) (red)

Interaction of Intense and ultrashort laser pulse with solids

We know the basic equation, but…

$$i\hbar\frac{\partial}{\partial t}\psi_i = \frac{1}{2m}\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right)^2\psi_i - e\phi\psi_i + \frac{\delta E_{xc}}{\delta n}\psi_i \qquad n = \sum_i |\psi_i|^2$$

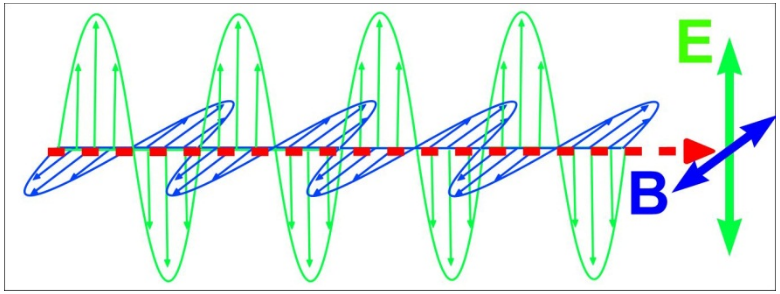
$$\frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} - \vec{\nabla}^2\vec{A} = \frac{4\pi}{c}\vec{j} \qquad \vec{\nabla}^2\phi = -4\pi\{en_{ion} - en_e\}$$

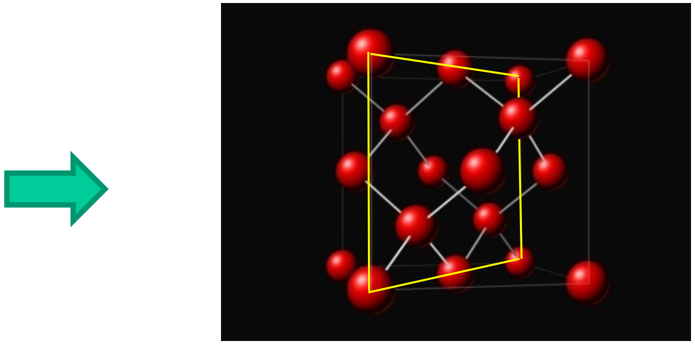
Light propagation in matter
described by Maxwell equation

$$E(\vec{r},t), \quad B(\vec{r},t)$$

Electron dynamics
described by time-dep. Kohn-Sham eq.

$$\psi_i(\vec{r},t)$$





For weak electromagnetic wave, we may apply perturbation theory for electron dynamics to obtain dielectric function $\varepsilon(\omega)$.
Then, Schroedinger and Maxwell equations decouple.

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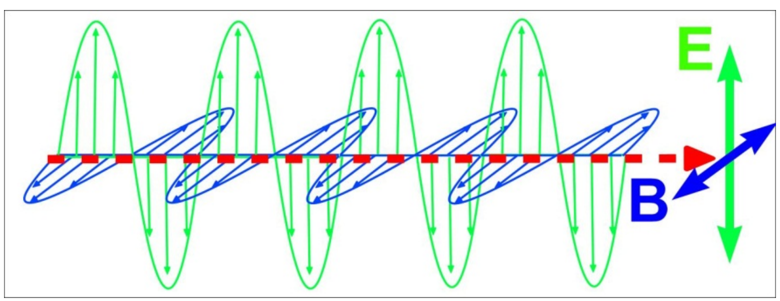
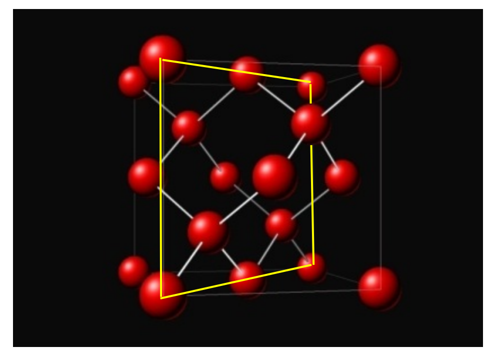


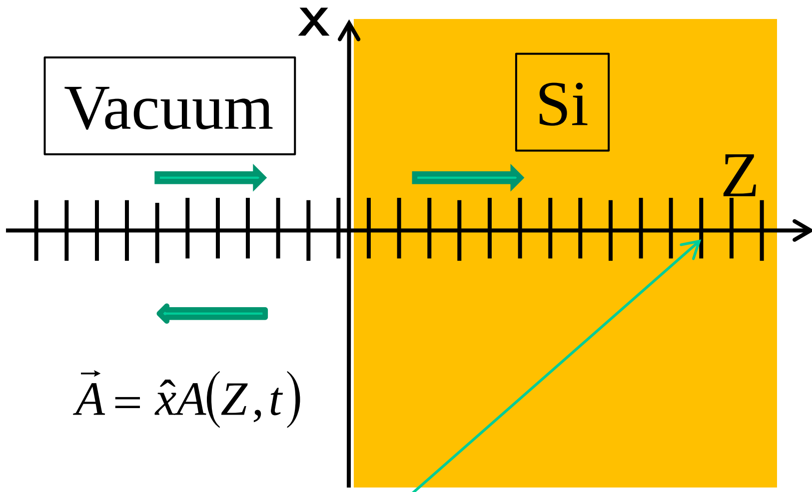


wave length [μm]

Electron dynamics [nm]

For intense electromagnetic field, $D \neq \varepsilon(\omega)E$.
We must solve “coupled Maxwell + Schroedinger eq”.
We also note that there are two different spatial scales, “multi-scale problem”

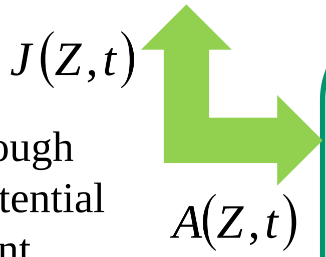
Coupled Maxwell + TDDFT multi-scale simulation
- 1D propagation of laser pulse incident normally on Si surface -



$$\vec{A} = \hat{x} A(Z,t)$$

Macroscopic vector potential
(discretized in μm scale)

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} A(Z,t) - \frac{\partial^2}{\partial Z^2} A(Z,t) = \frac{4\pi}{c} J(Z,t)$$



Coupled dynamics through macroscopic vector potential and macroscopic current

$$J(Z,t) = \int_{\Omega} d\vec{r}\, \vec{j}_{e,Z}$$

$$\vec{j}_{e,Z} = \frac{\hbar}{2mi} \sum_i \left(\psi^*_{i,Z} \vec{\nabla} \psi_{i,Z} - \psi_{i,Z} \vec{\nabla} \psi^*_{i,Z} \right) - \frac{e}{4\pi c} n_{e,Z} \vec{A}$$

At each macroscopic point, we assume dipole (uniform electric field) approximation.

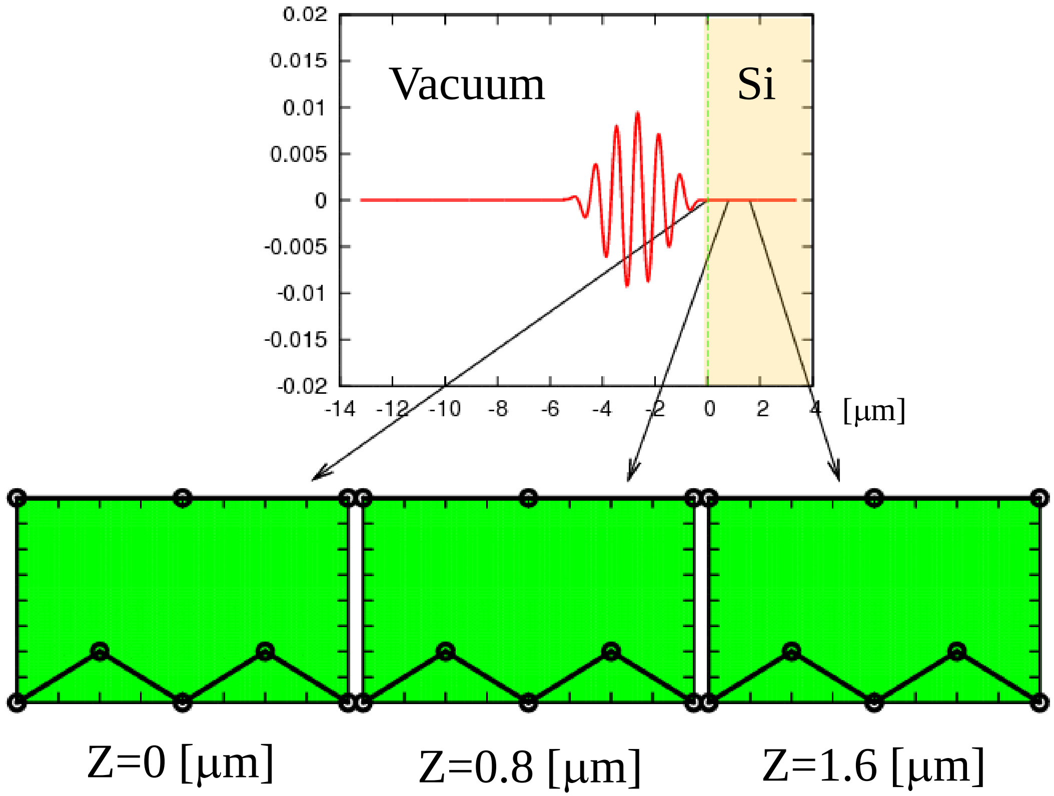
$$i\hbar \frac{\partial}{\partial t} \psi_{i,Z} = \frac{1}{2m} \left(-i\hbar \vec{\nabla} + \frac{e}{c} \vec{A} \right)^2 \psi_{i,Z} - e\phi_Z \psi_{i,Z} + \frac{\delta E_{xc}}{\delta n} \psi_{i,Z}$$

$$\vec{\nabla}^2 \phi_Z = -4\pi \left\{ e n_{ion} - e n_{e,Z} \right\}$$

Laser pulse on Si : Maxwell-TDDFT multi-scale calculation

Weak pulse, linear response regime

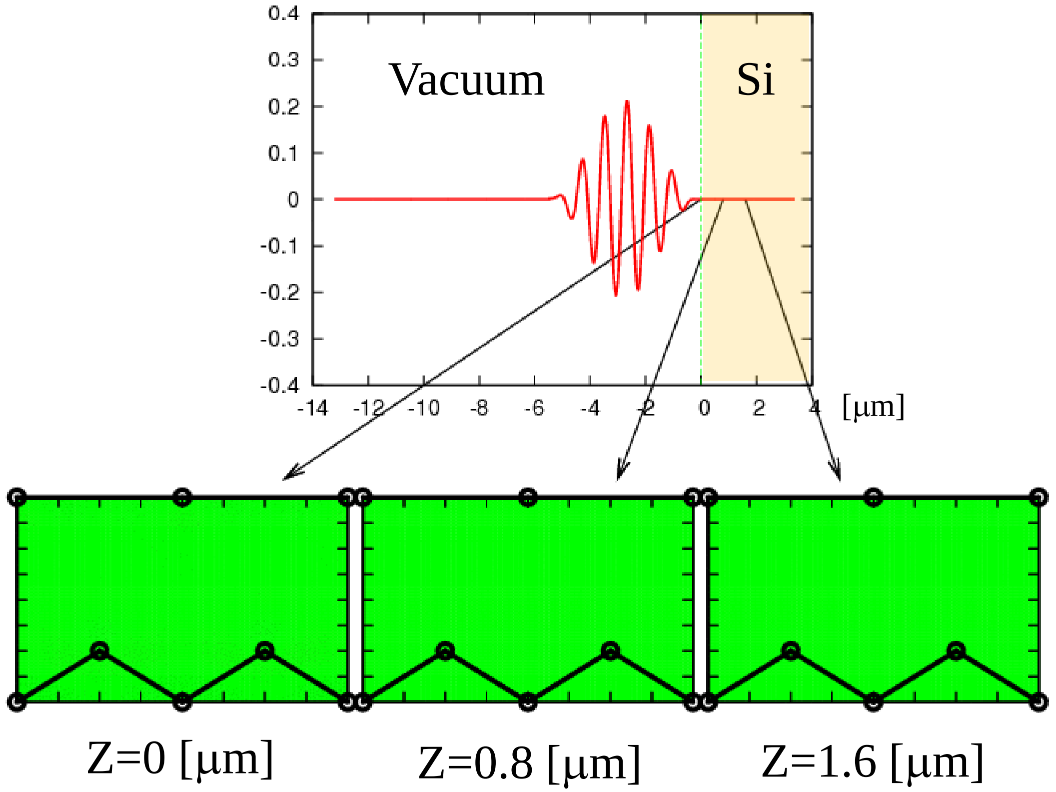
$I=10^{10}W/cm^2$



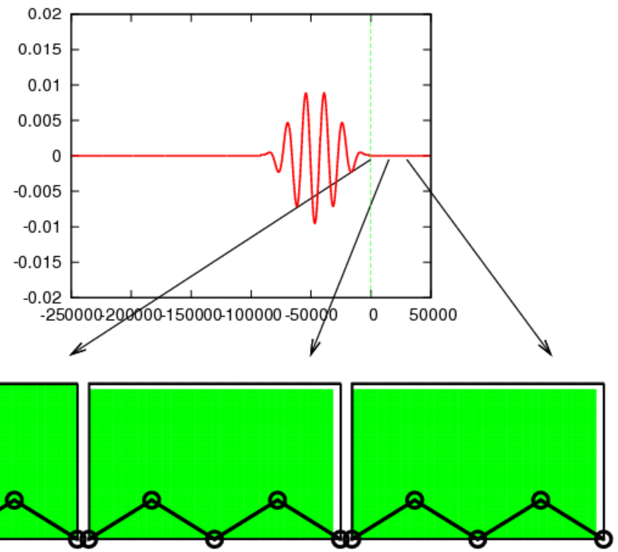
Laser pulse on Si : Maxwell-TDDFT multi-scale calculation

Intense pulse, nonlinear regime

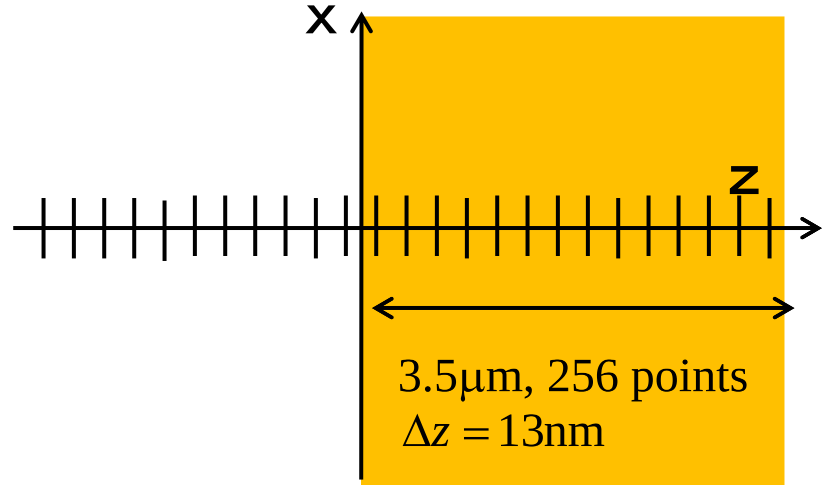
$I=5 \times 10^{12} W/cm^2$



Computational aspects



Microscopic (TDKS)
spatial grid: 16^3
k-points : 8^3 (reduced by symmetry)



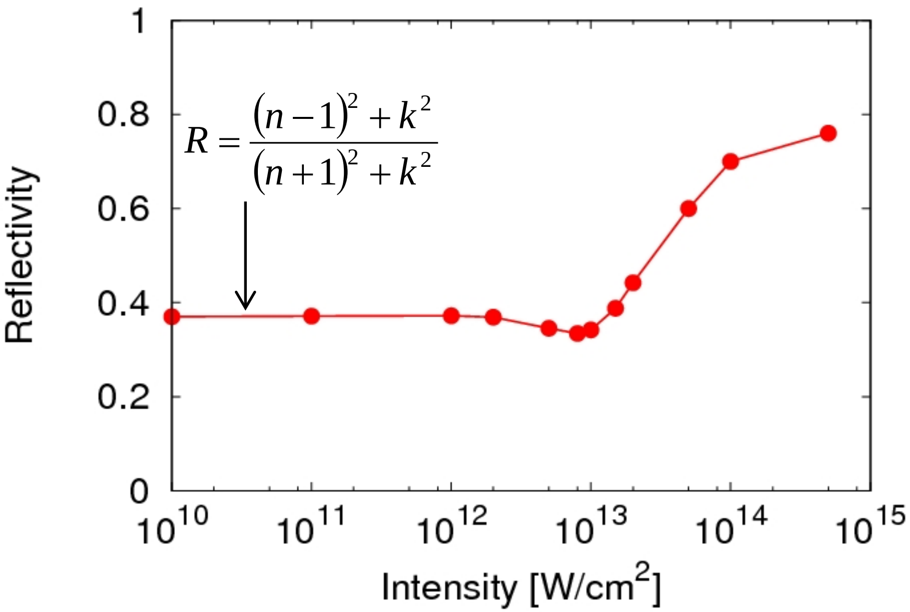
Macroscopic (Maxwell)
spatial grid: 256

Time step (commom) = 16,000

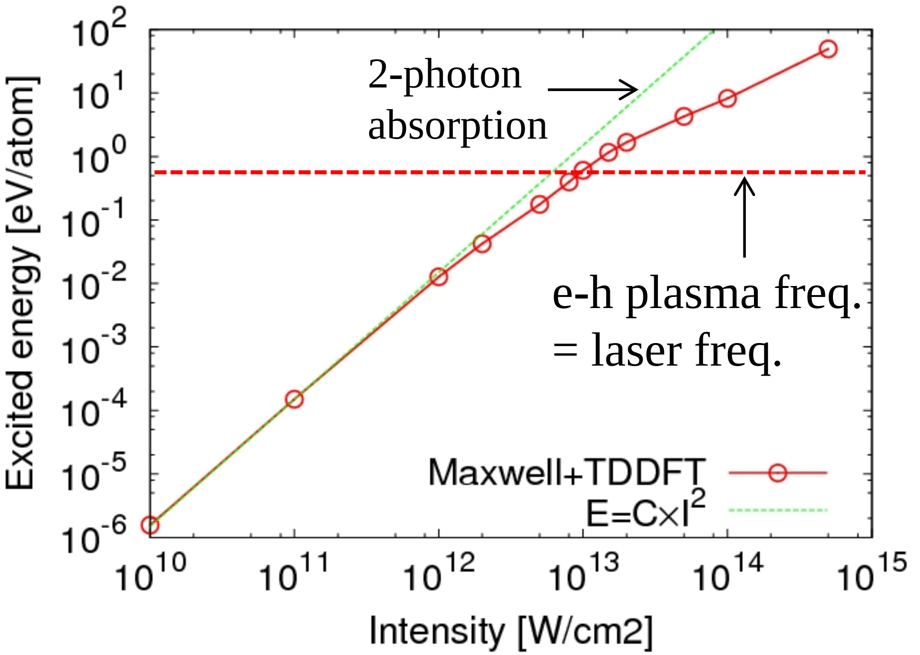
1024 Cores, 15 hours @ ISSP, Univ. Tokyo

Formation of electron-hole plasma at the surface of Si (under progress)

Reflection at Si surface



Excited electron density at the surface of Si

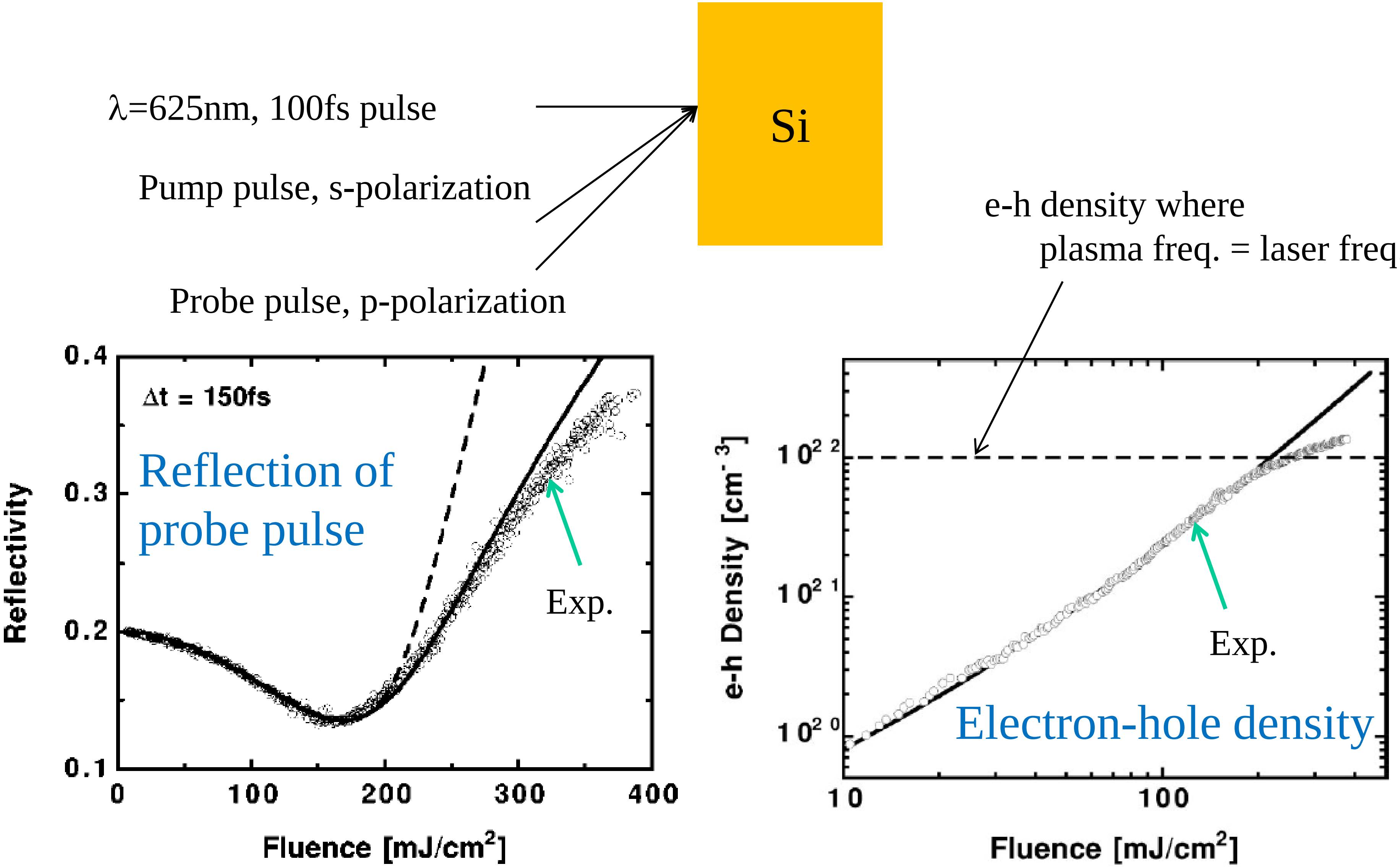


Laser Intensity	↓	Dielectric response
		Electron excitation by 2-photon absorption
		Formation of electron-hole plasma

Related measurement:

"Generation of dense electron-hole plasma in silicon"

K. Sokoowski-Tinten, D. von der Linde, Phys. Rev. B61, 2643 (2000)



Summary

Real-space, real-time TDDFT calculation

useful for linear and nonlinear dynamics of condensed many-fermion systems, isolated and periodic systems.

Linear response regime

- accurate description for oscillator strength distribution

Nonlinear electron dynamics in ultrashort and ultraintense laser field

- interaction of intense and ultrashort laser pulse with matter
- propagation of light: Maxwell + TDDFT multi-scale simulation

Future problems

- Collision effect is important,
  how to incorporate in systems with gap; Kadanoff-Baym eq?