Computational Approach for Dynamics of Many-Fermion Systems

- from Nuclear Physics to Optical Science -

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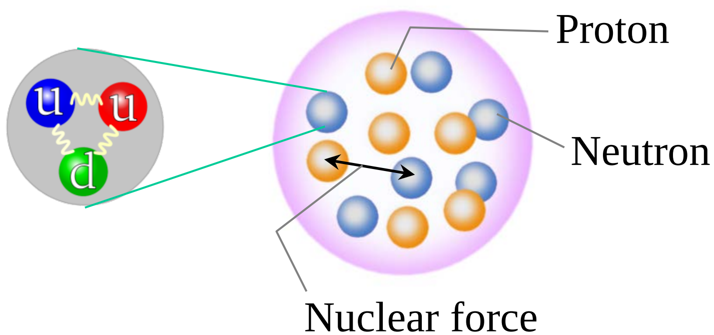
Links among Hierarchies in Nuclear Physics

Combining particle physics,
nuclear physics,
and astrophysics by computation

- Origin of elements

- Evolution of the universe

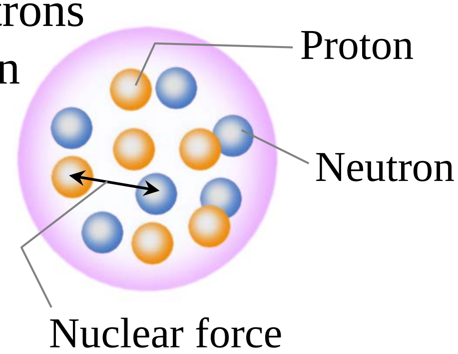



Fuel of Stars

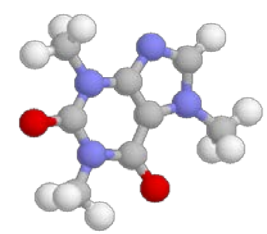

Origin of Elements

Quantum dynamics of
many-fermion systems

Nuclei
protons and neutrons
strong interaction



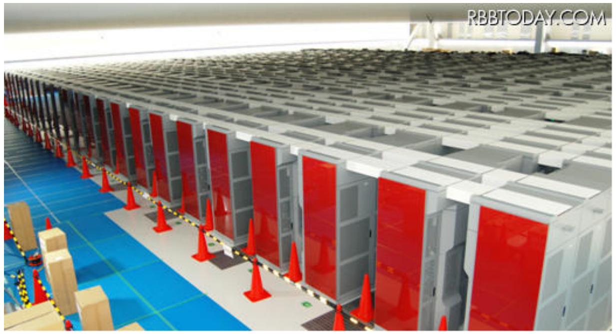
Atoms, molecules, solids
electron many-body system
Coulomb interaction



Computational Approach for Dynamics of Many-Fermion Systems:

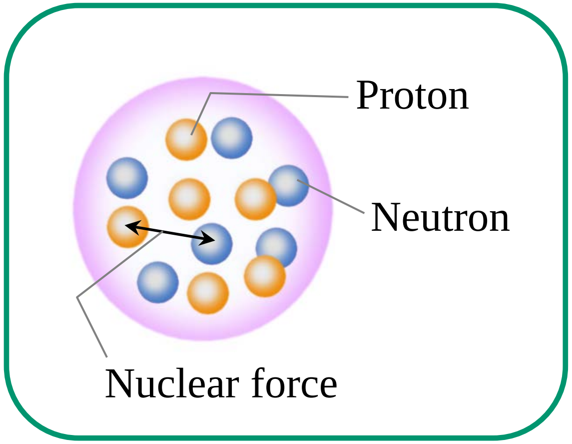
- from Nuclear Physics to Optical Science -

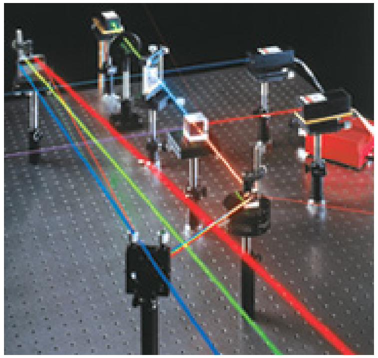
Large-scale computing has a high potential to link different hierarchies.



K-computer@Kobe

A number of concepts and methods on finite, quantum, fermion systems have been developed in nuclear physics.





Optical sciences developing as multi-disciplinary fields.
In particular, nonlinear electron dynamics by intense and ultrashort laser pulses.

Let me start to talk on

How I come to work on electron dynamics.

Quantum Simulation for Many-Fermion Systems: Nuclear Collision

Time-dependent Hartree-Fock theory.
3D time-dependent Schroedinger equation is solved with real-time and real-space method.

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

Time evolution of proton and neutron orbitals.

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)=h[n(\vec{r},t)]\psi_i(\vec{r},t)$$

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

$$\psi(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N,t)=A\{\psi_1(\vec{r}_1,t)\psi_2(\vec{r}_2,t)\cdots\psi_N(\vec{r}_N,t)\}$$

17 THREE-DIMENSIONAL TIME-DEPENDENT HARTREE-FOCK...

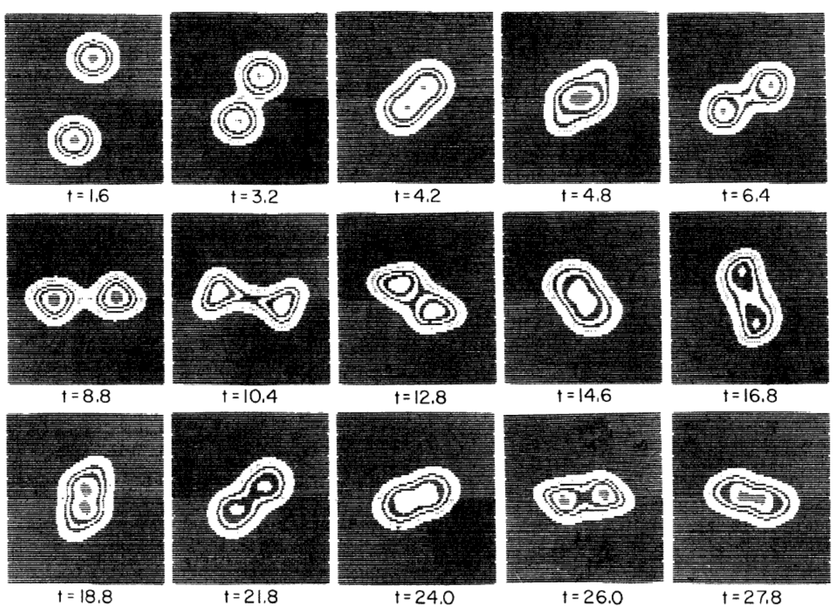
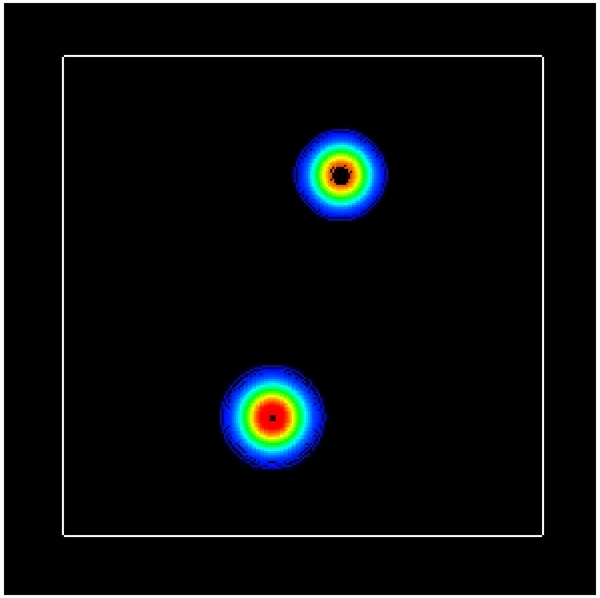


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{1ab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

Spatial grid 30x28x16, time step 4x10^2

^{24}O – ^{16}O collision at E=16 MeV



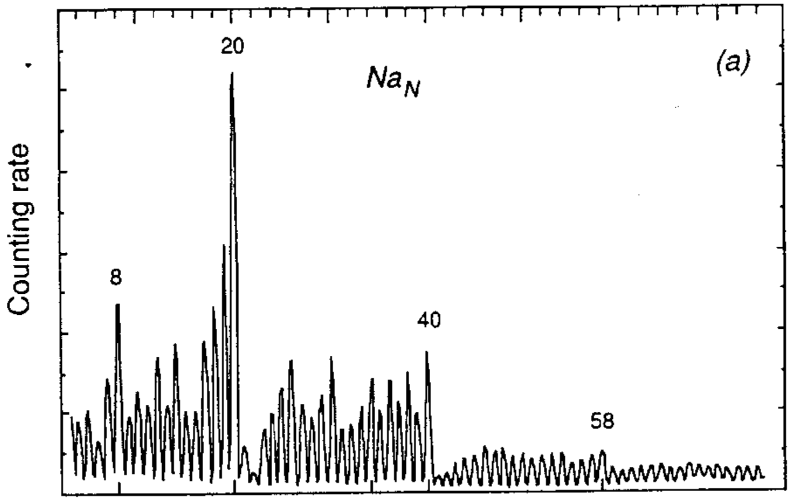
Time: 10^{-22}s, Length: 10^{-14}m

Crossover between nuclear physics and nanoscience: Atomic clusters

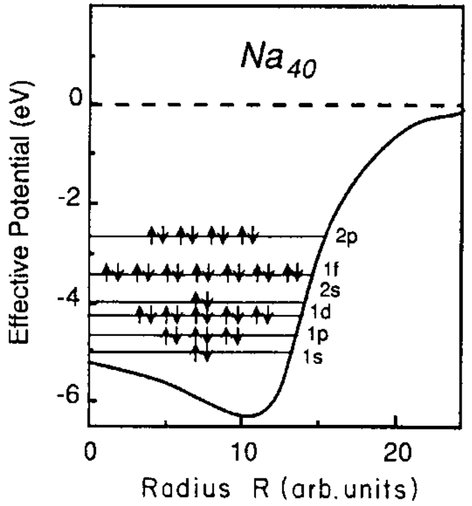
Synthesis of atomic clusters in cluster beam in the vacuum
- 1984: Discovery of magic numbers in metallic clusters
  Prediction of giant dipole resonance (soon observed)
- 1985: Discovery of fullerene C_{60} in cluster beam

(I was in graduate school during 1982-1987)

Abundance spectrum of Alkali metal clusters, electronic mean field and magic number



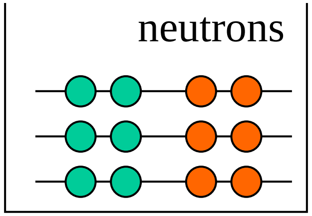
Magic number in Na clusters
Knight et.al.(1984)



Metallic clusters : 2,8,20,40,58,92,138, ...

Atomic nuclei : 2,8,20,28,50,82,126, ...

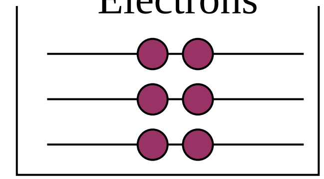
Protons and neutrons



Nuclei

Finite Fermion Systems confined in spherical potential

Electrons

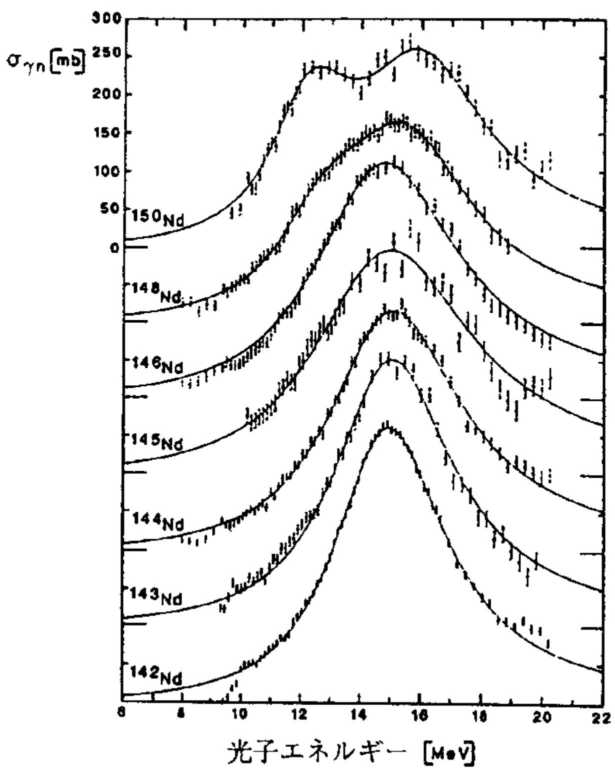


Metallic clusters

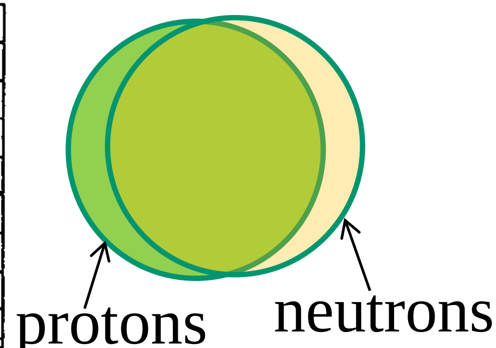
Common properties

- Magic number
- Deformation
- Collective excitation

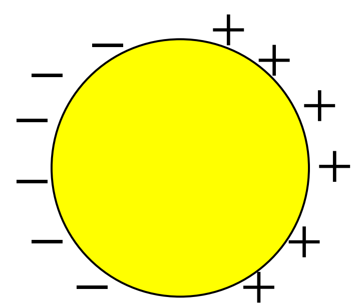
Giant Dipole Resonance

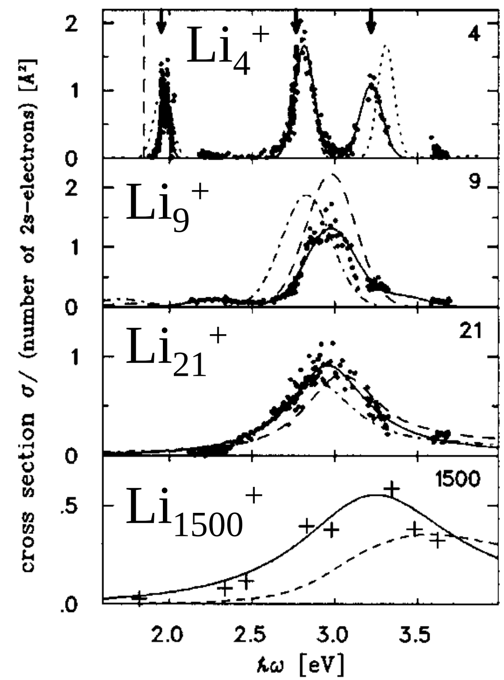


Optical absorption of atomic nuclei



Mie plasmon, a surface plasmon of spherical particle





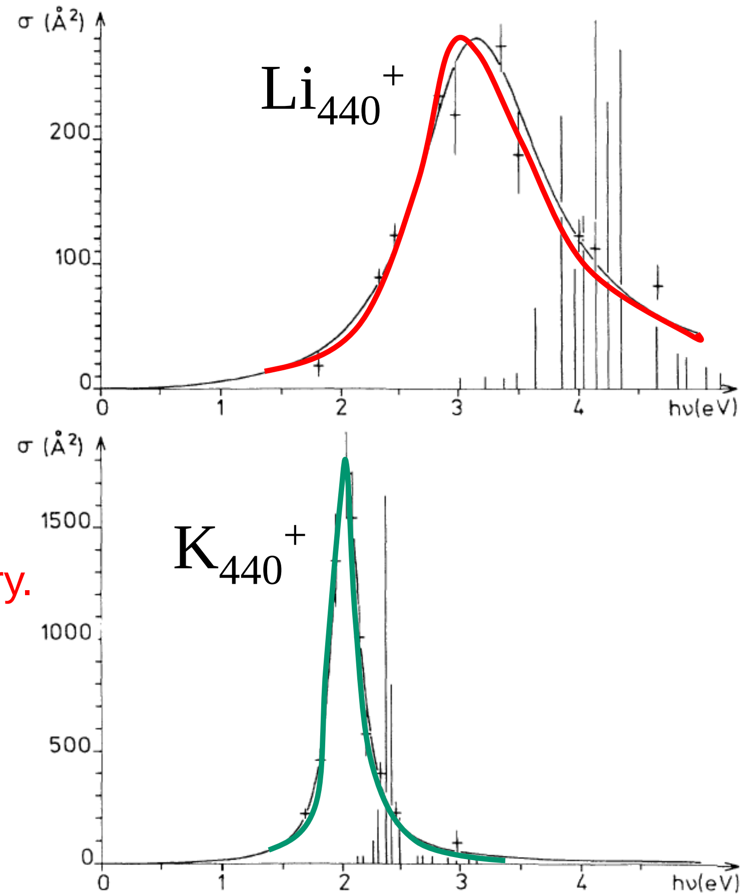
Optical absorption spectrum of Li clusters

I participated in atomic cluster physics in 1992.
There are a lot of interesting but “complex and difficult” problems.

- Different shape of absorption profiles among alkali metals, Li, Na, K. Why?

- Bulk concepts (e.g. dielectric function) effective for small systems?

How to describe optical response?
- Hundred of electrons.
- Roughly spherical but precisely having no symmetry.



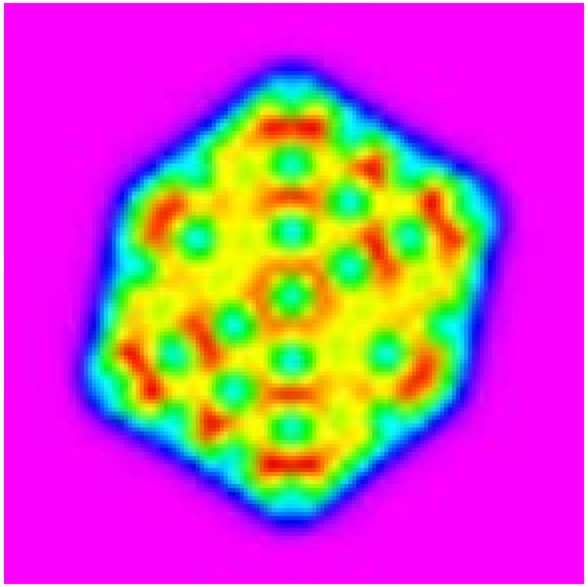
Absorption spectrum (Mie plasmon) of Alkali-metal clusters, Li and K

My answer was to combine - Nuclear time-dependent mean-field method –
and - First-principles density-functional theory in condensed matter physics -

$$i\hbar \frac{\partial}{\partial t}\psi_i(t) = \{h_{KS}[\rho(t)] + V_{ext}(t)\}\psi_i(t)$$

$$\rho(t) = \sum_i |\psi_i(t)|^2$$

Electron density change from that in the ground state.



Na_{147}^{+}

Assume icosahedral geometry

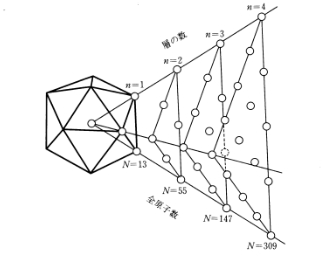
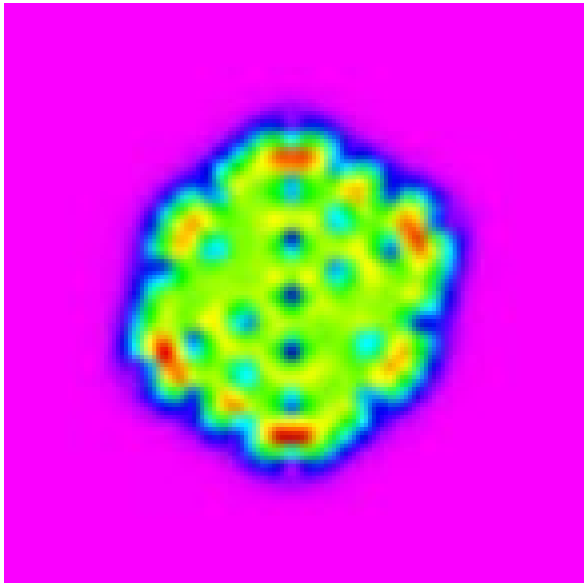
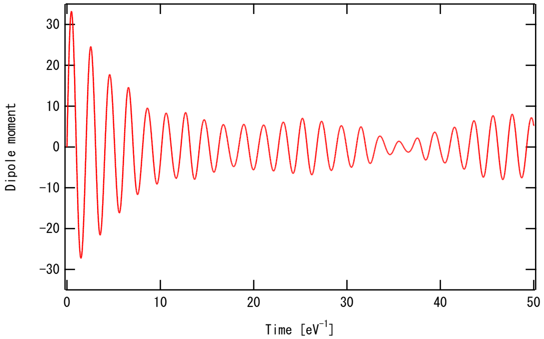
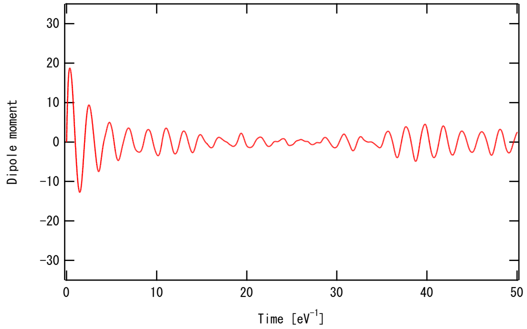


図 5·61 多層正二十面体構造(MIC)の概念図[104)]
n は MIC の層の数であり，N は全原子数である。1 層構造($n=1$)では原子数 $N=13$ に対応し，2 層構造($n=2$)では $N=55$，3 層構造($n=3$)では $N=147$…となる。



Li_{147}^{+}

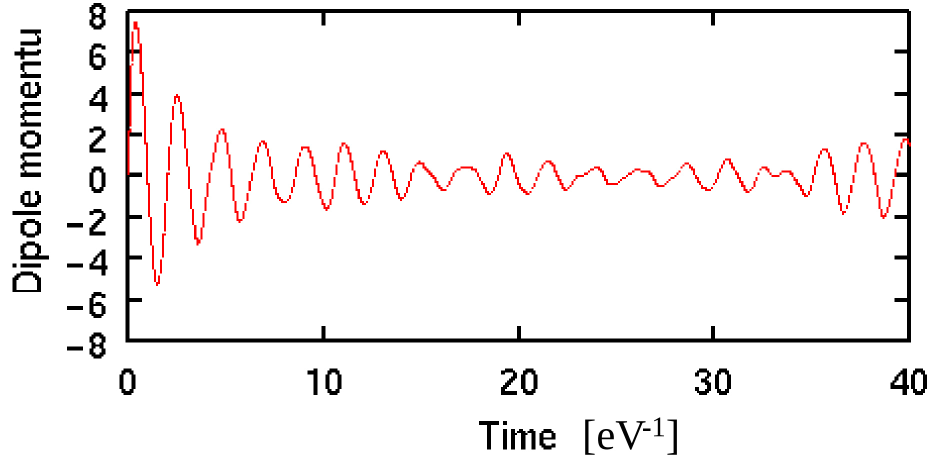




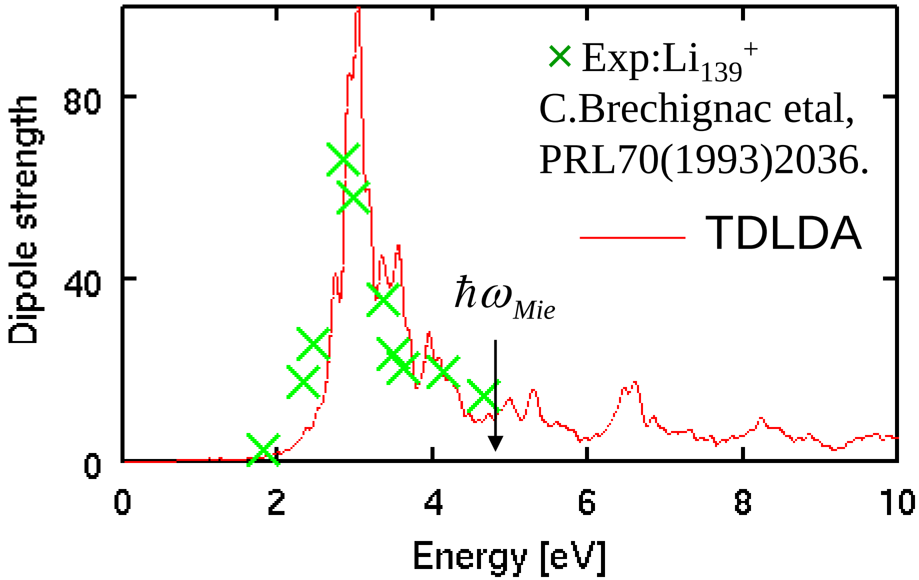
Optical absorption spectrum of Li_{147}^{+}

K. Y, G.F. Bertsch, Phys. Rev. B54, 4484 (1996).

$$\alpha(t) = \frac{e^2}{\hbar k} \int d\vec{r}\, z \rho(\vec{r}, t)$$



$$\alpha(\omega) = \int dt e^{-i\omega t} \alpha(t)$$



The width comes from electron-atom elastic scattering (Landau damping)

Time-dependent mean-field theory

$$i\hbar \frac{\partial}{\partial t}\psi_i(t) = \{h_{KS}[\rho(t)] + V_{ext}(t)\}\psi_i(t)$$

$$\rho(t) = \sum_i |\psi_i(t)|^2$$

Single-particle dynamics in mean-field potential

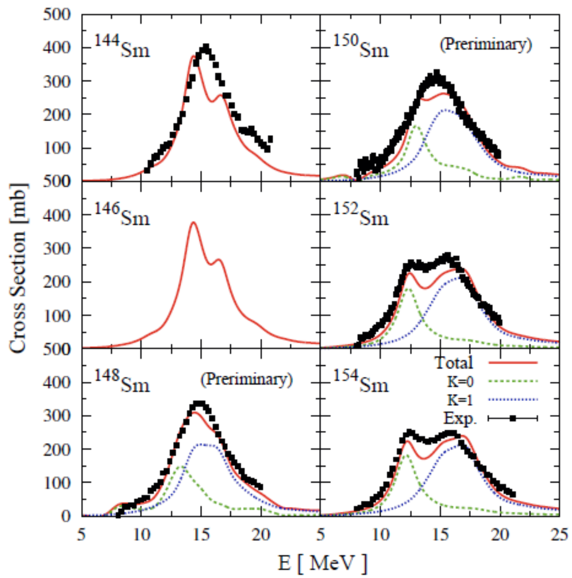
- Protons and neutrons in nuclei
- Electrons in atoms, molecules, and solids

TDHF (Time-dependent Hartree-Fock)
TDDFT (Time-dependent density-functional theory)

Universal tool for photoabsorption

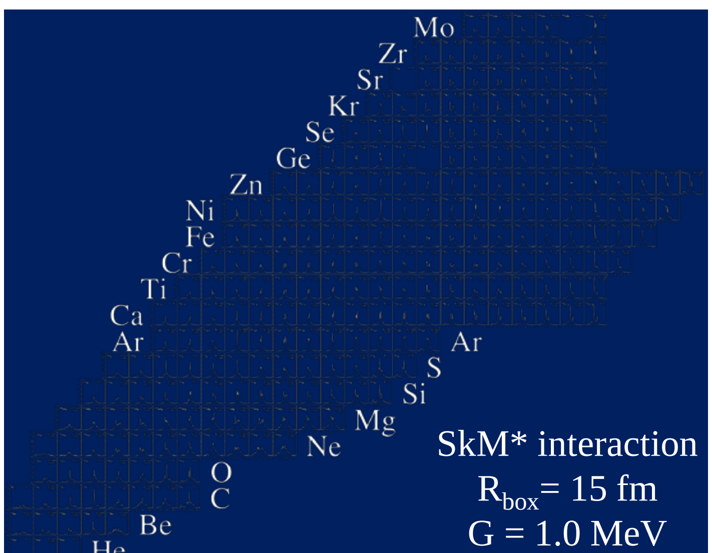
Nuclei

Real-time TDHF+BCS, S. Ebata Ph.D thesis (2010)



Attempt for systematic calculations

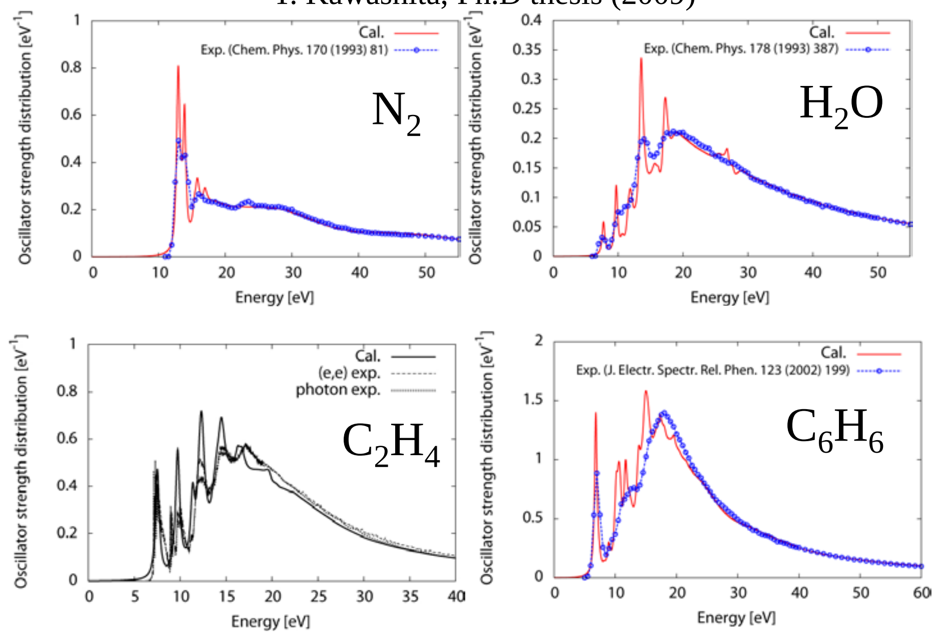
T. Inakura, T. Nakatsukasa, K.Y. Phys. Rev. C80, 044301 (2009)



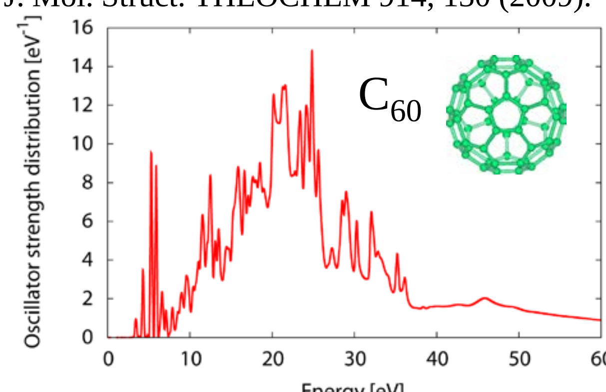
Molecules

Absorption spectra of molecules by real-time TDDFT

Y. Kawashita, Ph.D thesis (2009)



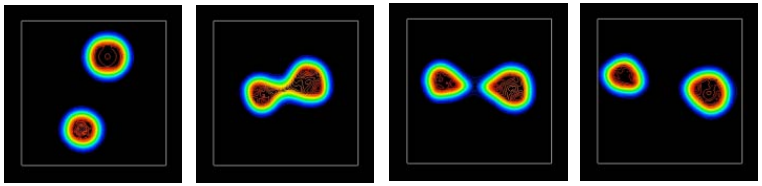
J. Mol. Struct. THEOCHEM 914, 130 (2009).



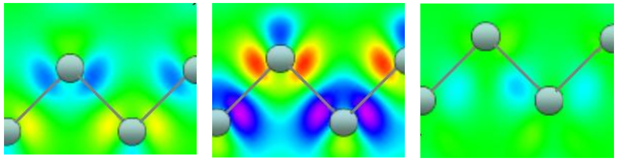
Optical absorption spectrum is a linear response property (within perturbation theory).
Next, on nonlinear fermion dynamics.

In low-energy nuclear physics, heavy-Ion collision has been the major phenomena of nonlinear nuclear dynamics.

In optical sciences, intense laser pulse induces a variety of phenomena reflecting nonlinear electron dynamics.

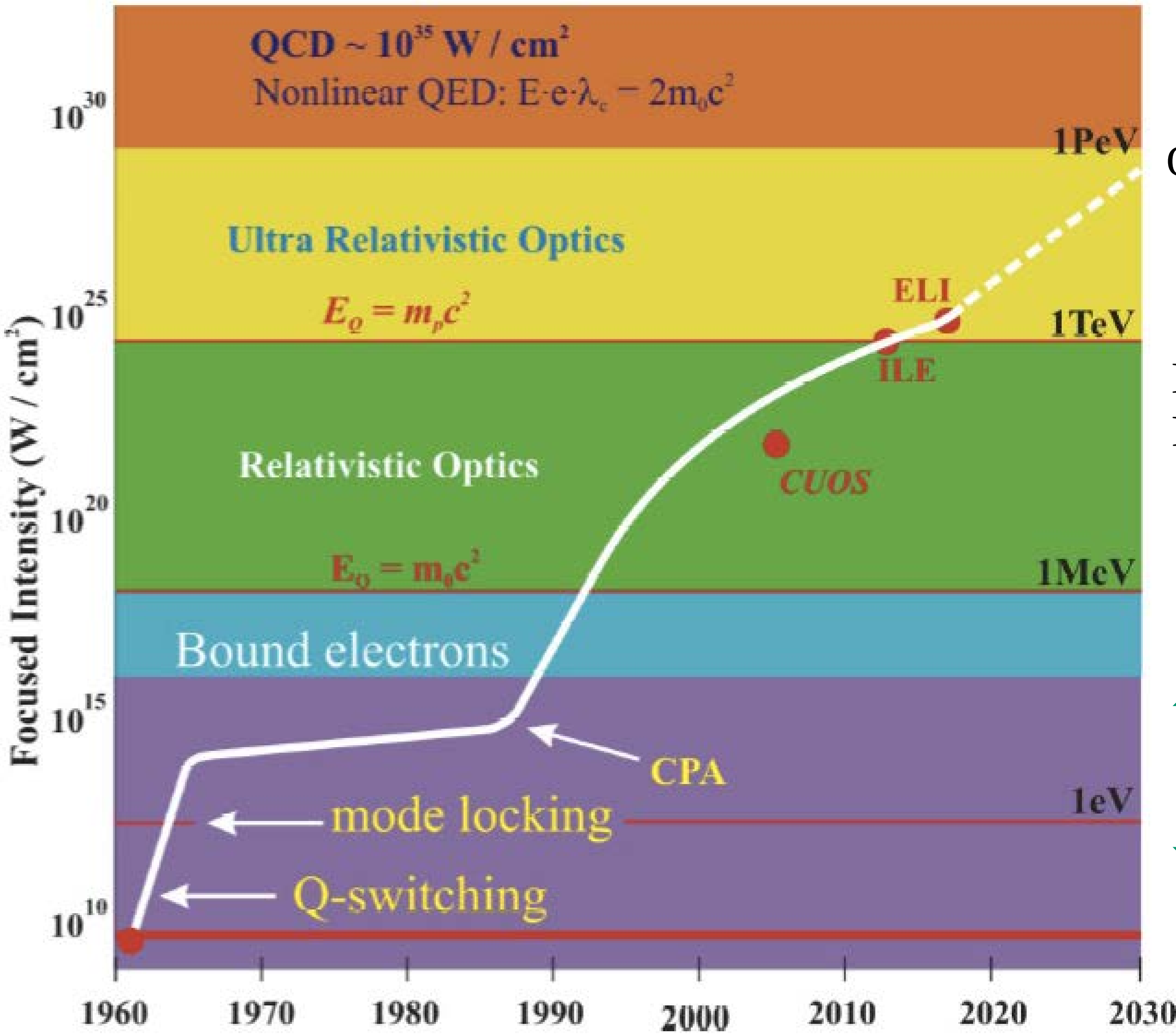


Nuclear TDHF simulation



Electron dynamics in solid, TDDFT simulation

Intense Laser Pulses: G. Mourou @ PIF2010



QED Vacuum breakdown

Nuclear reaction,
Particle Acceleration

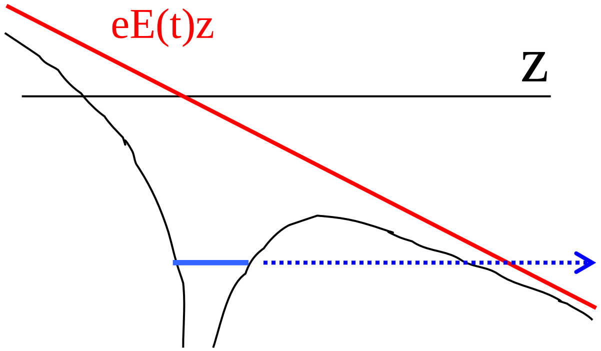
Relativistic
Classical

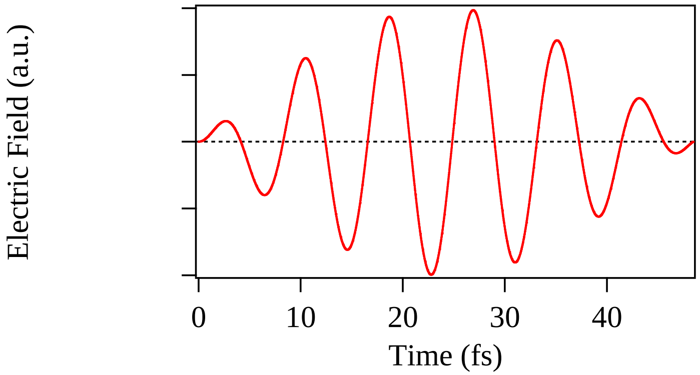
Nonlinear electron
dynamics

Nonrelativistic
Quantum

PIF2010 (International Conference on Physics in Intense Fields) (Nov. 24-26, 2010, KEK)

Intense and Ultrashort





10^{13}-10^{15}W/cm^2

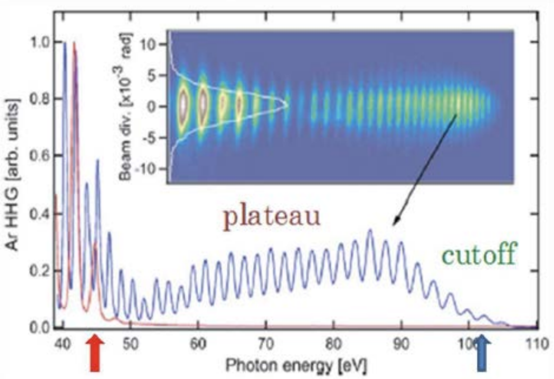
Intensity of applied laser pulse is comparable to electric field in matter which binds electrons.

10^{-15}s (1 femto sec)

Pulse duration shorter than molecular vibration comparable to electron dynamics.

Nonlinear Electron Dynamics
induced by intense and ultrashort laser pulse

Atoms:
High Harmonic Generation and Attosecond pulse generation



Solids:
Nonthermal laser machining, formation of electron-hole plasma by intense and ultrashort pulse

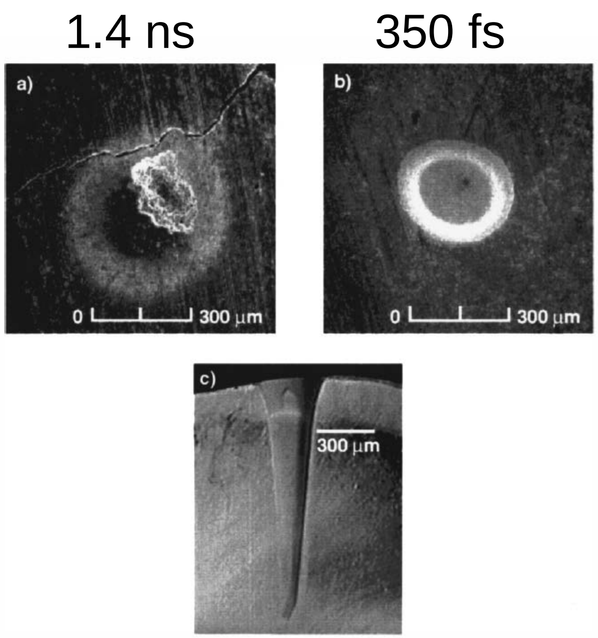
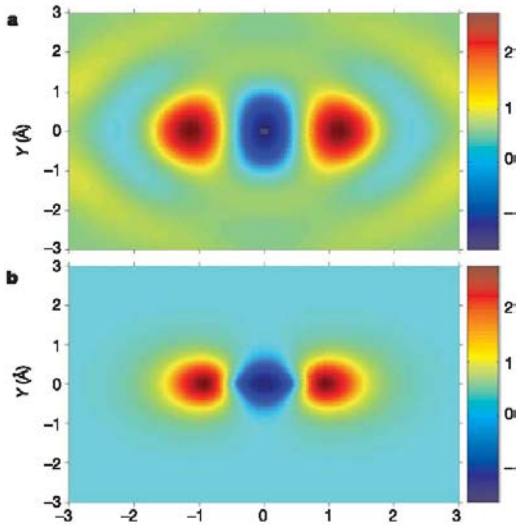


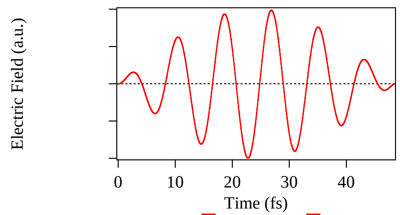
FIG. 1. (a) Drilling of enamel (tooth) with conventional 1053 nm, nanosecond pulses (ablation threshold=30 J/cm^2 for $\tau_p = 1.4$ ns). (b) Same as in (a) but with the pulse duration reduced to the ultrashort regime (ablation threshold=3 J/cm^2 for $\tau_p = 350$ fs). In both cases, the laser spot size was 300 μm. (c) cross section of hole made with 350 fs pulses.

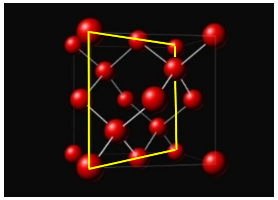
Molecules:
Tomographic imaging of molecular orbital by electron rescattering



Intense laser pulse propagation in solid
requires
undivided treatment of quantum mechanics and electromagnetism

Different length scales of light wavelength and atomic size
requires
multi-scale description





[μm] [nm]

Theoretical description of light propagation in matter
Electromagnetism and Quantum Mechanics

Maxwell equation	Constitutive relations	Schroedinger equation

$$\vec{\nabla}\cdot\vec{B}=0$$

$$\vec{\nabla}\times\vec{E}+\frac{\partial\vec{B}}{\partial t}=0$$

$$\vec{\nabla}\cdot\vec{D}=\rho$$

$$\vec{\nabla}\times\vec{H}-\frac{\partial\vec{D}}{\partial t}=\vec{j}$$

$$\vec{D}=\vec{D}\left[\vec{E},\vec{H}\right]\neq\varepsilon\vec{E}$$

$$\vec{B}=\vec{B}\left[\vec{E},\vec{H}\right]\neq\mu\vec{H}$$

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

$$\vec{\nabla}^2\phi=-4\pi\left\{en_{ion}-en_e\right\}$$

⇩ Linear response (perturbation) theory

$$\varepsilon(\omega),\ \mu(\omega)$$

For extremely intense field,
we need to solve coupled Maxwell + Schroedinger equations

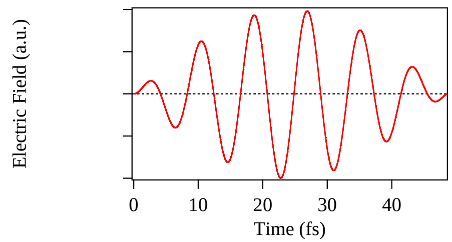
Two spatial scales, light wavelength [μm] and electron dynamics [nm]

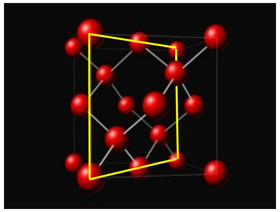
Microscopic Electron dynamics in crystalline Si under spatially uniform, time-dependent electric field

Time-dependent Bloch orbitals, an extension of band-theory for electron dynamics

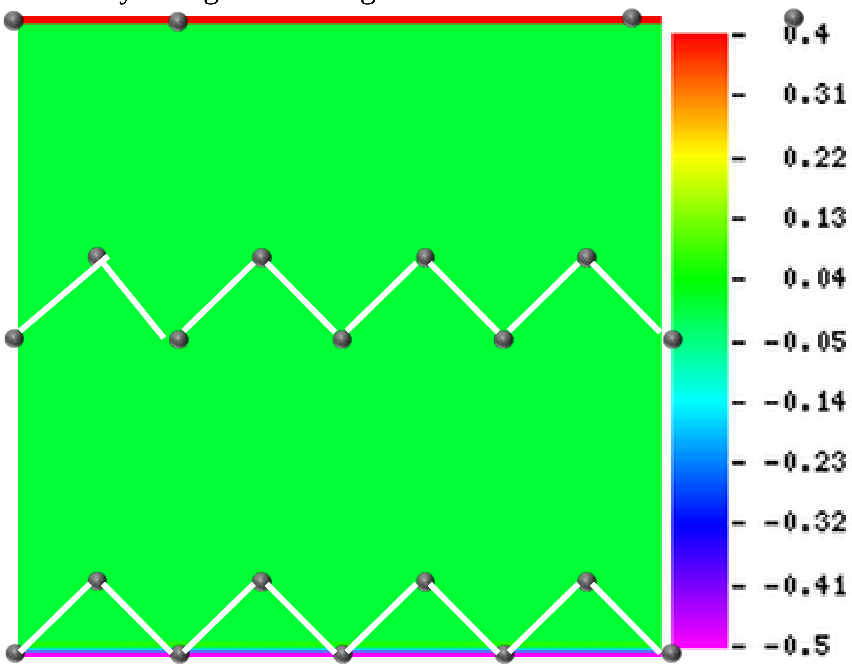
G.F. Bertsch, J.-I. Iwata, A. Rubio, K. Y., Phys. Rev. B62, 7998 (2000).

I= 3.5 × 10^{14} W/cm^2,
T=50 fs, ħω=0.5 eV

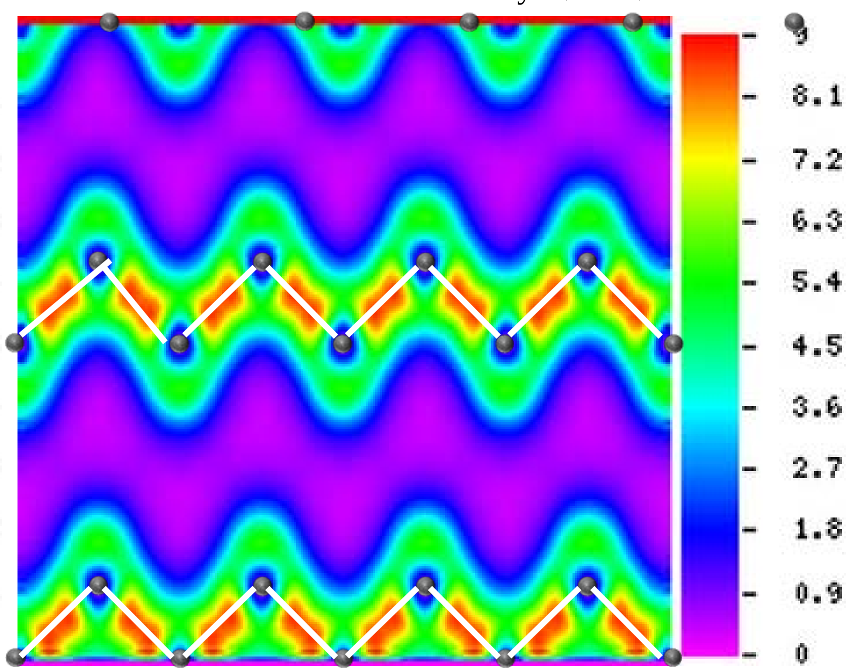




Density change from the ground state (110)



Ground state density (110)



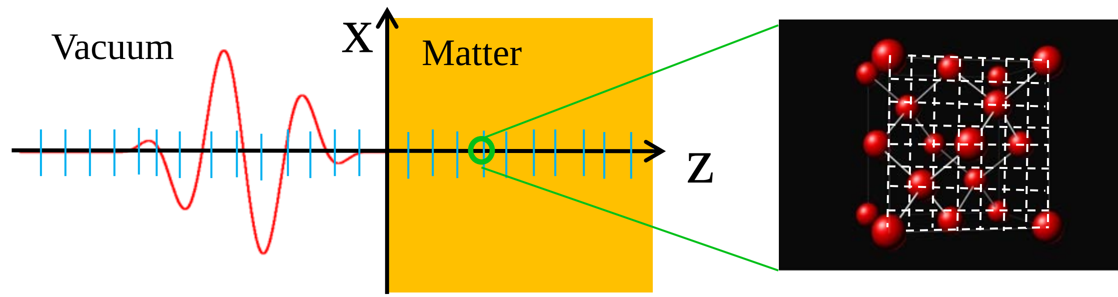
Coupled Maxwell + TDDFT multi-scale simulation

K. Y., T. Sugiyama, Y. Shinohara, T. Otobe, G.F. Bertsch, Phys. Rev. B85, 045134 (2012).

Two coordinates: Macroscopic and microscopic

Macroscopic grids for Z (μm scale) to calculate propagation of vector potential

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}A_Z(t)-\frac{\partial^2}{\partial Z^2}A_Z(t)=\frac{4\pi}{c}J_Z(t)$$



Electron orbitals: $\psi_{i,Z}(\vec{r},t)$

$J_Z(t)$

Coupled by macroscopic vector potential and current averaged over unit cell volume

$A_Z(t)$

At each macroscopic grid point Z, we consider Kohn-Sham orbital with microscopic grids (nm) to describe electron dynamics

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

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

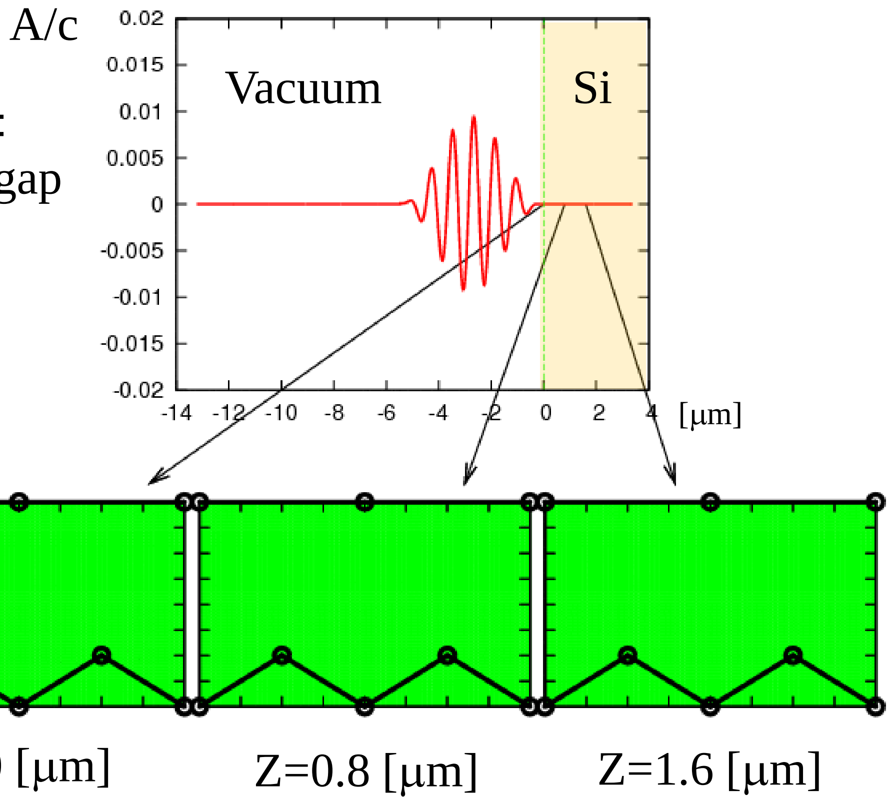
$$J(Z,t)=\int_\Omega d\vec{r}\,\vec{j}_{e,Z}$$

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

Propagation of weak pulse
(Linear response regime, separate dynamics of electrons and E-M wave)

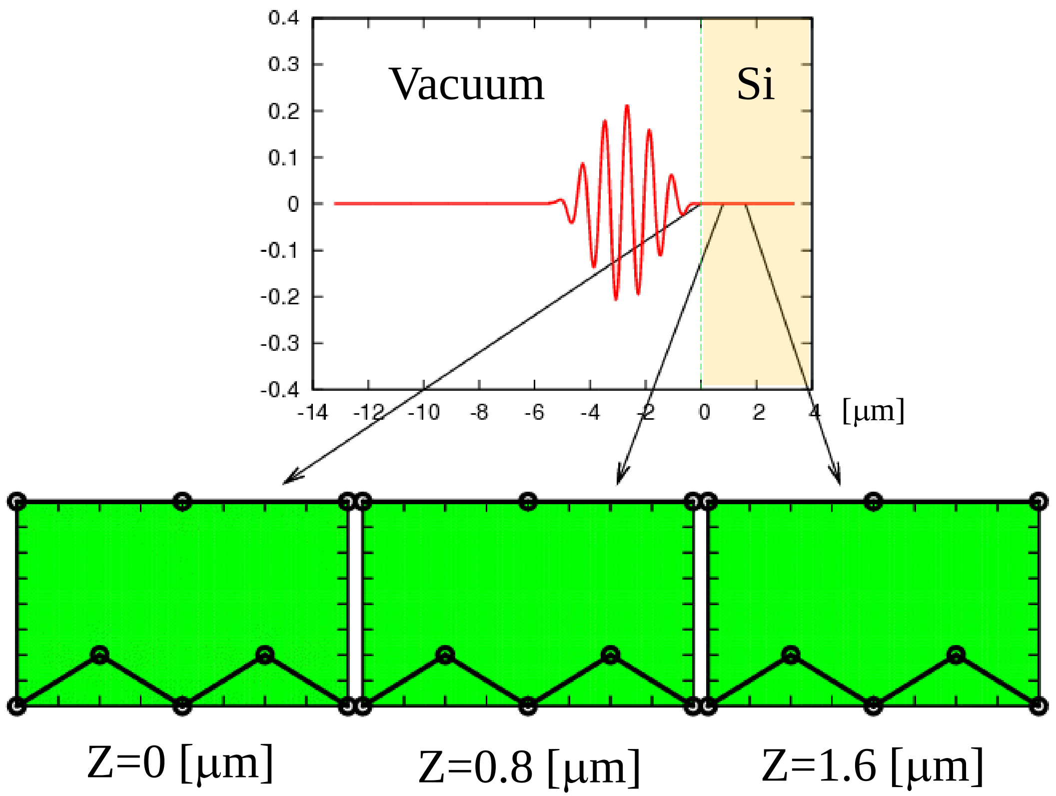
$I=10^{10} W/cm^2$

Laser frequency : 1.55eV :
lower than direct bandgap
2.4eV(LDA)



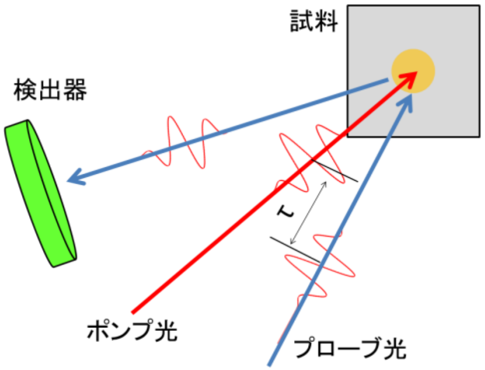
More intense laser pulse
Maxwell and TDKS equations no more separate.

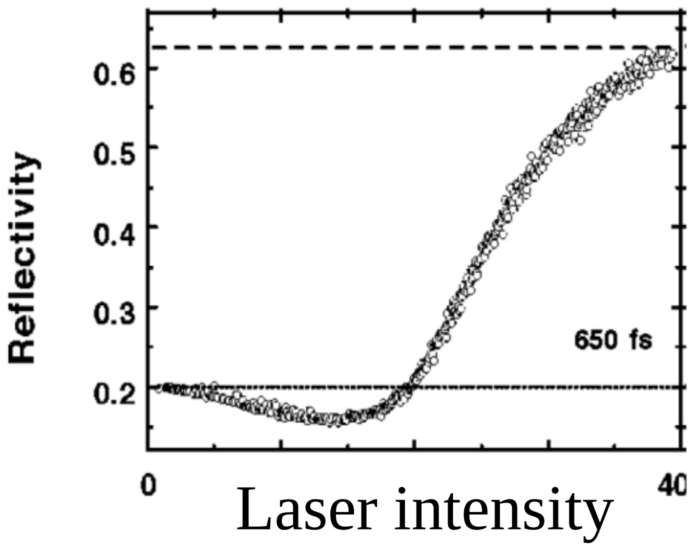
$I = 5 \times 10^{12} W/cm^2$



Reflectivity depends on laser intensity.

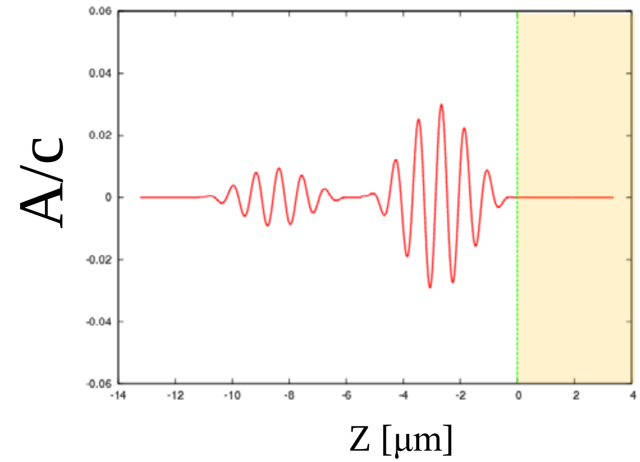
Pump-probe measurement

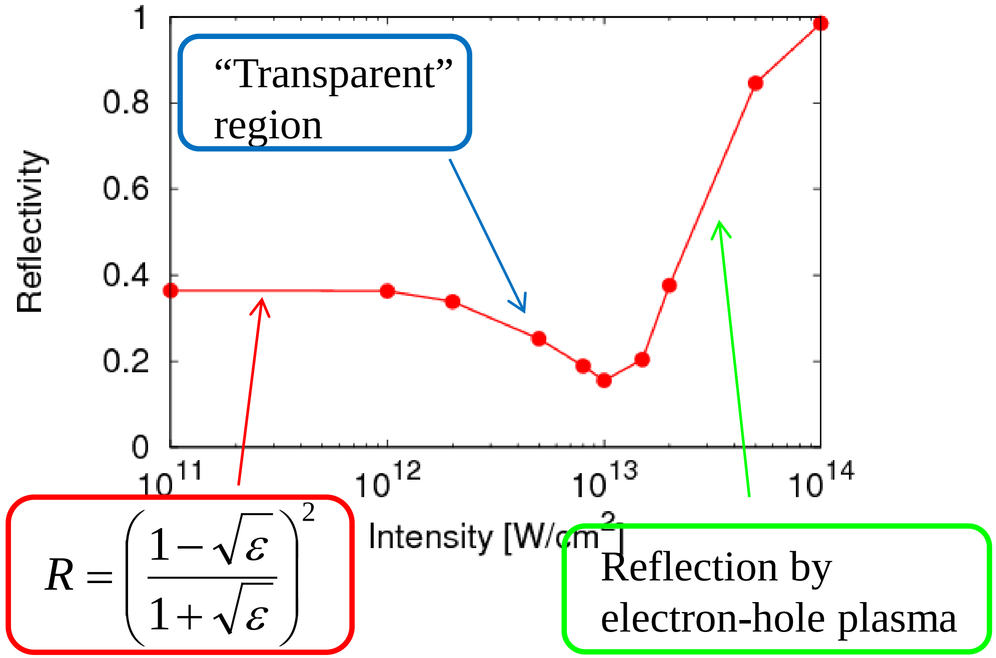




Generation of dense electron-hole plasmas in silicon
K. Sokolowski-Tinten and
D. von der Linde, Phys. Rev. B **61**, 2643 (2000)

Pump-probe simulation





Interpretation by Drude model

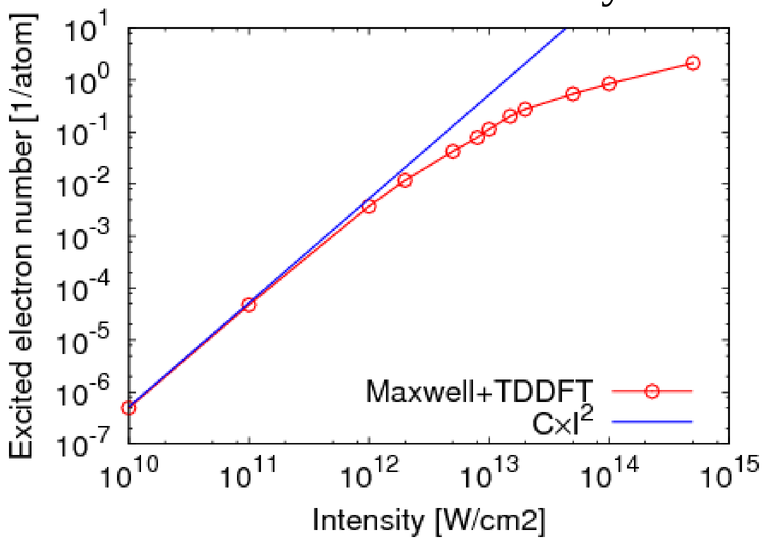
Laser pulse excites electrons.
Excited electrons behave metallic.

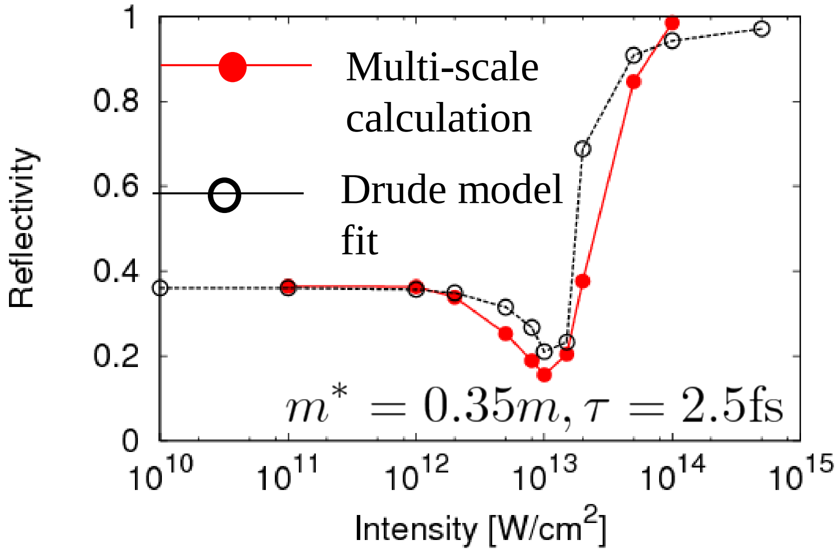
$$\varepsilon(n_{ph}) = \varepsilon_{GS} - \frac{4\pi e^2 n_{ph}}{m^*}\frac{1}{\omega(\omega + \frac{i}{\tau})}$$

n_{ph} electron-hole density

τ collision time

Electron-hole density





Time-dependent mean-field calculation includes collision effect !?

Summary

- Nuclear physics (has been and will) provide useful concepts/methods
  for new emergences in a variety of fields.

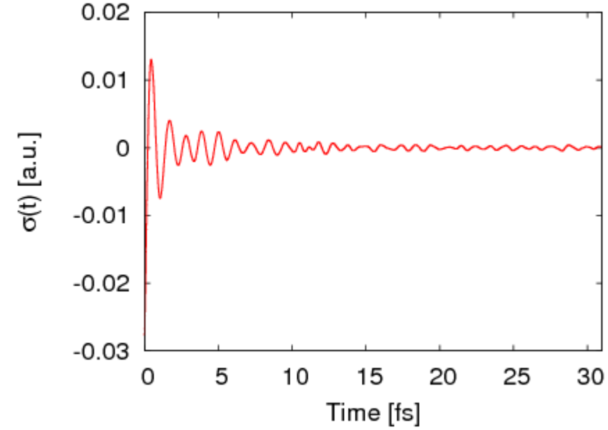
- Large scale computing has a high potential to link different hierarchies.

- I showed an example, the time-dependent mean-field theory
    - Universal tool for linear optical response
    - Maxwell / Schroedinger description for nonlinear electromagnetism
      (regarded as a new light source by computation
      after the laser, synchrotron radiation, XFEL, …)

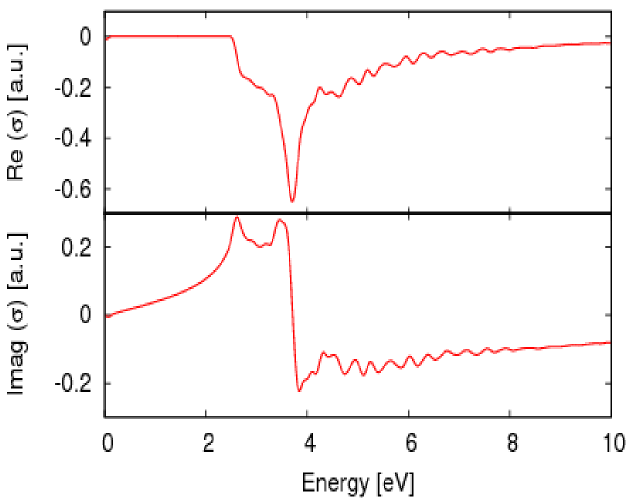
線形応答

$$\sigma(t)$$

$$j(t) = \int^{t} dt' \sigma(t - t') E(t')$$



$$\sigma(\omega)$$



$$\varepsilon(\omega) = 1 - \frac{4\pi i}{\hbar}\sigma(\omega)$$

$$\varepsilon(\omega)$$