Activities and Collaborations 8
Division of Materials and Life Sciences

# Quantum Many-Body Systems Group

K. Yabana

Quantum Many-Body Systems Group

# Members and research interests

| Atomic Nuclei | Atoms, Molecules | Solids |
|---|---|---|

Composed of protons and neutrons
strong interaction

Composed of electrons and ions
Coulomb interaction

Nuclear Physics

K. Yabana
Y. Hashimoto
T. Nakatsukasa ( -2007.7)

K. Hino ( -2007.3)
H. Koizumi
X.-M. Tong (2005.10- )

Atomic Physics
Material Science

*Common tool:*
*Quantum dynamics,*
*Wave mechanical simulation*

# Computational Quantum Dynamics
# Computational Optical Sciences

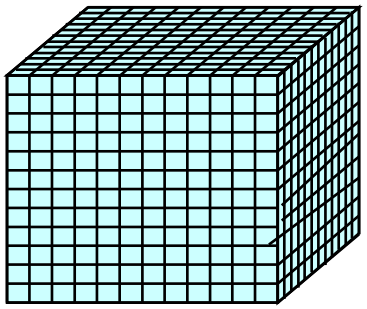
## Morning session: Yabana, Nakatsukasa

### Time-dependent Density-Functional Theory (TDDFT)

$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V_{eff}(\vec{r},t)\right\}\psi_i(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)$$

Real-space 3-dim grid representation
Real-time evolution of the wave function

$$\psi_m(x_i, y_j, z_k, t_l)$$



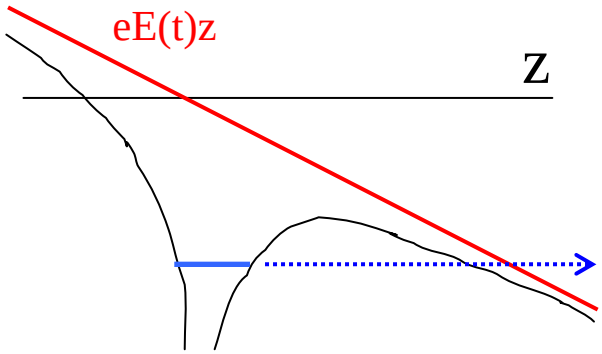
3 topics

1. Electronic dynamics under laser field
2. Nuclear density-functional theory
3. Developing real-time, real-space code

## Afternoon parallel session: Tong, Koizumi, Hashimoto

# Atoms, molecules, solid under intense, ultra-short pulse laser

One of the frontiers in current laser sciences




Laser intensity: $10^{13}$-$10^{15}$W/cm$^2$

laser electric field is comparable to field inside materials

⇩

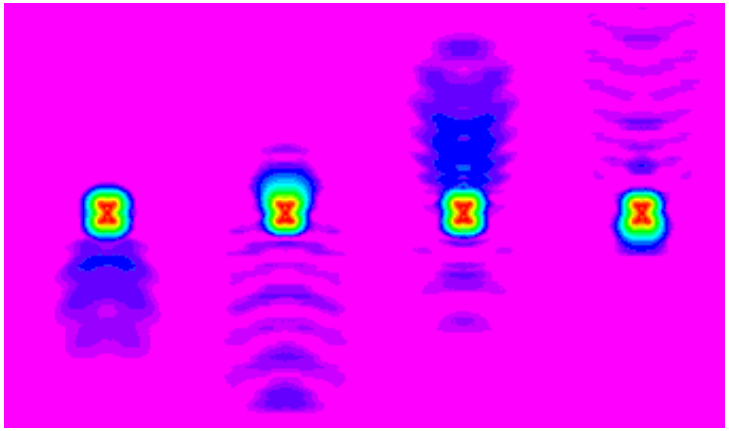
Nonlinear, nonperturbative nature in electron dynamics

Time resolution of
femto ($10^{-15}$s) to atto ($10^{-18}$s)-second

will be discussed by X.-M. Tong

Ethylene molecule under intense laser field

- Tunnel ionization,
- rescattering,
- high harmonic generation



TDDFT calculation

# Laser Induced breakdown in dielectrics

## Femtosecond laser machining

Non-thermal, precise cutting technique

M.D. Perry et.al,
J. Appl. Phys. 85, 6803 (1999)

1.4 ns 350 fs

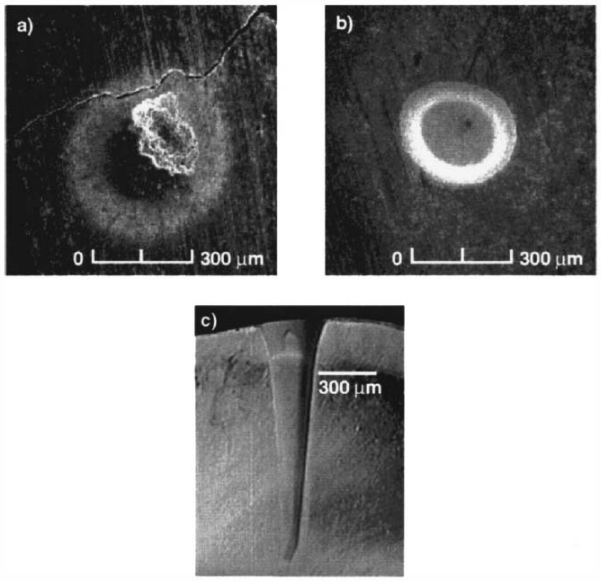


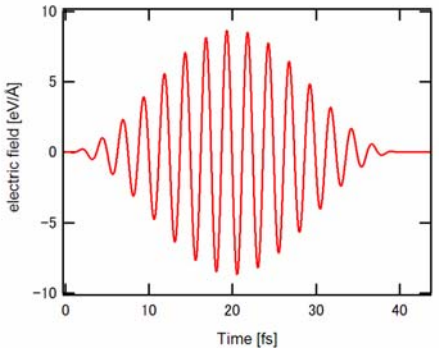

FIG. 1. (a) Drilling of enamel (tooth) with conventional 1053 nm, nanosecond pulses (ablation threshold=30 J/cm$^2$ for $\tau_p$=1.4 ns). (b) Same as in (a) but with the pulse duration reduced to the ultrashort regime (ablation threshold=3 J/cm$^2$ for $\tau_p$=350 fs). In both cases, the laser spot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

## We have achieved
## First-principles Electron Dynamics Simulation

-First calculation of electron dynamics in solid under intense pulse laser

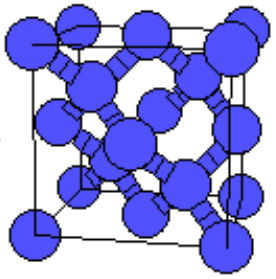
-First demonstration of optical breakdown within the time-dependent density-functional theory

Applied external field $E_{ext}(t)$




Pulse laser

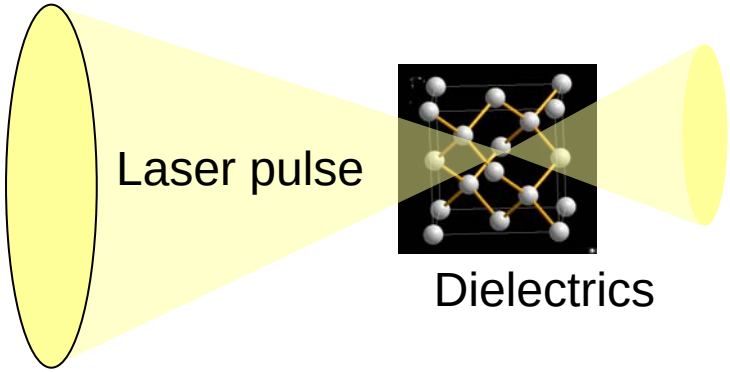
Insulator

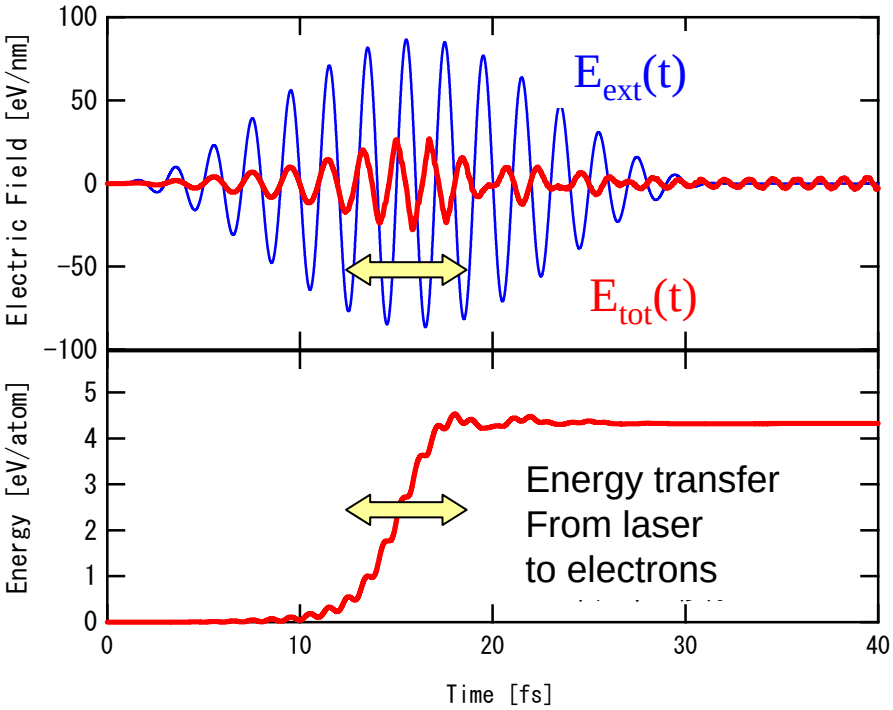


Collaboration with JAEA

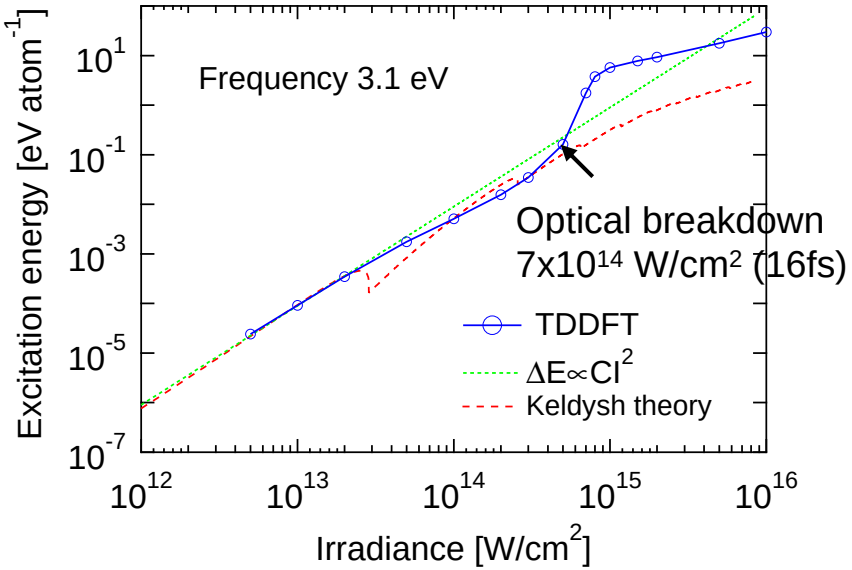
# Irradiation of intense, ultra-short pulse laser on dielectrics

Calculations are achieved partly on PACS-CS.



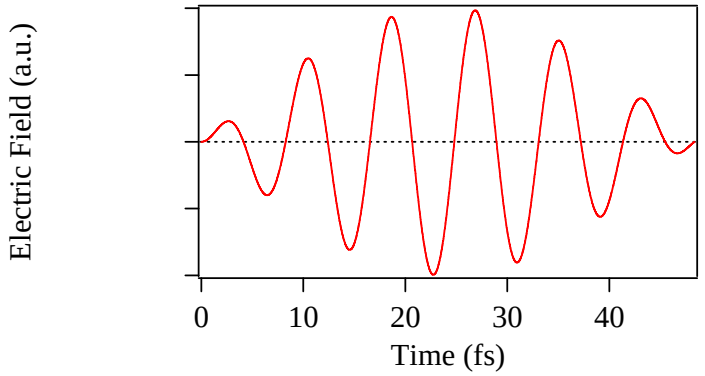

Energy transfer from laser to electrons



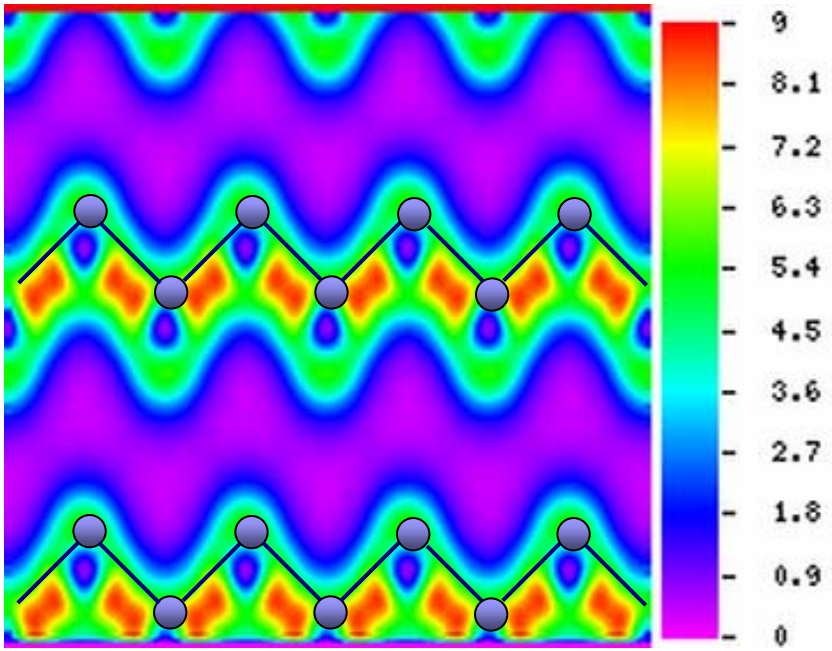

2 photon absorption
Keldysh theory (1965)

# Electron dynamics inside bulk material

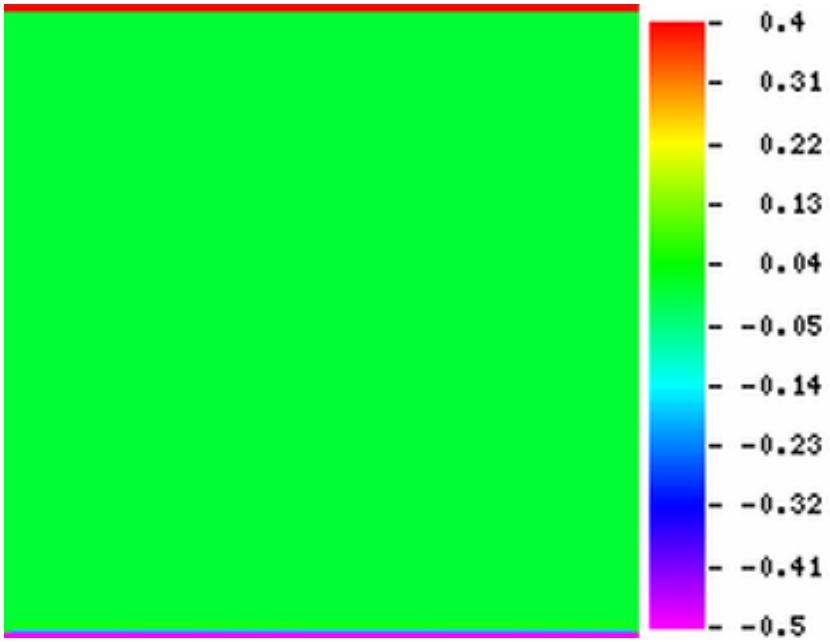
Intensity $I = 3.5 \times 10^{14}$ ( $W/cm^2$ )
Frequency $\omega = 0.5$ (eV)




Total electron density （110）




Density difference from ground state （110）



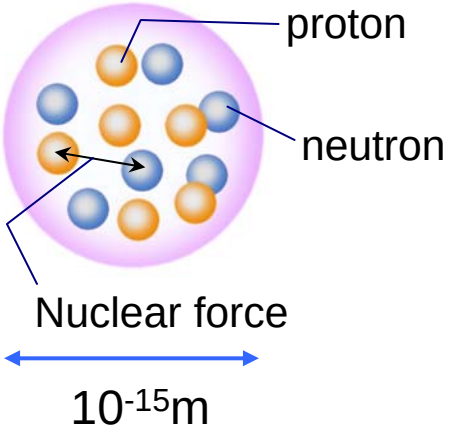

Calculation: J.-I. Iwata

# Density functional theory for nuclear structure

## Nuclei

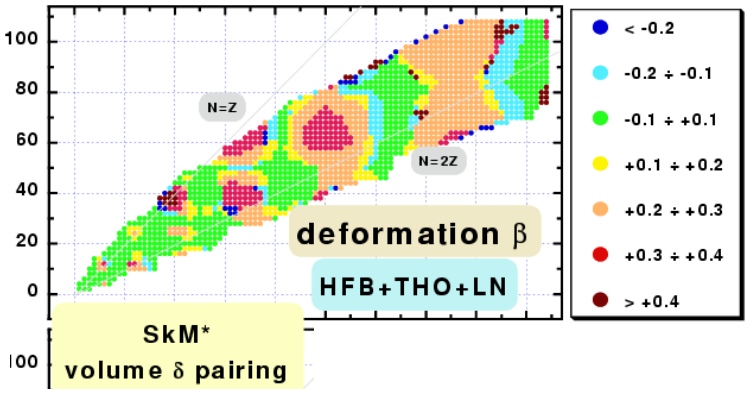
- Quantum liquid of two kinds of fermions (protons and neutrons)

- Strong interaction

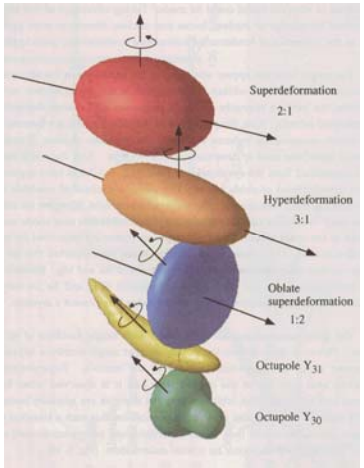



## Success of density functional theory for

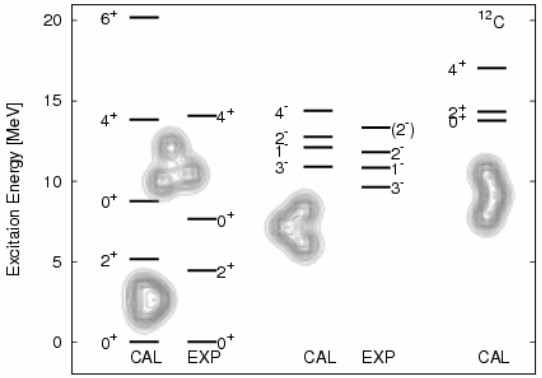
### Masses




### Shapes




### Excitations



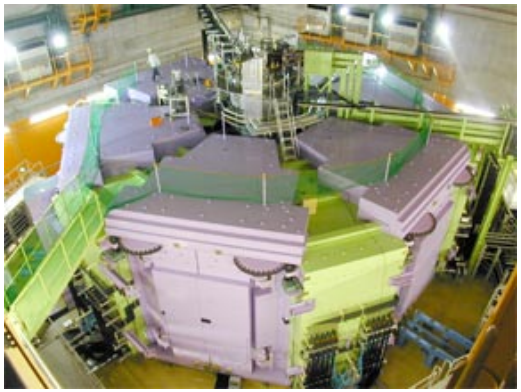
# Current hot issues:

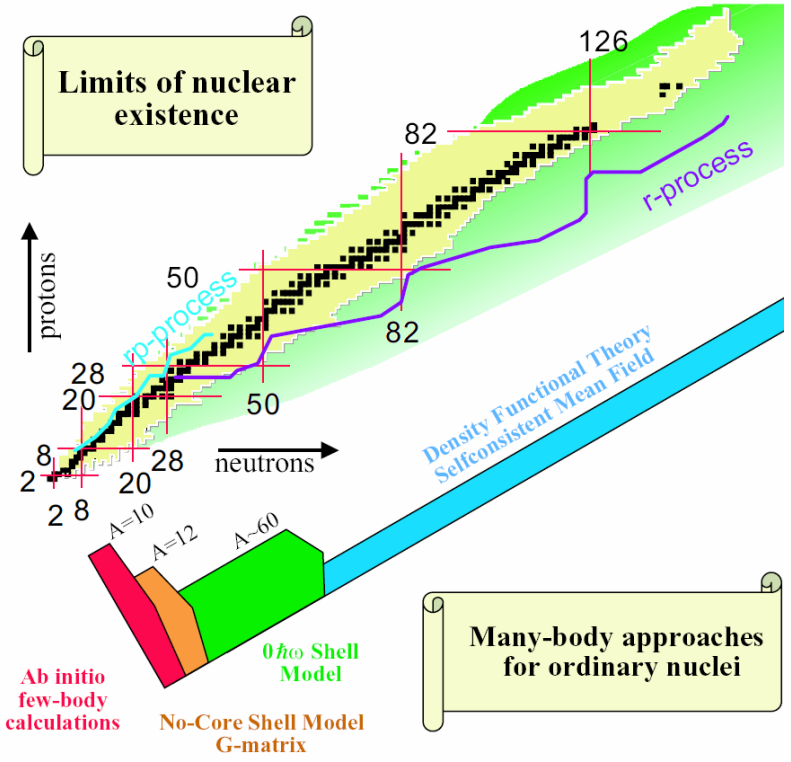
1. How and where the elements (nuclei) are created?
2. Find universal nuclear energy density functional of nuclei.

(UNEDF project, SciDAC, Yabana and Nakatsukasa take part in as foreign collaborator.)

- First principle calculation of nuclear force. (Ishii, Aoki)
- Green function Monte Carlo for light nuclei (Argonne, USA)
- Phenomenological construction of energy functional.

RIBF at RIKEN (T. Nakatsukasa, 2007.8-)
(Radioactive Ion Beam Factory, 2007-)



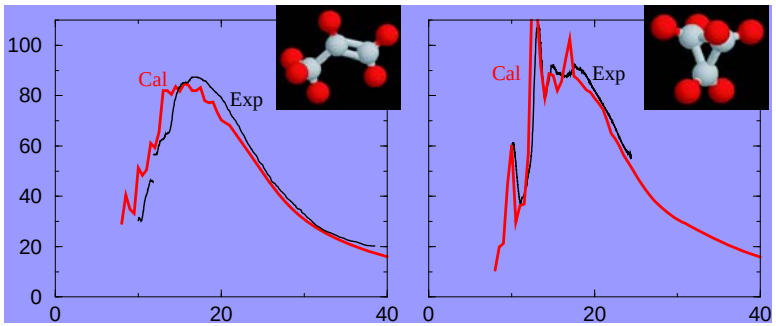


# Shape, excitation (optical response), and density-functional.

TDDFT for electronic and nuclear systems

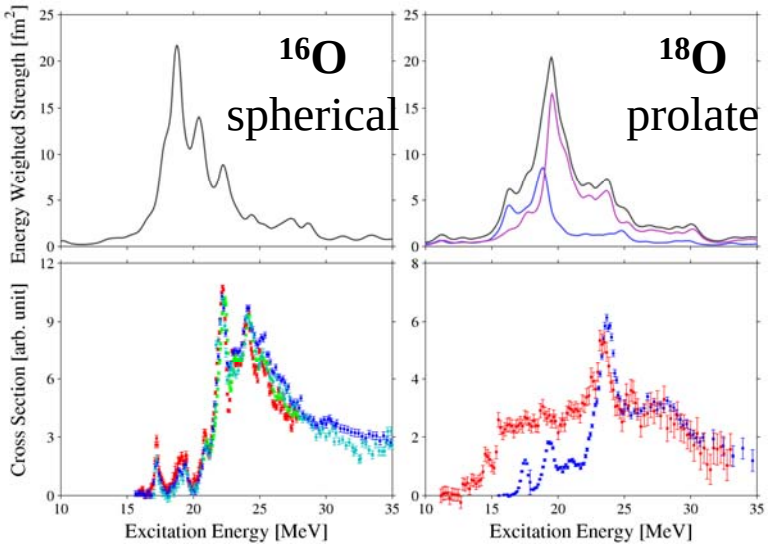
Nuclear density-functional

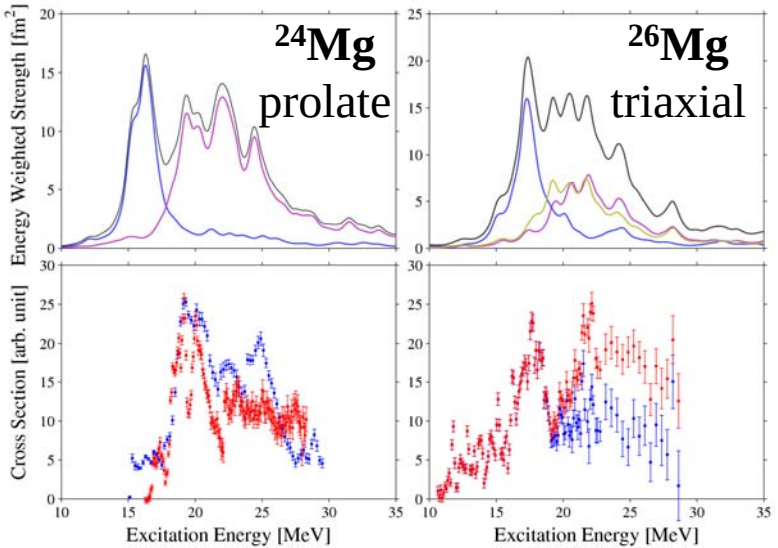
Electronic density-functional
for molecules




Photon energy [ eV ]

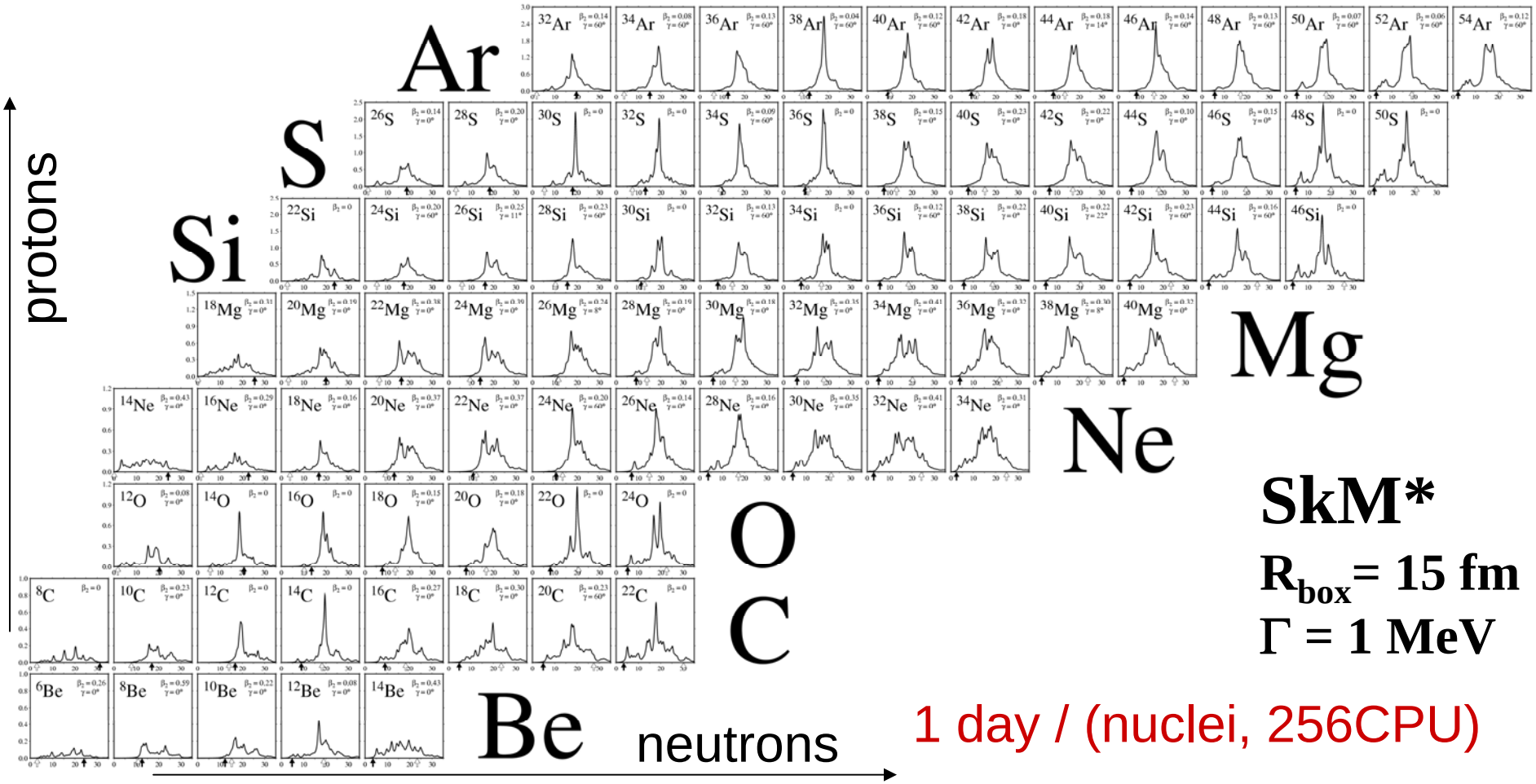
Optical absorption of organic molecule,
$C_3H_6$



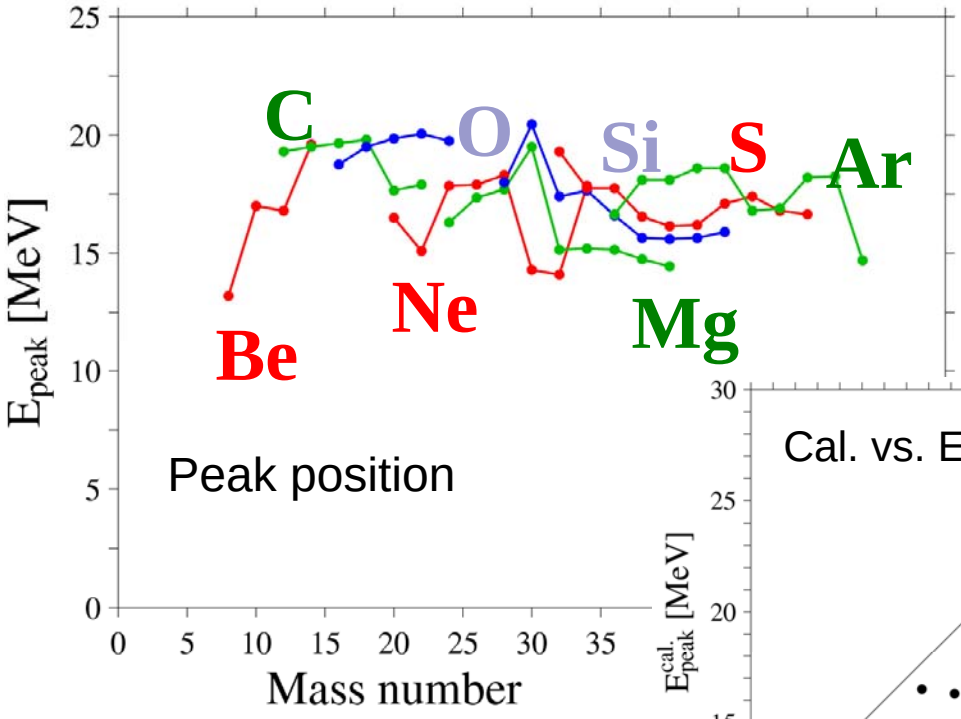



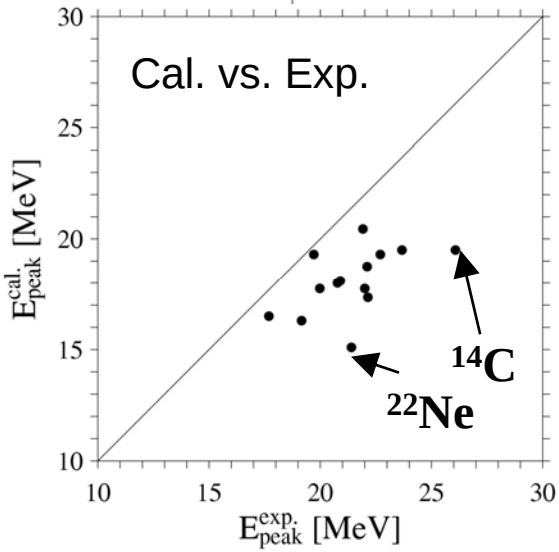
# Toward "Computational Nuclear Data Table"

First attempt for comprehensive calculation
for optical responses of atomic nuclei (PACS-CS)



# Systematic investigation



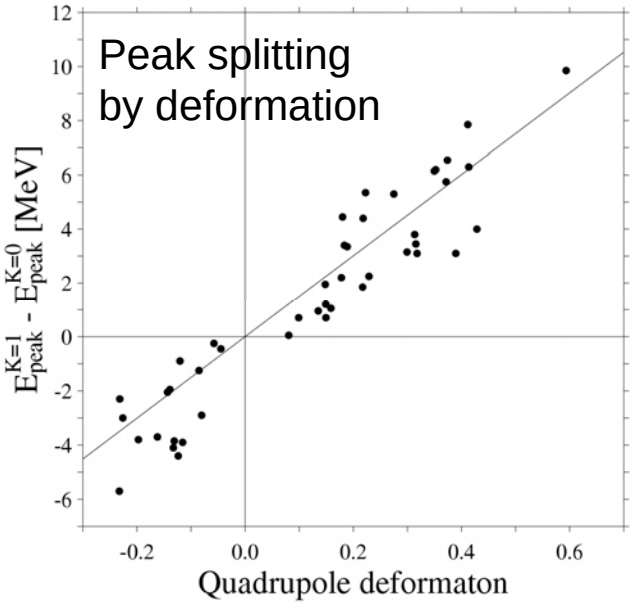




Excitation energy too low
(indication for energy
density functional)

$$\beta_{2m} = \frac{4\pi}{3}\frac{\langle r^2 Y_{2m}\rangle}{\frac{5}{3}\langle r^2\rangle}$$

$$\beta_2 = \sqrt{\beta_{20}^2 + \beta_{22}^2}$$

$$\gamma = \mathrm{Arctan}\left(\frac{\beta_{22}}{\beta_{20}}\right)$$



# Computation for large systems:

developing efficient MPI code for massively-parallel machine
under cooperation with

- computational condenced matter group (real-space DFT code)
- high performance computing group

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

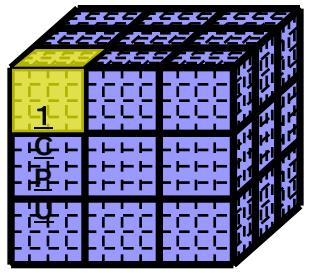
$$\psi_m(x_i,y_j,z_k,t_l)$$

## orbital parallel

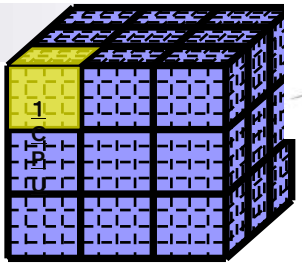
- Simple coding
- Communication among whole processors in constructing density from orbitals.

## space division

- communication only with adjacent processors
- good balance among processors



# Present status of space-division parallel

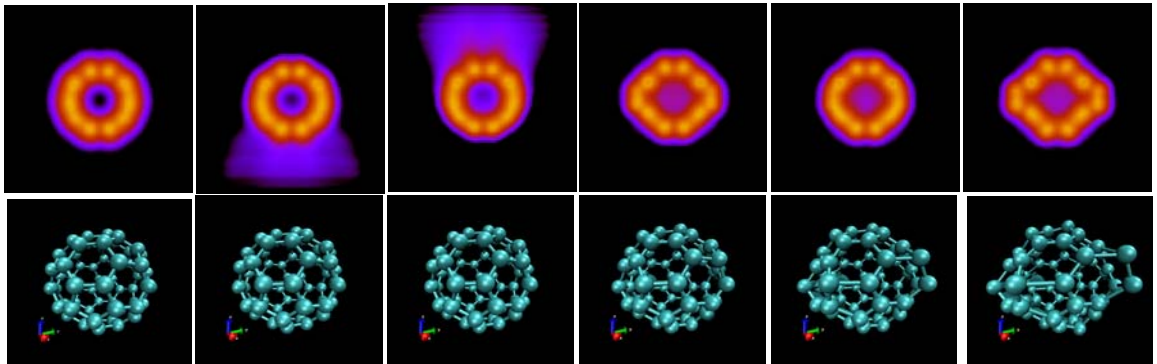



$N_2$ molecule 5 orbitals
# of grid points $30^3$/CPU
# of CPU 256 = 4x8x8
# of time step 10,000

$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{r},t)\right\}\psi_i(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)$$

| | Computational time | Communication time (adjacent) | Communication time (Allreduce) |
|---|---|---|---|
| $-\frac{\hbar^2}{2m}\Delta\psi_m(x,y,z,t)$ | 959 s (23.9%) | 333 s (8.3%) | |
| $V(x,y,z,t)\psi_m(x,y,z,t)$ | 306 s (7.6%) | 102 s (2.5%) | |
| $\Delta\phi(x,y,z)=-4\pi\rho(x,y,z)$ | 1290 s (32.2%) | 227 s (5.7%) | 378 s (9.4%) |

In total, computation 71.2% + communication 28.8%



Example:
Coulomb explosion of fullerene ($C_{60}$) under intense laser pulse

# Summary

## Quantum Many-Body Systems Group

- Quantum dynamics simulation
- Computational optical sciences

Condenced matter physics
High performance computing
- Real-time, -space DFT
Efficient parallel code

Particle physics
Lattice QCD
Nuclear force

Time-dependent density-functional theory

Nuclear systems
- construct DF
- systematics

Electronic systems
- Intense field
- excited states

Astrophysics
Origin of elements
Evolution of stars

Computational Life Sciences
- Excited states, Optical response of bio-molecules
- Electron dynamics in XFEL