



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

Composed of protons and neutrons
strong interaction

Atoms, Molecules

Composed of electrons and ions
Coulomb interaction

Solids

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)

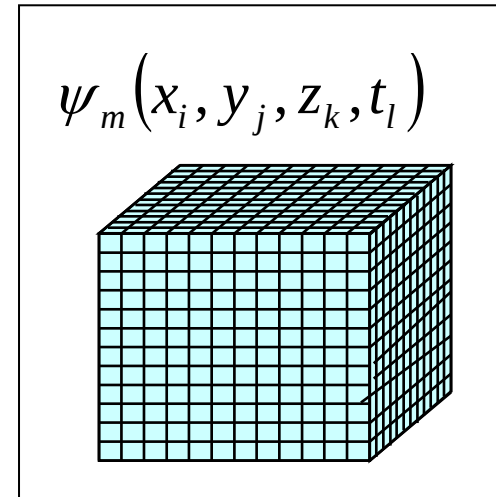
$$\left\{ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V_{\text{eff}}(\vec{r}, t) \right\} \psi_i(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi_i(\vec{r}, t)$$

Real-space 3-dim grid representation

Real-time evolution of the wave function

3 topics

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

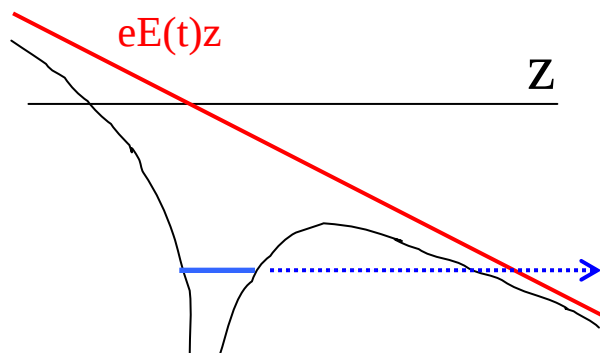


Afternoon parallel session: Tong, Koizumi, Hashimoto



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

One of the frontiers in current laser sciences



Laser intensity: 10^{13} - 10^{15} W/cm²

laser electric field is comparable
to field inside materials



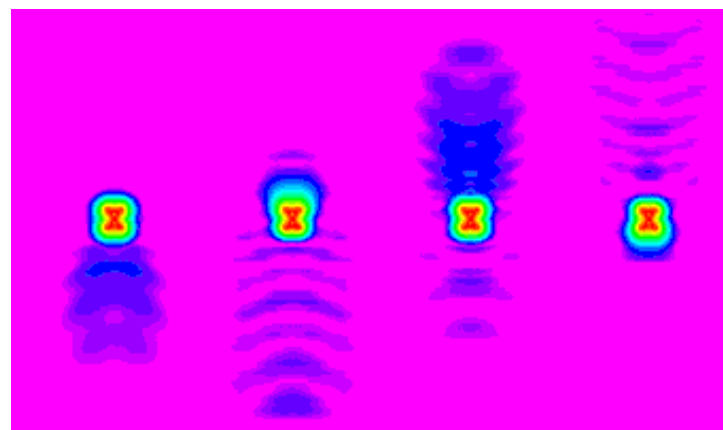
Nonlinear, nonperturbative nature
in electron dynamics

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

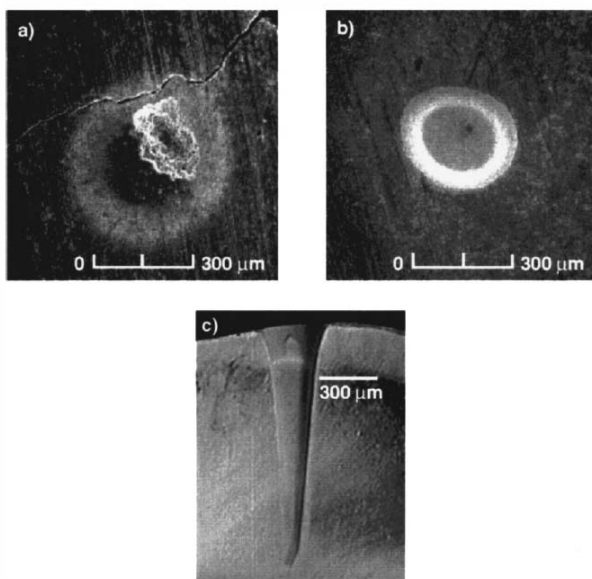
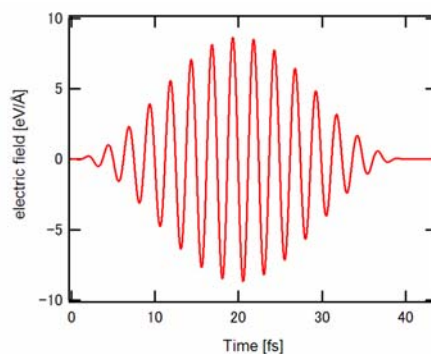


FIG. 1. (a) Drilling of enamel (tooth) with conventional 1053 nm, nanosecond pulses (ablation threshold=30 J/cm² for $\tau_p=1.4$ ns). (b) Same as in (a) but with the pulse duration reduced to the ultrashort regime (ablation threshold=3 J/cm² for $\tau_p=350$ fs). In both cases, the laser spot size was 300 μm. (c) cross section of hole made with 350 fs pulses.

We have achieved First-principles Electron Dynamics Simulation

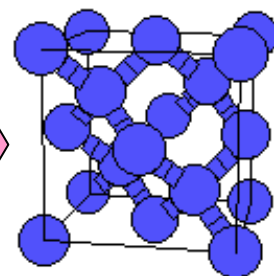
- First calculation of electron dynamics in solid under intense pulse laser
- First demonstration of optical breakdown within the time-dependent density-functional theory

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



Pulse laser

Insulator

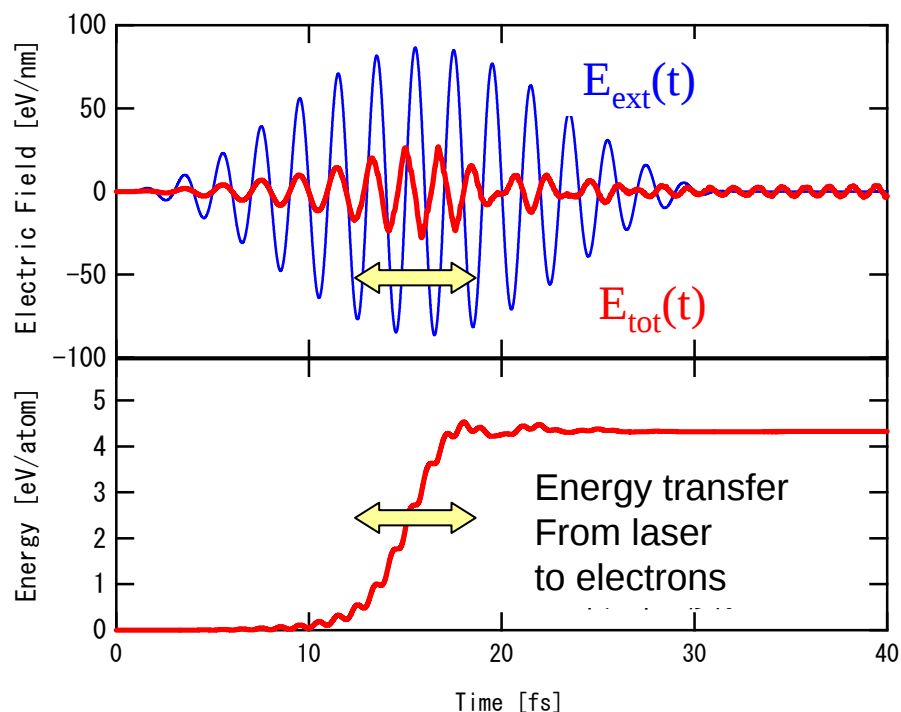
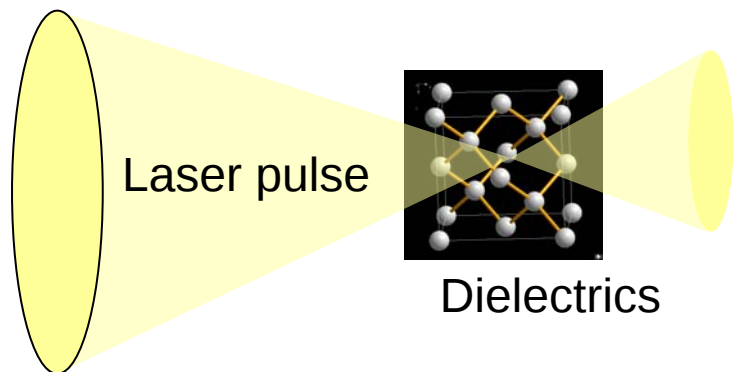


Collaboration with JAEA

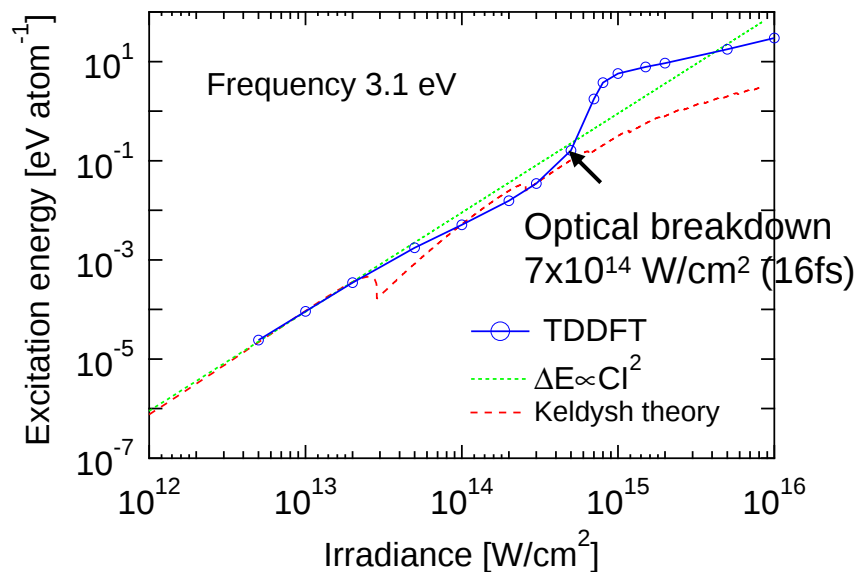


Irradiation of intense, ultra-short pulse laser on dielectrics

Calculations are achieved partly on PACS-CS.



Energy transfer from laser to electrons



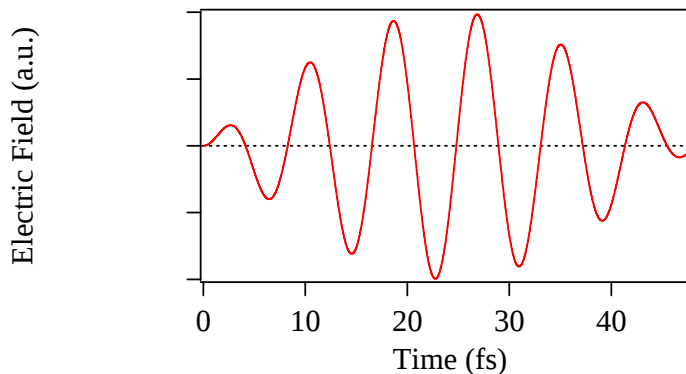
2 photon absorption
Keldysh theory (1965)



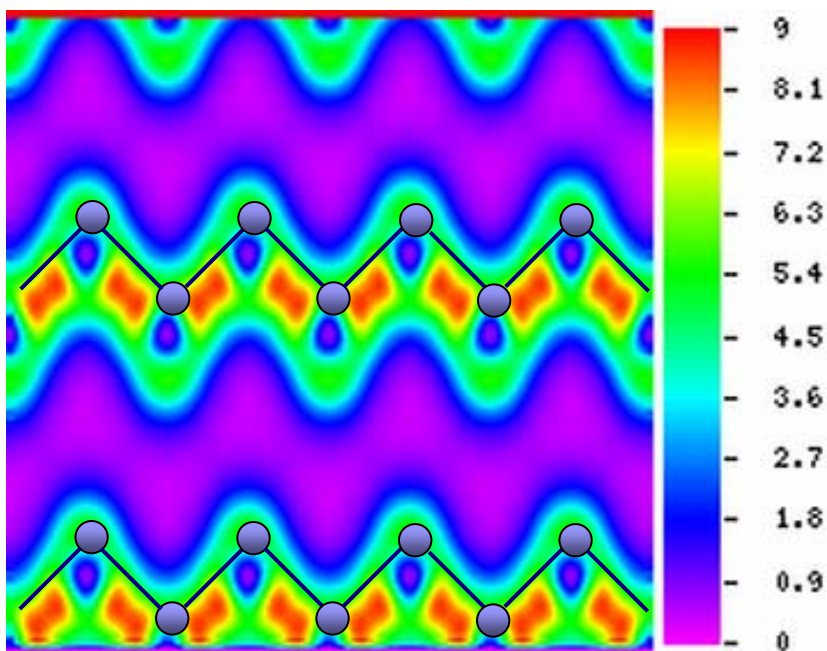
Electron dynamics inside bulk material

Intensity $I = 3.5 \times 10^{14}$ (W/cm²)

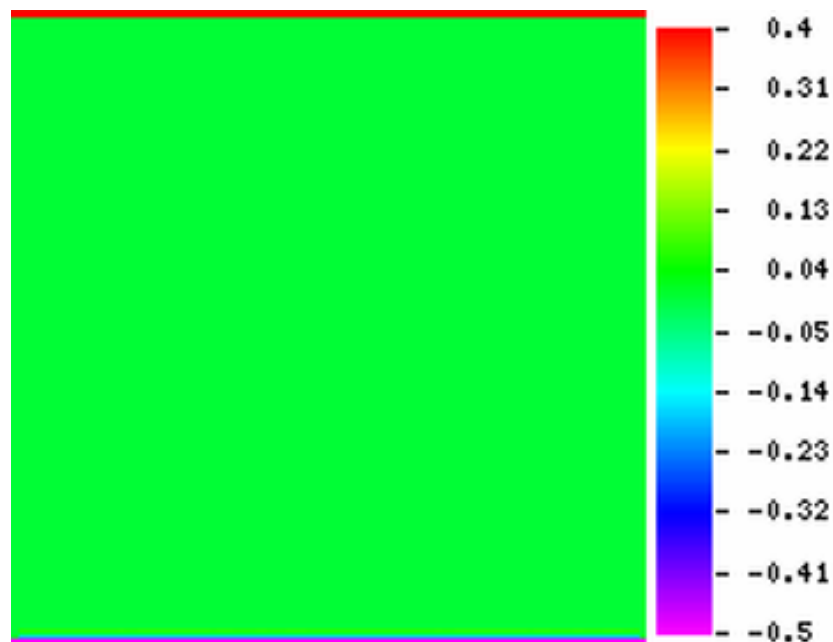
Frequency $\omega = 0.5$ (eV)



Total electron density (110)



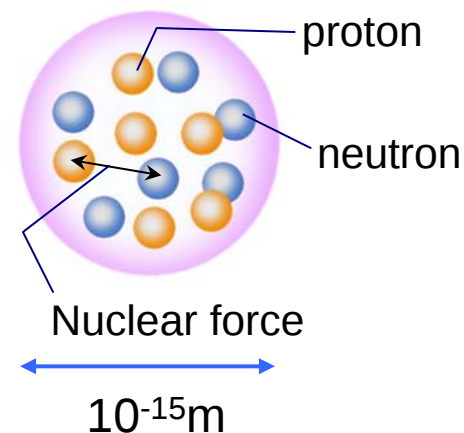
Density difference from ground state (110)



Density functional theory for nuclear structure

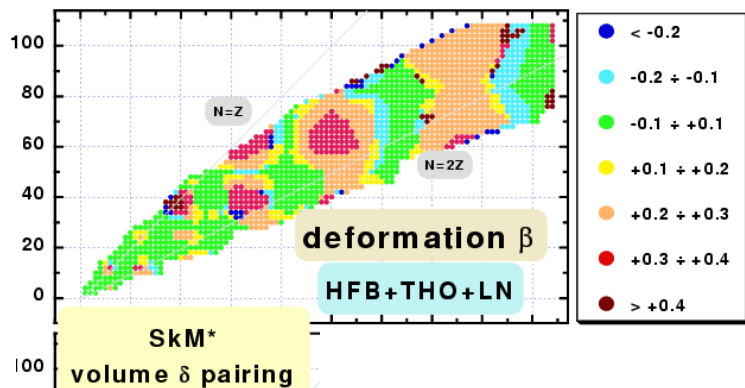
Nuclei

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

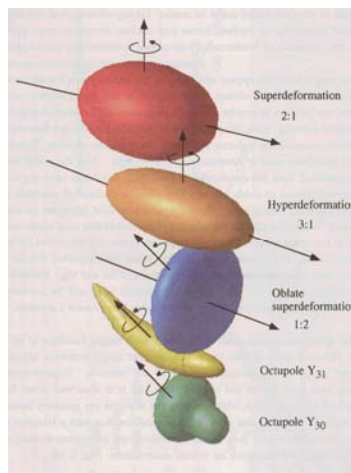


Success of density functional theory for

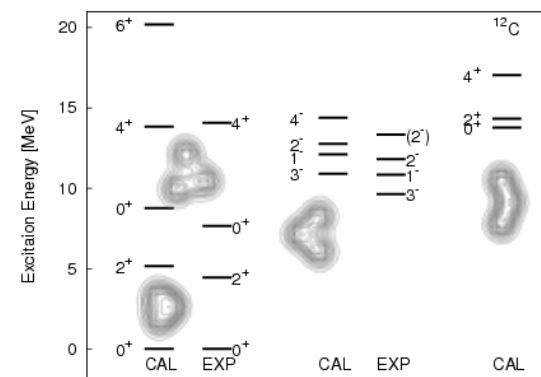
Masses



Shapes



Excitations





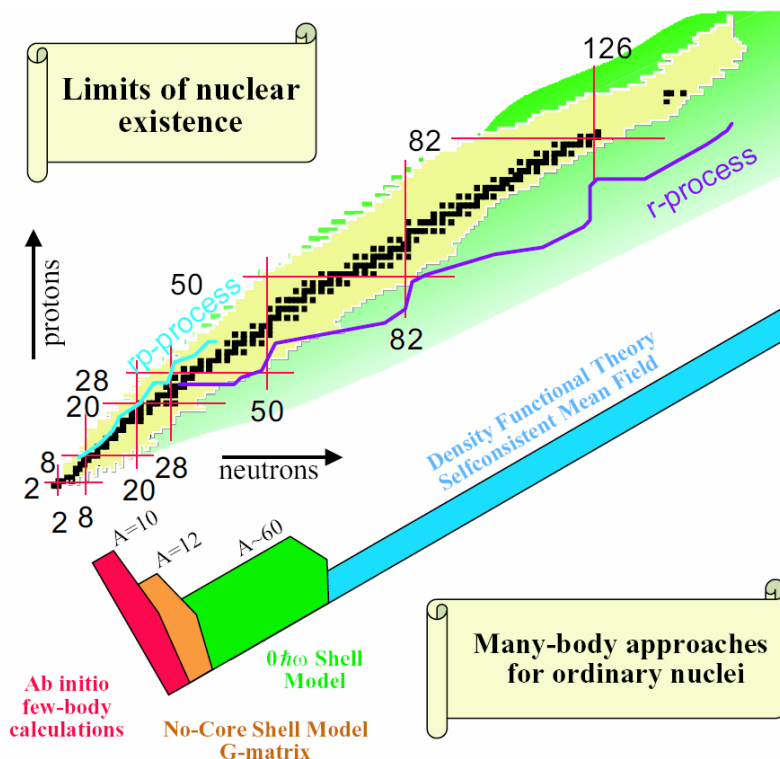
Current hot issues:

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-)



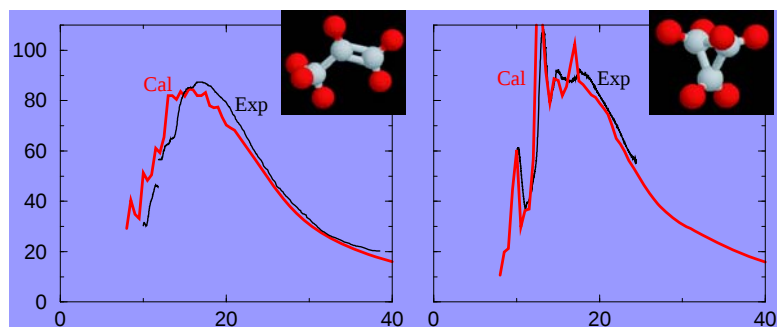


Shape, excitation (optical response), and density-functional.

TDDFT for electronic and nuclear systems

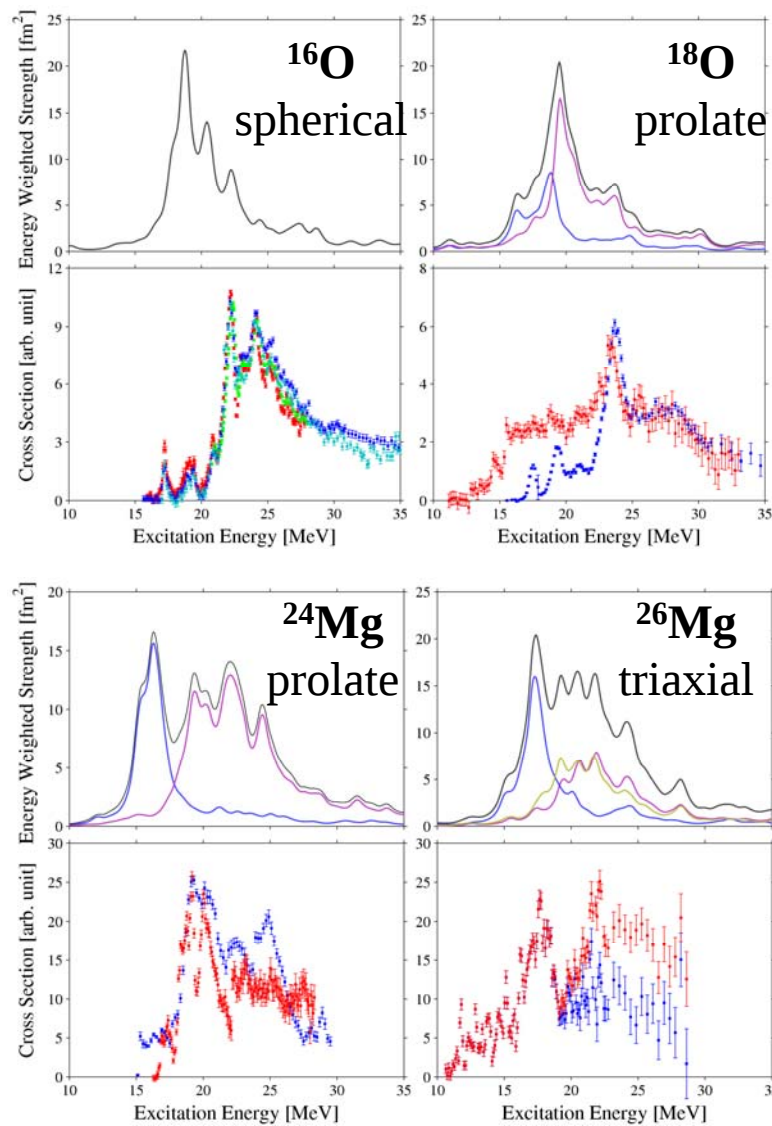
Nuclear density-functional

Electronic density-functional
for molecules



Photon energy [eV]

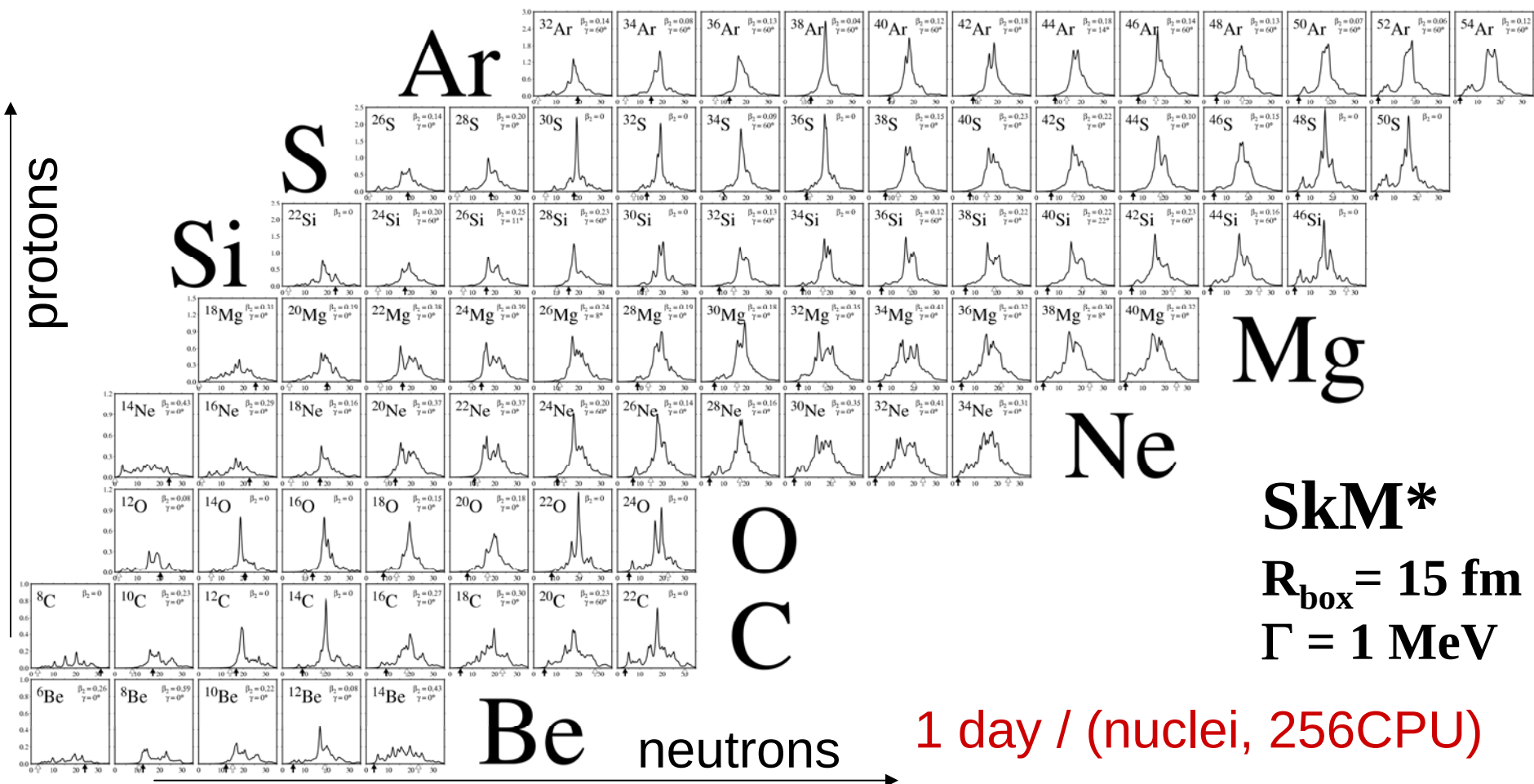
Optical absorption of organic molecule,
 C_3H_6





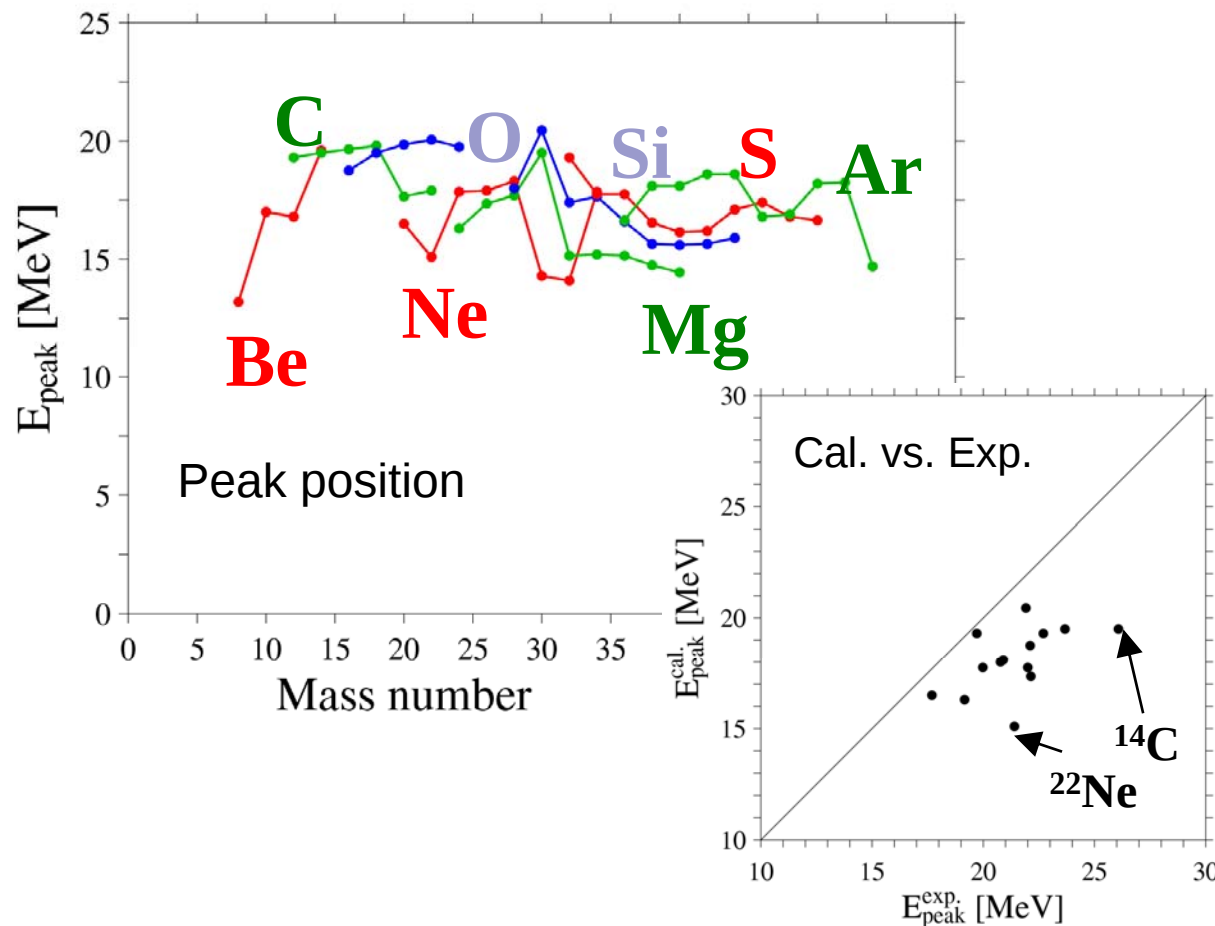
Toward “Computational Nuclear Data Table”

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

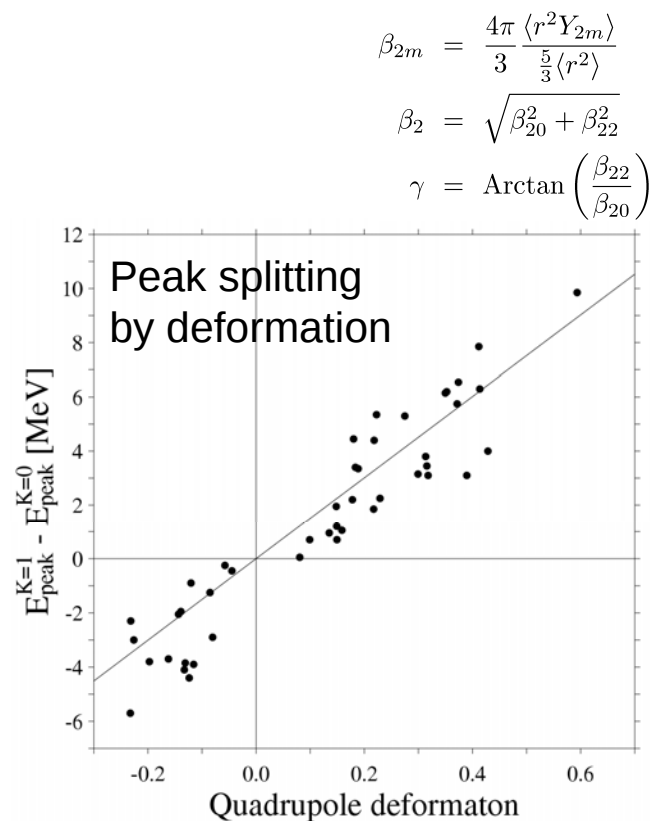




Systematic investigation



Excitation energy too low
(indication for energy
density functional)



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

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

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

Computation for large systems:

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

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

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

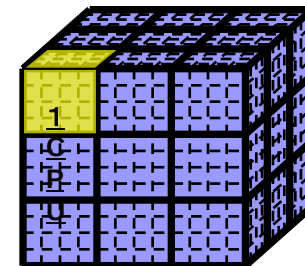
$$\psi_m(x_i, y_j, z_k, t_l)$$

orbital parallel

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

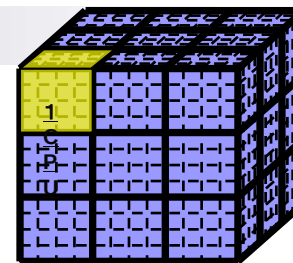
space division

- communication only with adjacent processors
- good balance among processors





Present status of space-division parallel

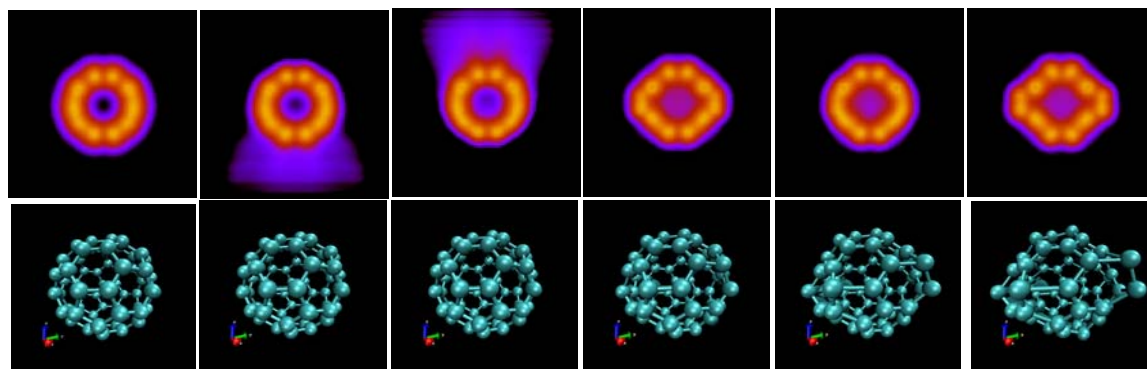


N_2 molecule 5 orbitals
 # of grid points $30^3/\text{CPU}$
 # of CPU $256 = 4 \times 8 \times 8$
 # of time step 10,000

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

	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

Particle physics

Lattice QCD
Nuclear force

Astrophysics

Origin of elements
Evolution of stars

Time-dependent density-functional theory

Nuclear
systems

- construct DF
- systematics

Electronic
systems

- Intense field
- excited states

Condensed matter physics High performance computing

- Real-time, -space DFT
- Efficient parallel code

Computational Life Sciences

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