第5回クラスター階層領域研究会

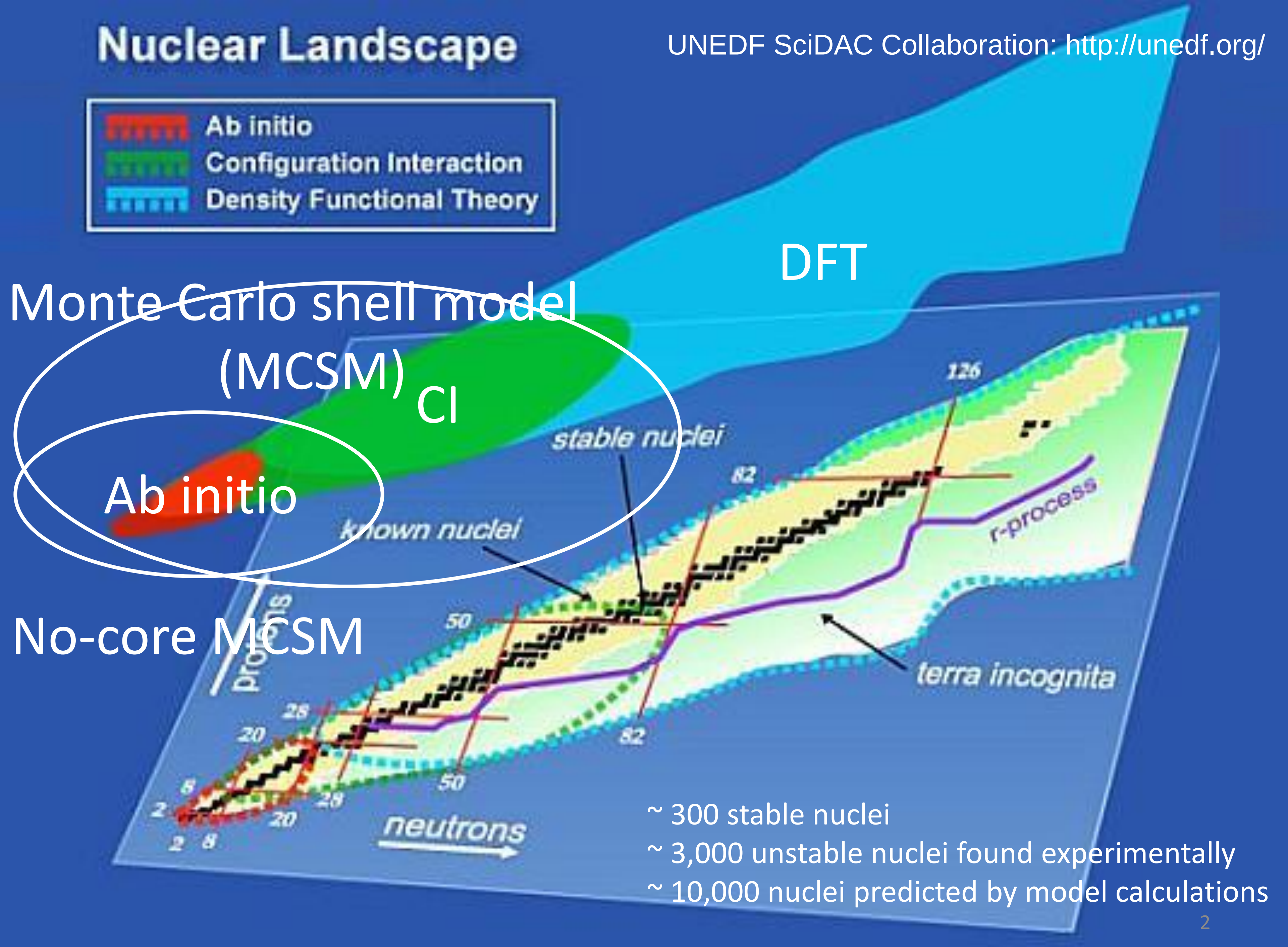
Ab initio description of light nuclei from no-core Monte Carlo shell model

Takashi Abe (RIKEN Nishina Center)

Collaborators:
P. Maris (Iowa State U), T. Otsuka (RIKEN/U Tokyo),
N. Shimizu (U Tokyo), Y. Tsunoda (U Tokyo), Y. Utsuno (JAEA),
J. P. Vary (Iowa State U), T. Yoshida (RIST)

ZOOM

September 25, 2020


Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
Monte Carlo shell model (MCSM)
CI
Ab initio
No-core MCSM
stable nuclei
known nuclei
r-process
terra incognita
protons
neutrons
126
82
50
28
20
8
2
~ 300 stable nuclei
~ 3,000 unstable nuclei found experimentally
~ 10,000 nuclei predicted by model calculations

Configuration Interaction (CI)

- Eigenvalue problem of large and sparse Hamiltonian matrix

$$H|\Psi\rangle = E|\Psi\rangle$$

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & E_3 & \\ & & & \ddots \\ 0 & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

Large and sparse real symmetric

$\sim \mathcal{O}(10^{11})$

non-zero MEs $\sim \mathcal{O}(10^{13-14})$

Lanczos method for diagonalization

Slater determinants

$$\begin{cases} |\Psi_1\rangle = a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle = a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle = \cdots \\ \vdots \end{cases}$$

Monte Carlo shell model (MCSM)

Standard shell-model calculation

$$
H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix}
\;\Longrightarrow\;
\begin{pmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & E_2 & \\ 0 & & & \ddots \end{pmatrix}
$$

Diagonalization

Spanned by Slater determinants

$$d \lesssim \mathcal{O}(10^{11})$$

Monte Carlo shell model

Importance truncation

$$
H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix}
\;\Longrightarrow\;
\begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}
$$

Diagonalization

Spanned by important bases
selected stochastically and variationally

$$d_{\mathrm{MCSM}} \sim \mathcal{O}(10^2)$$

Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

MCSM wave function

- Superposition of quantum-number projected SDs

\# of MCSM basis states ~ 100

$$|\Psi^{J M \pi}(N_b)\rangle = \sum_{d=1}^{N_b} f^{(d)} \sum_{K=-J}^{J} g_K^{(d)} \hat{P}^{\pi} \hat{P}^{J}_{MK} |\Phi(D^{(d)})\rangle$$

Superposition — Projection on to good spin & parity — Deformed SD

$$|\Phi(D^{(d)})\rangle = \prod_i \hat{a}_i^\dagger (D^{(d)}) |\mathrm{core}\rangle \qquad \hat{a}_i^\dagger (D^{(d)}) = \sum_\ell D^{(d)}_{\ell i} \hat{c}_\ell^\dagger$$

$$|\mathrm{vacuum}\rangle$$

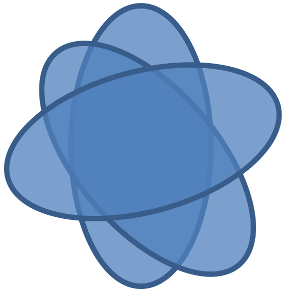
- Angular momentum projection

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2} \int D^{I*}_{MK}(\Omega) \hat{R}(\Omega) d\Omega$$

$$\rightarrow \sum_\Omega W(\Omega) \cdots$$

O(~10^4)

Restoration of symmetries

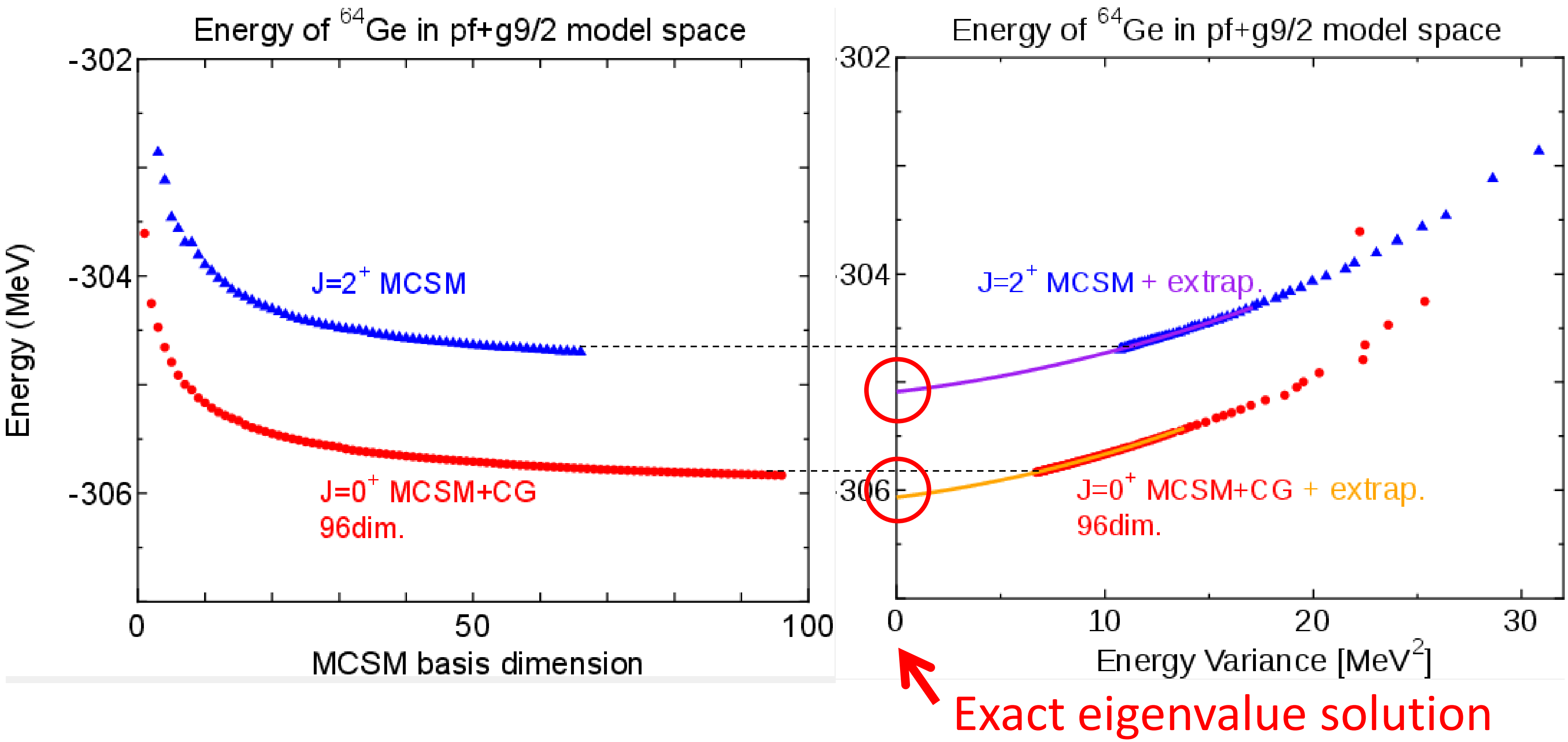


Favorable for massively parallel computation

Towards exact solution for eigenvalue

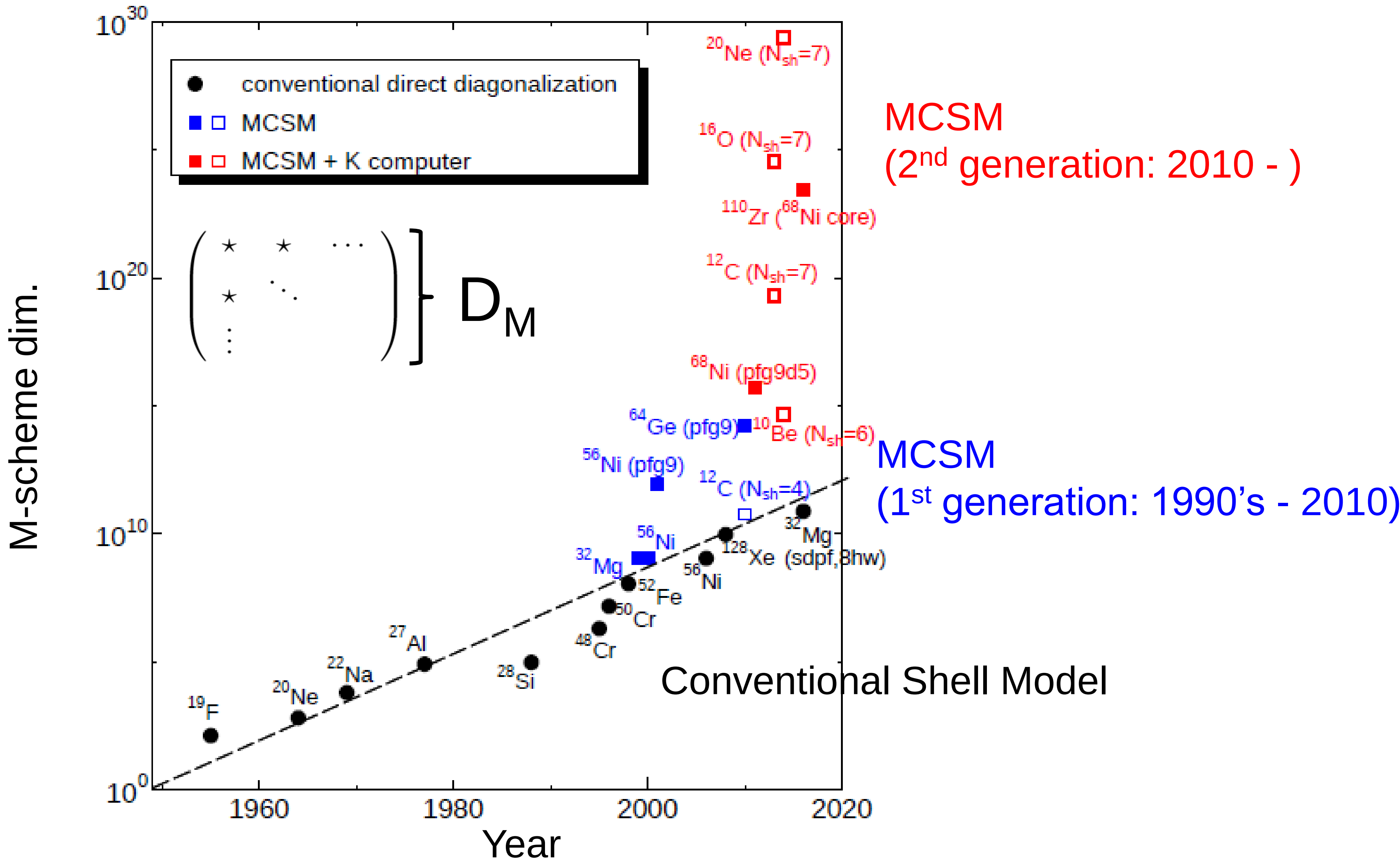
- Example for the energy-variance extrapolation in the MCSM

  ^{64}Ge (Z=32,N=32), pf+g9/2 model space (^{40}Ca core)



N. Shimizu et al., Phys. Rev. C85, 021301 (2012). + …

Dimensionality of shell-model calculations



N. Shimizu et al., Phys. Scr. 92, 063001 (2017).

“Ab initio” in low-energy nuclear structure physics

- Major challenge in nuclear physics

  - Nuclear structure & reactions directly from *ab-initio* calc. w/ nuclear forces

  - *ab-initio* approaches in nuclear structure calculations (A > 4):

  Light mass: Green’s Function Monte Carlo, No-Core Shell Model (A ~ 12),

  Medium/heavy mass: Coupled Cluster, IM-SRG,

  Self-consistent Green’s Function theory, Lattice EFT, UMOA, …

- Solve the non-relativistic many-body Schroedinger eq.

  and obtain the eigenvalues and eigenvectors.

$$H|\Psi\rangle = E|\Psi\rangle$$

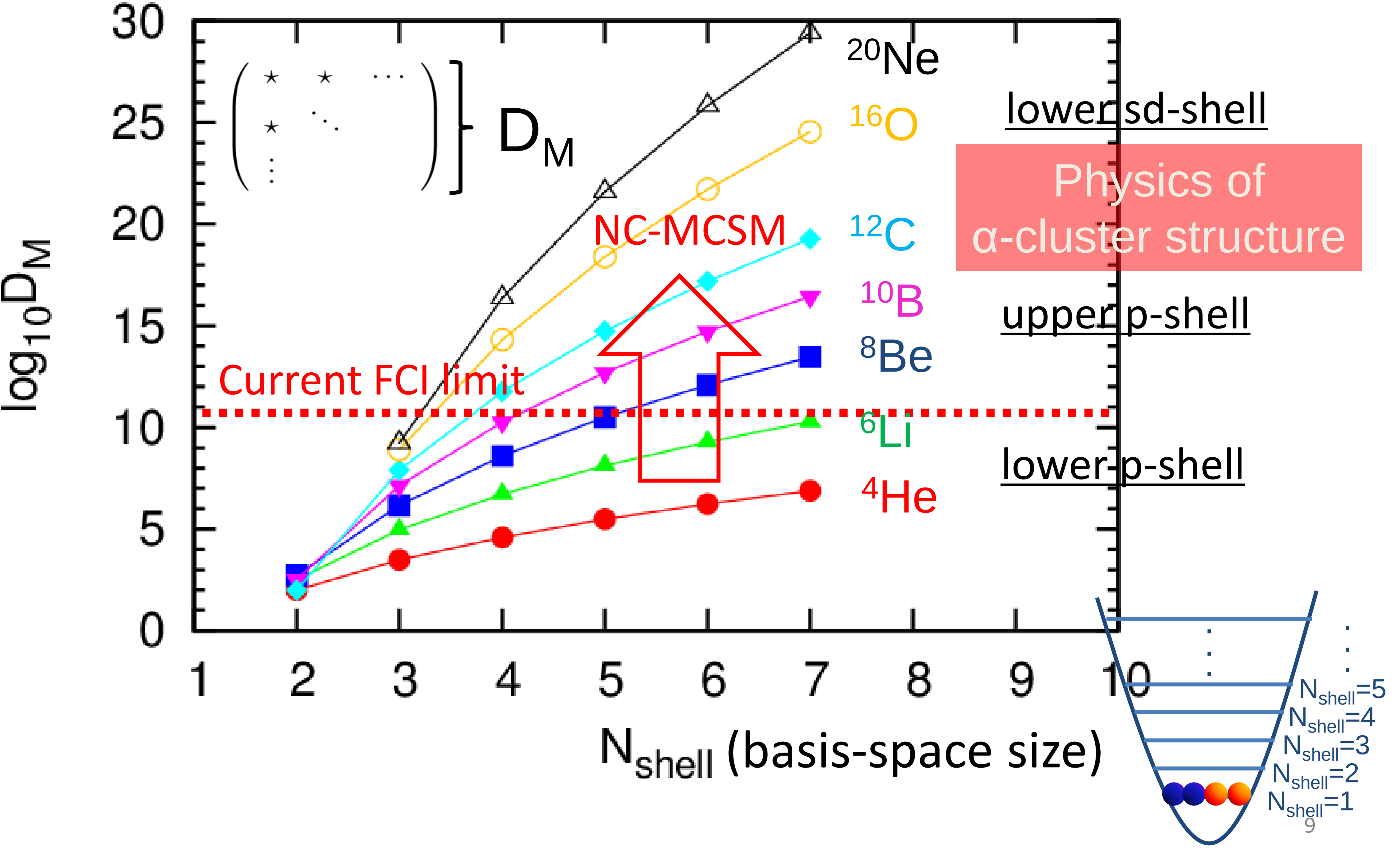
$$H = T + V_{\mathrm{NN}} + V_{\mathrm{3N}} + \cdots + V_{\mathrm{Coulomb}}$$

  – Ab initio: All nucleons are active, and Hamiltonian consists of realistic NN (+ 3N + …) potentials.

→ Computationally demanding → Monte Carlo shell model (MCSM)

M-scheme dimension

Ab initio calculations w/ NN int only



How to obtain ab-initio results from no-core MCSM

- Two steps of the extrapolation

Same as in the MCSM w/ an inert core

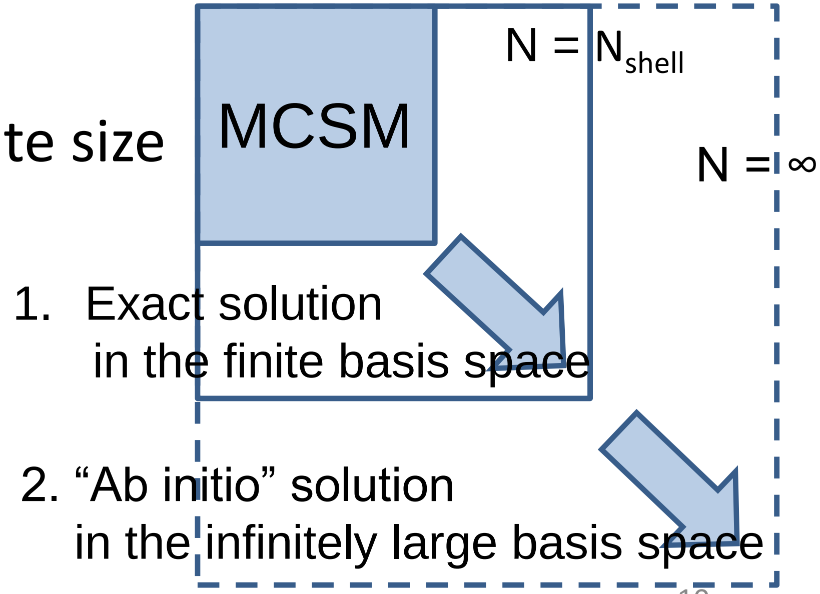
1. Extrapolation of our MCSM (approx.) results
   to exact results in the finite size of model space

   Energy-variance extrapolation

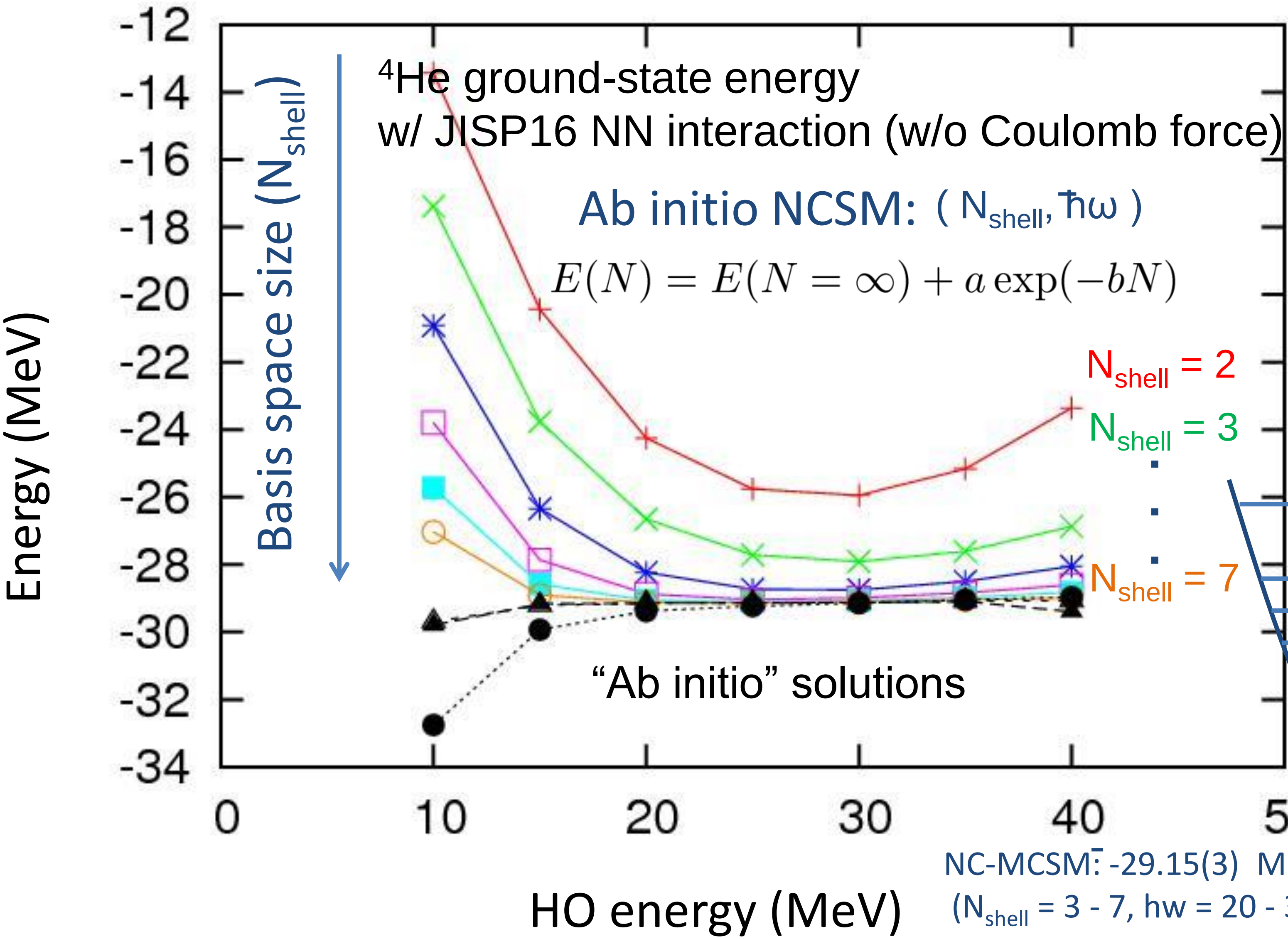
N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

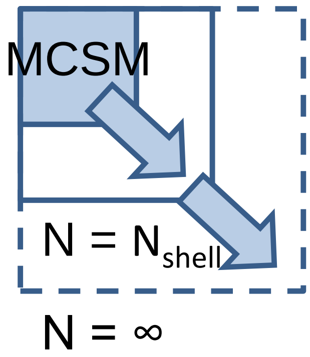
2. Extrapolation of the results in the finite size
   to the infinitely large basis space
   - Empirical extrapolation w.r.t. N_{shell}
   - IR- & UV-cutoff extrapolations

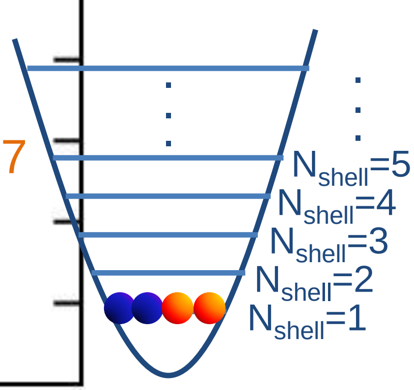
→ Ab initio solution



Extrapolation to the infinitely large basis space







NC-MCSM: -29.15(3) MeV
(N_{shell} = 3 - 7, hw = 20 - 30 MeV)

c.f.) NCFC: -29.164(2) MeV

Inter-nucleon potentials

- JISP16:

  J-matrix Inversion Scattering Potential tuned up to O-16

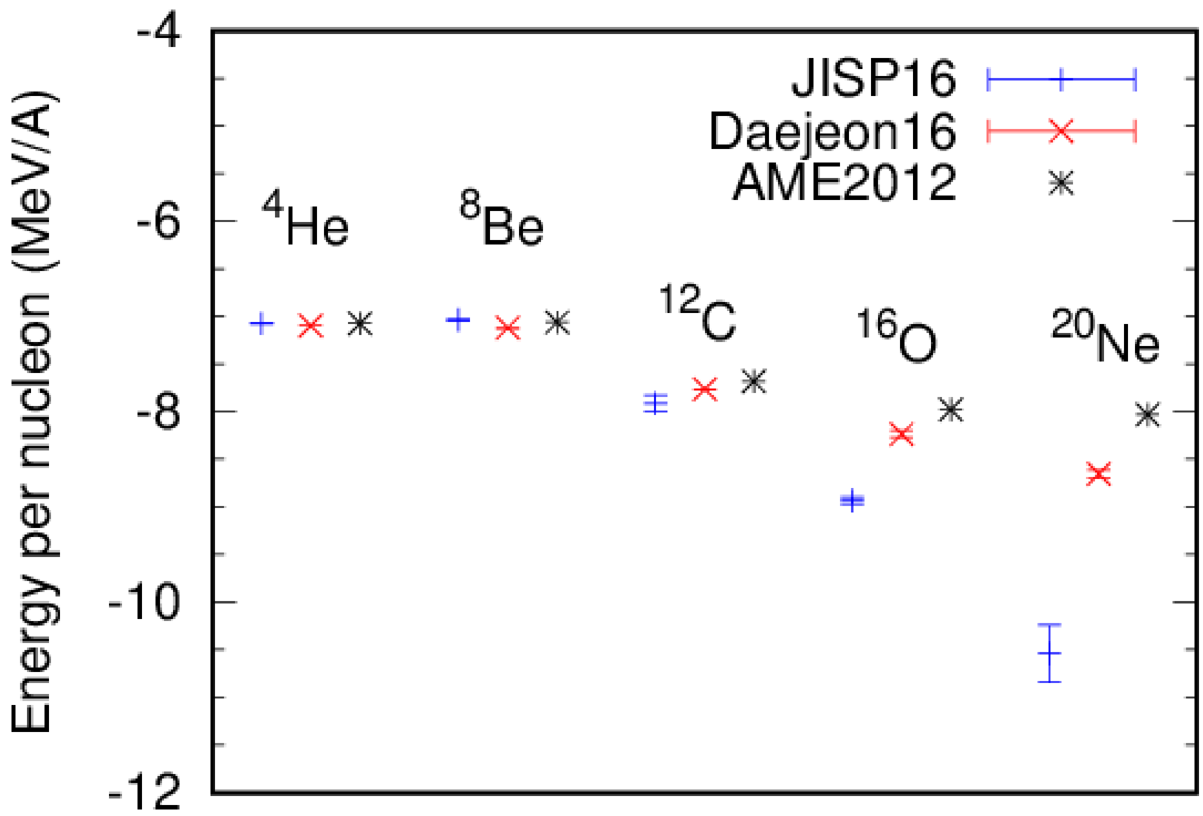
  - Derived from nucleon-nucleon scattering phase shifts by J-matrix inversion scattering method. Then, adjusted via a phase-shift equivalent transformations (PETs) to better describe light nuclei with $A < 16$

  A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, PLB644, 33 (2007)

- Daejeon16:
  - Starting from χEFT N3LO NN interaction (EM) + PETs

  A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris and J. P. Vary, PLB761, 87 (2016).

Ground-state energies of light nuclei

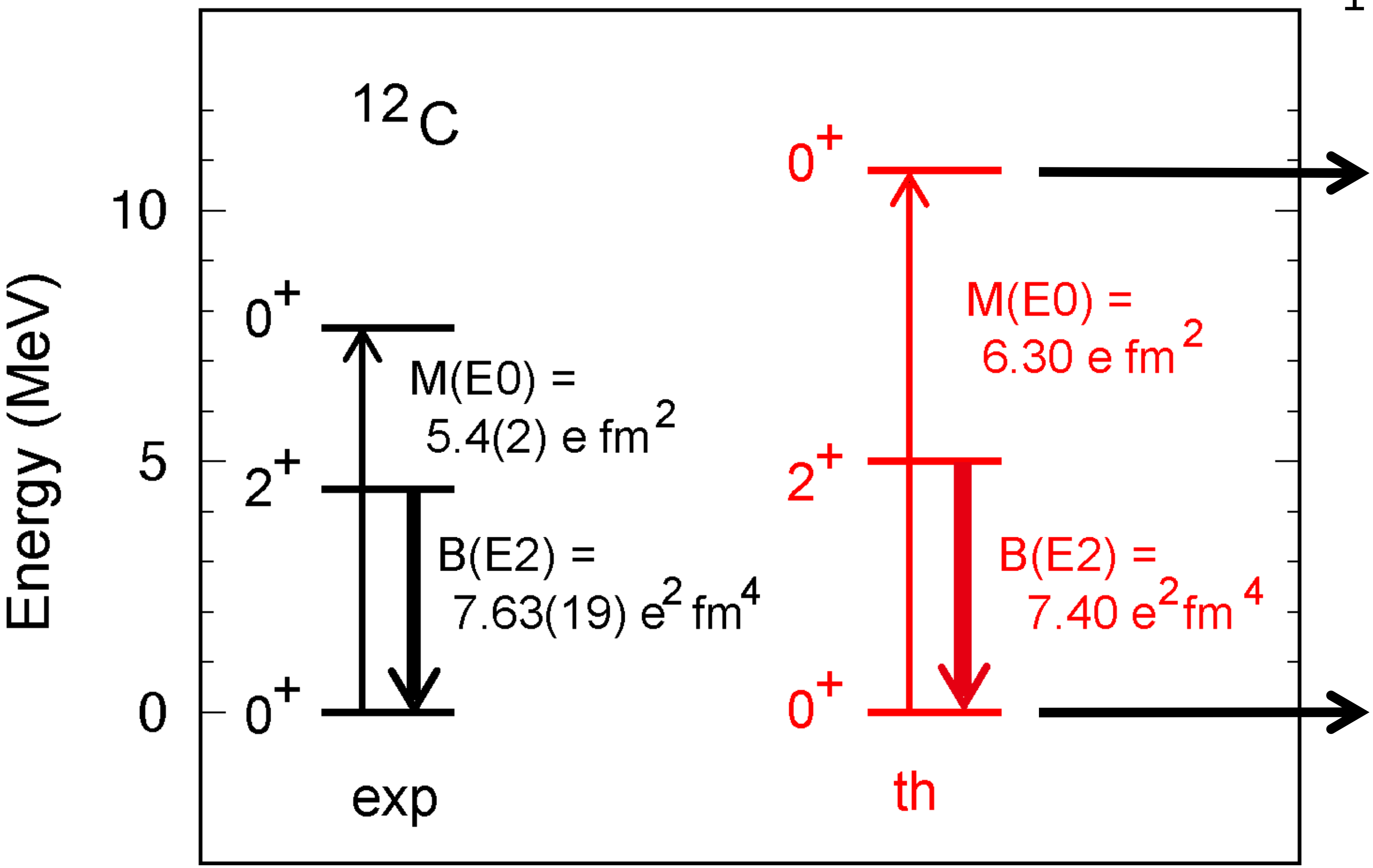


MCSM results are obtained using K computer by traditional extrapolation w/ optimum harmonic oscillator energies.

JISP16 results show good agreements w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

Daejeon16 results show good agreements w/ experimental data up to ^{20}Ne.

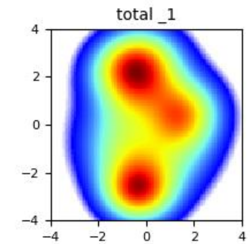
^{12}C excitation spectra and transitions



Daejeon16 NN, N_{shell} = 7, hw = 20 MeV
w/o energy-variance extrapolation

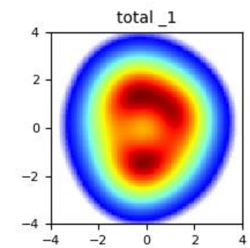
“Intrinsic” density

1st excited 0^+ state
(Hoyle state?)



r_{pp} = 2.60 fm

Ground state



r_{pp} = 2.28 fm

r_{pp} = 2.32(2) fm (exp)

Summary

- Ab initio calculations by NC-MCSM can be performed in light nuclei (A <= 20).
- NC-MCSM results can be extrapolated to the infinitely large basis space to obtain ab initio solution.
  - Daejoen16 NN interaction provides good agreement w/ experimental data for light nuclei.

Future perspective

- Alpha-cluster structure in light nuclei (p- & sd-shell region)

  ⟶ Next talk by T. Otsuka

- Neutron(proton)-rich nuclei in p-shell nuclei
- Heavier (sd-shell) N~Z nuclei beyond ^{20}Ne