

Alpha-clustering in atomic nuclei from first principles

Takashi Abe (RCNP, Osaka)

Collaborators:

T. Otsuka(U Tokyo/RIKEN/JAEA), T. Yoshida (RIST), Y. Tsunoda (U Tsukuba),
N. Shimizu (U Tsukuba), N. Itagaki (OMU), Y. Utsuno (JAEA),
J. P. Vary (Iowa State U), P. Maris (Iowa State U), H. Ueno (RIKEN)

References:

Nat. Commun. 13, 2234 (2022), Phys. Rev. C 104, 054315 (2021)

[nature](#) > [nature communications](#) > [articles](#) > [article](#)

Article | Open Access | Published: 27 April 2022

α -Clustering in atomic nuclei from first principles with statistical learning and the Hoyle state character

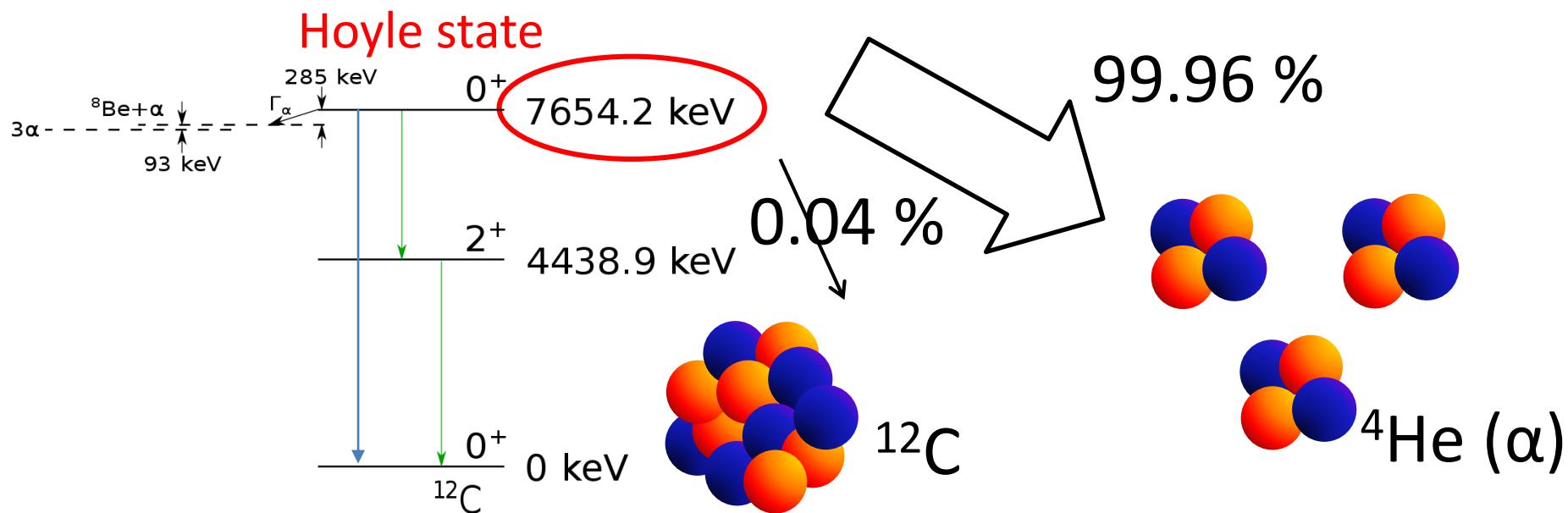
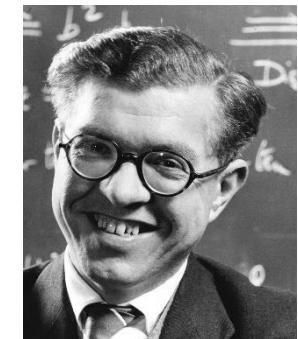
[T. Otsuka](#) , [T. Abe](#), [T. Yoshida](#), [Y. Tsunoda](#), [N. Shimizu](#), [N. Itagaki](#), [Y. Utsuno](#), [J. Vary](#), [P. Maris](#) & [H. Ueno](#)[Nature Communications](#) 13, Article number: 2234 (2022) | [Cite this article](#)578 Accesses | 2 Altmetric | [Metrics](#)

Abstract

A long-standing crucial question with atomic nuclei is whether or not α clustering occurs there. An α particle (helium-4 nucleus) comprises two protons and two neutrons, and may be the building block of some nuclei. This is a very beautiful and fascinating idea, and is indeed plausible because the α particle is particularly stable with a large binding energy. However, direct experimental evidence has never been provided. Here, we show whether and how α -like objects emerge in atomic nuclei, by means of state-of-the-art quantum many-body simulations formulated from first principles, utilizing supercomputers including K/Fugaku. The obtained physical quantities exhibit agreement with experimental data. The appearance and variation of the α clustering are shown by utilizing density profiles for the nuclei beryllium-8, -10 and carbon-12. With additional insight by statistical learning, an unexpected crossover picture is presented for the Hoyle state, a critical gateway to the birth of life.

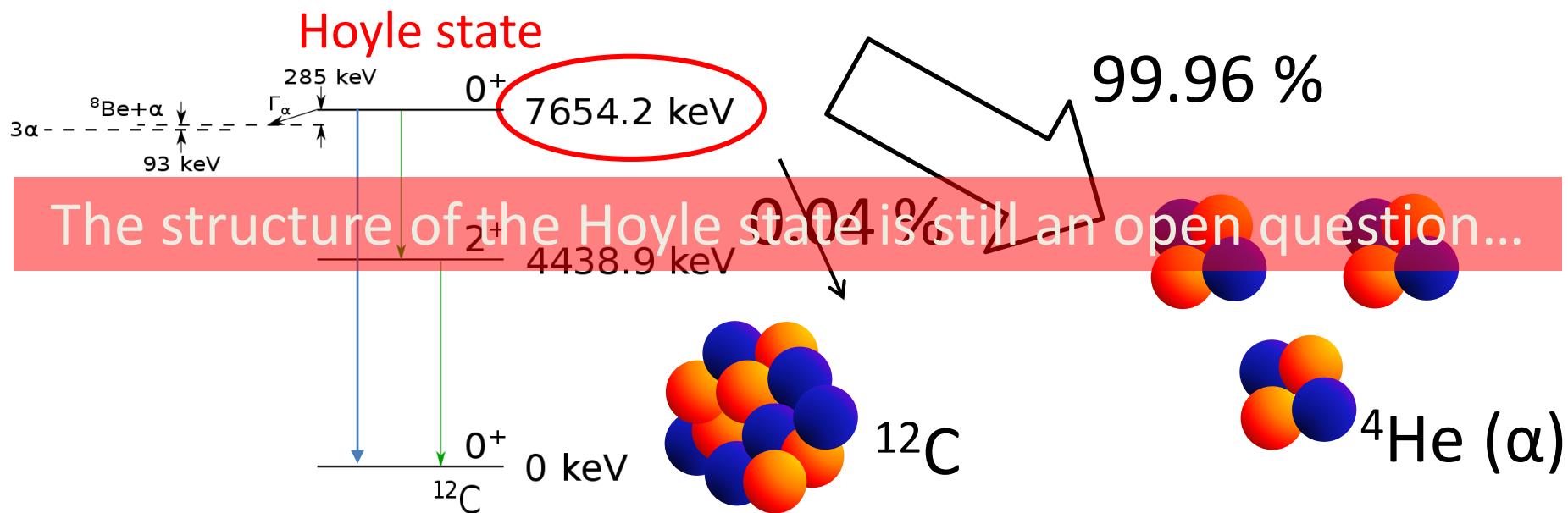
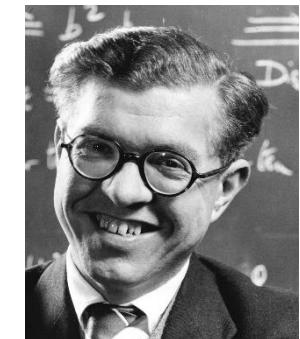
Hoyle state

- This state was predicted by Fred Hoyle in 1954.
- The existence of the Hoyle state is essential for the nucleosynthesis of carbon in helium-burning red giant stars, where $T \sim 10^8$ K and $\rho_{^{4\text{He}}} \sim 10^5$ g/cm³.
- This state is produced by the triple-alpha reaction. It primarily decays back into three alpha particles, but 0.0413% of decays occurs into the ground state.



Hoyle state

- This state was predicted by Fred Hoyle in 1954.
- The existence of the Hoyle state is essential for the nucleosynthesis of carbon in helium-burning red giant stars, where $T \sim 10^8$ K and $\rho_{^{4\text{He}}} \sim 10^5$ g/cm³.
- This state is produced by the triple-alpha reaction. It primarily decays back into three alpha particles, but 0.0413% of decays occurs into the ground state.



Alpha-cluster hypothesis

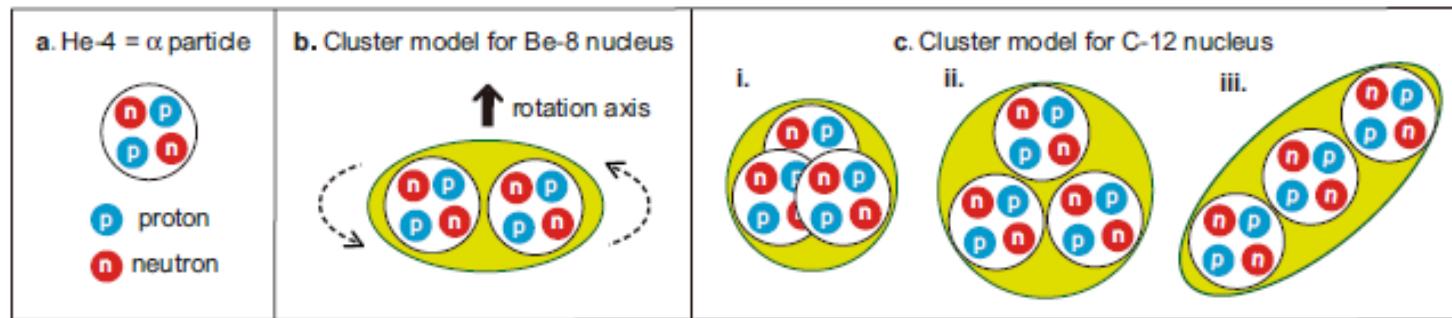


Fig. 1 Schematic illustrations of α clustering in atomic nuclei. **a** ${}^4\text{He} = \alpha$ particle, **b** ${}^8\text{Be}$, and **c** ${}^{12}\text{C}$ (three possible cases, i, ii, and iii). The green areas represent atomic nuclei allowing some movements of α clusters.

References

1. Wefelmeier, W. V. Ein geometrisches Modell des Atomkerns. *Z. Phys. Hadrons Nucl.* **107**, 330 (1937).
2. Wheeler, J. A. Molecular viewpoints in nuclear structure. *Phys. Rev.* **52**, 1083 (1937).
3. Morinaga, H. Interpretation of some of the excited states of $4n$ self-conjugate nuclei. *Phys. Rev. C* **101**, 254 (1956).
4. Brink, D. Alpha-particle model of light nuclei. *Proc. Int. Sch. Phys. Enrico Fermi. Course* **36**, 247 (1966).
5. Ikeda, K., Takigawa, N. & Horiuchi, H. The systematic structure-change into the molecule-like structures in the self-conjugate $4n$ nuclei. *Prog. Thoer. Phys. Suppl.* **E68**, 464 (1968).
6. Arima, A., Horiuchi, H., Kubodera, K. and Takigawa, N. Clustering in Light Nuclei. In: Baranger M. and Vogt E. (ed) *Advances in Nuclear Physics*, 5, 345 (Springer, Boston, MA, 1973).
7. Freer, M., Horiuchi, H., Kanada-En'yo, Y., Lee, D. & Meißner, U.-G. Microscopic clustering in light nuclei. *Rev. Mod. Phys.* **90**, 035004 (2018).

Alpha-cluster hypothesis

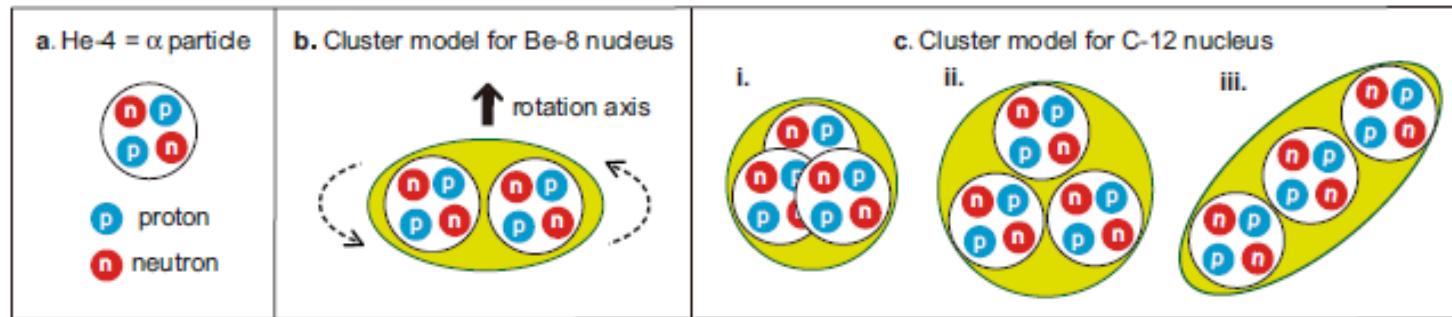


Fig. 1 Schematic illustrations of α clustering in atomic nuclei. **a** ${}^4\text{He} = \alpha$ particle, **b** ${}^8\text{Be}$, and **c** ${}^{12}\text{C}$ (three possible cases, i, ii, and iii). The green areas represent atomic nuclei allowing some movements of α clusters.

References

1. Wefelmeier, W. V. Ein geometrisches Modell des Atomkerns. *Z. Phys. Hadrons Nucl.* **107**, 330 (1937).
2. Wheeler, J. A. Molecular viewpoints in nuclear structure. *Phys. Rev.* **52**, 1083 (1937).
3. Morinaga, H. Interpretation of some of the excited states of $4n$ self-conjugate nuclei. *Prog. Phys.* **1**, 131 (1956).
4. Brink, D. Alpha-particle model of light nuclei. *Proc. Int. Sch. Phys. Enrico Fermi. Course* **36**, 247 (1966).
5. Ikeda, K., Takigawa, N. & Horiuchi, H. The systematic structure-change into the molecule-like structures in the self-conjugate $4n$ nuclei. *Prog. Thoer. Phys. Suppl.* **E68**, 464 (1968).
6. Arima, A., Horiuchi, H., Kubodera, K. and Takigawa, N. Clustering in Light Nuclei. In: Baranger M. and Vogt E. (ed) *Advances in Nuclear Physics*, 5, 345 (Springer, Boston, MA, 1973).
7. Freer, M., Horiuchi, H., Kanada-En'yo, Y., Lee, D. & Meißner, U.-G. Microscopic clustering in light nuclei. *Rev. Mod. Phys.* **90**, 035004 (2018).

How does it look like from an ab-initio point of view?
It is hard or impossible to observe in the experiments,
though...

“Ab initio” in low-energy nuclear structure physics

- Major challenge in nuclear theory
 - Nuclear structure & reactions directly from *ab initio* calculations
 - In terms of nucleon degrees of freedom w/ nuclear forces

→ Various *ab initio* approaches → No core shell model (full CI)

- Solve the non-relativistic many-body Schroedinger eq.
and obtain the eigenvalues and eigenvectors.

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

$$H = T + V_{\text{NN}} + V_{\text{3N}} + \dots + V_{\text{Coulomb}}$$

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

→ Computationally demanding → Monte Carlo shell model (MCSM)

Monte Carlo shell model (MCSM)

Standard shell-model calculation

$$H = \begin{pmatrix} * & * & * & * & * & \cdots \\ * & * & * & * & & \\ * & * & * & & & \\ * & * & & \ddots & & \\ * & & & & & \\ * & & & & & \\ \vdots & & & & & \end{pmatrix} \xrightarrow{\text{Diagonalization}} \begin{pmatrix} E_0 & & & & & 0 \\ & E_1 & & & & \\ & & E_2 & & & \\ & & & \ddots & & \\ 0 & & & & & \end{pmatrix}$$

Spanned by Slater determinants

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

Monte Carlo shell model

Importance truncation

$$H' \sim \begin{pmatrix} * & * & \cdots \\ * & \ddots & \\ \vdots & & \end{pmatrix} \xrightarrow{\text{Diagonalization}} \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Spanned by “important” bases
selected stochastically and variationally

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

MCSM wave function

- Superposition of quantum-number projected SDs

of MCSM basis states ~ 100

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

Superposition
Projection on to
good spin & parity
Deformed SD

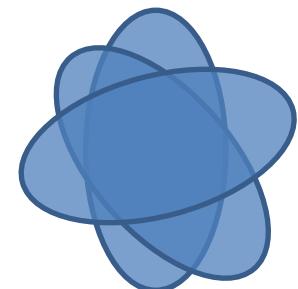
$$|\Phi(D^{(d)})\rangle = \prod_i \hat{a}_i^\dagger(D^{(d)}) | \begin{array}{l} \text{core} \\ \text{vacuum} \end{array} \rangle \quad \hat{a}_i^\dagger(D^{(d)}) = \sum_\ell D_{\ell i}^{(d)} \hat{c}_\ell^\dagger$$

- Angular momentum projection

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

Restoration of symmetries

$\sum_\Omega W(\Omega)$... **Favorable for**
 $O(\sim 10^4)$ **massively parallel computation**



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**

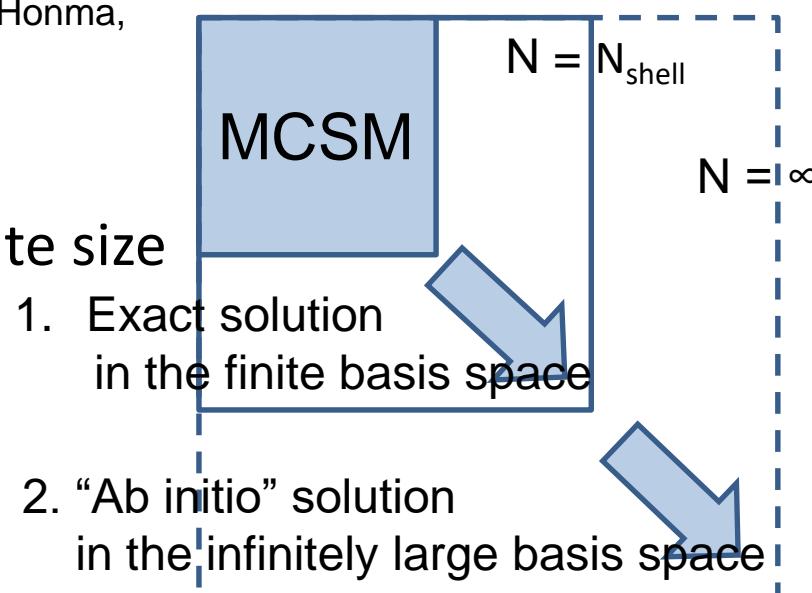
T. Mizusaki, M. Imada, Phys. Rev. C 65, 064319 (2002); 67, 041301 (2003).

T. Mizusaki, Phys. Rev. C 70, 044316 (2004).

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

→ **Ab initio solution**



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 $A < 16$

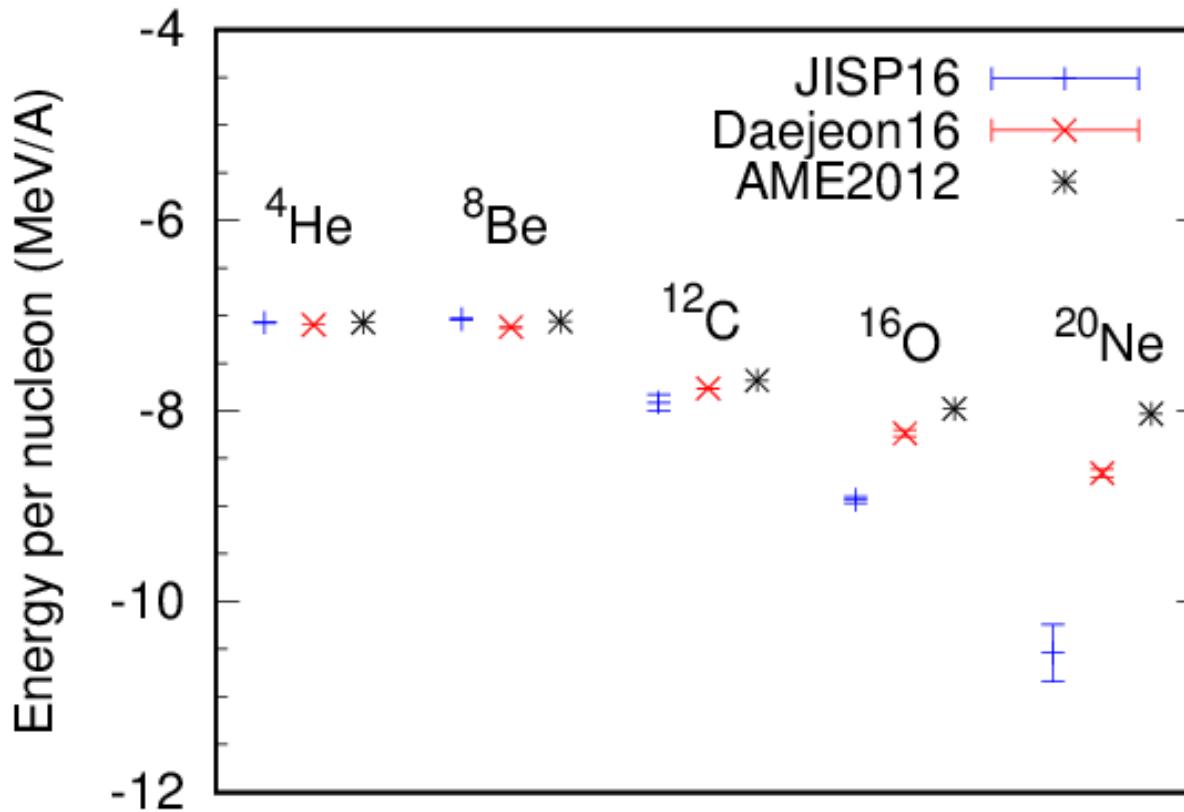
A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, PLB644, 33 (2007).

- Daejeon16:

- Starting from χ EFT 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



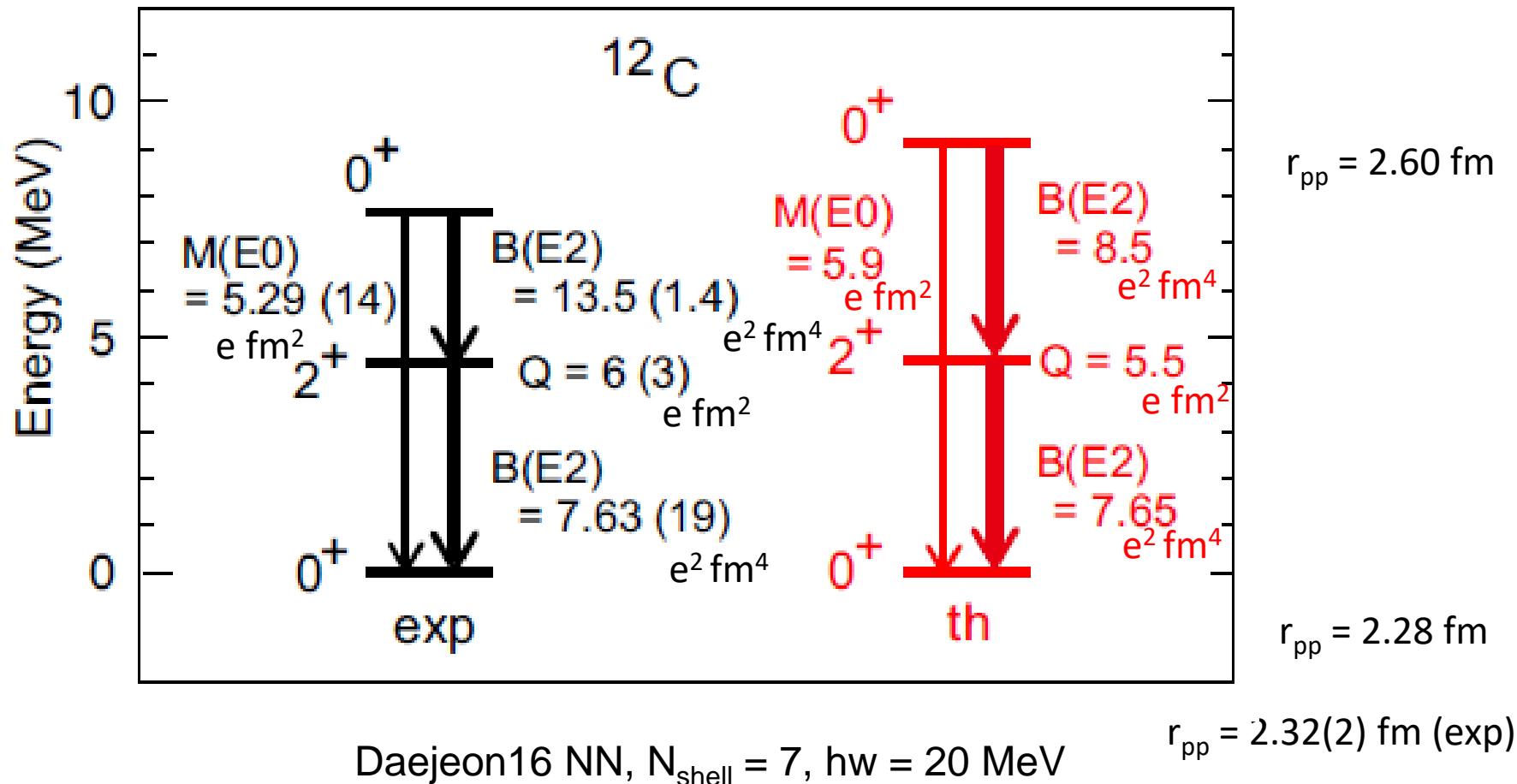
MCSM results are obtained using K computer by traditional extrapolation w/ optimum harmonic oscillator energies.

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

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, Phys Rev C 104, 054315 (2021).

^{12}C excitation spectra and transitions

K computer / Supercomputer Fugaku

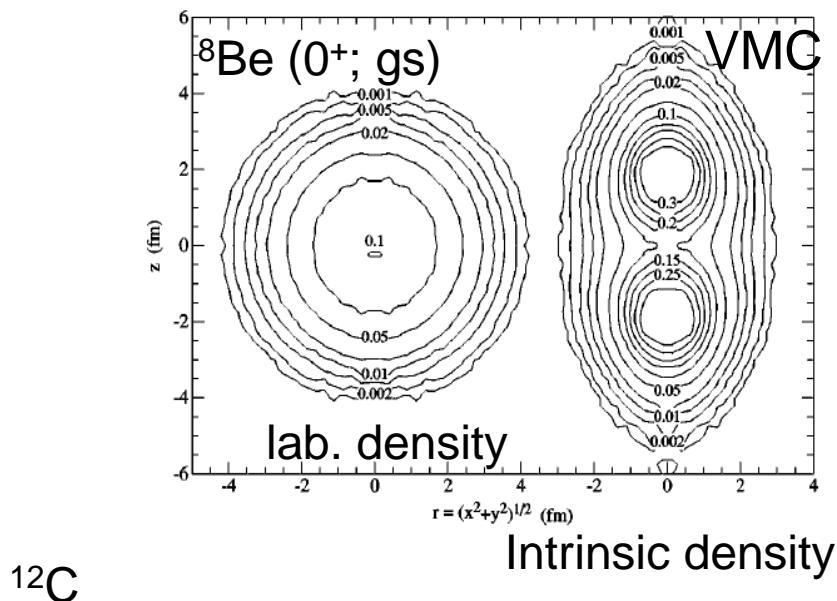
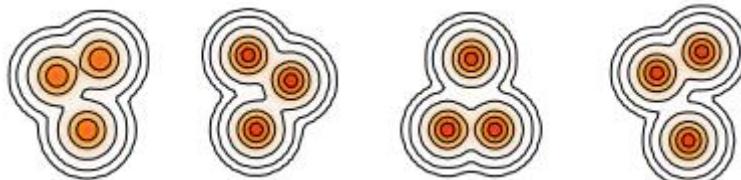


T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno,
J. P. Vary, P. Maris, H. Ueno, Nat. Commun. 13, 2234 (2022).

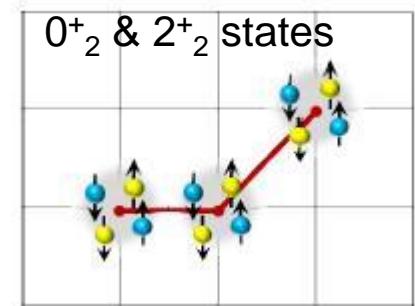
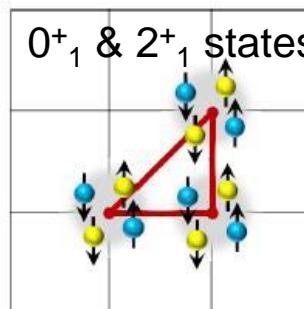
Density distribution from ab initio calc.

- Green's function Monte Carlo (GFMC)
 - "Intrinsic" density is constructed by aligning the moment of inertia among samples
- R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)

- Lattice EFT
 - Triangle structure of carbon-12
- E. Epelbaum, H. Krebs, T. A. Lahde, D. Lee, & U.-G. Meissner, Phys. Rev. Lett. 109, 252501 (2012), ...
- FMD (AMD)
 - H. Feldmeier, Nucl. Phys. A515, 147 (1990),
 - M. Chernkh, et al., Phys Rev Lett. 98 032501 (2007), ...



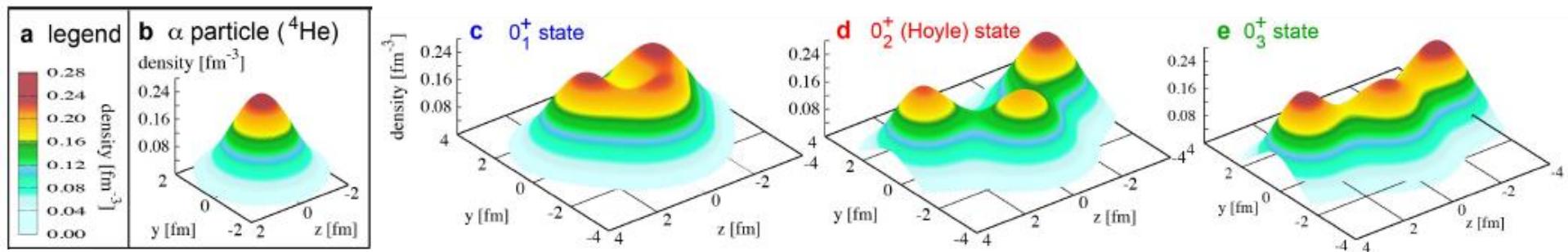
^{12}C



^{12}C 0^+_2 states (Hoyle state)

Density distribution of carbon-12

Daejeon16 NN interaction



⁰⁺₁ (ground) state

Compact (quantum liquid-like) structure

⁰⁺₂ (Hoyle) state

Emergence of 3 α -cluster structure
(without any assumptions of α clusters)

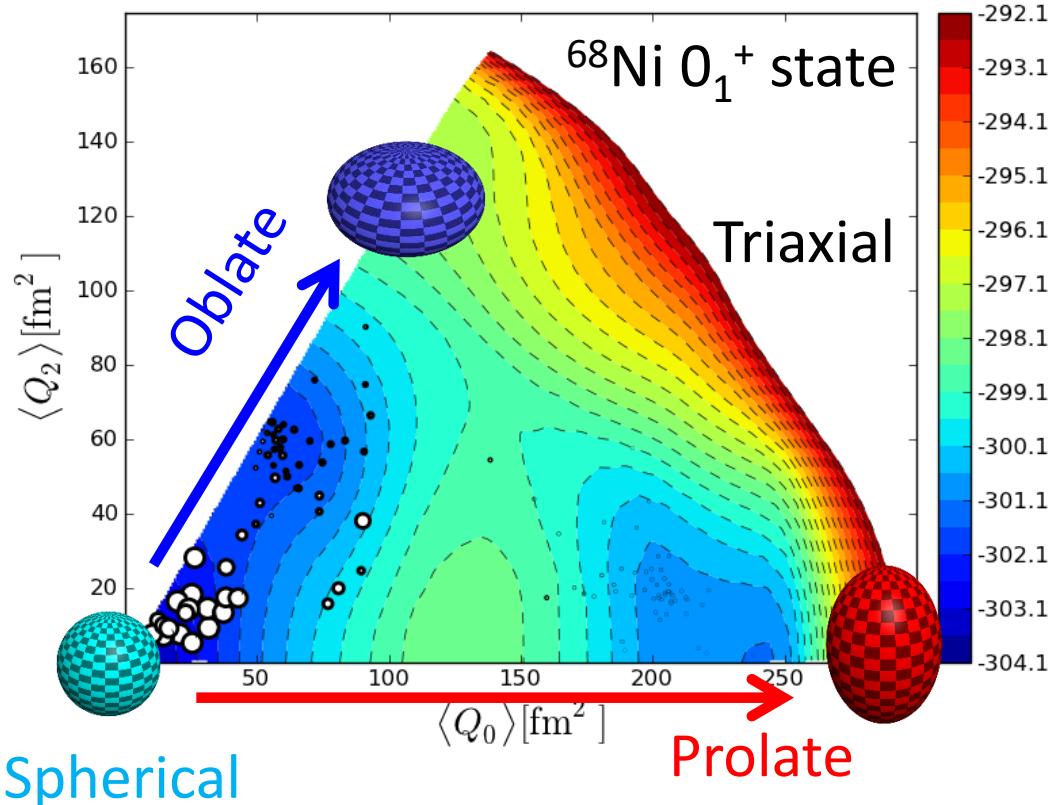
⁰⁺₃ state

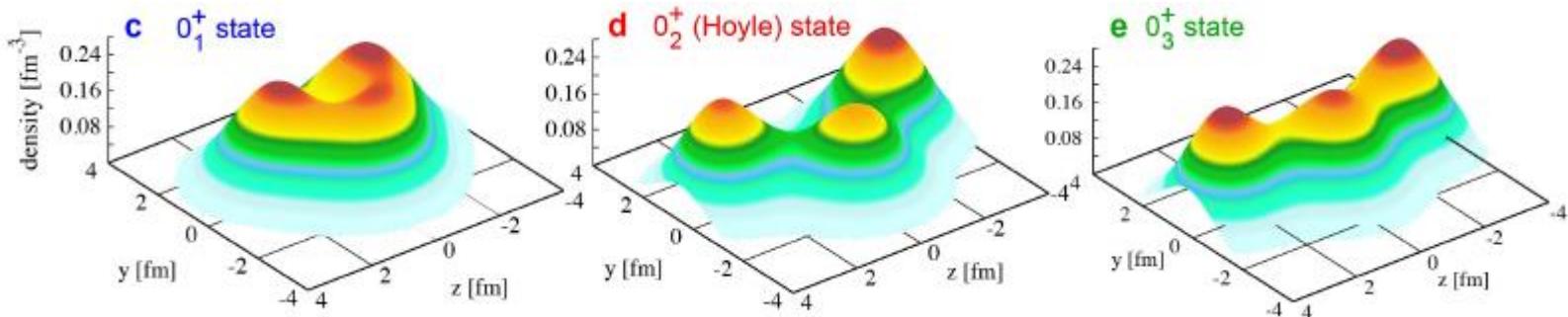
Linear chain of 3 α -clusters

T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno, J. P. Vary, P. Maris, H. Ueno, Nat. Commun. 13, 2234 (2022).

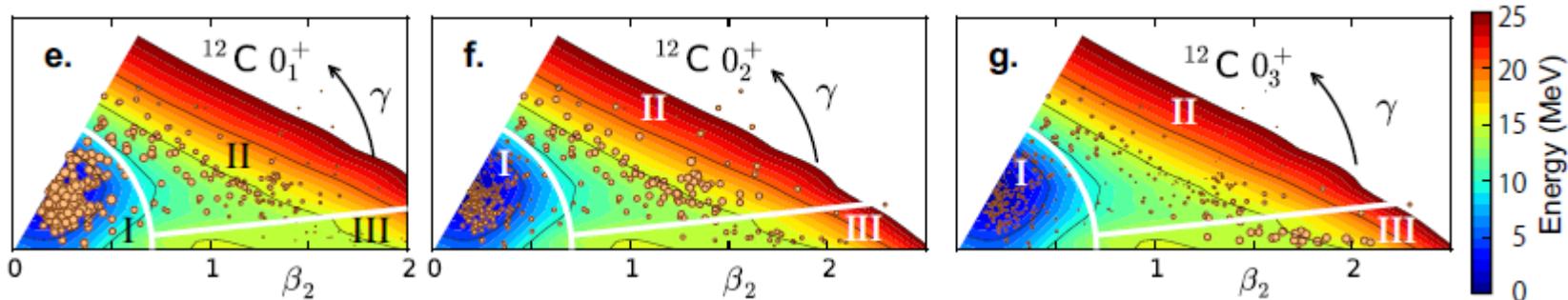
T-plot in MCSM

- MCSM wf: $|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$ ← Deformed SD
→ info of intrinsic shape
- Potential Energy Surface (PES): Calculated by Q-constrained HF
- Location of circles:
Quadrupole deformation of unprojected deformed SDs
- Area of circles:
Overlap probability btw deformed SD & total MCSM





Classification by T-plot analysis (in quadrupole-deformation DoF)



0_1^+ (ground) state

Region I (Quantum-liquid like): **94%**

Region II (Alpha-cluster like): **6%**

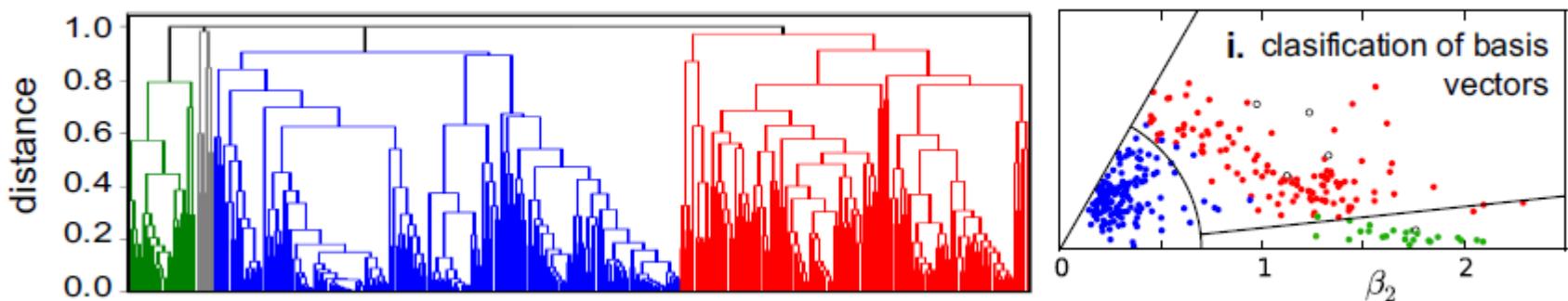
0_2^+ (Hoyle) state

Region I: **33% (~ 1/3)**

Region II: **61% (~ 2/3)**

Mixture of alpha-cluster
& quantum-liquid like structures
(crossover)

Classification by cluster analysis (with dendrogram)



Summary

- Ab initio calculations in NC-MCSM can be performed up to $A \sim 20$ on state-of-the-art supercomputers like K computer and Fugaku.
- NC-MCSM results can be extrapolated to the infinitely large basis space to obtain an ab initio solution.
 - Daejoen16 NN interaction provides good agreement w/ experimental data for light nuclei.

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, Phys Rev C 104, 054315 (2021).

K computer

K computer

Fugaku

- Low-lying level structure of ^{12}C can be examined by NC-MCSM, including alpha-cluster structure of the Hoyle state.

T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno, J. P. Vary, P. Maris, H. Ueno, Nat. Commun. 13, 2234 (2022).

Future perspective

- Application to the triple alpha reaction...