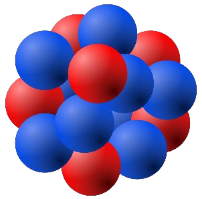
Papers discussed : A. Tichai, P. Demol, T. Duguet, PLB **851** 138571 (2024)
P. Demol, T. Duguet, A. Tichai, PLB **878** 140524 (2026)
U. Vernik, P. Demol, T. Duguet, A. Tichai, arXiv:2607:05086 (2026)

Tin isotopes from ab initio nuclear structure calculations

***Pepijn Demol**, T. Duguet, A. Tichai, U. Vernik*

Colloque GANIL, 21 - 25 Sept 2026

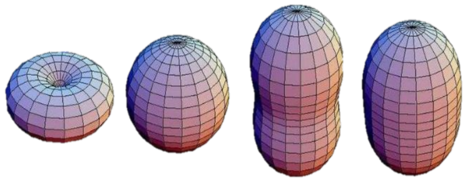
Broad nuclear phenomenology



Nucleus: bound system of Z **protons** and N **neutrons** (nucleons)

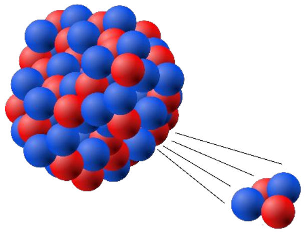
Ground-state properties

Mass, binding energy, shape, moments, ...



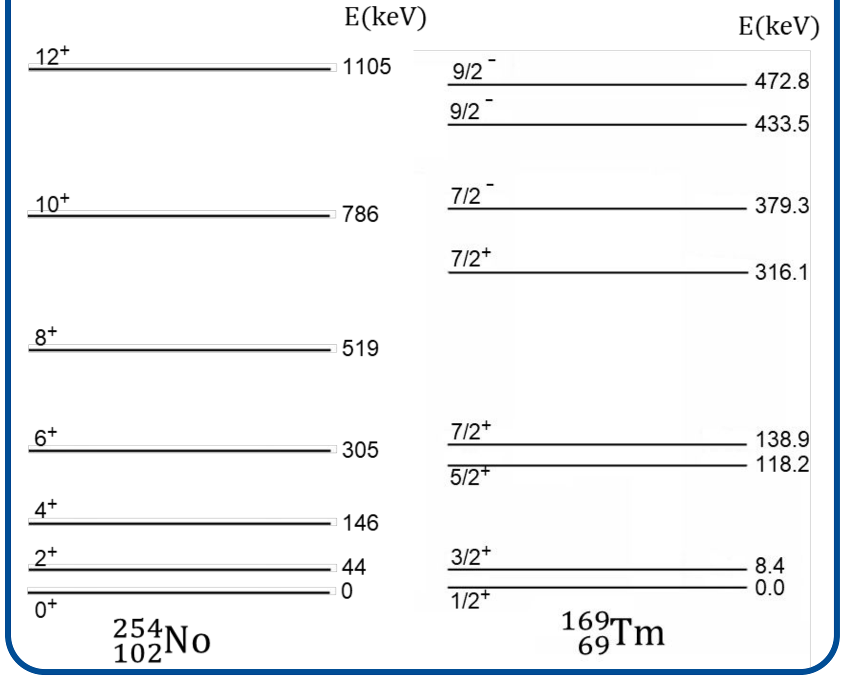
Radioactive decay

α, $\beta^{+/-}$, p, fission, ...



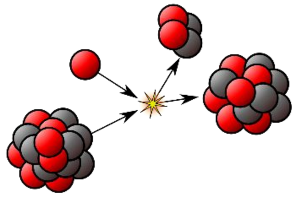
Spectroscopy

Collective (rotational/vibrational), Single-particle dominated



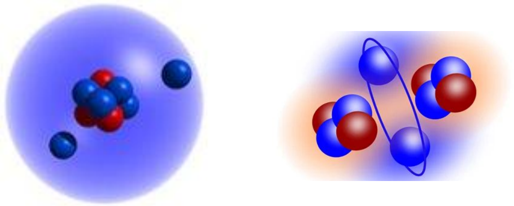
Nuclear reactions

Compound, knockout, transfer, ...



Exotic structures

Halo, clustering, ...



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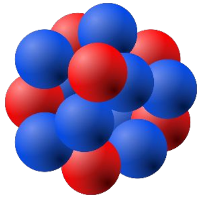

Nucleus: bound system of Z **protons** and N **neutrons** (nucleons)

Ground-state properties	Spectroscopy	Nuclear reactions

The atomic nucleus is a **correlated self-bound many-body quantum system** and therefore **intrinsically complex**

⬇️

Requires **systematic** theoretical framework with **high predictive power** = aim of *ab initio* nuclear theory

Ab initio approach to nuclear structure

Assumption: protons and neutrons are relevant degrees of freedom

Solve the A-body Schrödinger equation

$$H|\Psi_n^A\rangle = E_n^A|\Psi_n^A\rangle$$

1) Chiral effective field theory (EFT)

$$H = T + V_{\mathrm{LO}} + V_{\mathrm{NLO}} + V_{\mathrm{N^2LO}} + \cdots$$

- Rooted into QCD
- Up to A-body interactions

2) many-body method

$$|\Psi_n^A\rangle = \mathcal{W}_n|\Phi_n\rangle = |\Phi_n^{(0)}\rangle + |\Phi_n^{(1)}\rangle + |\Phi_n^{(2)}\rangle + \cdots$$

- All nucleons active (no core)
- Controlled approximations

Systematically improvable double expansion

$\longrightarrow$ allows for uncertainty quantification

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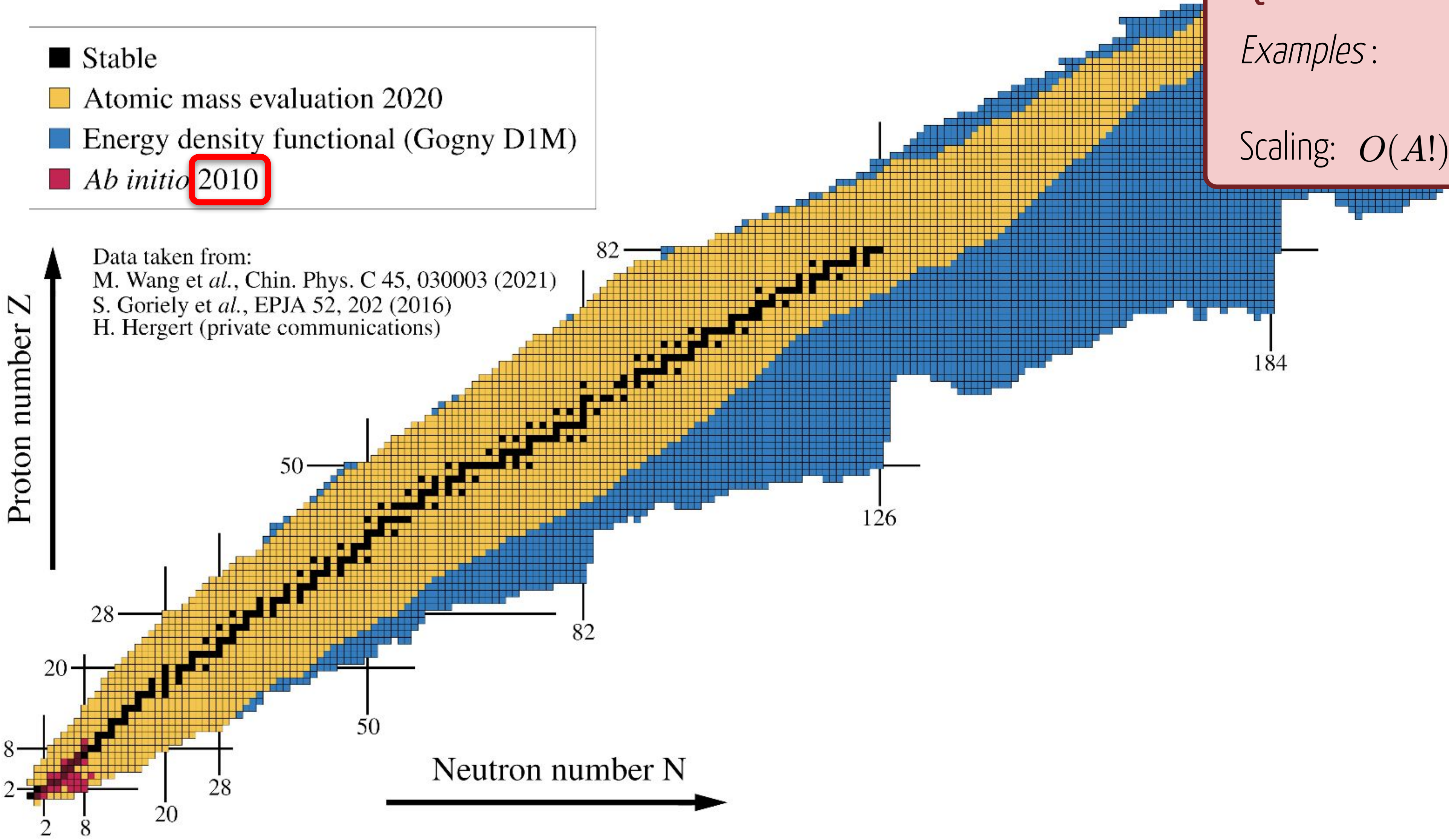
Recent progress of ab initio



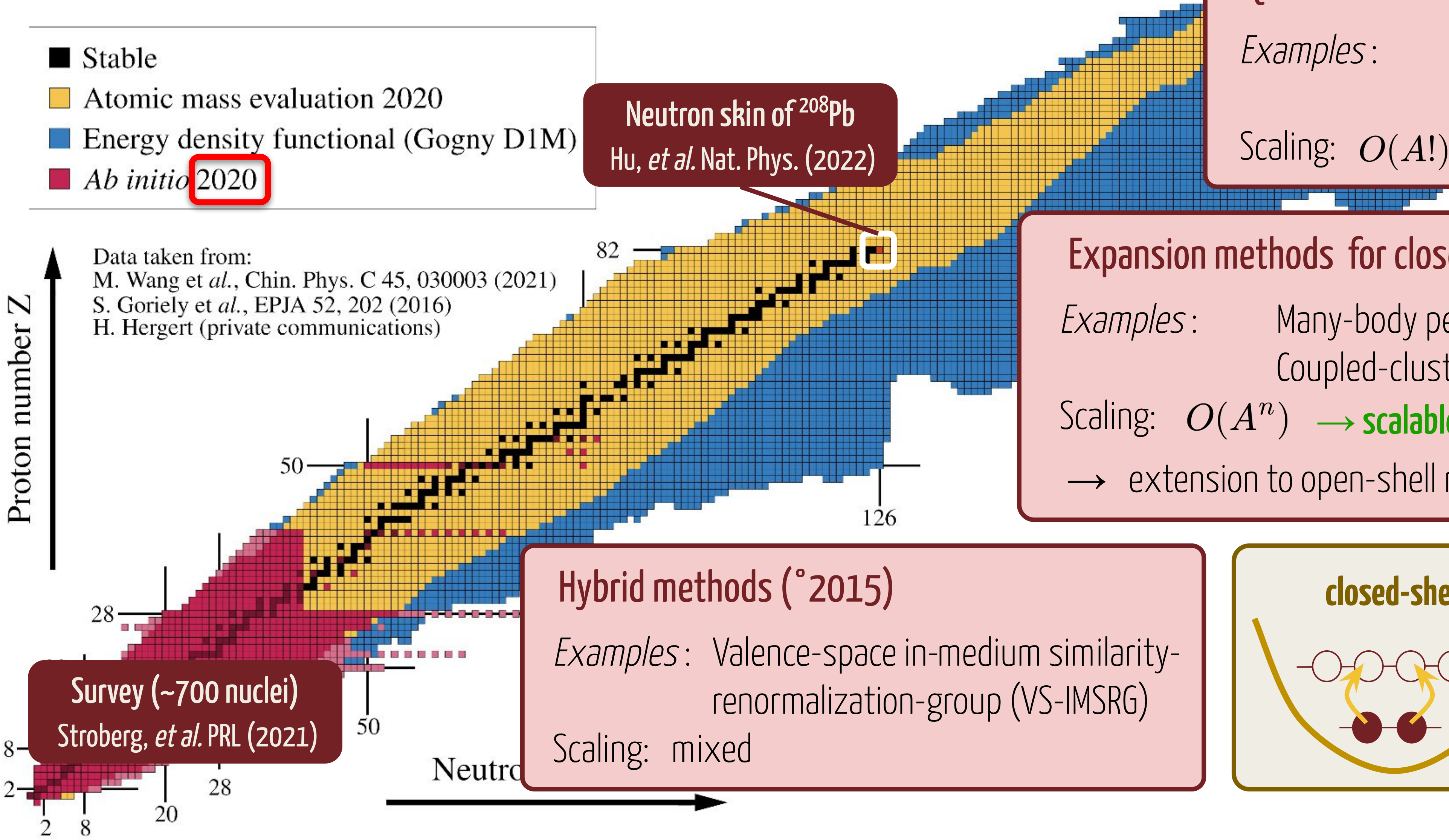
Quasi-exact methods (˚2000)

Examples : Diagonalization
Monte-Carlo

Scaling: $O(A!)$ $\longrightarrow$ light nuclei only

Nuclear charts courtesy of B. Bally

Recent progress of ab initio



Neutron skin of ^{208}Pb
Hu, *et al.* Nat. Phys. (2022)

Survey (~700 nuclei)
Stroberg, *et al.* PRL (2021)

Quasi-exact methods (˚2000)

Examples : Diagonalization
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Scaling: $O(A!)$ → light nuclei only

Expansion methods for closed-shell nuclei (˚2010)

Examples : Many-body perturbation theory (MBPT)
Coupled-cluster theory (CC)

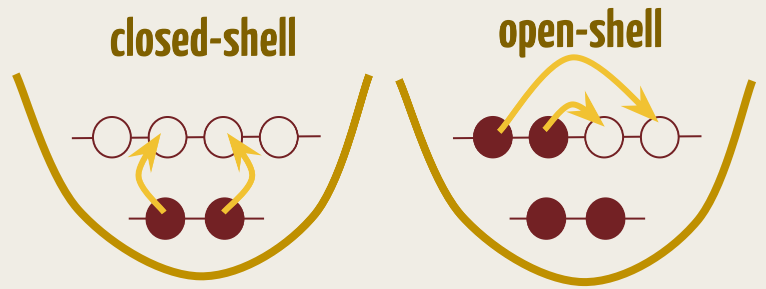
Scaling: $O(A^n)$ → scalable

→ extension to open-shell nuclei (˚2015)

Hybrid methods (˚2015)

Examples : Valence-space in-medium similarity-renormalization-group (VS-IMSRG)

Scaling: mixed



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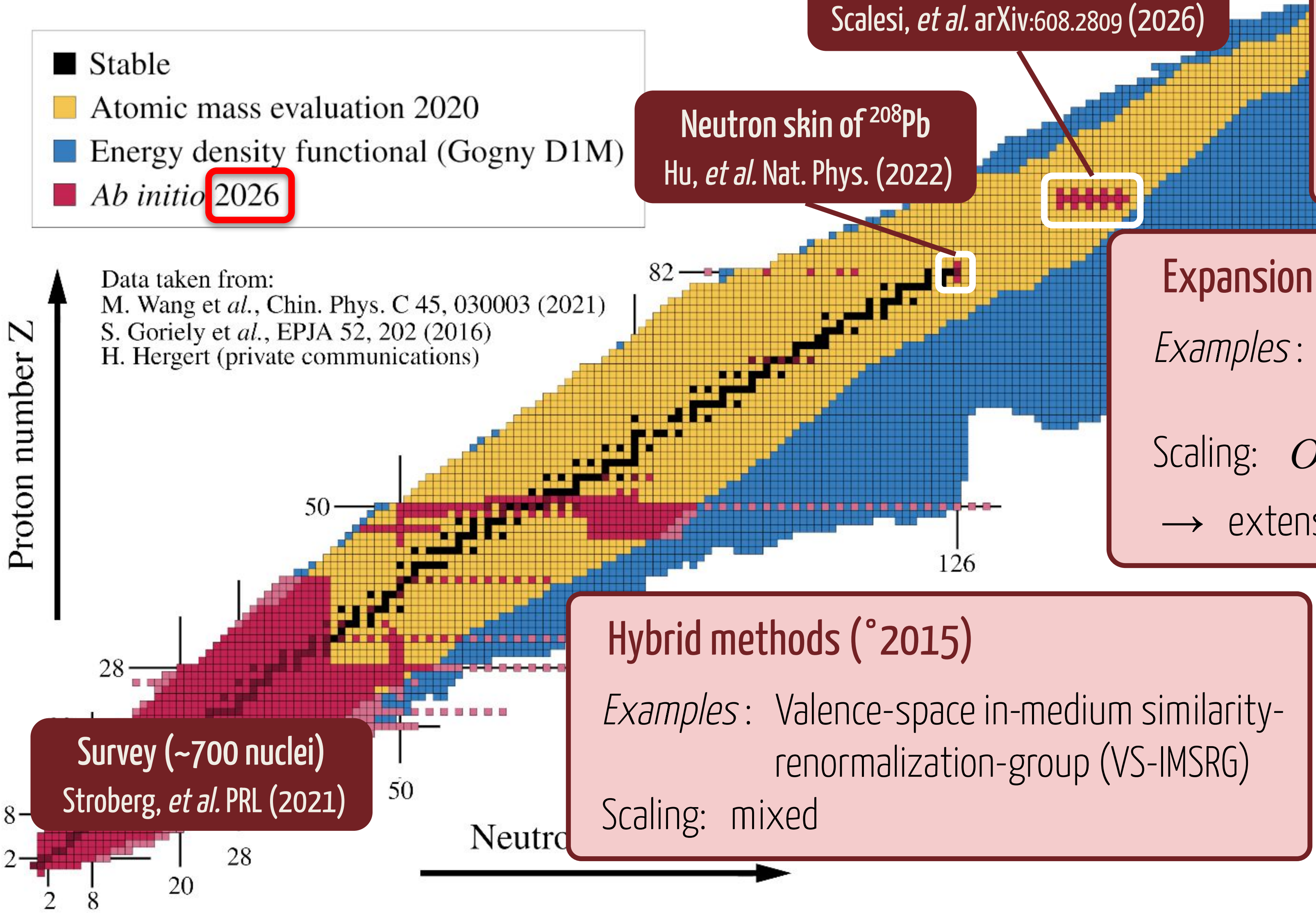

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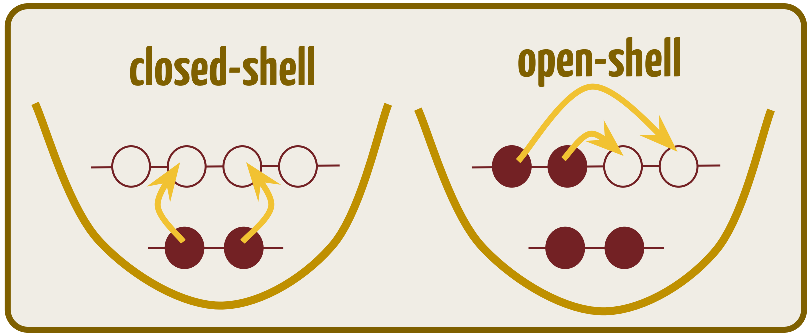
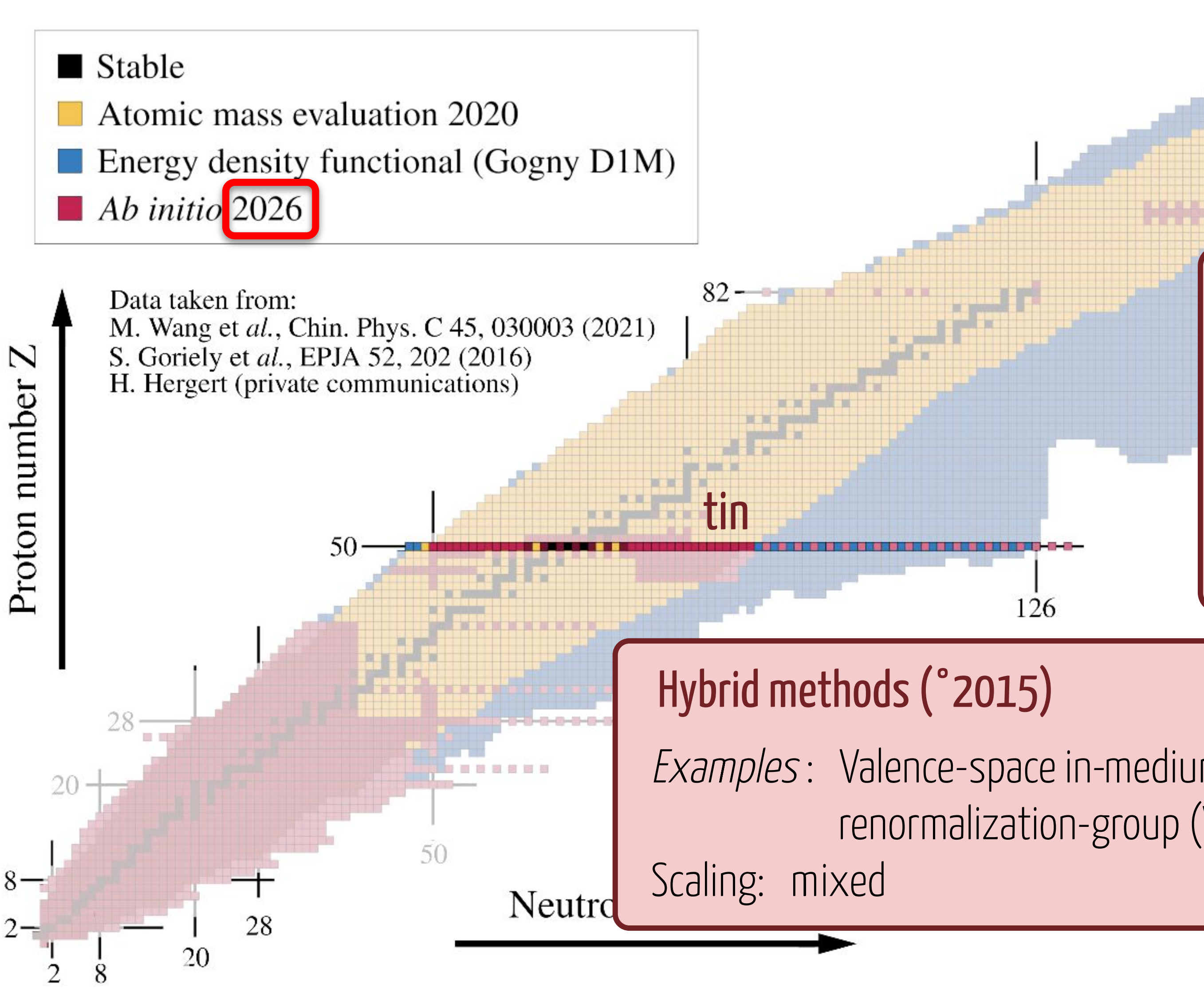


Recent progress of ab initio



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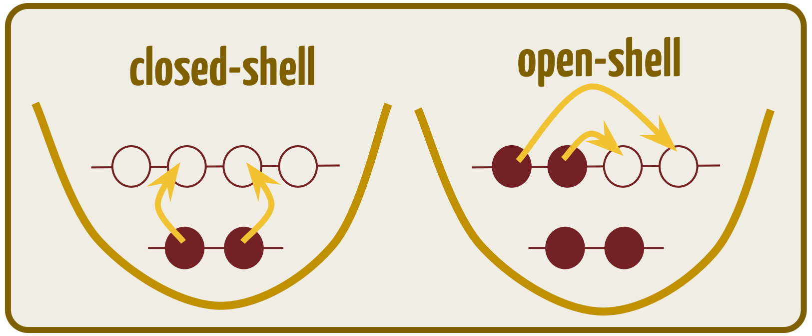


Many-body expansion methods

$$H\left|\Psi_n^A\right\rangle = E_n\left|\Psi_n^A\right\rangle$$

Mean-field: Hartree-Fock $H_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle$

<u>Partitioning:</u> $H = H_0 + H_1$ → Correlation expansion $|\Psi_n^A\rangle = \mathcal{W}_n|\Phi_n\rangle$

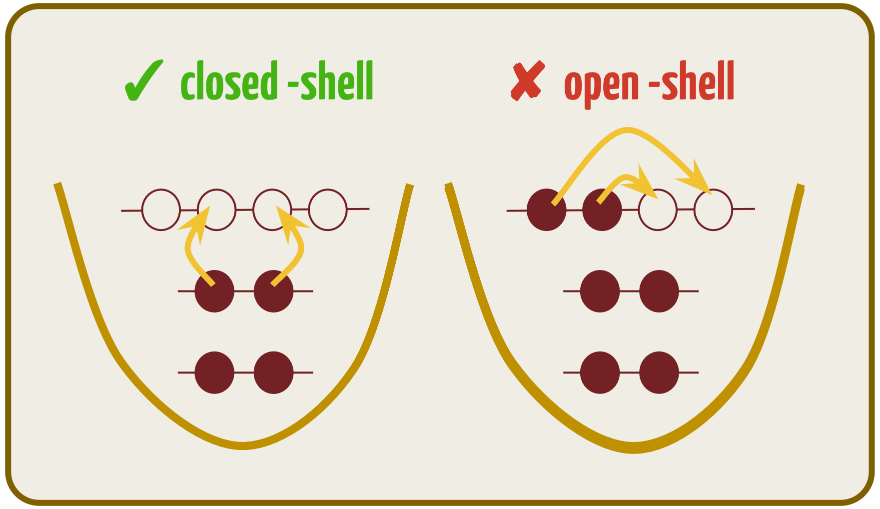
Many-body perturbation theory (MBPT)

$\mathcal{W}$: Taylor expansion in powers of H_1

Coupled-cluster theory (CC)

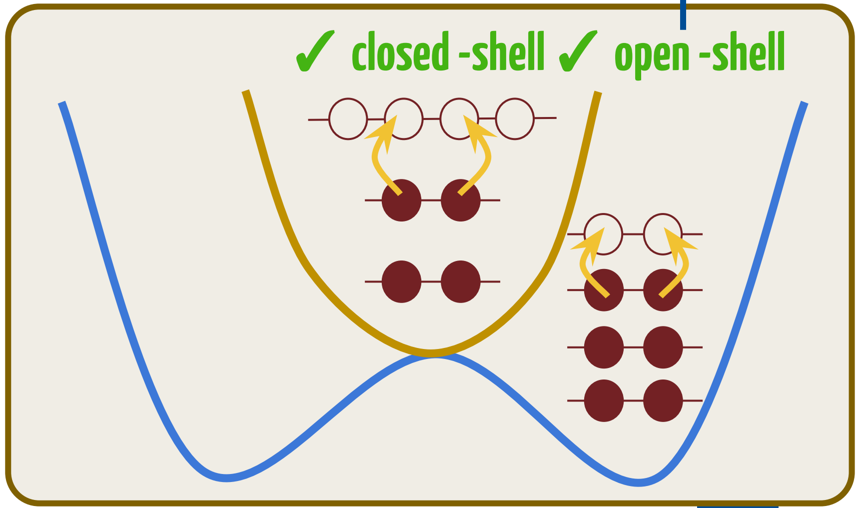
$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(H_1)$

Semi-magic nuclei spontaneously break particle-number symmetry related to pairing



Symmetry breaking of H_0 & H_1

Lifts degeneracy



BLU-ULB BRUSSELS LABORATORY OF THE UNIVERSE ULB fnrs FREEDOM TO RESEARCH

$$H\left|\Psi_n^A\right\rangle = E_n\left|\Psi_n^A\right\rangle$$

Many-body expansion methods

Mean-field: Hartree-Fock-Bogoliubov (HFB) $H_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle$

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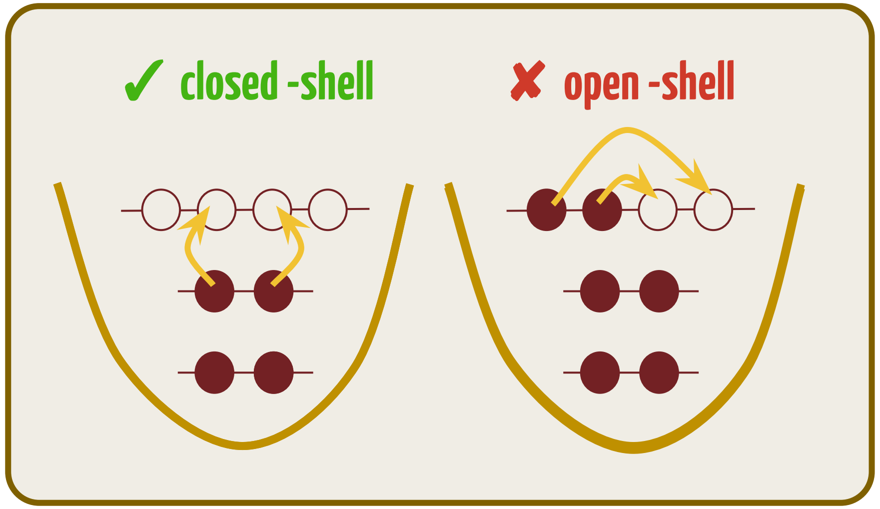
Bogoliubov coupled-cluster theory (BCC)

$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(H_1)$

Semi-magic nuclei spontaneously break **particle-number symmetry** related to **pairing**



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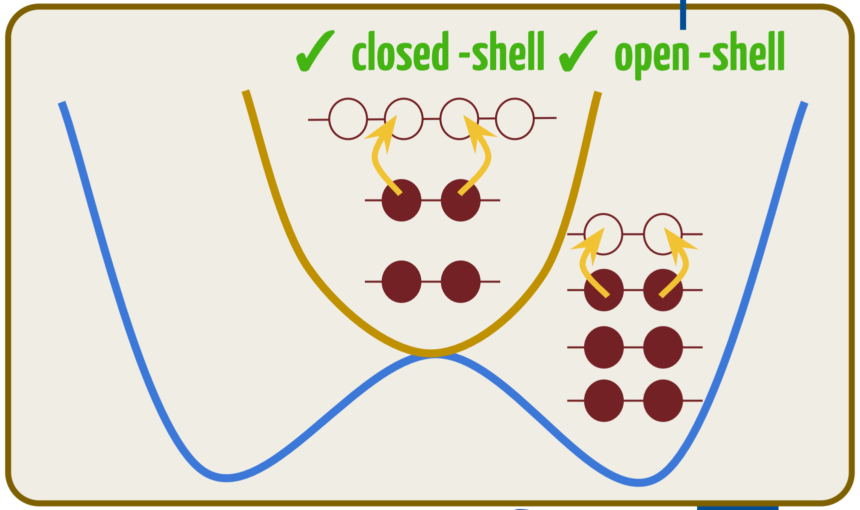

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Symmetry breaking of H_0 & H_1

Lifts degeneracy

A. Signoracci, et al. PRC **91** (2015).

Bogoliubov coupled-cluster (BCC) theory

Bogoliubov coupled-cluster theory (BCC)

$\mathcal{W} = e^{\mathcal{T}}$ with cluster excitation operator $\mathcal{T}(H_1)$

Exponential ansatz: $|\Psi_0^A\rangle = e^{\mathcal{T}}|\Phi\rangle$

Quasi-particle cluster operator: $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \cdots$

BCCSD

$$\mathcal{T}_1 \equiv \frac{1}{2!}\sum_{k_1 k_2} t_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$ [singles]

$$\mathcal{T}_2 \equiv \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$ [doubles]

$$\mathcal{T}_3 \equiv \frac{1}{6!}\sum_{k_1 k_2 k_3 k_4 k_5 k_6} t_{k_1 k_2 k_3 k_4 k_5 k_6} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} \beta^\dagger_{k_5} \beta^\dagger_{k_6}$$ [triples]

Quasi-particle excitation operators : mix of ordinary single-particle creation and annihilation operators $\beta^\dagger_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p$

Excitation amplitudes : solutions of set of non-linear algebraic equations which must be solved iteratively

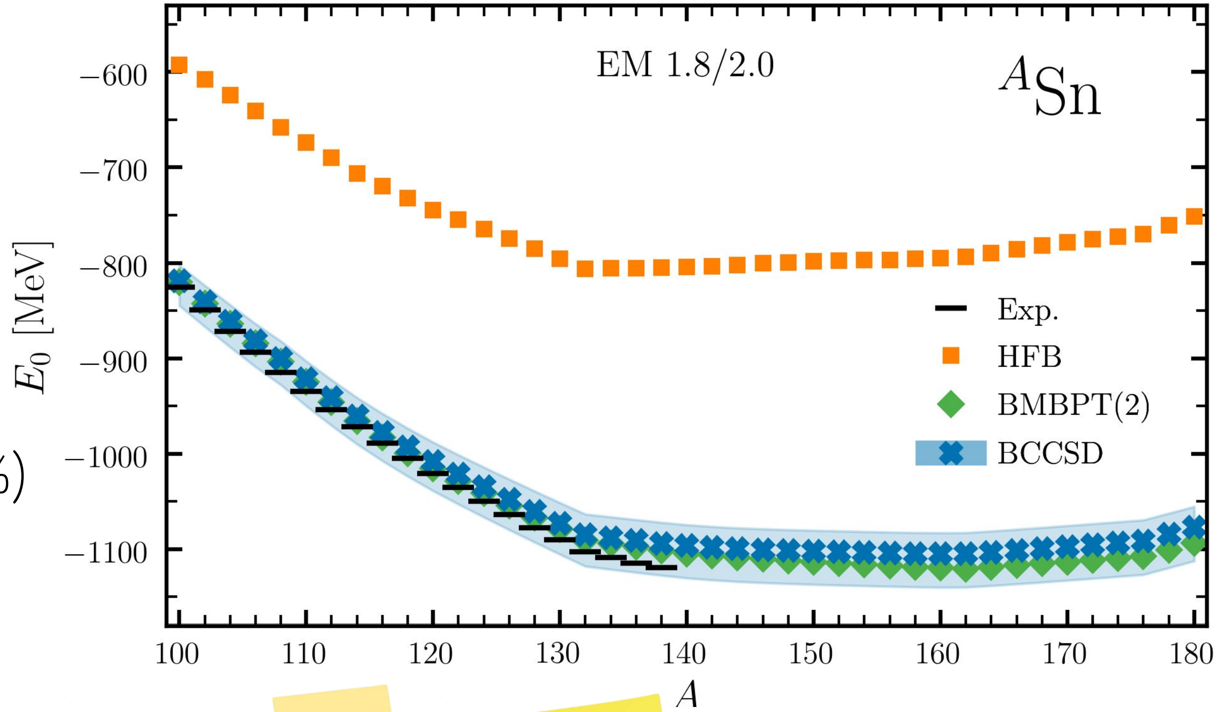
Application of BCC to binding energies of tin isotopes

A. Tichai, PD, T. Duguet, PLB **851** (2024).

BCCSD applied total binding energy

- Ground-state energy along Sn chain: ^{100}Sn – ^{180}Sn
- BCCSD agrees with experiment within uncertainty* (2–3%)
- BMBPT(2) performs well (soft interaction)
- BCCSD uncertainty dominated by lacking triples excitations

$$\boxed{\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2} + \mathcal{T}_3 + \cdots$$



***Uncertainties**

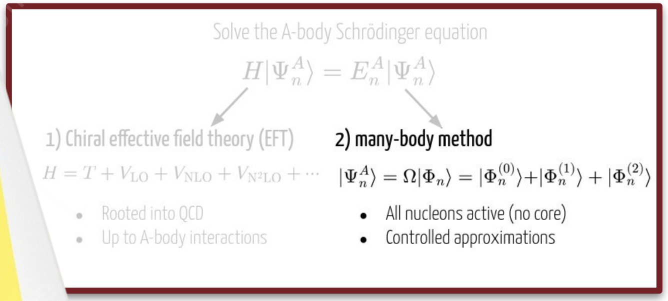
Many-body error only

- computational basis

- many-body expansion

- particle-number breaking

- normal-ordering



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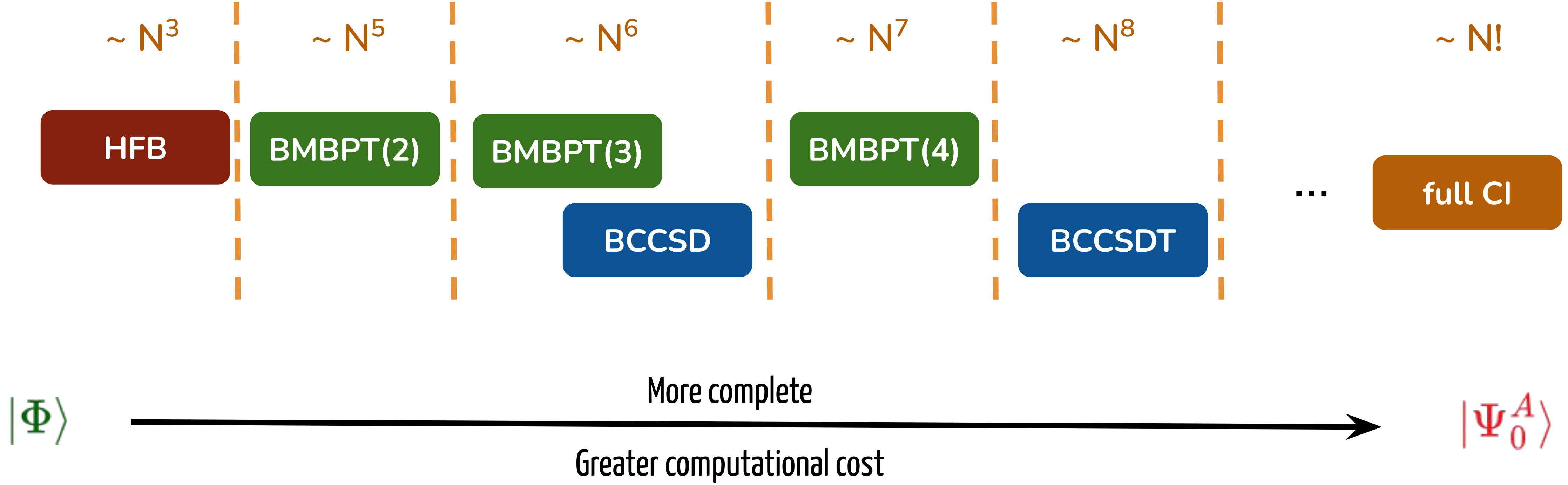
Towards a more complete account of correlations



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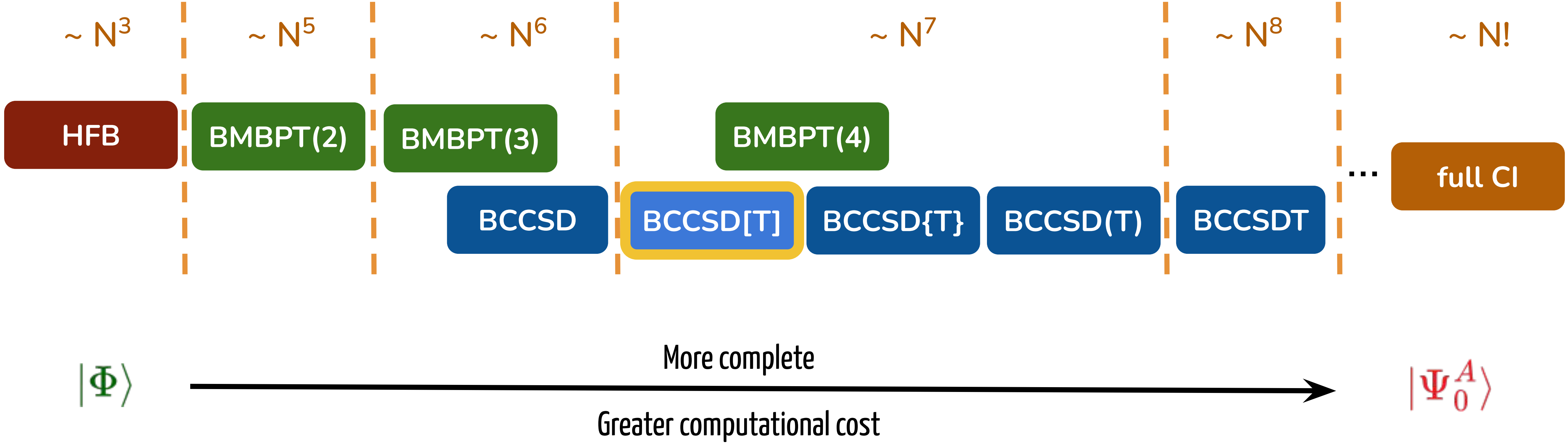
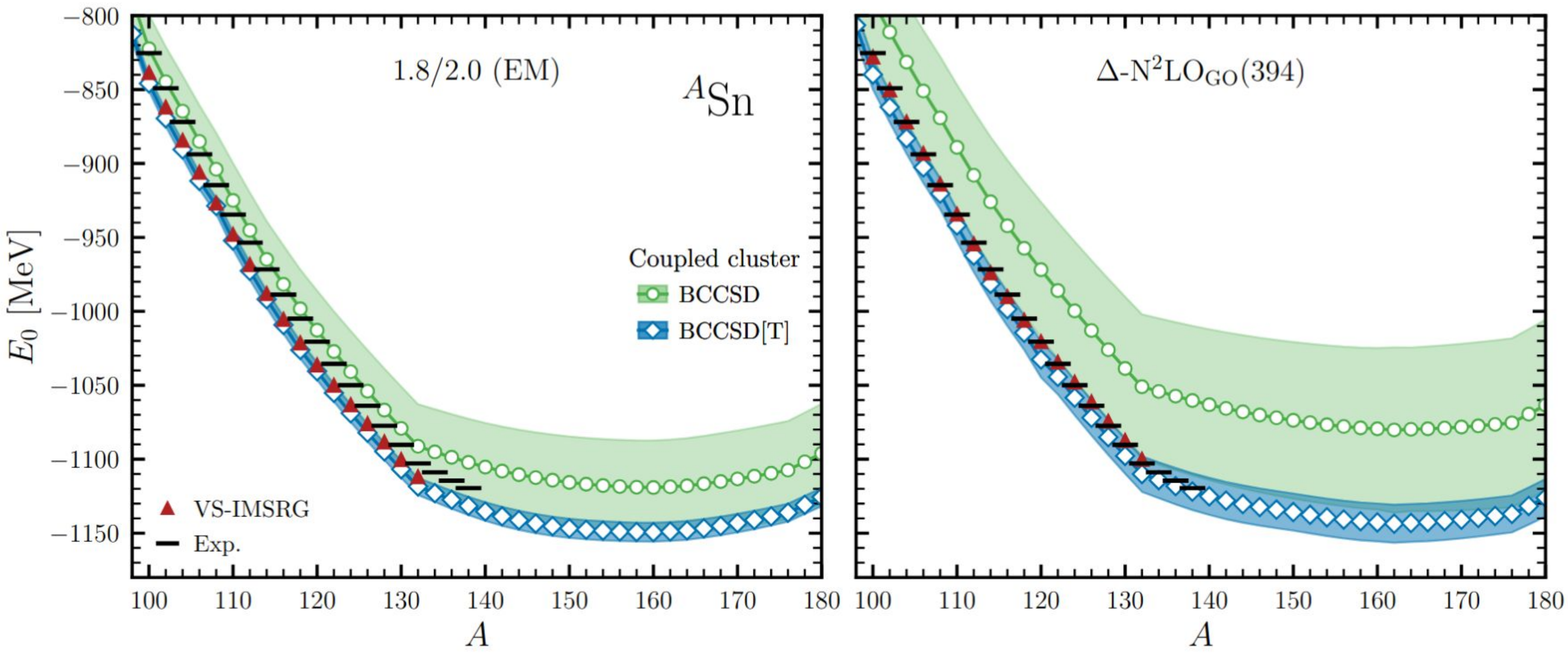


U. Vernik, PD, T. Duguet, A. Tichai, arXiv:2607.05086 (2026).

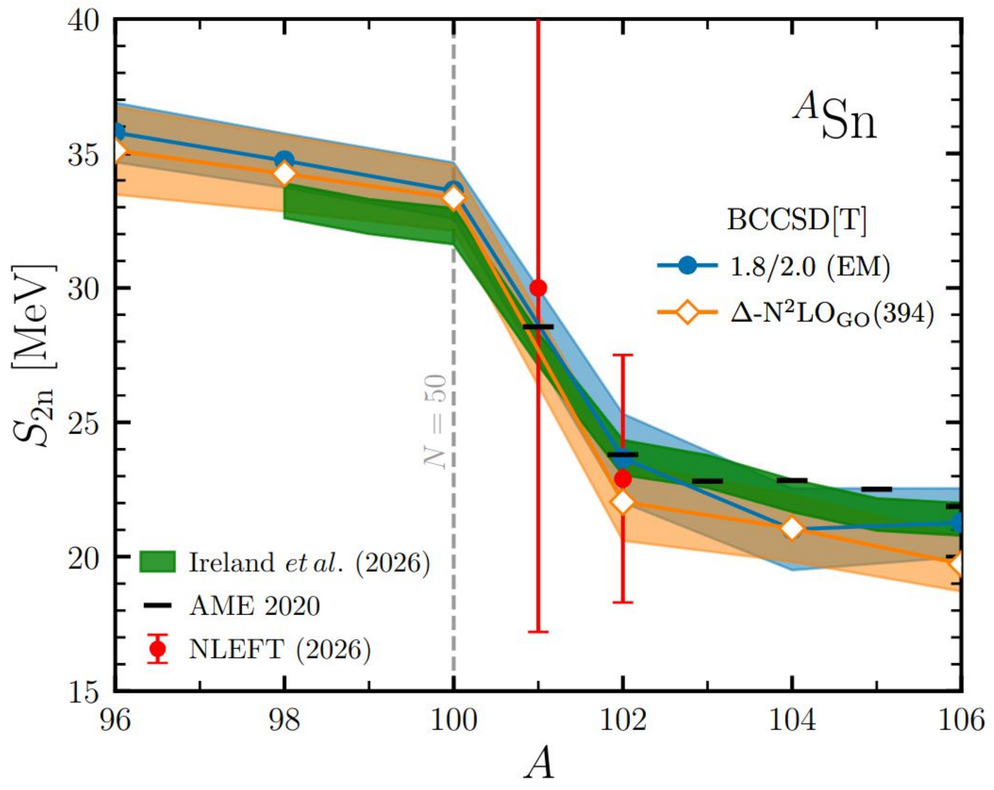
High-precision BCCSD[T] prediction of total binding energy

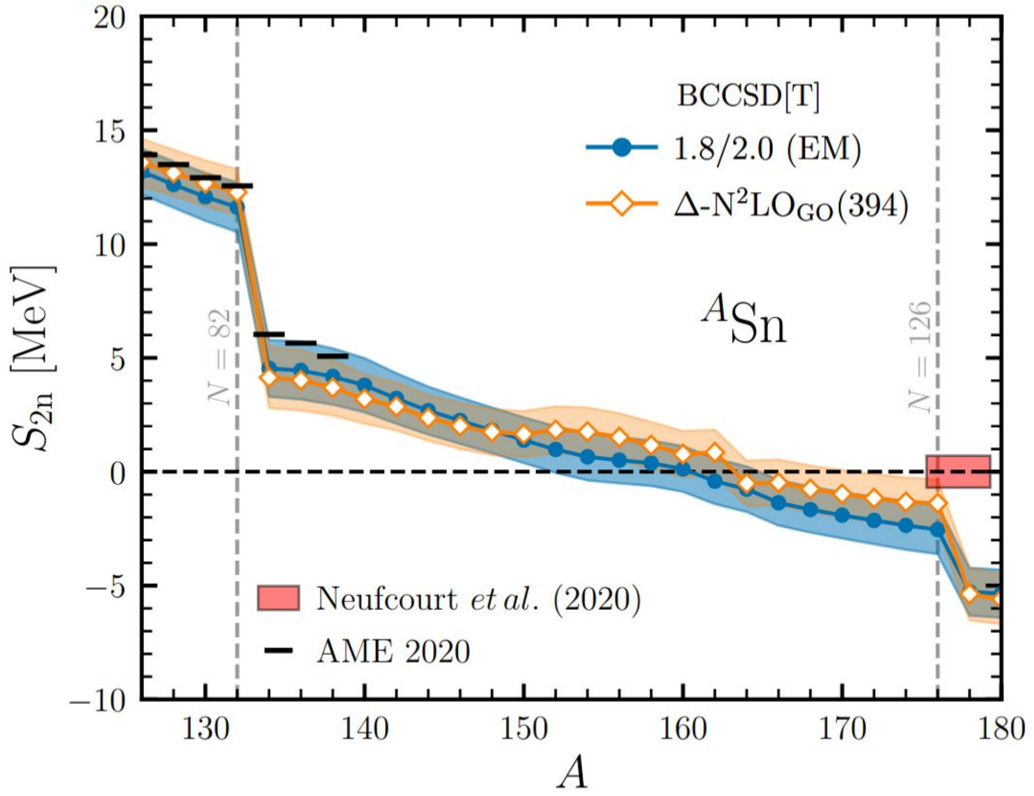


- Many-body uncertainty reduced by factor 5 ⟶ sub percent level
- 1.8/2.0 (EM) chiral EFT interaction overbinds tins by 18 MeV

BCCSD[T] : U. Vernik, PD, T. Duguet, A. Tichai, arXiv:2607.05086 (2026)
NLEFT : F. Hildenbrand *et al.*, PRL **136** (2026)
Mass extr. : C. M. Ireland *et al.* PRC **103** (2026)

High-precision BCCSD[T] two-neutron separation energies





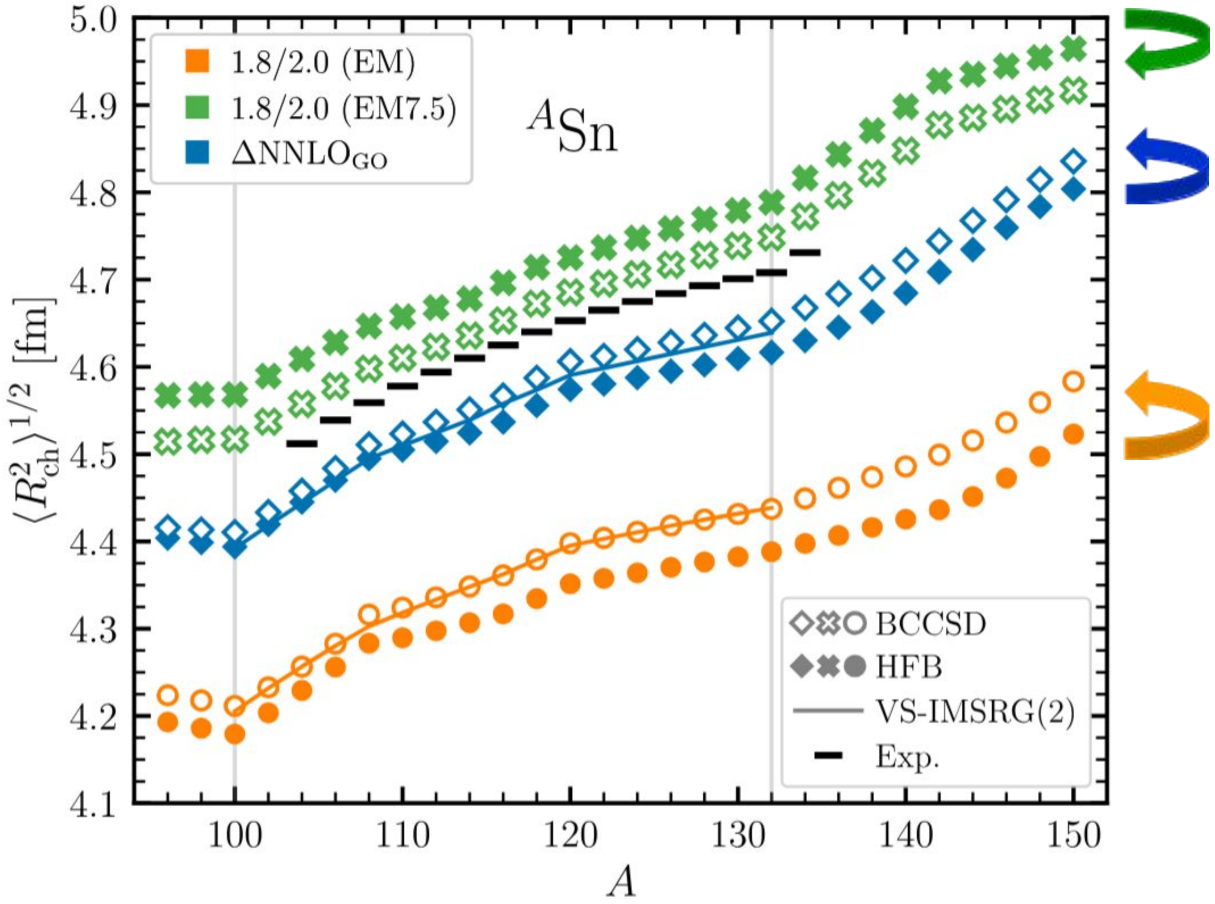
- BCCSD[T] in good agreement with
  - recent Bayesian mass extrapolation
  - nuclear lattice EFT

- Flat trend in $S_{2n} \rightarrow$ drip line location is fine tuned
- BCCSD[T] in tension with EDF predictions

Application of BCC to radii of tin isotopes

BCCSD : PD, T. Duguet, A. Tichai, PLB **878** (2026)
Hamil : K. Hebeler *et al.*, PRC **83** (2011)
W.G. Jiang *et al.* PRC **102** (2020)
P. Arthuis *et al.*, EPJA **62** (2026)
Exp. : F. P. Gustafson *et al.*, PRL **135** (2025)
C. Gorges *et al.* PRL **122** (2019)

BCCSD applied absolute charge radii of tin



rms error BCCSD - Exp.	
1.8/2.0 (EM)	**5.6 %**
ΔNNLO$_{\mathrm{GO}}$	**1.2 %**
1.8/2.0 (EM7.5)	**0.7 %**

- **1.8/2.0 (EM)** strongly underestimates absolute radii
- **ΔNNLO$_{\mathrm{GO}}$** largely improves but still underestimates
- **1.8/2.0 (EM7.5)** further improves but sightly overestimates
- BCCSD correlations always in the right direction

BCCSD applied to isotopic shifts of tin

BCCSD : PD, T. Duguet, A. Tichai, PLB **878** (2026)
Hamil : K. Hebeler *et al.*, PRC **83** (2011)
W.G. Jiang *et al.* PRC **102** (2020)
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Exp. : F. P. Gustafson *et al.*, PRL **135** (2025)
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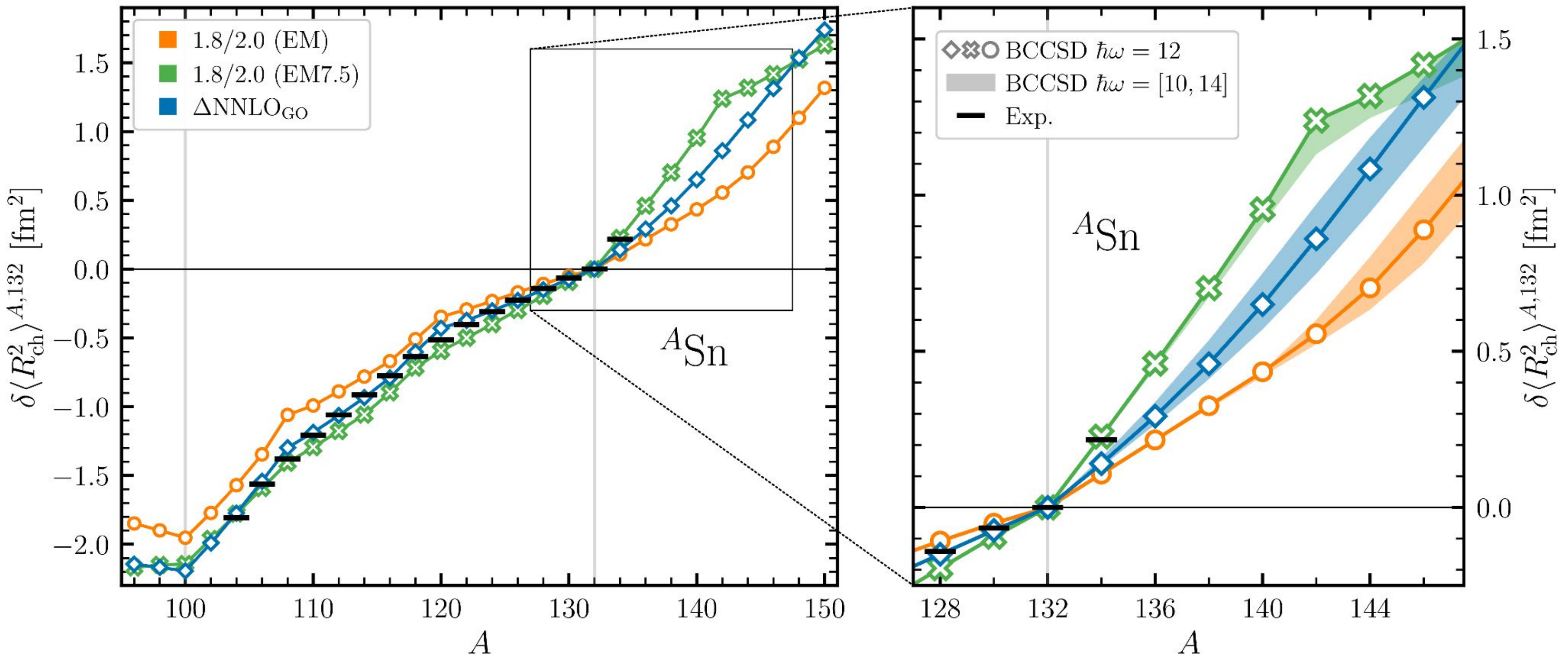
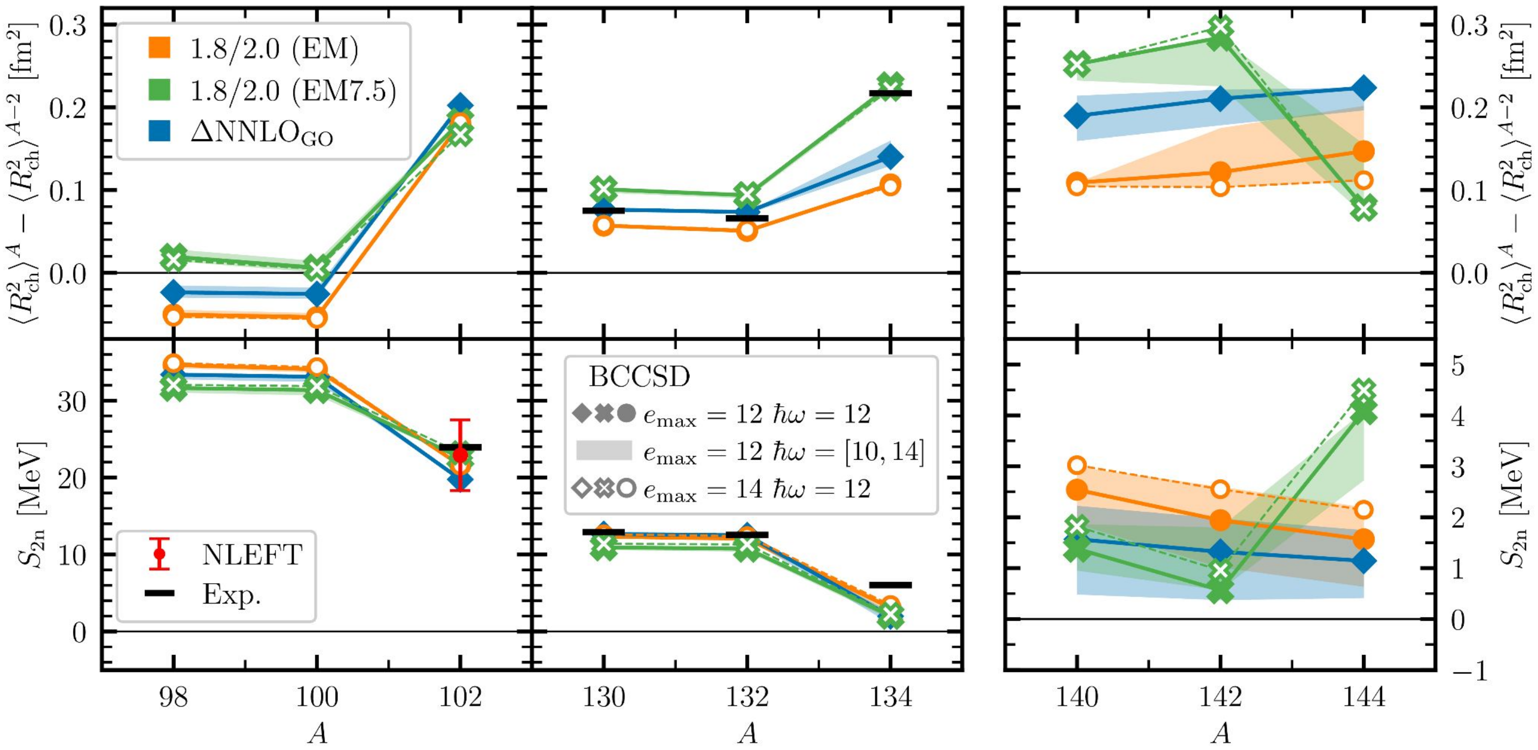


Isotopic shift ^{132}Sn – ^{134}Sn (fm^2)	
Exp	0.22
1.8/2.0 (EM)	0.11
ΔNNLO$_{GO}$	0.14
1.8/2.0 (EM7.5)	0.23

- **1.8/2.0 (EM7.5)** seems to be superior regarding the kink at ^{132}Sn

  … and predicts inverted kink for ^{142}Sn

BCCSD applied to isotopic shifts of tin



^{100}Sn

R_{ch} : all interactions predict kink

S_{2n} : drop consistent with NLEFT & data

^{132}Sn

R_{ch} : **EM7.5** captures kink best

S_{2n} : all interactions overestimate drop

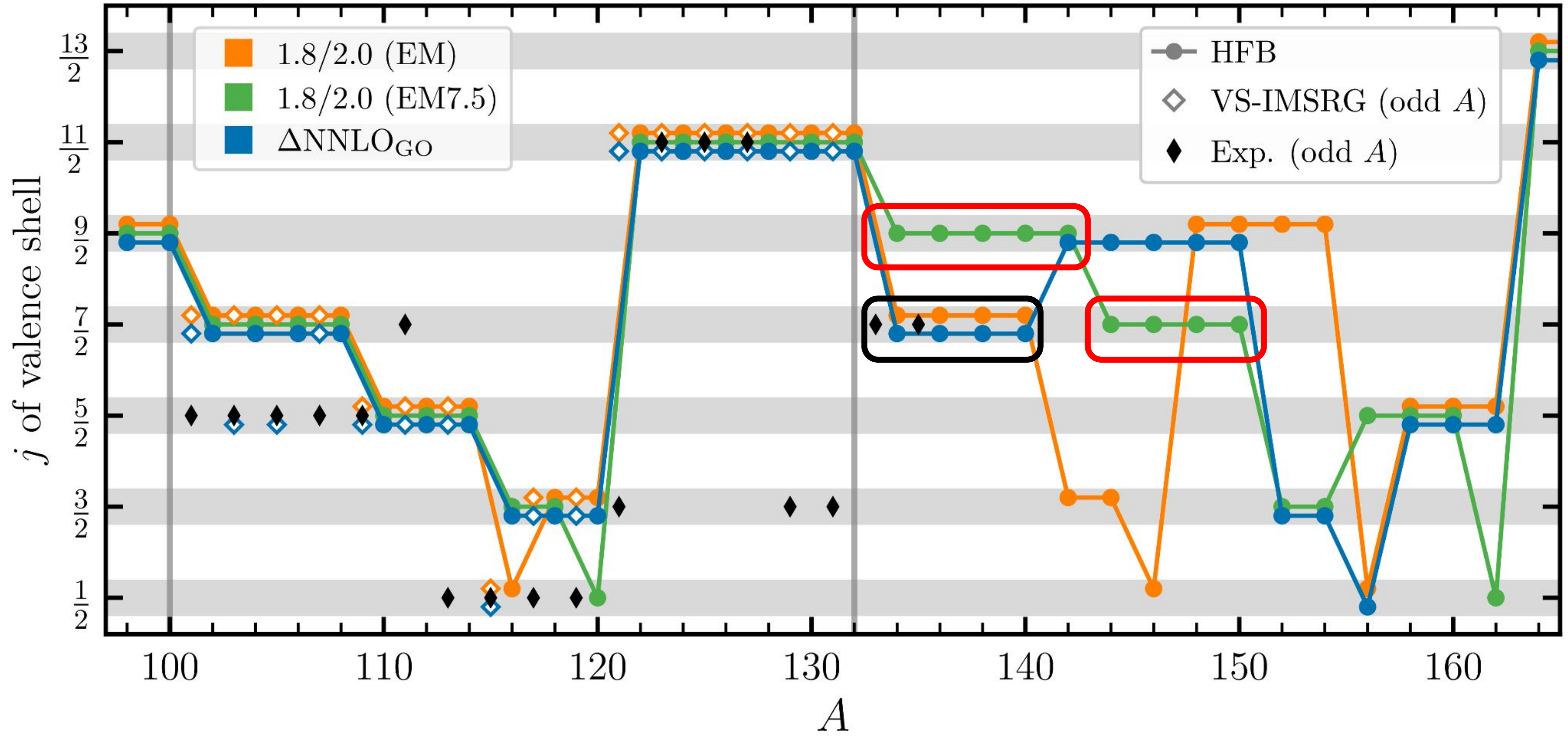
^{142}Sn

R_{ch} : **EM7.5** predicts inverted kink

S_{2n} : dubious large jump up for **EM7.5**

PD, T. Duguet, A. Tichai, PLB **878** (2026)

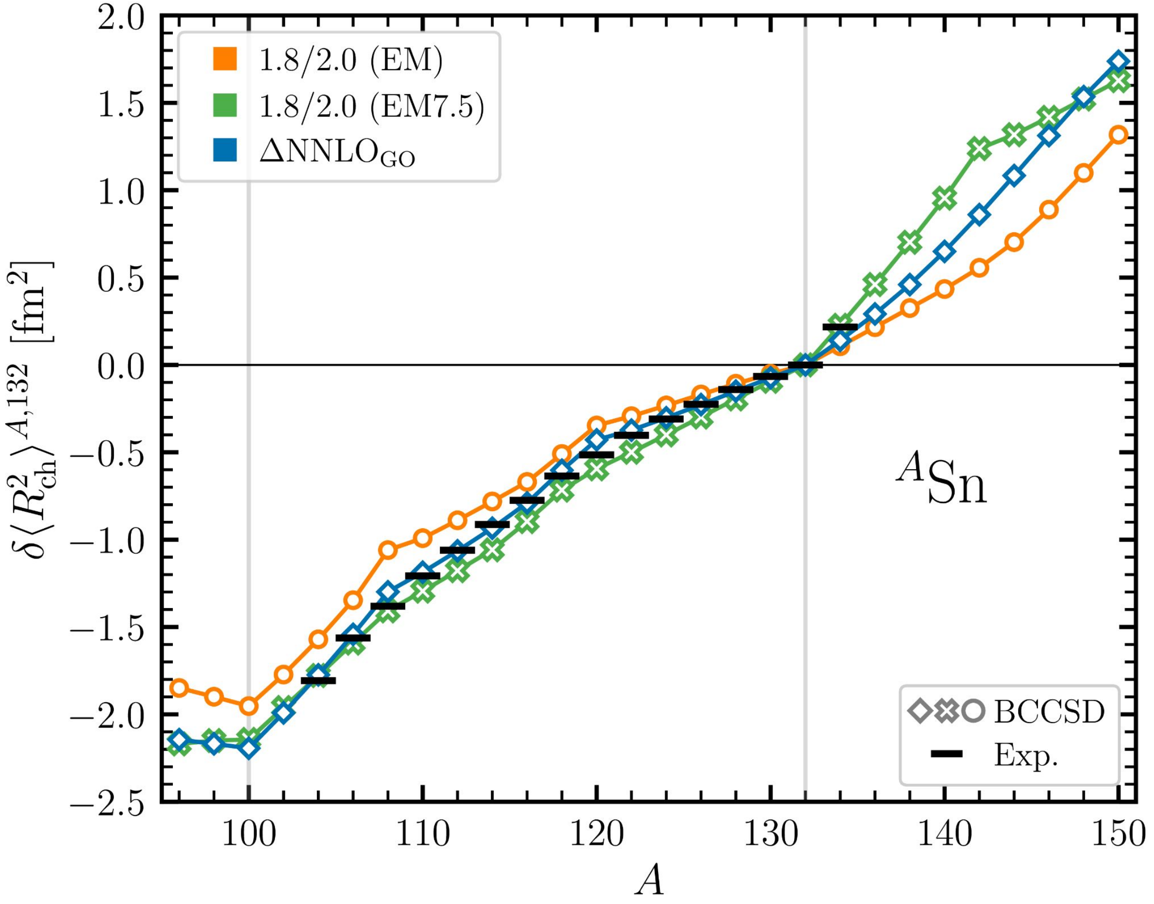
BCCSD applied to isotopic shifts of tin



- VS-IMSRG retains strong memory of single-particle shells and rarely agrees with odd-A ground-state spins
- Robust shell ordering upto ^{132}Sn *vs* large sensitivity to chiral EFT hamiltonian beyond
- **EM7.5** reorders $1h_{9/2}$ and $1f_{7/2}$ causing the R_{ch} kink in ^{132}Sn and ^{142}Sn

PD, T. Duguet, A. Tichai, PLB **878** (2026)

Global trend between ^{100}Sn and ^{132}Sn : linear slope



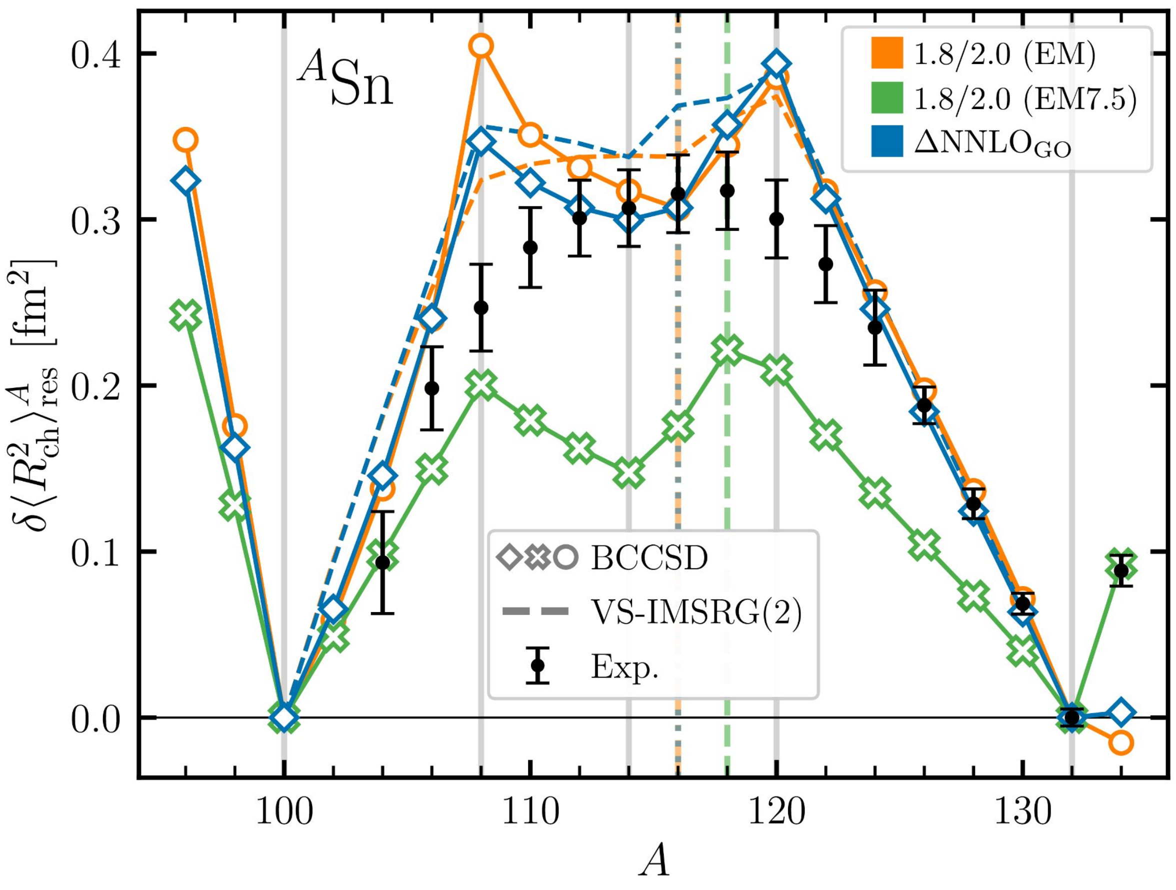
Extract the approximate linear trend

$$\delta\langle R^2_{\mathrm{ch}}\rangle^{A,132} \approx a(A-132)$$

Linear slope a (fm^2)	
Exp	**0.070**
1.8/2.0 (EM)	**0.061**
ΔNNLO$_{\mathrm{GO}}$	**0.069**
1.8/2.0 (EM7.5)	**0.067**

PD, T. Duguet, A. Tichai, PLB **878** (2026)

Global trend between ^{100}Sn and ^{132}Sn : quadratic arch



Residual arch by subtracting dominant linear part:

$$\delta\langle R^2_{\mathrm{ch}}\rangle^{A,132}_{\mathrm{res}} \equiv \delta\langle R^2_{\mathrm{ch}}\rangle^{A,132} - a(A-132)$$

- **1.8/2.0 (EM)** and **ΔNNLO$_{\mathrm{GO}}$** in good overall agreement with data
- **1.8/2.0 (EM7.5)** strongly underestimates arch
- Underlying subshell closures overpronounced in BCCSD
  → additional VS-IMSRG correlations smooths trend
  … but more correlations are still missing

Conclusion

- **Bogoliubov coupled-cluster** theory pushes *ab initio* frontiers to :
    - heavy nuclei thanks to its polynomial scaling
    - open-shell systems via the breaking of $U(1)$ symmetry
    - high precision by incorporating (leading-order) triples excitations

- Binding energies and charge radii along tin isotopic chain offers stringent test for chiral EFT interaction

  $\longrightarrow$ strong motivation to extend measurements beyond ^{100}Sn and ^{134}Sn

Next steps

- Improve BCC accuracy of radii by including triples and two-body charge density

- Extend BCC odd isotopes & excited states via its equation-of-motion techniques

Thanks to all my collaborators

KU LEUVEN
T. Duguet
R. Raabe

TECHNISCHE UNIVERSITÄT DARMSTADT
A. Tichai
M. Aytekin
R. Roth
U. Vernik

ULB
W. Ryssens
S. Goriely

cea
T. Duguet
L. Zurek

OAK RIDGE National Laboratory
G. Hagen

Funding fwo fnrs