TRIUMF

Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Ab Initio Theory for All Medium-Mass Nuclei

Jason D. Holt

INPC September 12, 2016

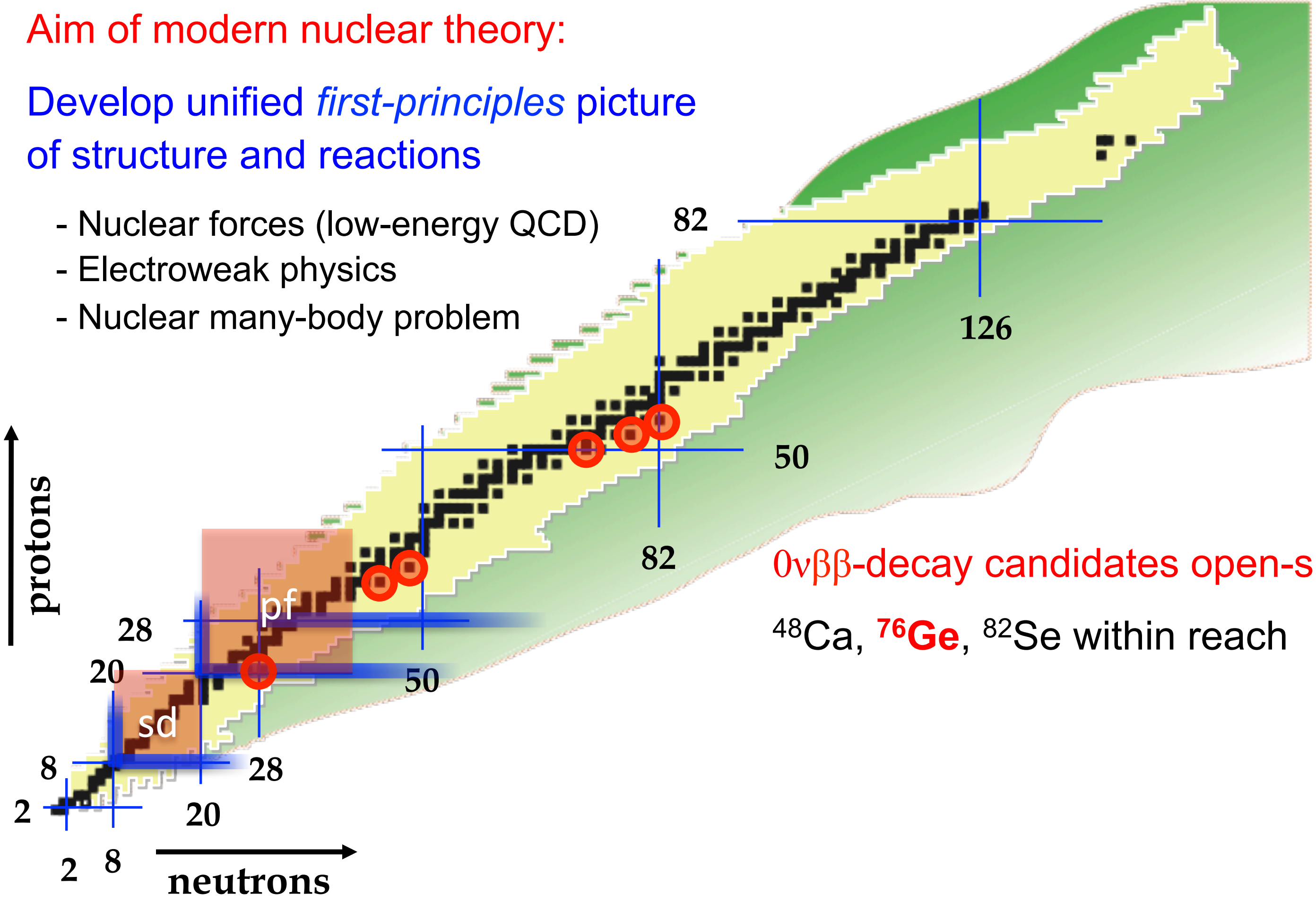
Collaborators
S. R. Stroberg
S. Bogner
H. Hergert
T. Morris
N. Parzuchowski
A. Schwenk

The Nuclear Landscape

Aim of modern nuclear theory:

Develop unified *first-principles* picture of structure and reactions

- Nuclear forces (low-energy QCD)
- Electroweak physics
- Nuclear many-body problem



0νββ-decay candidates open-shell medium/heavy-mass

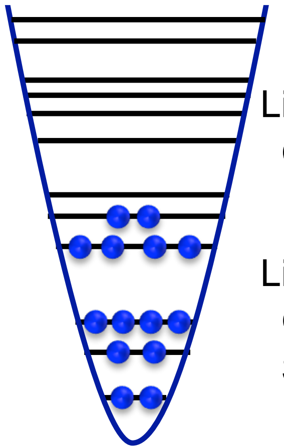
^{48}Ca, **^{76}Ge**, ^{82}Se within reach

The Nuclear Many-Body Problem

Nucleus strongly interacting many-body system – full A-body problem impossible

$$H\psi_n = E_n\psi_n$$

Large space: controlled approximation to full Schrödinger Equation



Limited range:
Closed shell ±1
Even-even (spherical)

Limited properties:
Ground states
Some excited states

Coupled Cluster
In-Medium SRG
Green's Function
Perturbation Theory

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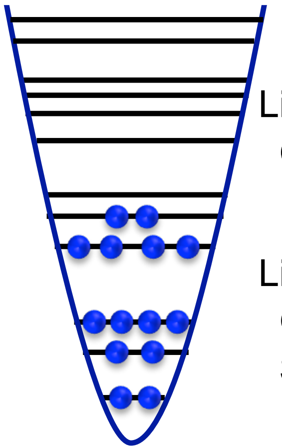
Valence space: diagonalize *effective valence-space Hamiltonian*

Large-space approach



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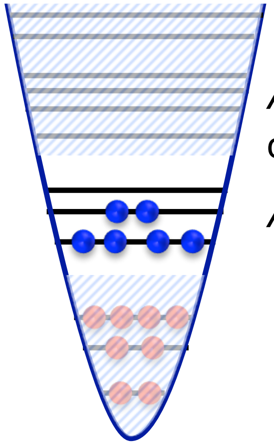

All nuclei near closed shells

All properties
  Ground states
  Excited states
  Transitions

Nucleus strongly interacting many-body system – full A-body problem impossible

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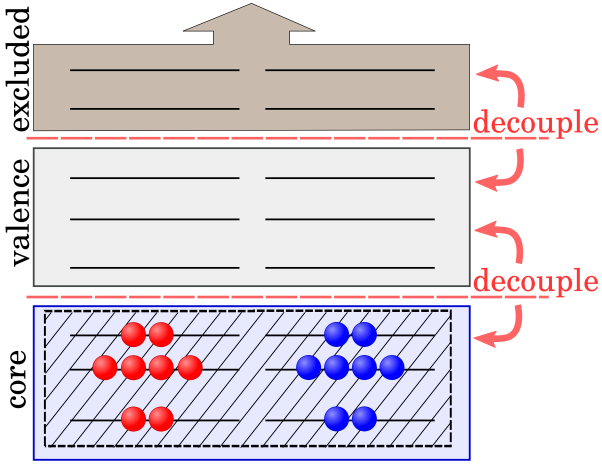


$|\Phi_0\rangle = |^{16}\mathrm{O}\rangle$

In-Medium SRG

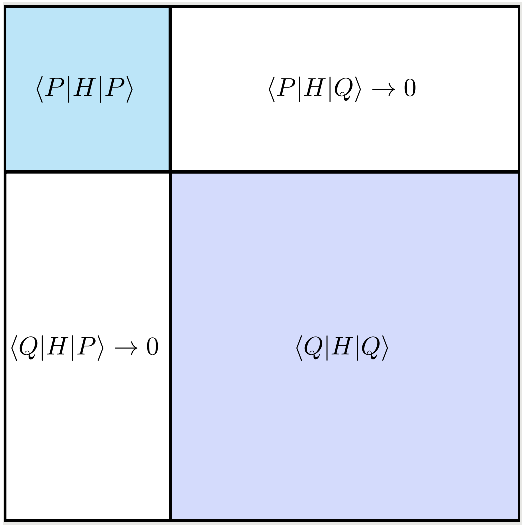
Can we achieve accuracy of large-space methods?

$$U = e^{\Omega}$$

$$\tilde{H} = e^{\Omega} H e^{-\Omega}$$

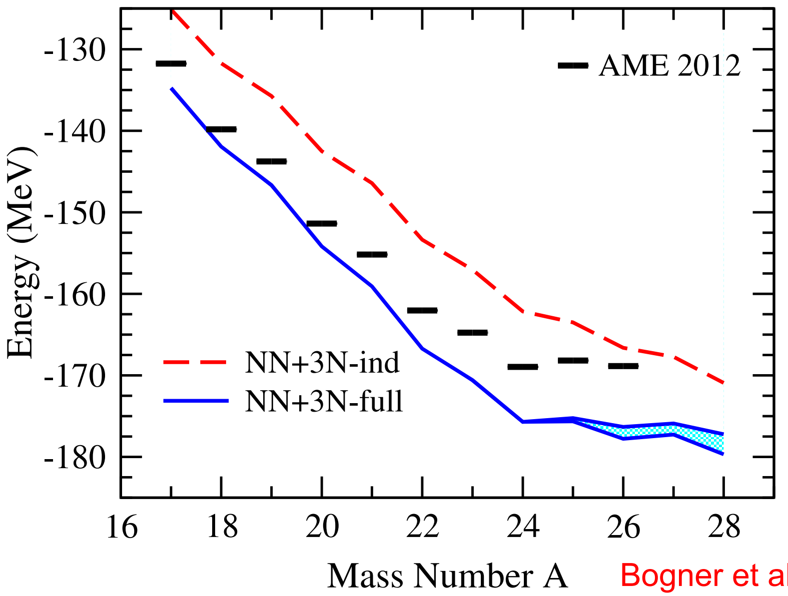
$$\langle \tilde{\Psi}_n | P\tilde{H}P | \tilde{\Psi}_n \rangle = \langle \Psi_i | H | \Psi_i \rangle$$

Tsukiyama, Bogner, Schwenk, PRC 2012
Morris, Parzuchowski, Bogner, PRC 2015

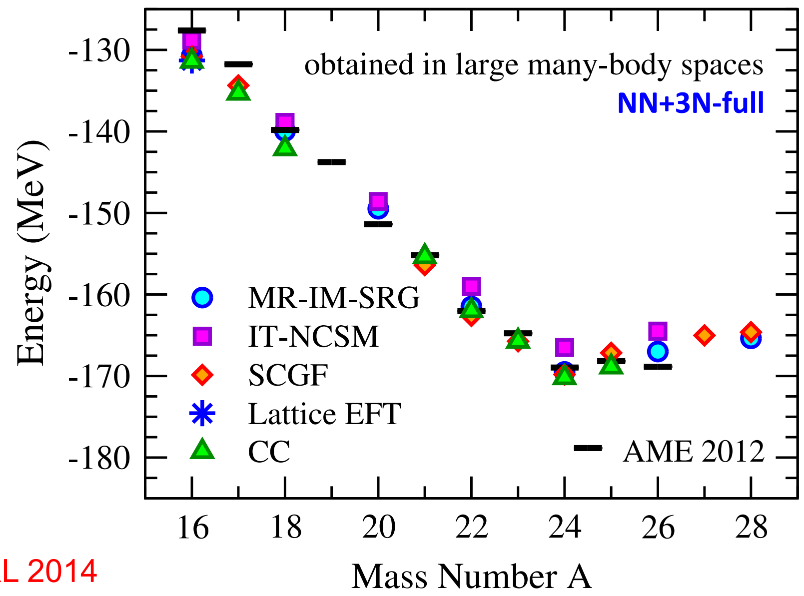


Ground States: Oxygen Isotopes

Large/valence-space methods with **same SRG-evolved NN+3N-full forces**



Bogner et al., PRL 2014



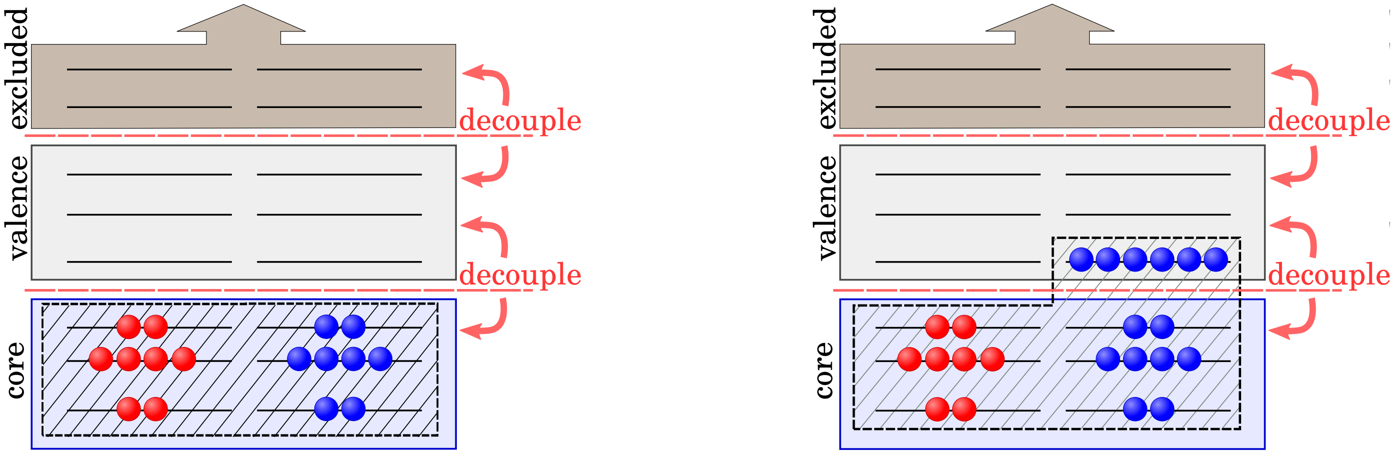
Agreement between all methods with same input forces

Hebeler, JDH, Menéndez, Schwenk, ARNPS 2015

Discrepancy between valence/large-space results

Targeted Normal Ordering

With more valence nucleons, new reference becomes more accurate



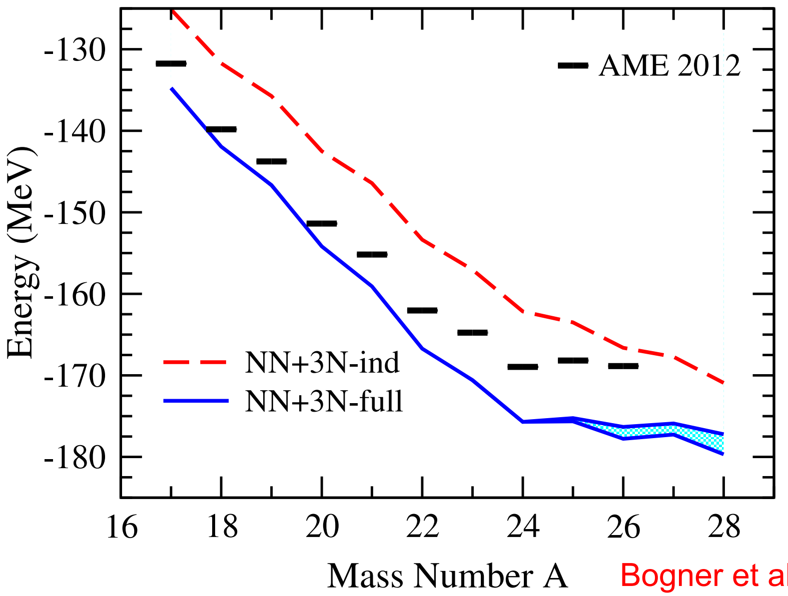
$|\Phi_0\rangle = |^{16}\mathrm{O}\rangle$ $|\Phi_0\rangle = |^{22}\mathrm{O}\rangle$

Targeted Normal Ordering: take nearest closed shell as new reference

Still decouple sd valence space in IMSRG

Ground States: Oxygen Isotopes

Large/valence-space methods with **same SRG-evolved NN+3N-full forces**



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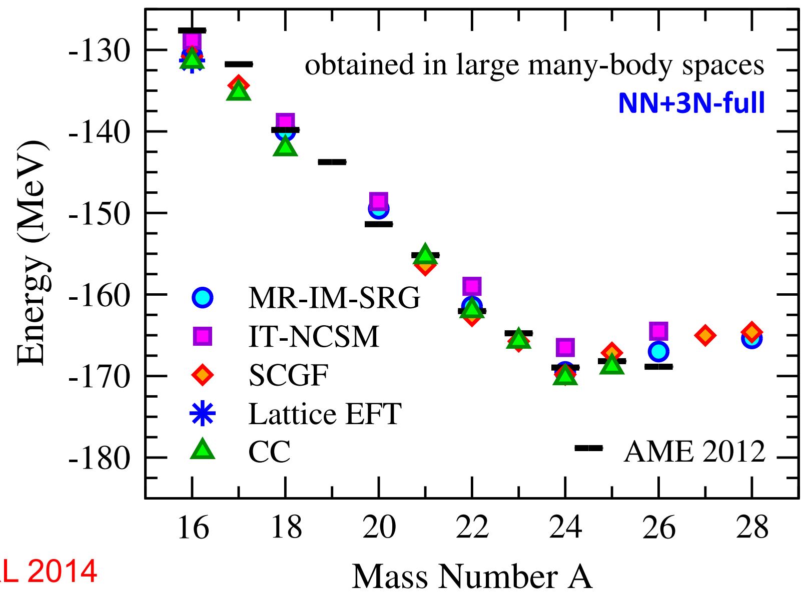

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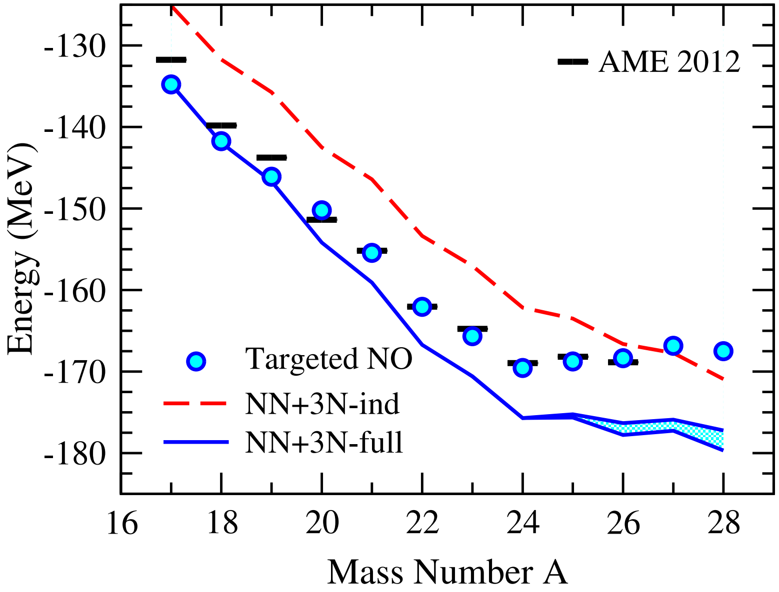
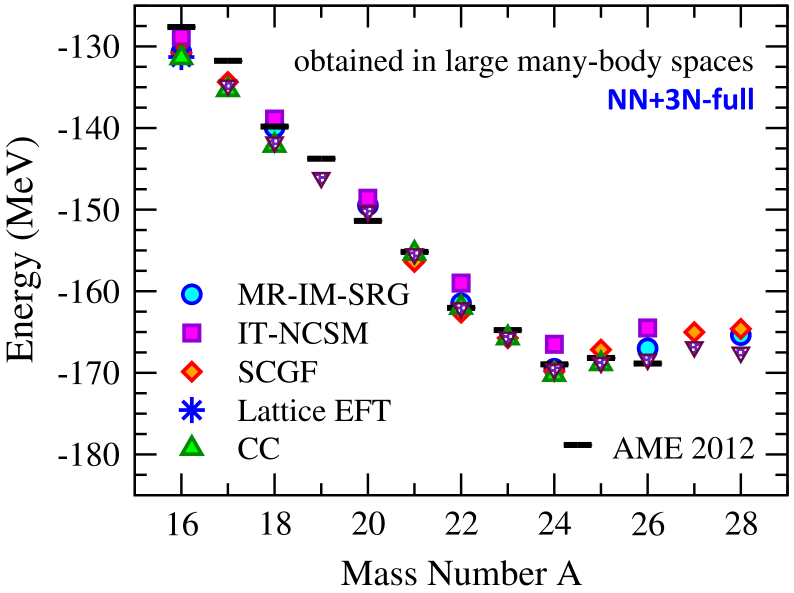




Agreement between all methods with same input forces

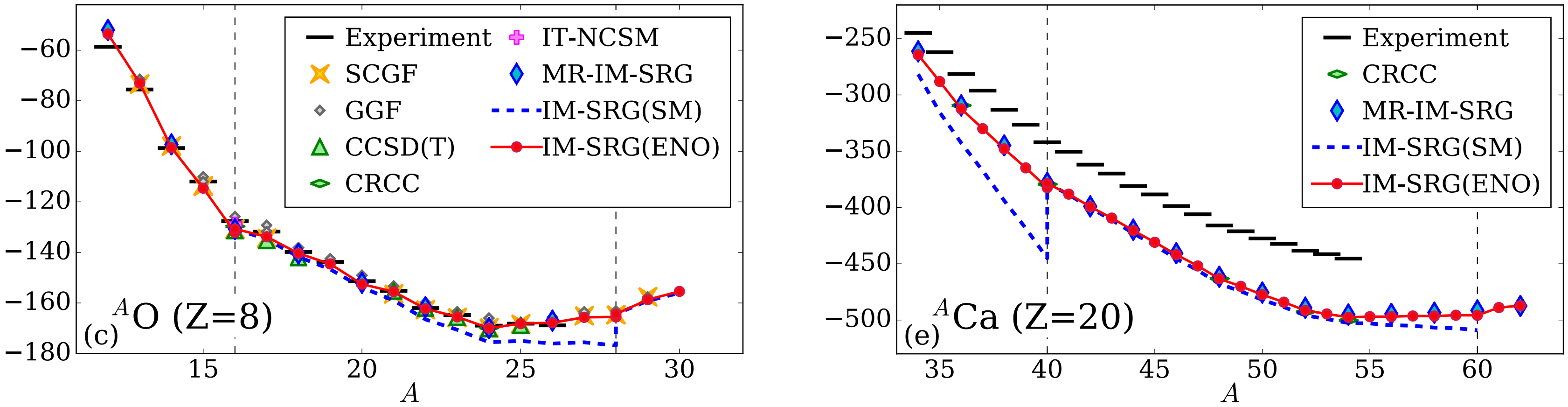
Hebeler, JDH, Menéndez, Schwenk, ARNPS 2015

Capture 3N forces between valence nucleons

"Targeted normal ordering" results agree well with large-space methods

Ground States: From Oxygen to Nickel

Targeted valence space agrees to 1% with all large-space methods (where calculations exist)



Stroberg et al., arXiv:1607.03229

Extend beyond standard *sd*/*pf* shells

Agreement with experiment deteriorates for heavy chains (due to input Hamiltonian)

Significant gain in applicability with little/no sacrifice in accuracy

Low computational cost: ~1 node-day/nucleus

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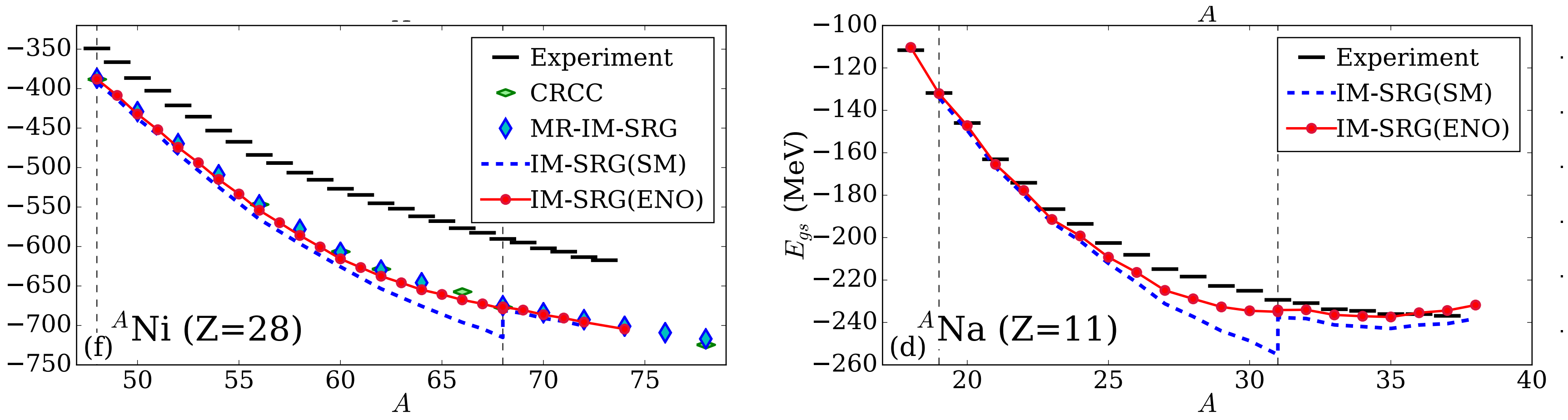

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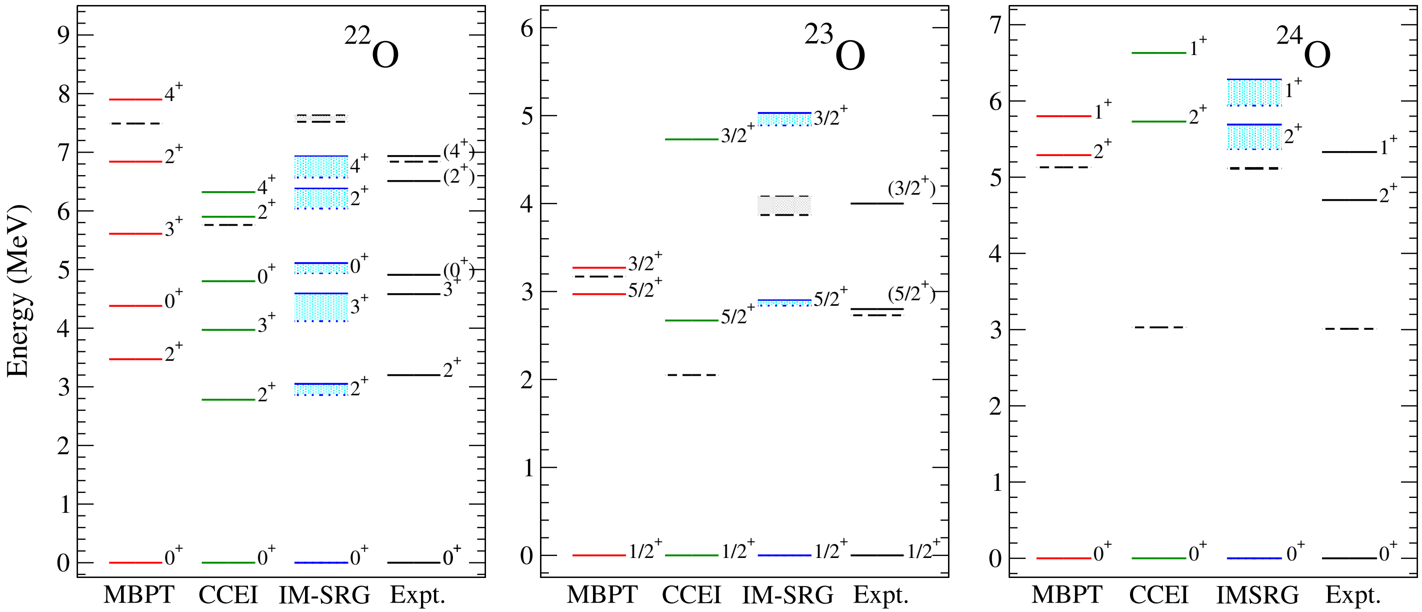
Excited States in Exotic Oxygen Isotopes

Neutron-rich oxygen spectra from existing shell-model approaches



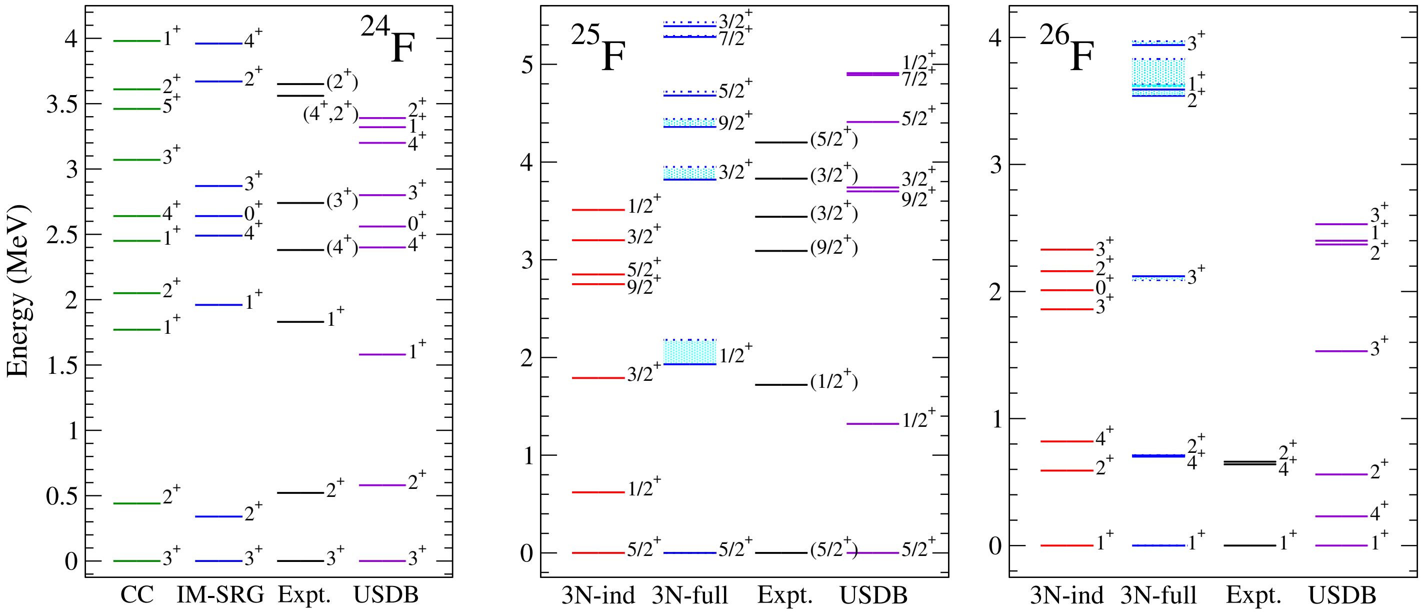
Hebeler, JDH, Menéndez, Schwenk, ARNPS 2015

MBPT in extended valence space

IM-SRG/**CCEI** spectra agree within ~300 keV

Excited States in Exotic Fluorine Isotopes

Fluorine spectroscopy: **NN+3N-ind** and **NN+3N-full**, **Full CC**



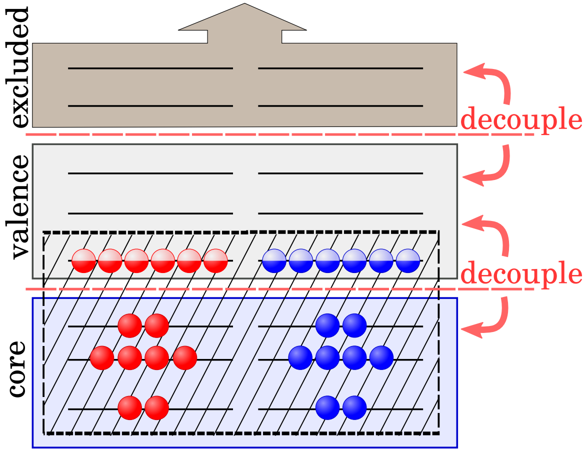
Stroberg et al., PRC 2016

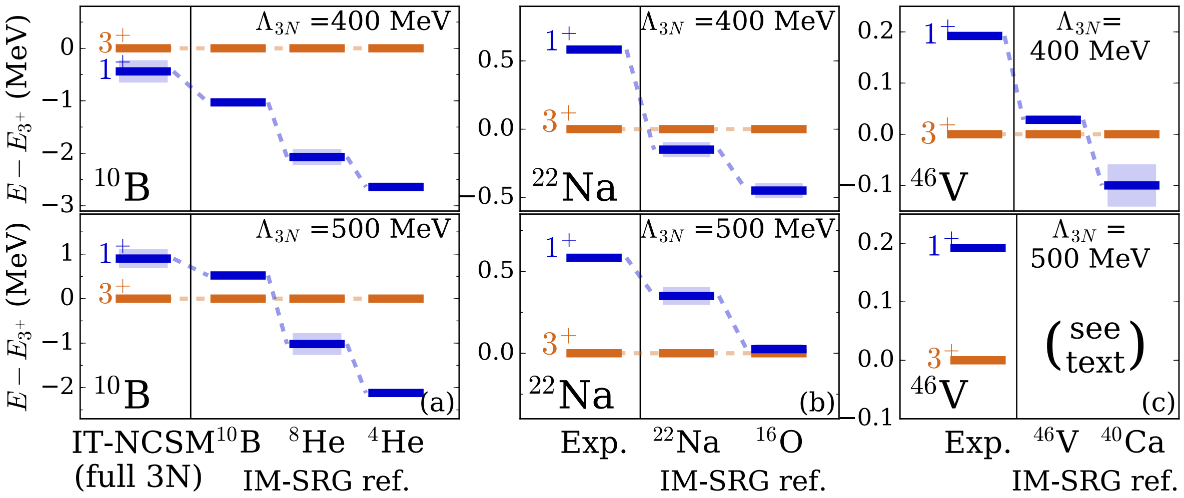
IMSRG: competitive with phenomenology, good agreement with data

Ground-State Inversion: A Puzzle in ^{22}Na/^{46}Va

Long-standing puzzle: 3p+3n above ^{16}O/^{40}Ca: same $1^+/3^+$ inversion as in ^{10}B

Clear improvement with targeted valence space approach – agreement with NCSM for ^{10}B



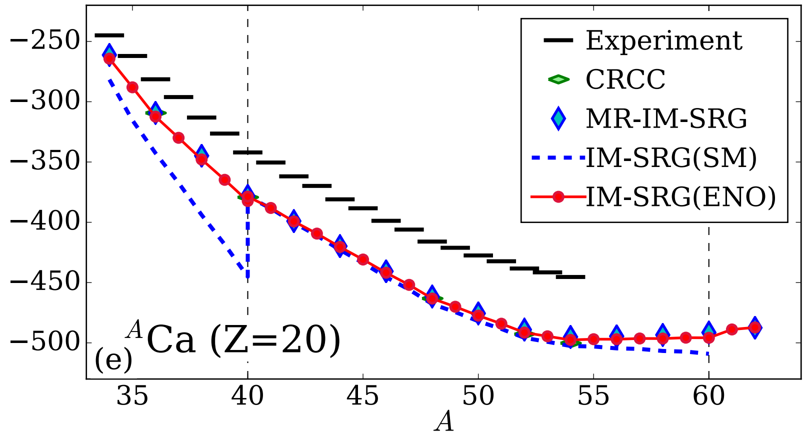


Stroberg et al., arXiv:1607.03229

Similar improvement in medium mass: first ab initio prediction of $3^+/1^+$ ordering in ^{22}Na, ^{46}V

Improved Input NN+3N Forces

New input NN+3N forces which reproduce saturation



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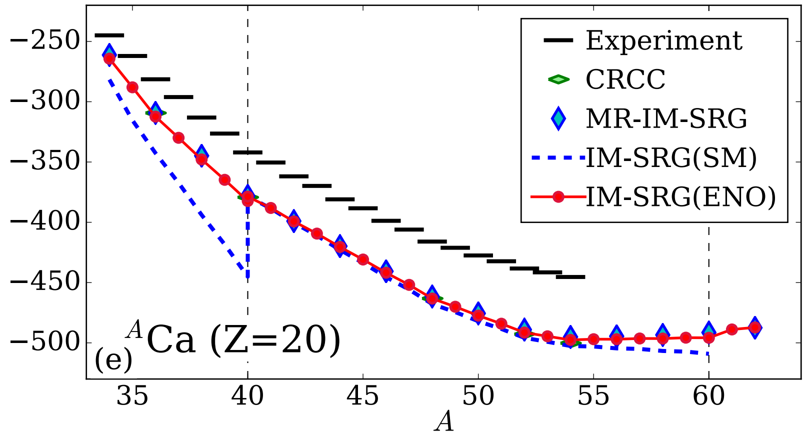

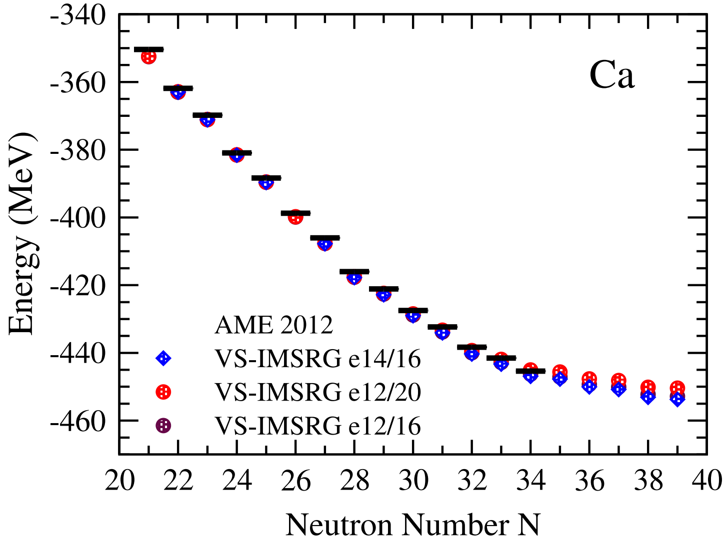

Find remarkable improvement with respect to experimental data

Shell Closures in Neutron-Rich Ca

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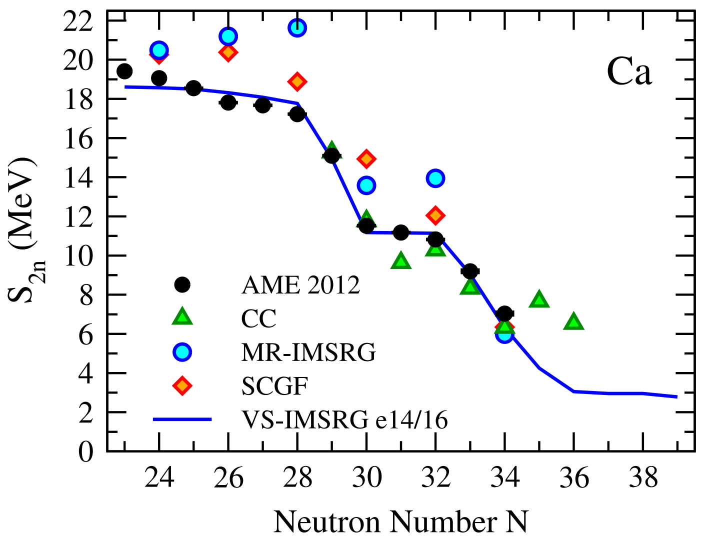

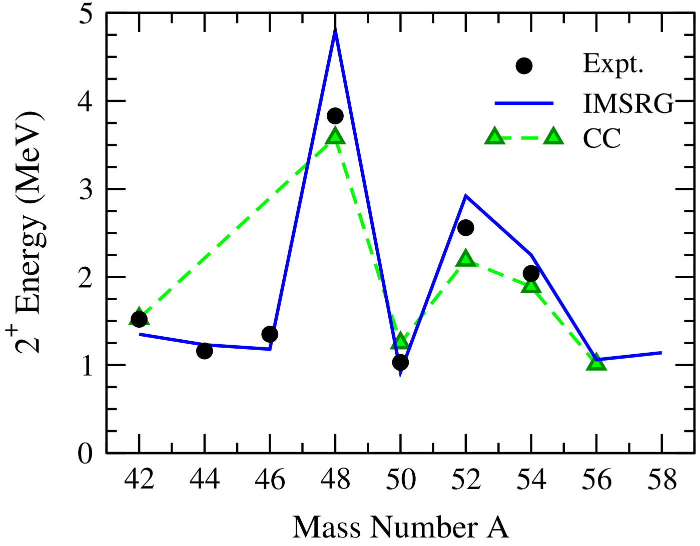

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New ab initio predictions for shell closures in neutron-rich Ca

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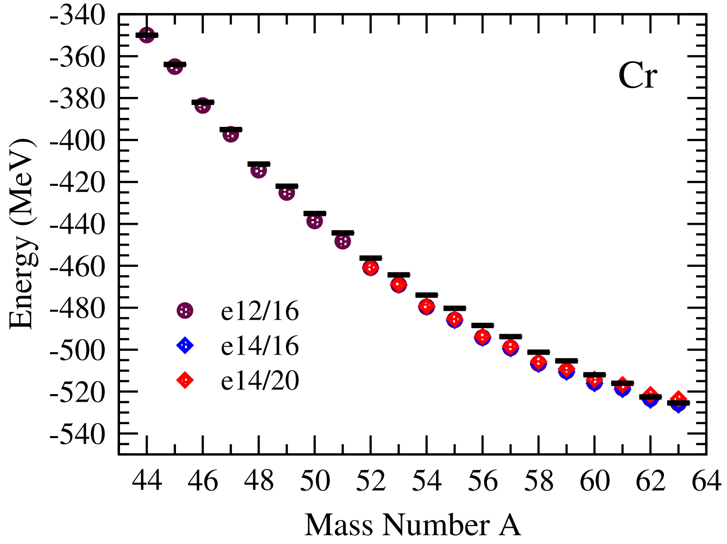
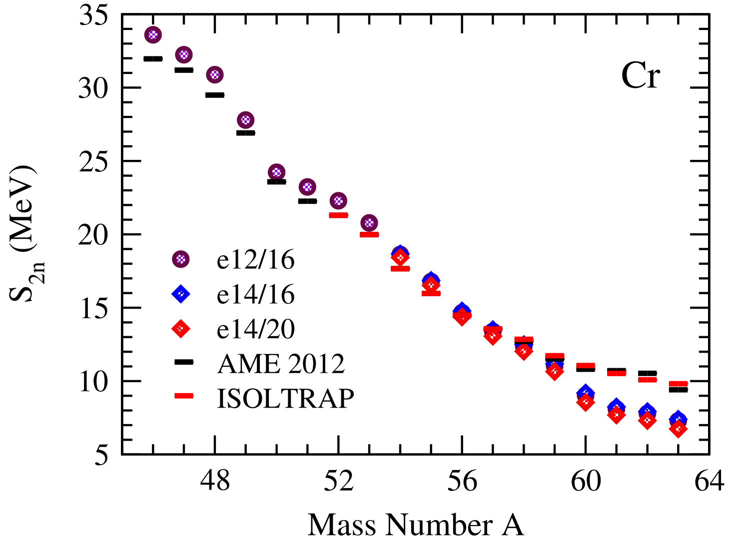




Find remarkable improvement for experimental data

New ab initio predictions in Cr isotopes – compares well with new ISOLTRAP data

Outlook: Towards ^{76}Ge

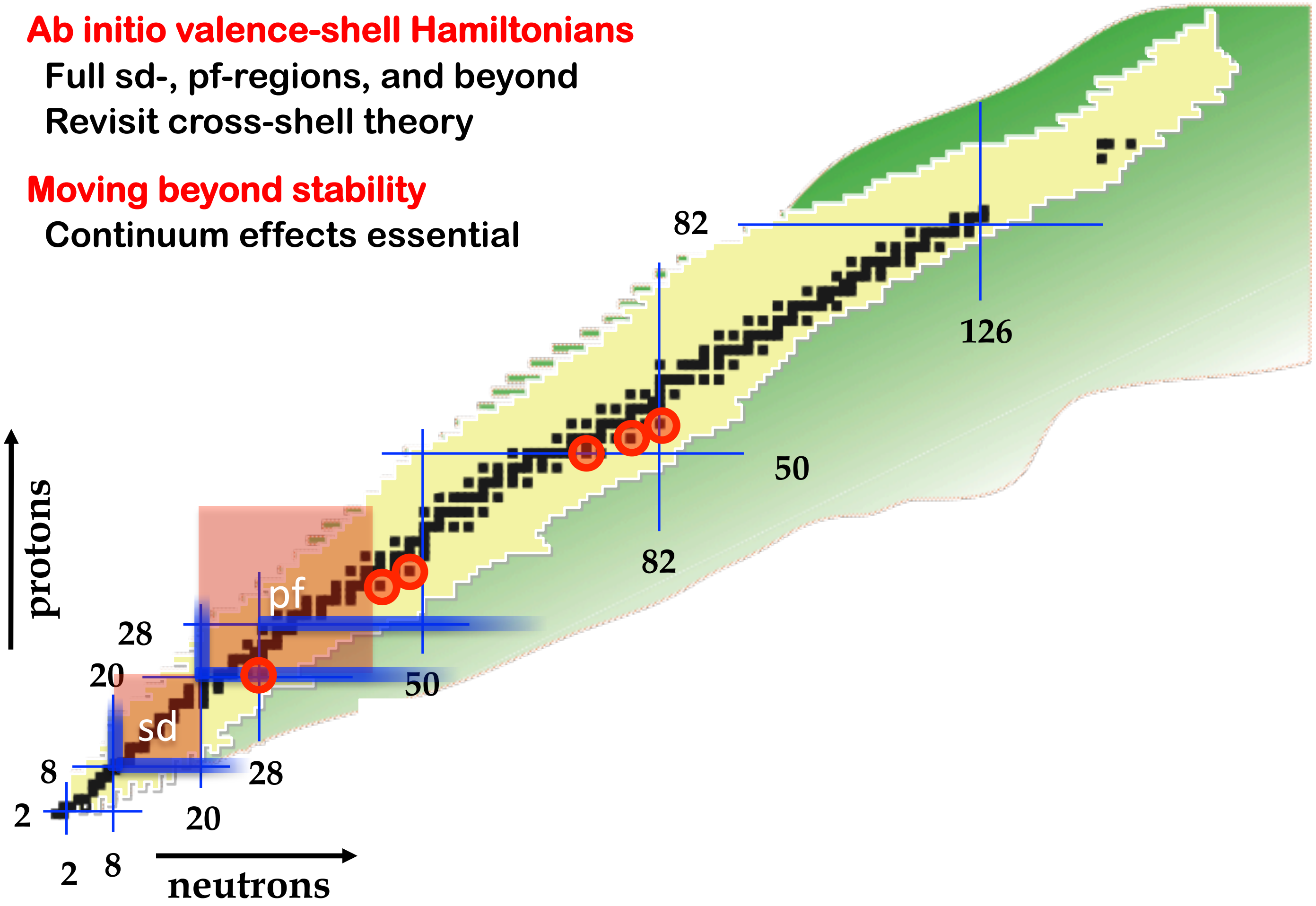
Ab initio valence-shell Hamiltonians

Full sd-, pf-regions, and beyond

Revisit cross-shell theory

Moving beyond stability

Continuum effects essential



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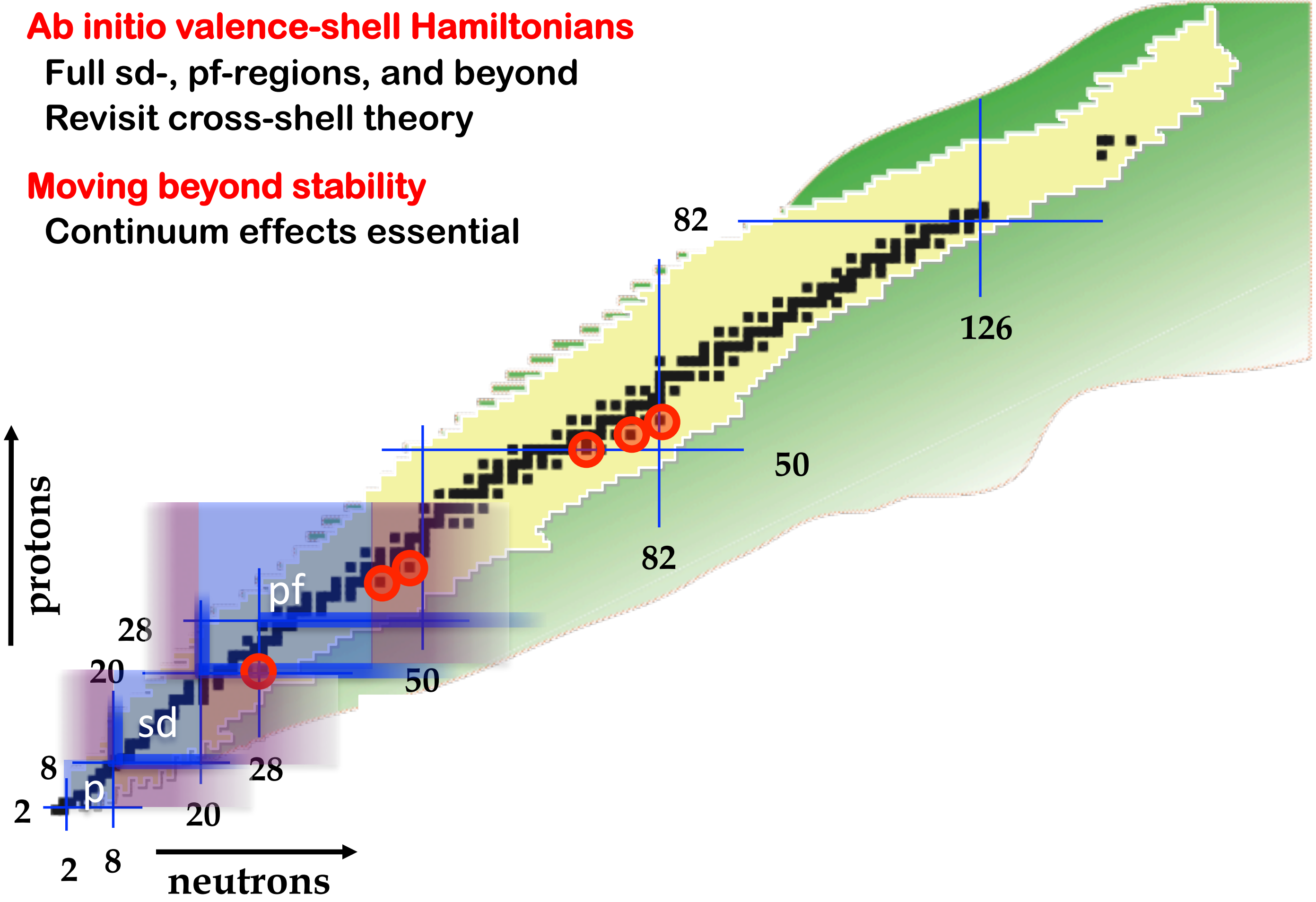

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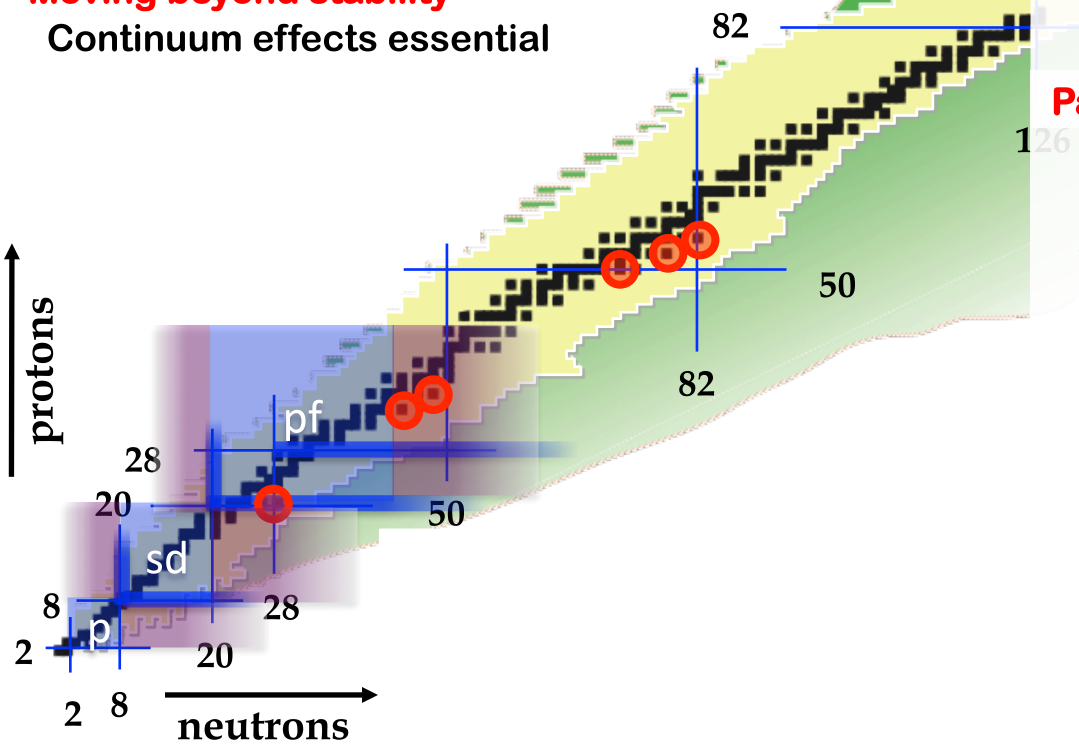
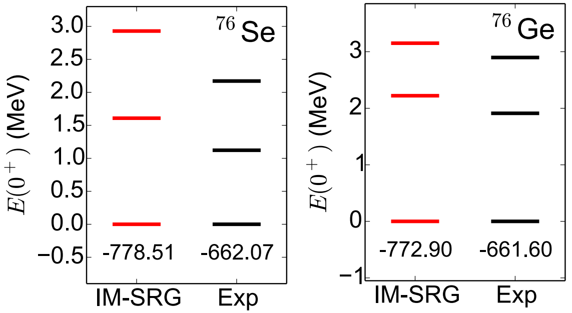


Fundamental physics

- Effective electroweak operators underway
- Effective $0\nu\beta\beta$ decay operator
- Superallowed β decay
- Dark-matter scattering

Path to ab initio ^{76}Ge NME

- Benchmark with large-space for ^{48}Ca ($2\nu\beta\beta$)
- Multiple predictions for $0\nu\beta\beta$ in ^{48}Ca
- Valence-space IMSRG calculation of ^{76}Ge
- Quantify uncertainties



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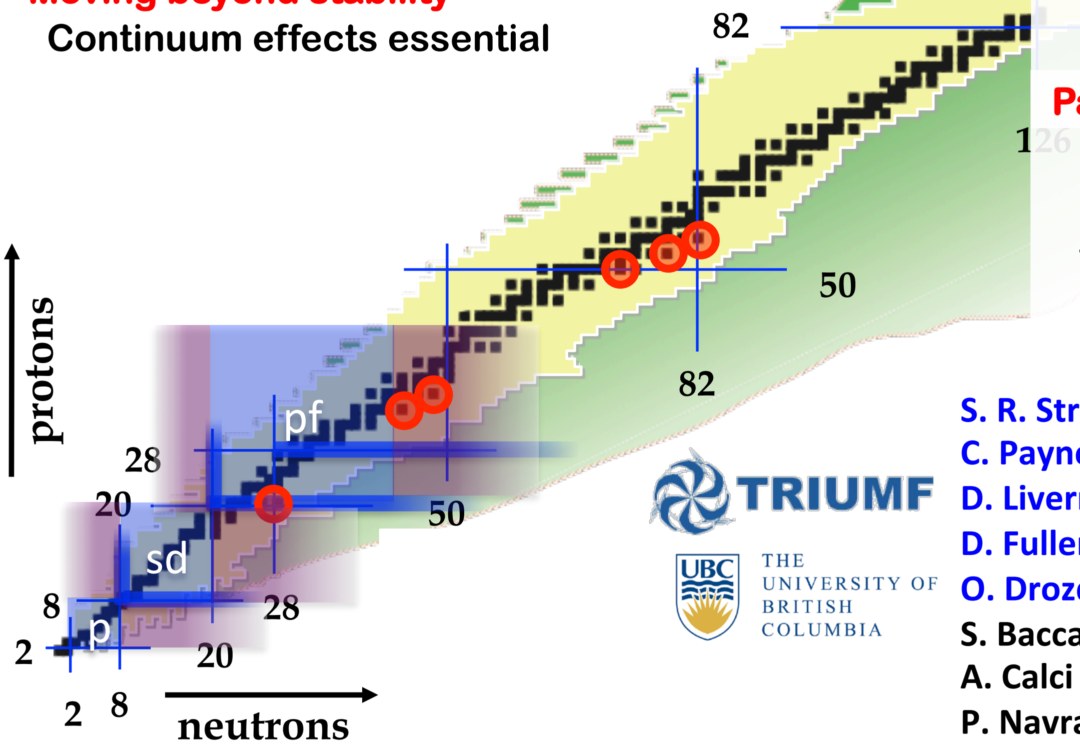

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THE UNIVERSITY OF BRITISH COLUMBIA

S. R. Stroberg
C. Payne
D. Livermore
D. Fullerton
O. Drozdowski
S. Bacca
A. Calci
P. Navrátil

MICHIGAN STATE UNIVERSITY
H. Hergert
S. Bogner
T. Morris
N. Parzuchowski

TECHNISCHE UNIVERSITÄT DARMSTADT
J. Simonis
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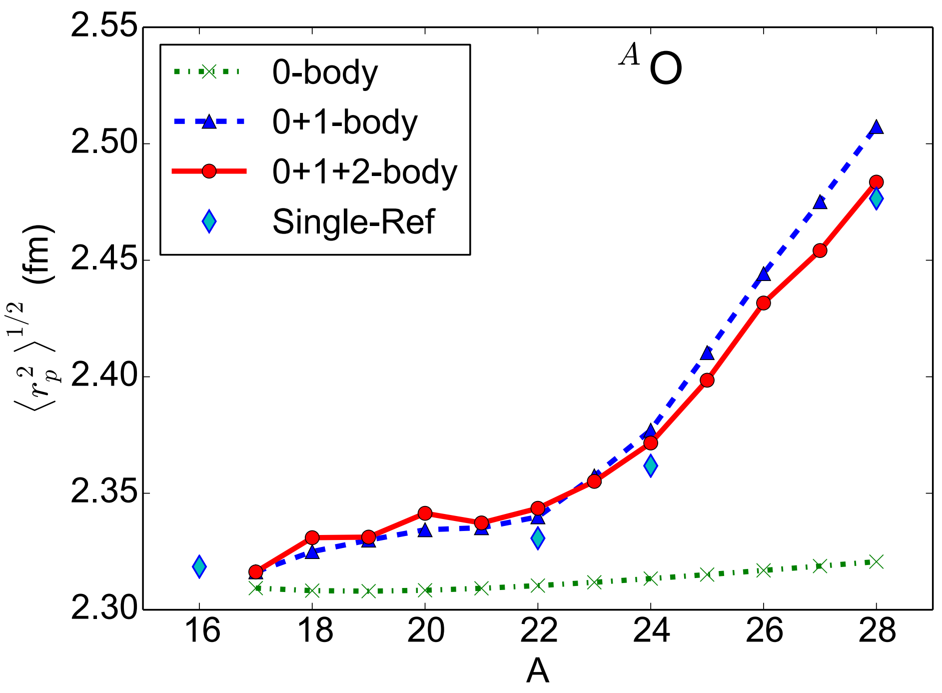
東京大学 THE UNIVERSITY OF TOKYO
J. Menéndez

Radii in sd shell

General **scalar operators** developed for valence-space IMSRG

$$\tilde{R}^2 = U R^2 U^\dagger \qquad \langle R^2 \rangle = \left\langle \Phi_0 \mid \tilde{R}^2 \mid \Phi_0 \right\rangle + \left\langle \Phi_{\rm SM} \mid \tilde{R}^2 \mid \Phi_{\rm SM} \right\rangle$$



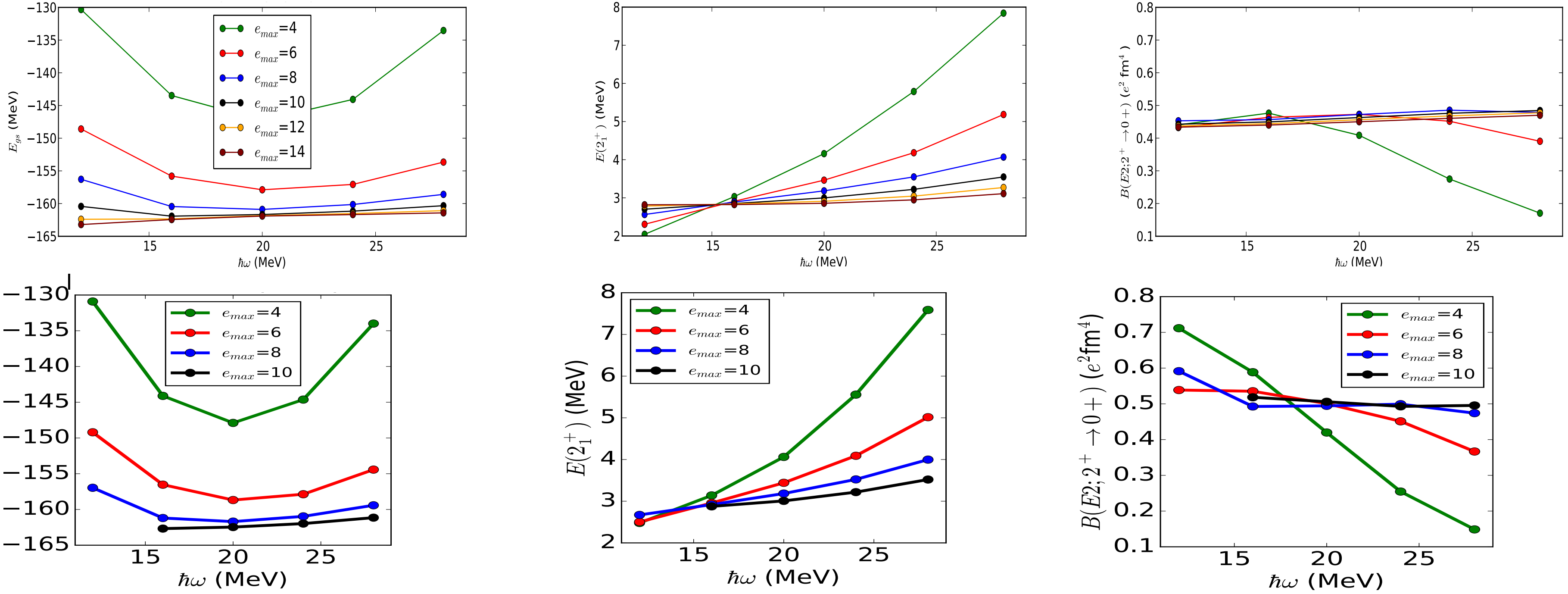
Agreement with SR-IMSRG; two-body contribution minor

EOM-IMSRG Benchmark: E2 Transition in ^{22}O

General **one-body tensor operators** developed for valence-space IMSRG

$$\tilde{\mathcal{O}} = e^{\Omega}\mathcal{O}e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + [\Omega, [\Omega, \mathcal{O}]] + \ldots$$

Parzuchowski, Stroberg et al., in prep



Agreement with EOM-IMSRG; benchmarks also underway with EOM Coupled-Cluster

Ab Initio GT Transitions from Valence-Space IMSRG

General **one-body tensor operators** developed for valence-space IMSRG: Gamow-Teller

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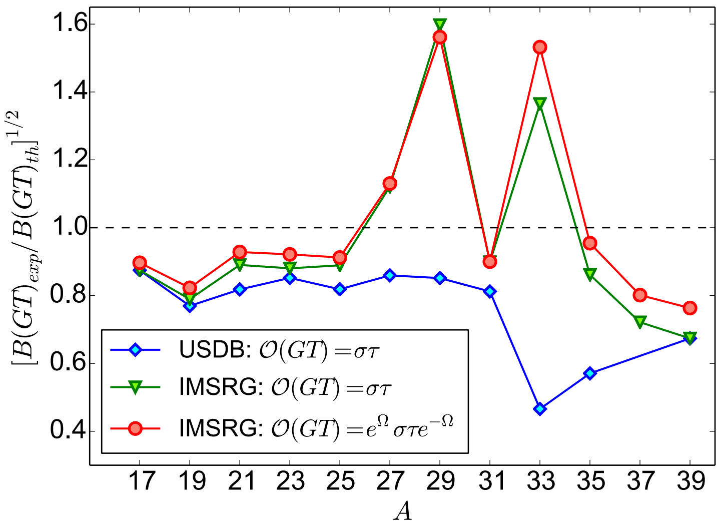

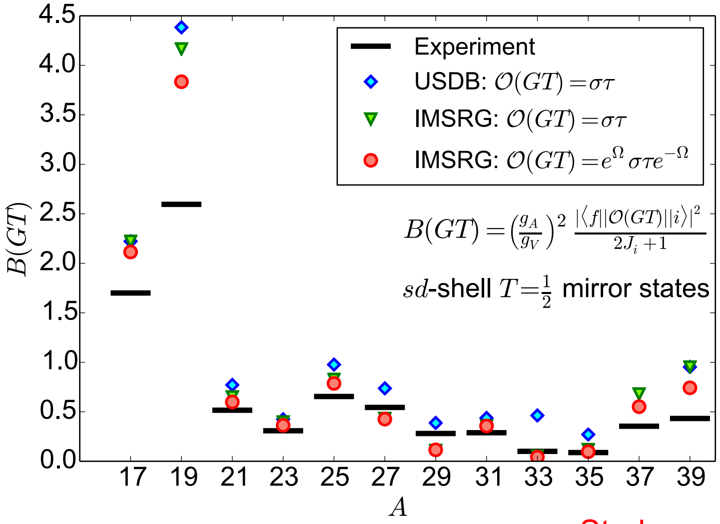

Stroberg et al., in prep

First ab initio valence-space calculations of GT transition rates

Small renormalization effect, but (mostly) reasonable agreement with experiment

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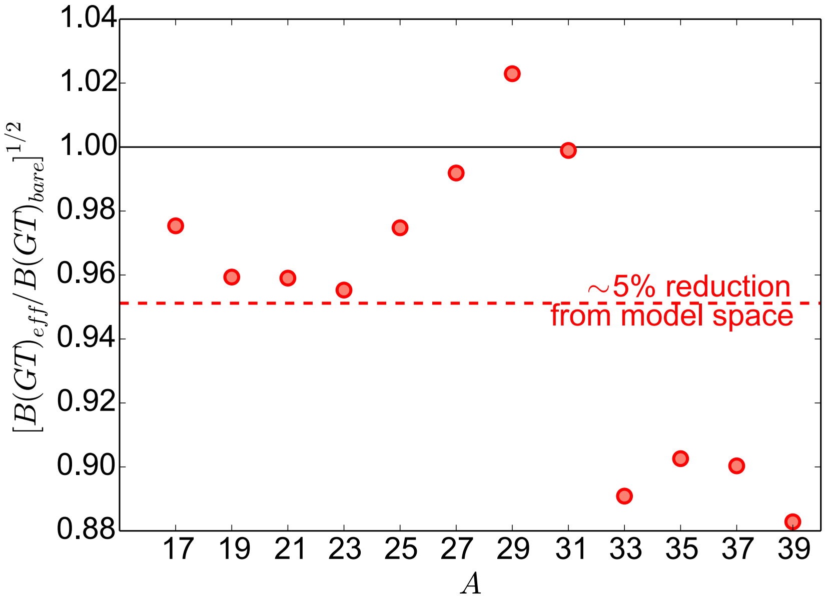

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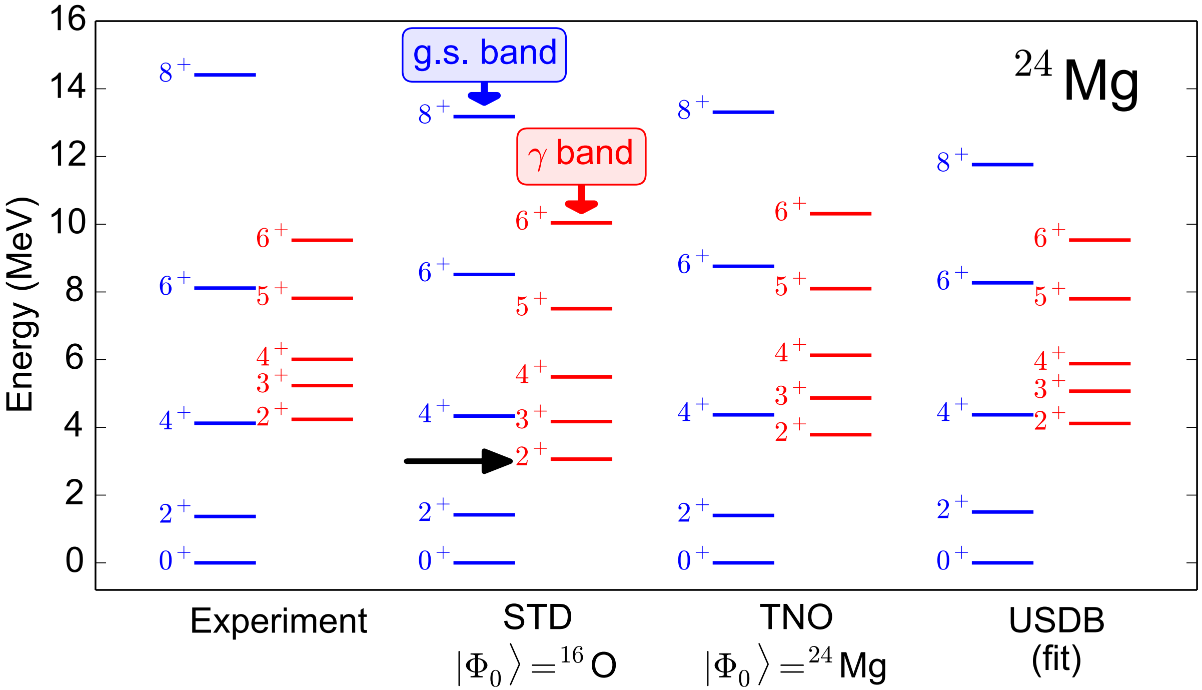
Deformation in Ab Initio Framework

Prediction of ground-state and gamma bands

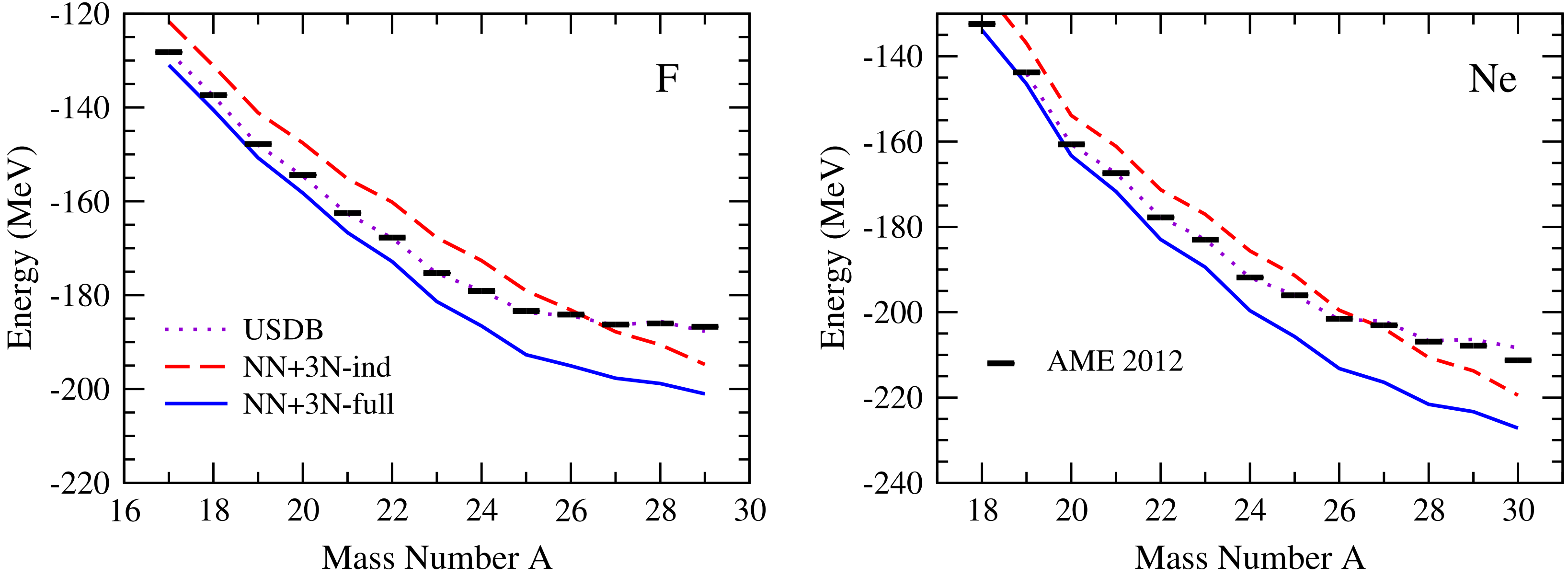
Compare with phenomenology in sd-shell nuclei



Stroberg et al., in prep

Ground States: Fluorine and Neon

Valence-space IMSRG results for open-shell fluorine and neon isotopes



3N forces improve experimental agreement; significant overbinding

Stroberg et al., PRC 2016

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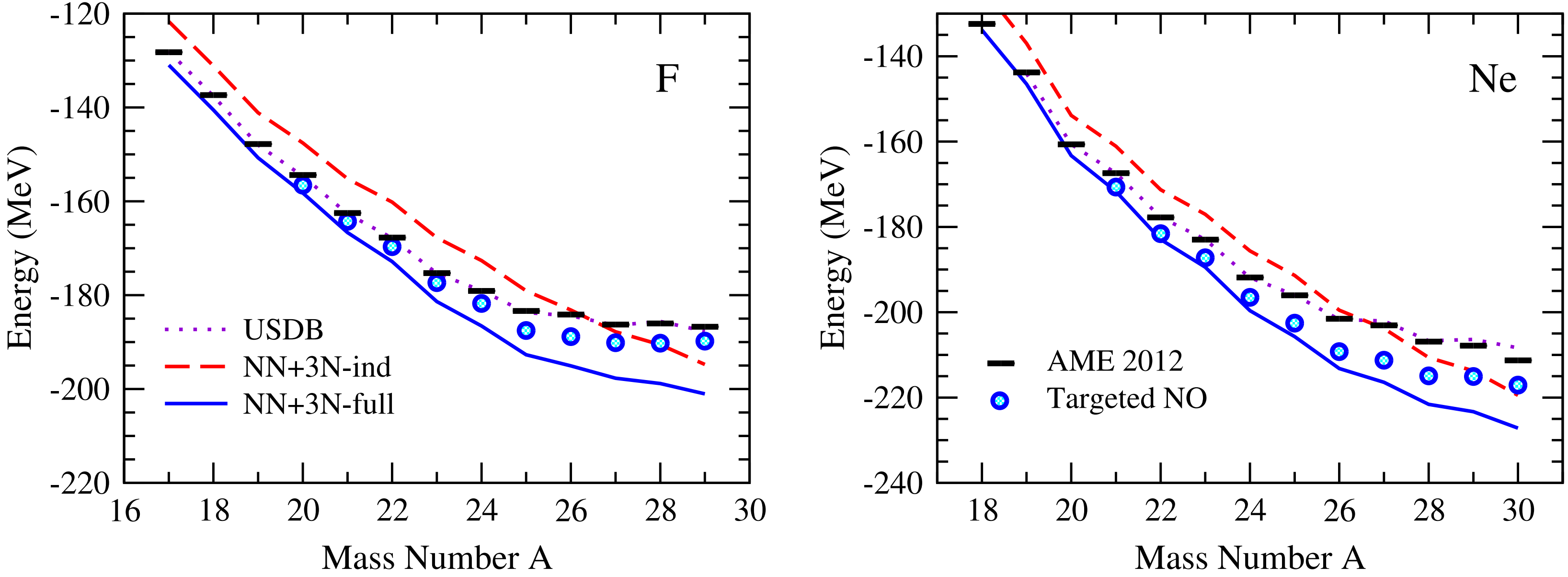

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Further improvement from Targeted Normal Ordering

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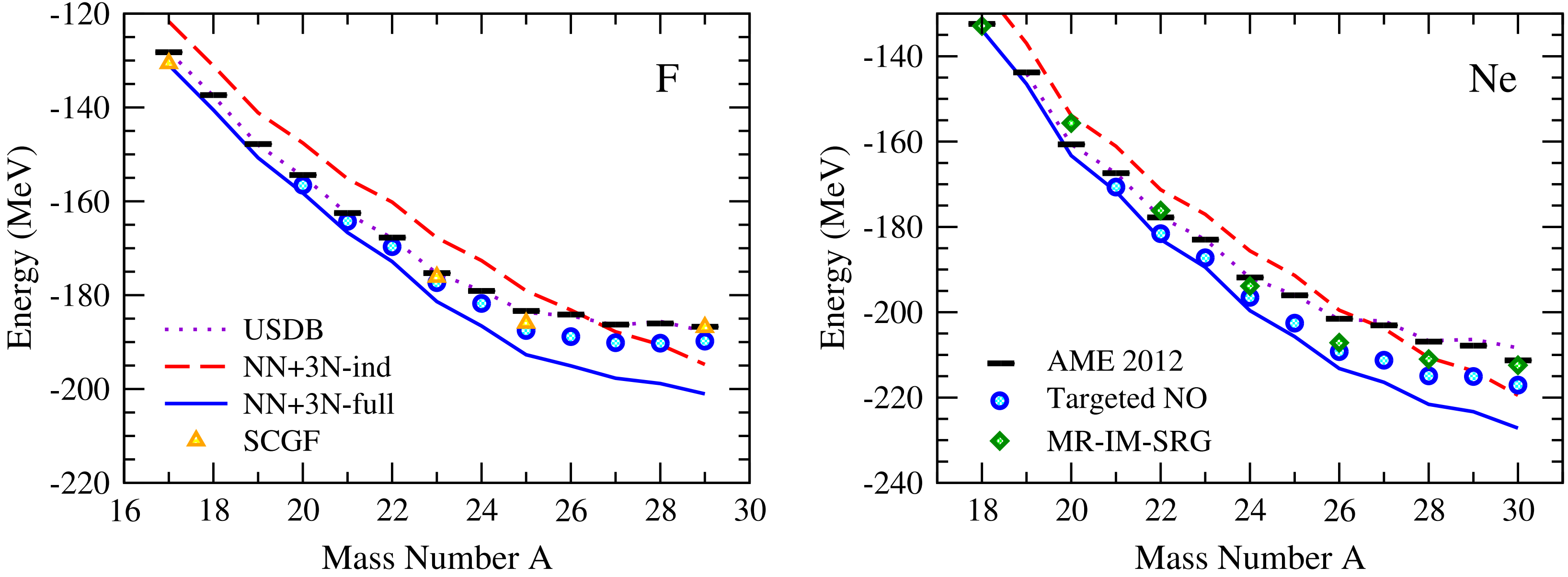


Stroberg et al., PRC 2016

3N forces improve experimental agreement; significant overbinding

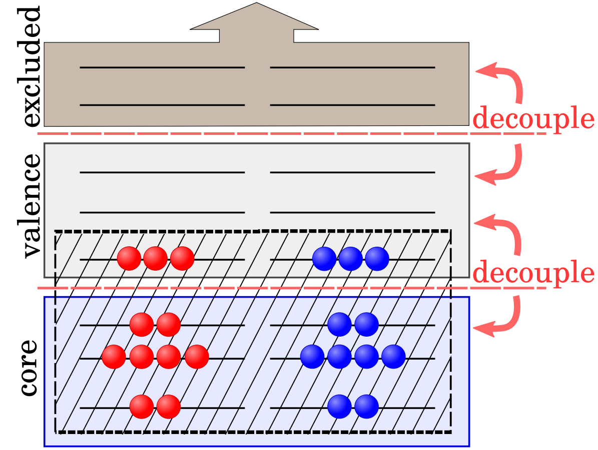
Further improvement from Targeted Normal Ordering

Minor loss in accuracy compared to SCGF and MR-IMSRG

Ground-State Inversion: A Puzzle in $^{22}Na/^{46}Va$

Long-standing puzzle: 3p+3n from $^{16}O/^{40}Ca$, same $1^+/3^+$ ground-state inversion as in ^{10}B

With 3N forces ab initio valence space (IMSRG, CCEI) still incorrect ground state

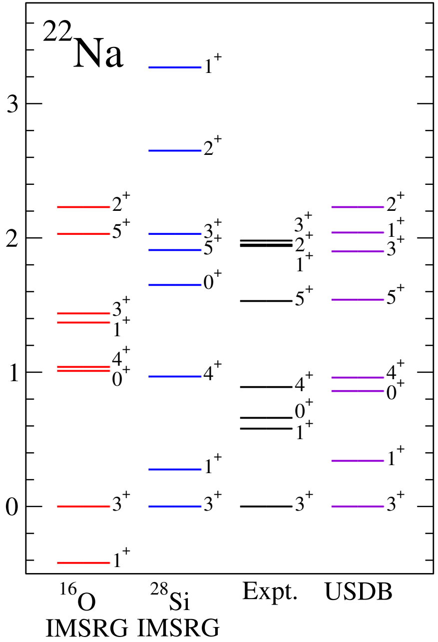


$$|\Phi_0\rangle = |^{28}\mathrm{Si}\rangle$$

A fundamental te
energy observables c
principle does not m
fact, it implies that v
large cutoff, with no
offers the possibility
of freedom. This deco
to handle similar pro
The general purpo
by David Gross [63]:

6 For an early discussion

Navrátil, PRL (2007)

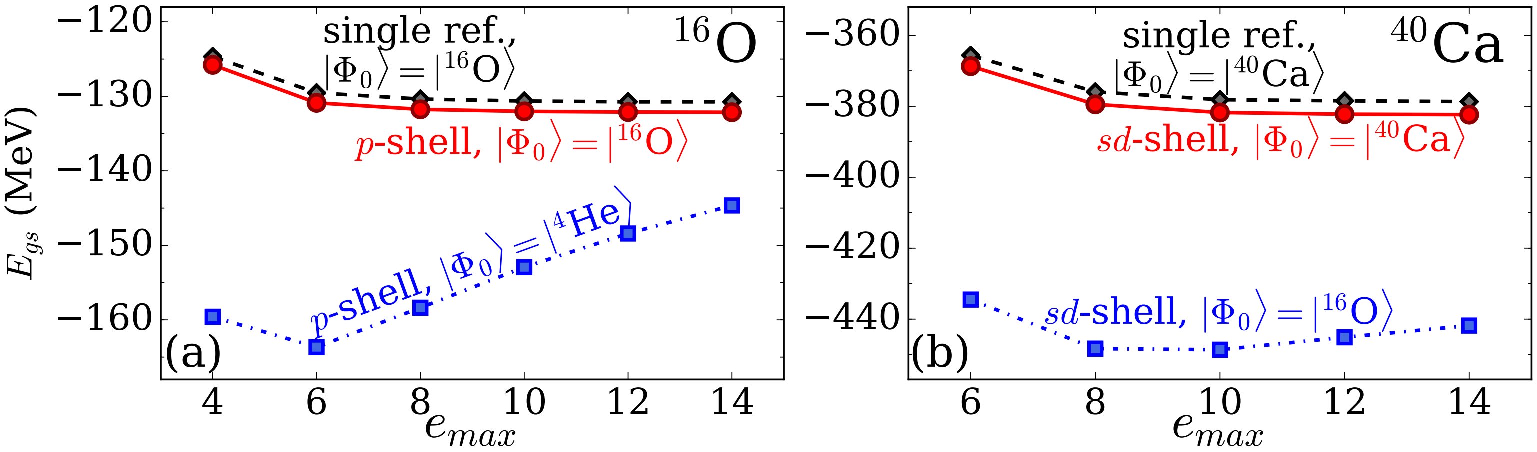


Far from closed shell – ^{28}Si reference overestimates 3N

Convergence with Ensemble Normal Ordering

Results not converged with standard core reference

ENO converges as expected – small difference from single-reference



Stroberg et al., in prep

Ensemble Normal Ordering

Use ensemble state as new reference, defined by the density matrix

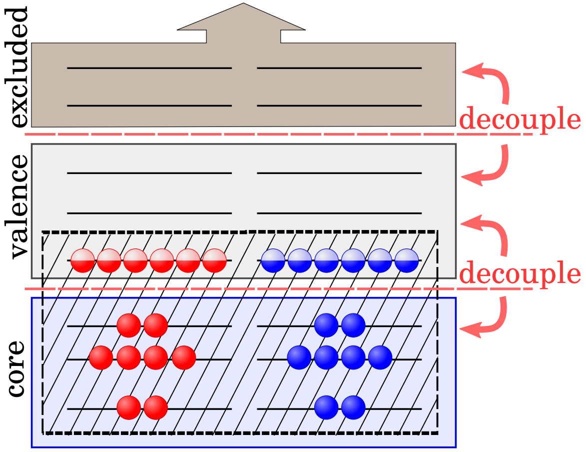
$$\rho = \sum_i \alpha_i \left|\Phi_i\right\rangle \left\langle\Phi_i\right| \quad \langle\mathcal{O}\rangle = \mathrm{Tr}\left(\rho\mathcal{O}\right) \implies \sum_p \mathrm{Tr}(\rho\, a_p^\dagger a_p) = A$$

New definition of normal ordering:

$$\mathrm{Tr}(\rho\,\{a_1^\dagger \dots a_N\}) = \sum_i \alpha_i \left\langle\Phi_i\right| \{a_1^\dagger \dots a_N\} \left|\Phi_i\right\rangle = 0$$

And Wick contraction

$$\{\overline{a_p^\dagger a_q}\} = \sum_\alpha c_\alpha \langle\Phi_\alpha|a_p^\dagger a_q|\Phi_\alpha\rangle \equiv n_p\delta_{pq}$$



$$\rho = \frac{1}{2}\left|{}^{16}\mathrm{O}\right\rangle\left\langle{}^{16}\mathrm{O}\right| + \frac{1}{2}\left|{}^{28}\mathrm{Si}\right\rangle\left\langle{}^{28}\mathrm{Si}\right|$$

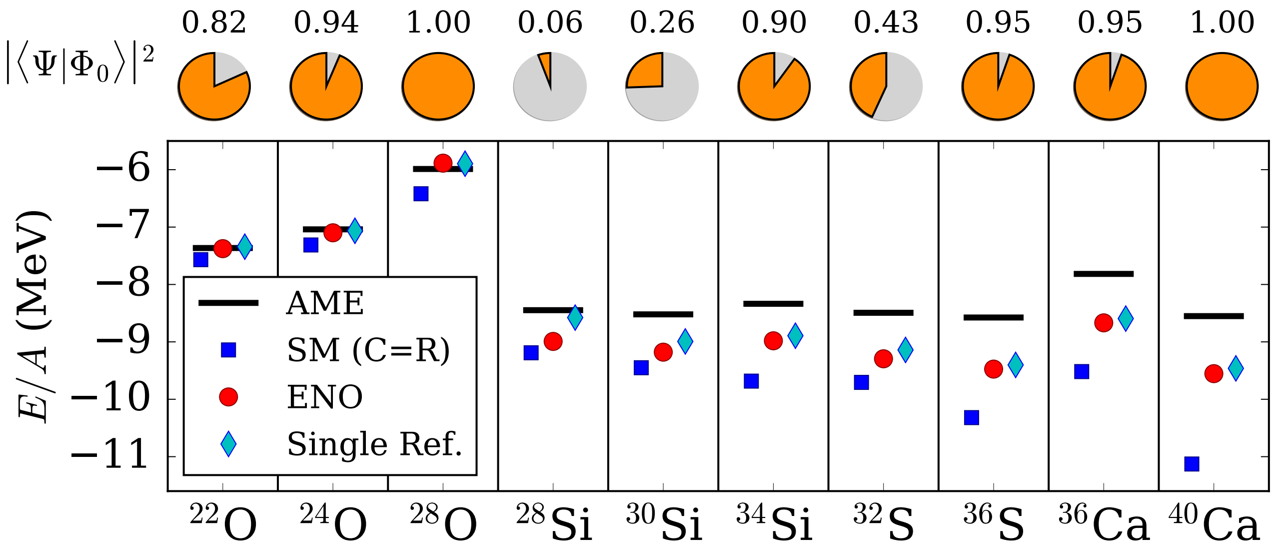
Can have fractional occupations

No N-representability problem!

Benchmarking Ground States from Oxygen to Calcium

Benchmark against SR-IMSRG results for closed sd-shell nuclei

Error from using core as reference grows far from core



Stroberg et al., arXiv:1607.03229

Targeted NO finds good agreement with SR-IMSRG

Experimental discrepancies due to deficiencies in initial Hamiltonians