Ab initio spectroscopy (and related topics) with the VS-IMSRG

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ESNT
May 22, 2024

Discovery, accelerated

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

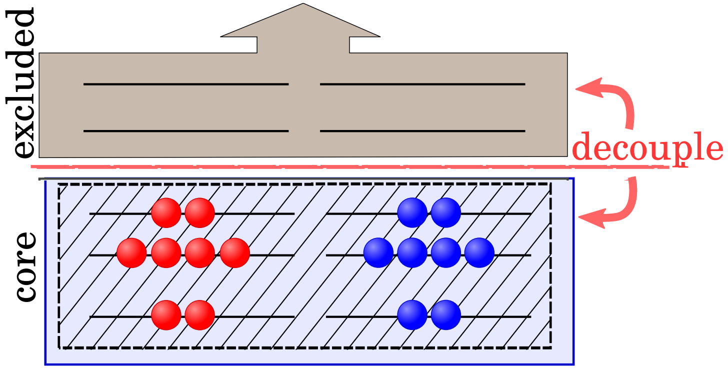
$$U = e^{\Omega} = e^{\eta_n} \ldots e^{\eta_1} \qquad \eta = \frac{1}{2}\arctan\left(\frac{2H_{\mathrm{od}}}{\Delta}\right) - \mathrm{h.c.}$$

$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

All operators truncated at two-body level IMSRG(2)
IMSRG(3) in progress

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

Step 1: Decouple core



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

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

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

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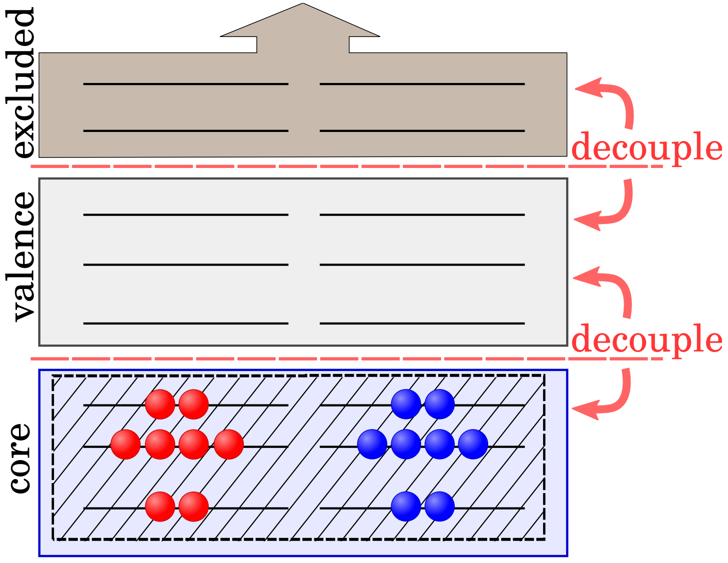
All operators truncated at two-body level IMSRG(2)
IMSRG(3) variants in progress (Heinz, Stroberg)

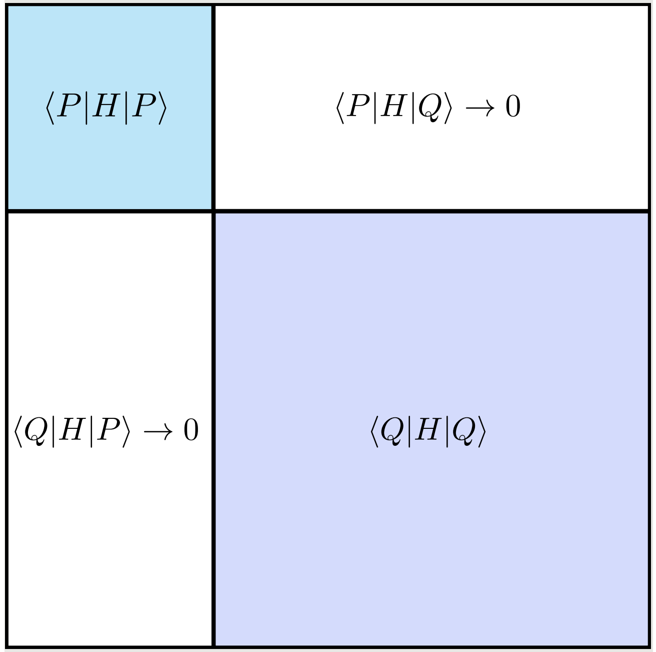
Tsukiyama, Bogner, Schwenk, PRC 2012
Morris, Parzuchowski, Bogner, PRC 2015



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

Step 1: Decouple core
Step 2: Decouple valence space

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



$\langle P\|H\|P\rangle$	$\langle P\|H\|Q\rangle \to 0$
$\langle Q\|H\|P\rangle \to 0$	$\langle Q\|H\|Q\rangle$

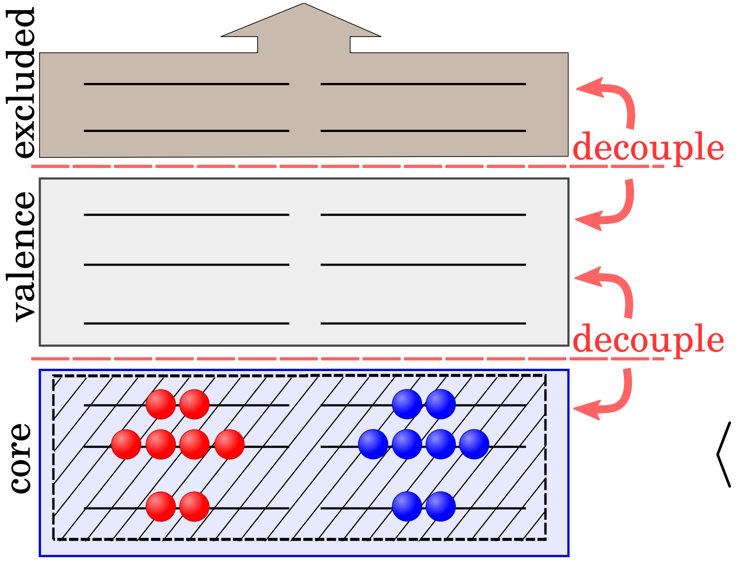
Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

$$U = e^{\Omega} = e^{\eta_n} \ldots e^{\eta_1} \qquad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\mathrm{od}}}{\Delta}\right) - \mathrm{h.c.}$$

$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2} [\Omega, [\Omega, H]] + \cdots$$

$$\tilde{\mathcal{O}} = e^{\Omega} \mathcal{O} e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2} [\Omega, [\Omega, \mathcal{O}]] + \cdots$$



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

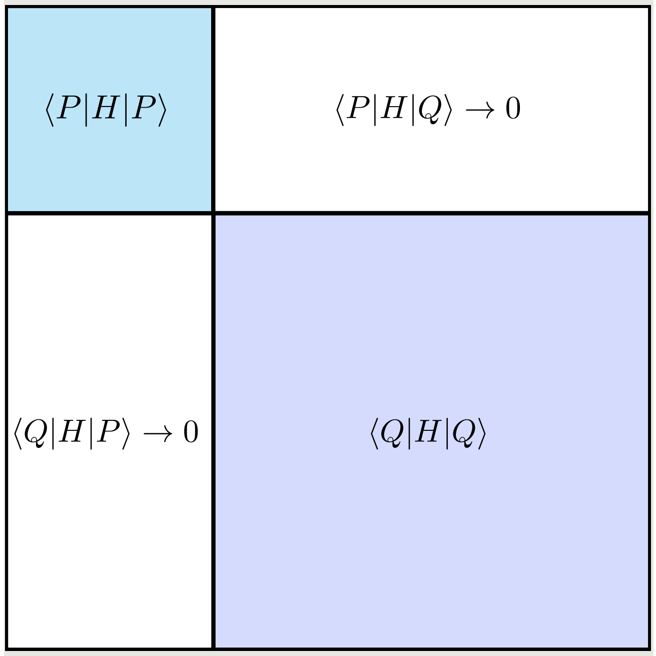
Step 1: Decouple core

Step 2: Decouple valence space

Step 3: Decouple additional operators

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

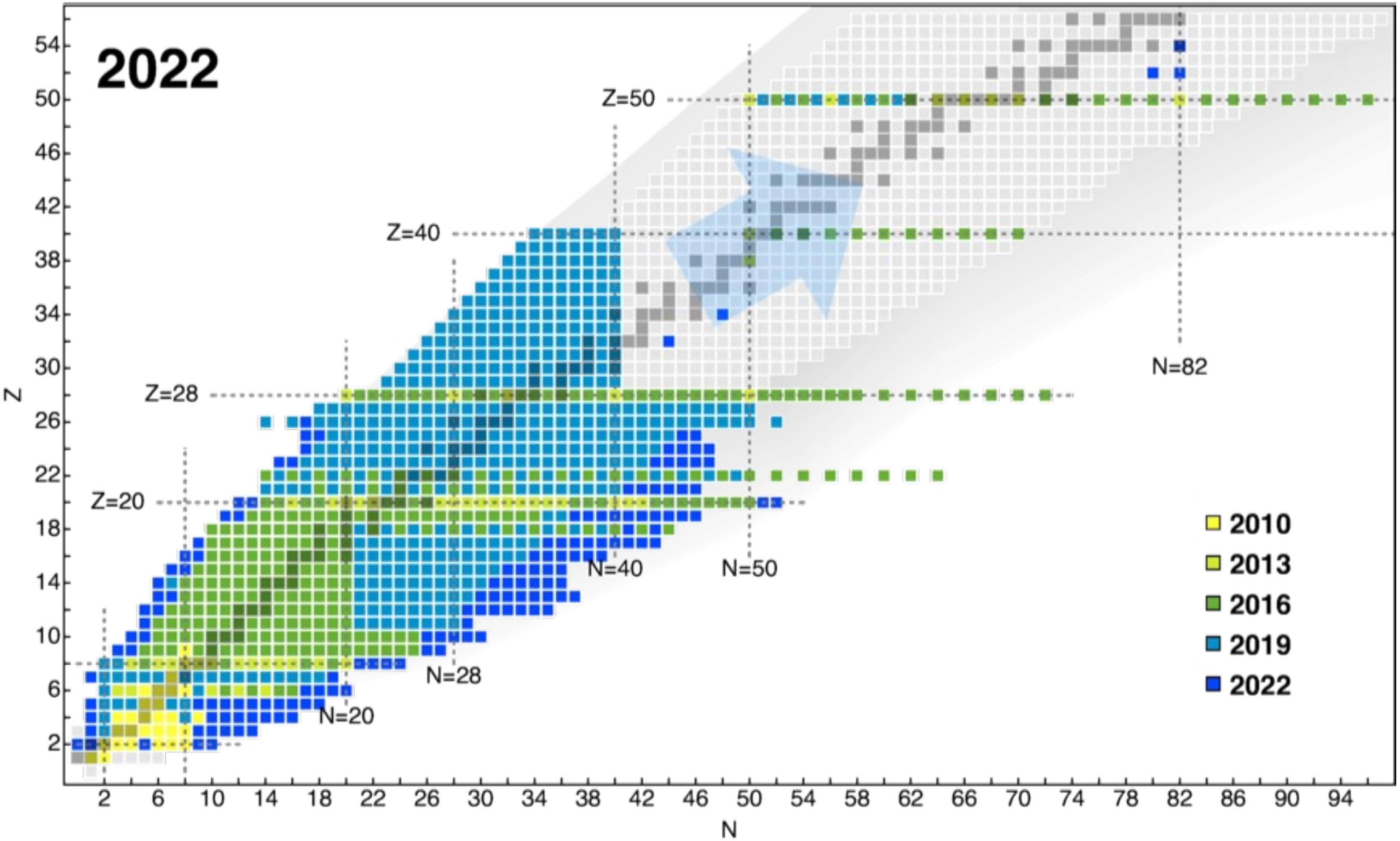
$$\langle \tilde{\Psi}_n | P \tilde{M}_{0\nu} P \mid \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$



$\langle P\vert H\vert P\rangle$	$\langle P\vert H\vert Q\rangle \to 0$
$\langle Q\vert H\vert P\rangle \to 0$	$\langle Q\vert H\vert Q\rangle$

Ab Initio Progress: How Heavy Can We Go?

Tremendous progress in ab initio reach, largely due to polynomially scaling methods!



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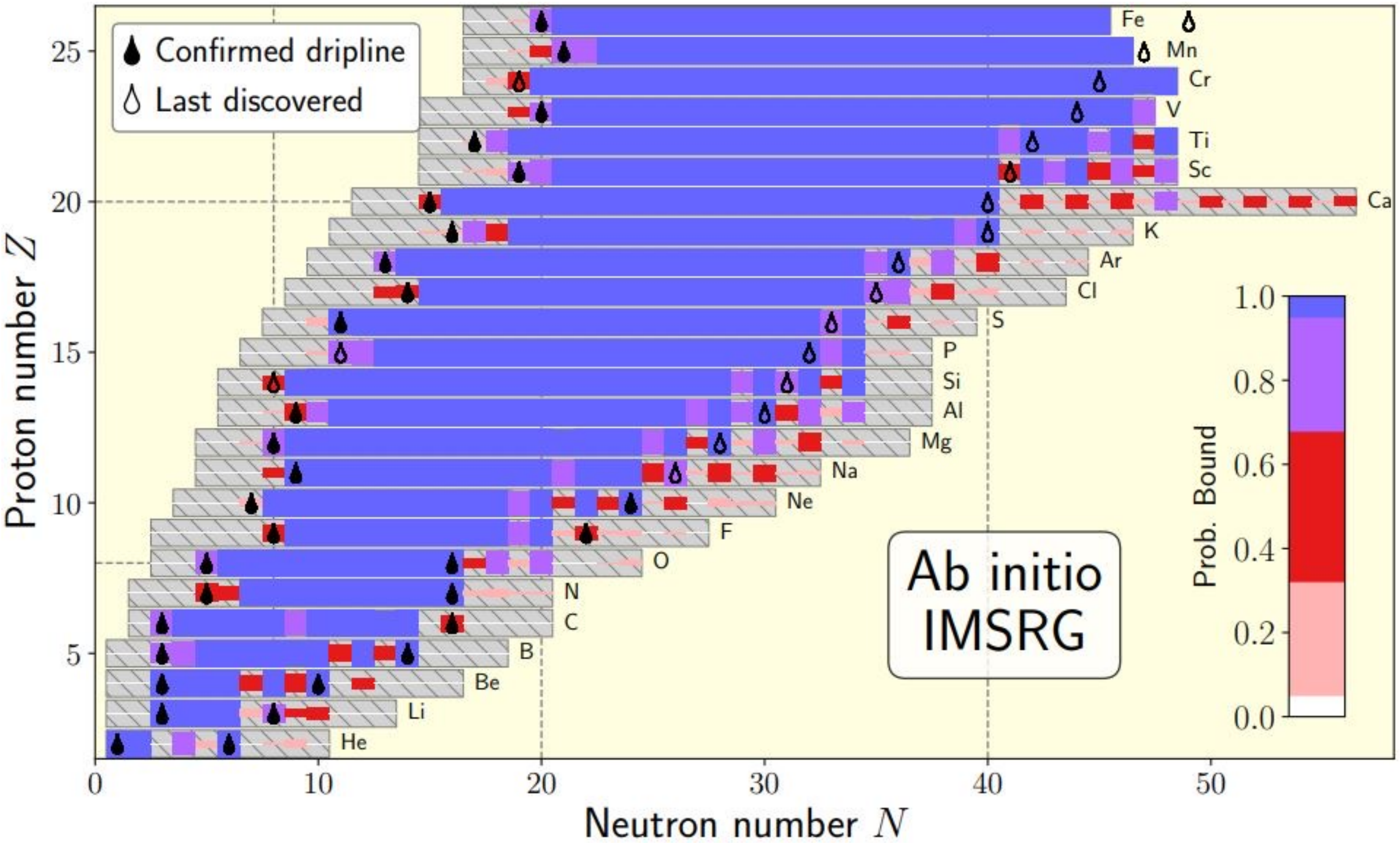
Limits of Existence in Medium-Mass Region

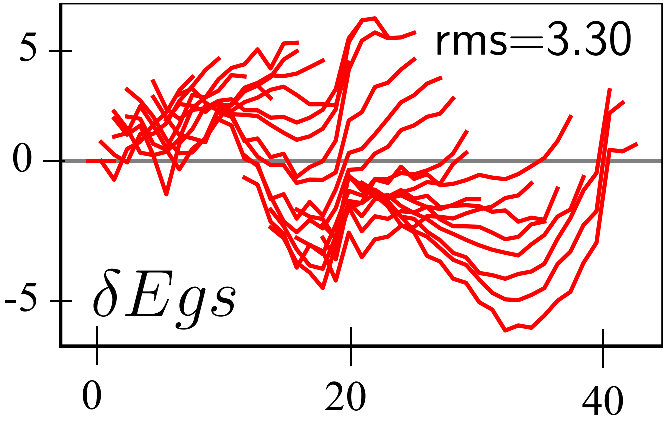
Ab initio calculations of ~700 nuclei from He to Fe



Known drip lines predicted within uncertainties

Ab initio guide for neutron-rich driplines

$$\delta\mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$



Input H fit to 2,3,4-body
Not biased towards existing data

Featured in Physics **Editors' Suggestion**

Ab Initio Limits of Atomic Nuclei

S. R. Stroberg, J. D. Holt, A. Schwenk, and J. Simonis
Phys. Rev. Lett. **126**, 022501 – Published 12 January 2021

Physics See synopsis: Predicting the Limits of Atomic Nuclei

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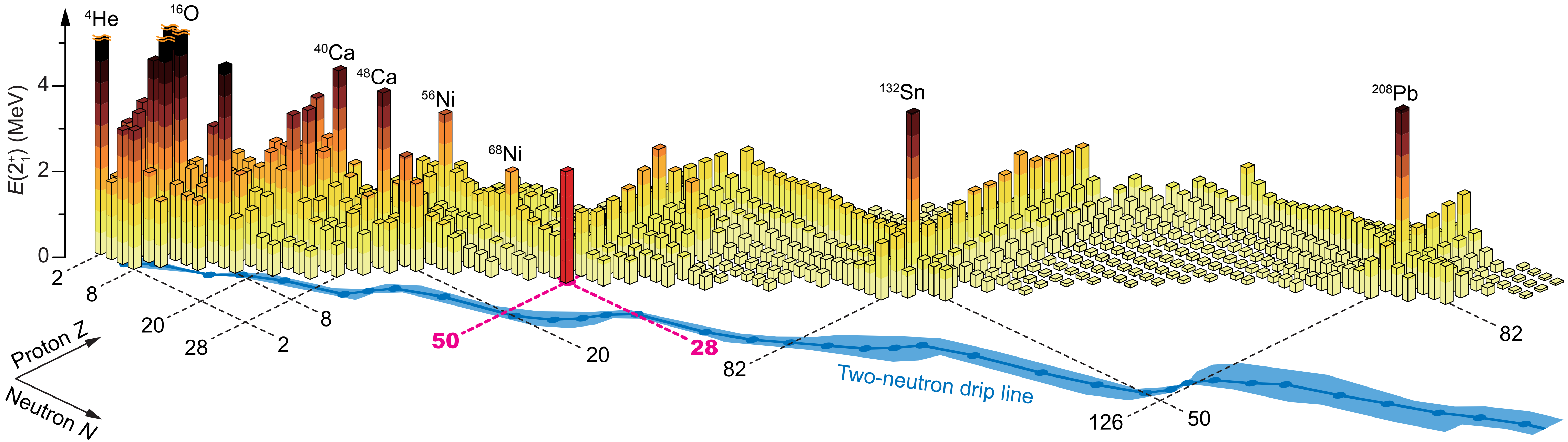
Magic Numbers in Nuclei

Magic numbers: pillars of nuclear structure, novel evolution in exotic nuclei



Signatures of Magic Numbers

Sharp decrease in separation energy (masses)

Elevated first excited 2+ energy (spectroscopy)

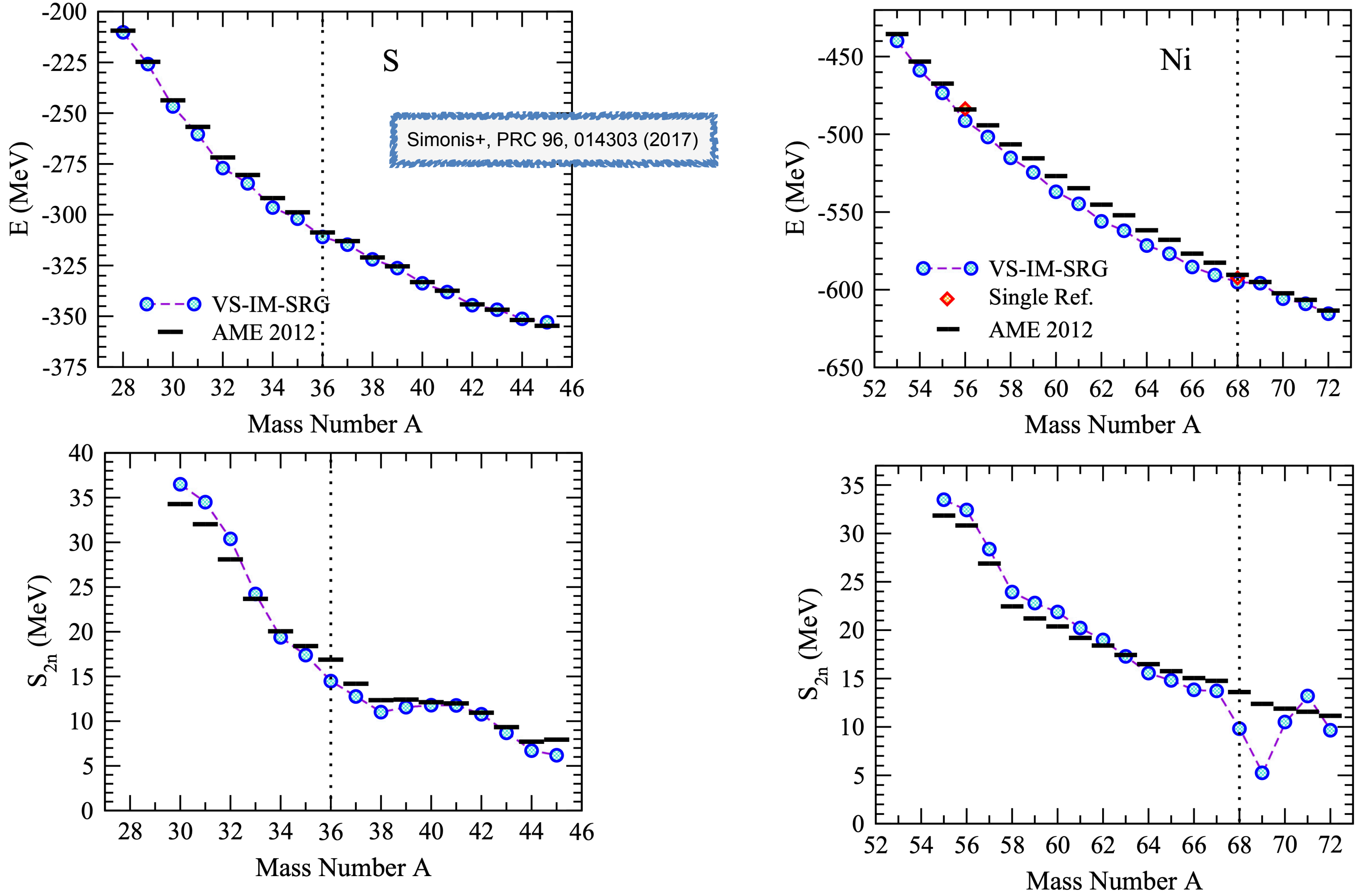
Tightly bound (decreased radii)

EM Moments

Q – collectivity; μ single-particle nature

Prediction of Energies Across Chains

Energies: Generally excellent agreement along isotopic chains to limits of existence



Simonis+, PRC 96, 014303 (2017)

Prediction of Energies Across Chains

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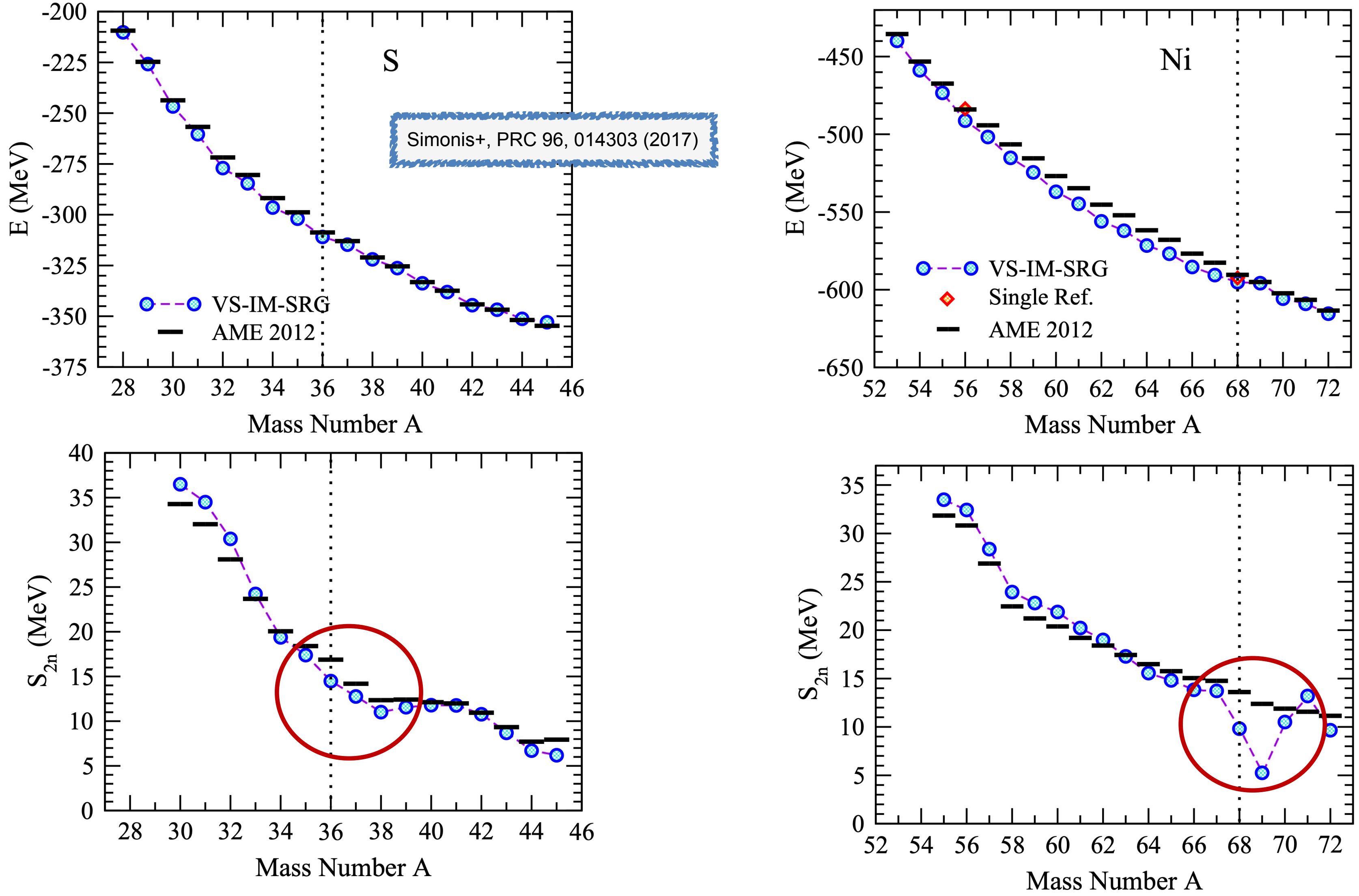


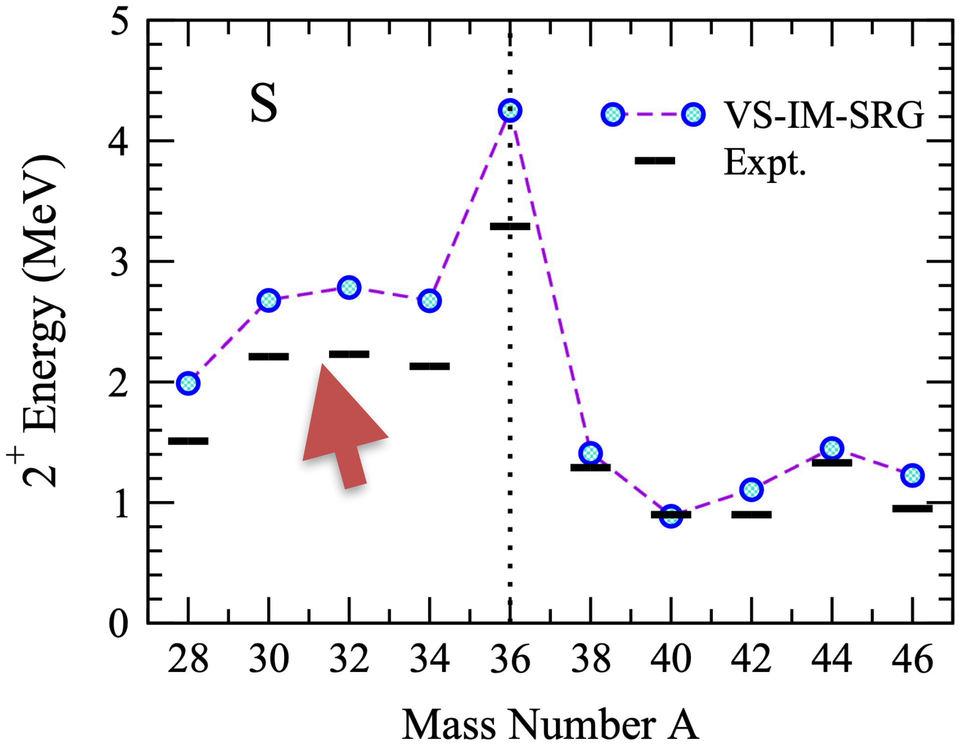
Simonis+, PRC 96, 014303 (2017)

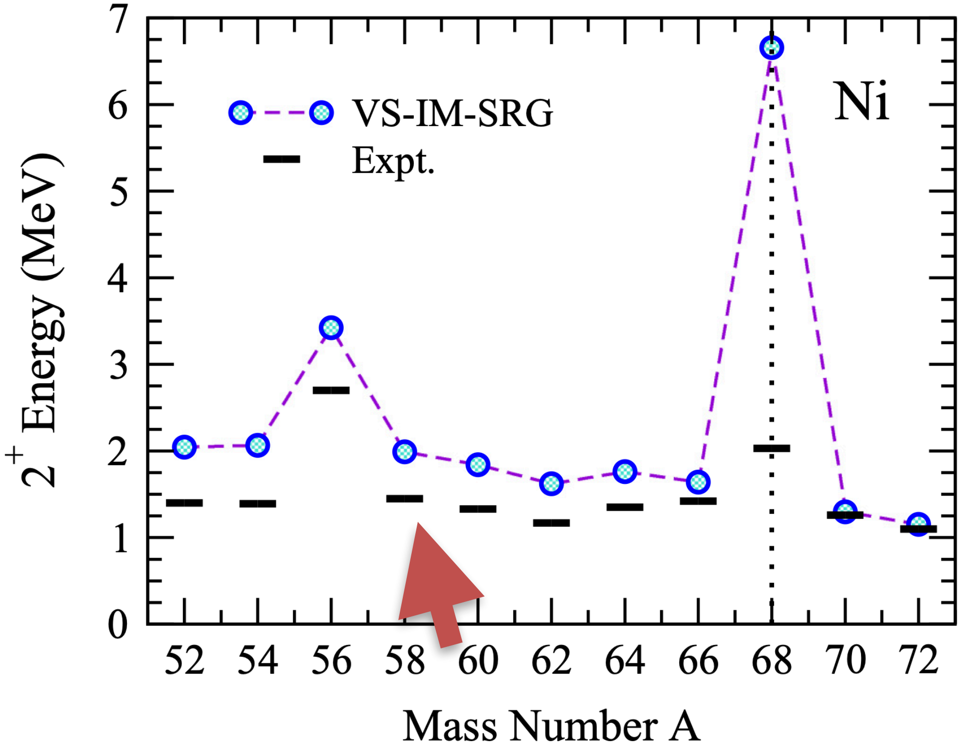
Artifacts across major shells

Prediction of Excitation Energies Across Chains

Energies: Generally good agreement along isotopic chains

Overpredict 2+ at shell closures… what might help?

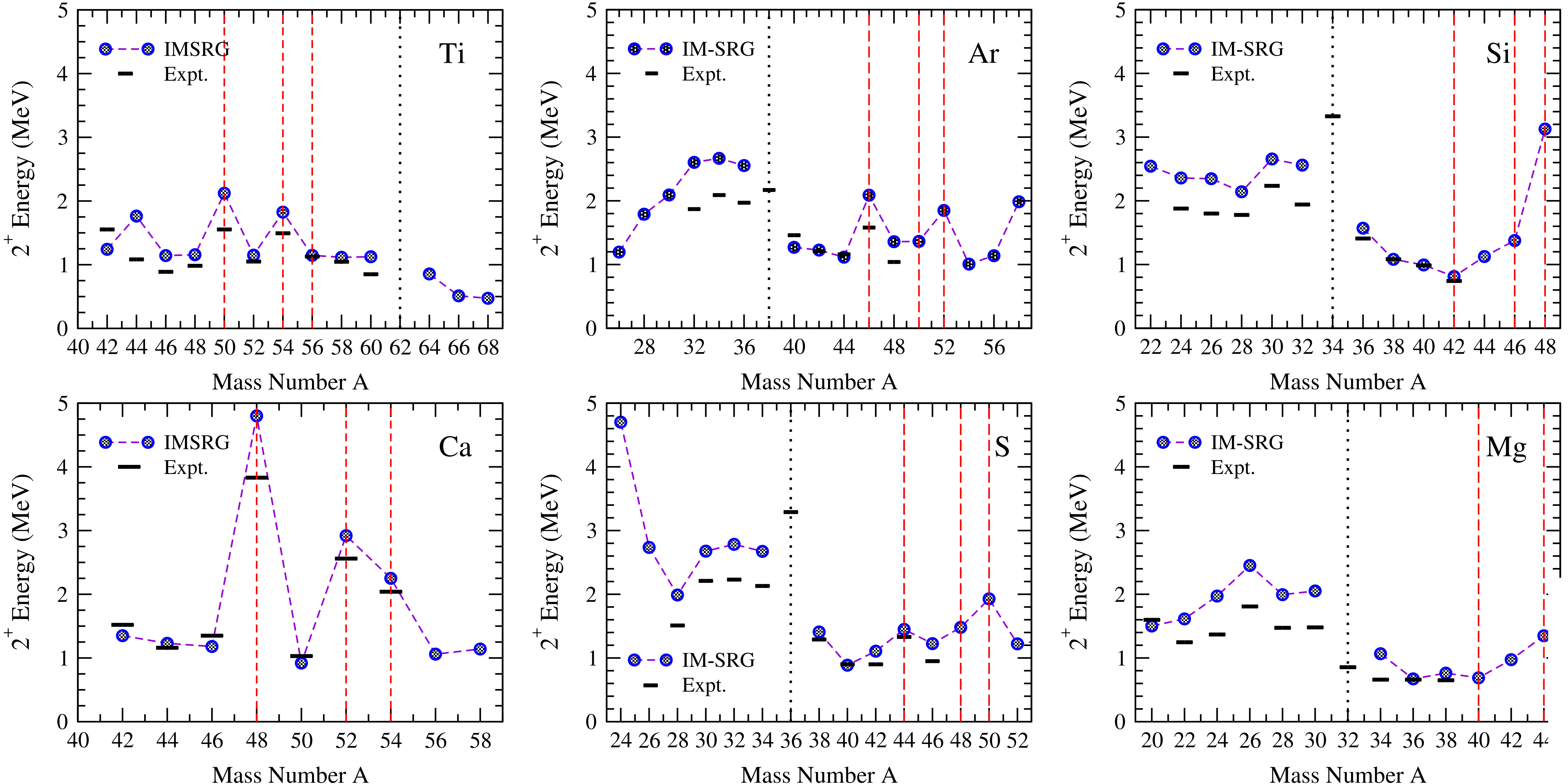




Too large shell gap – IMSRG(3) – or missing cross-shell physics?

Future: Evolution of N=28,32,34 Magic Numbers

Ab initio predictions from above calcium towards oxygen – **persistence of N=34**

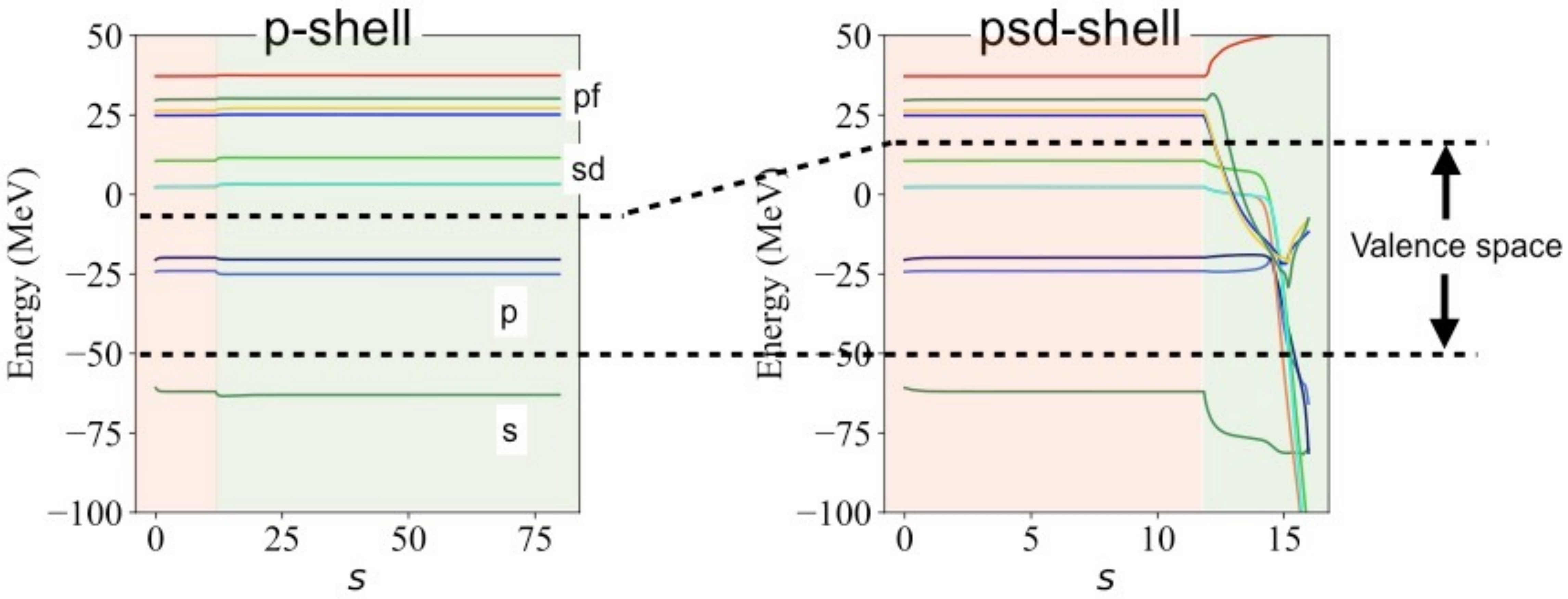


Improve Cross-Shell Physics: Multi-Shell Spaces

Essential for many applications: island of inversion, forbidden transitions, heavier beta decay cases

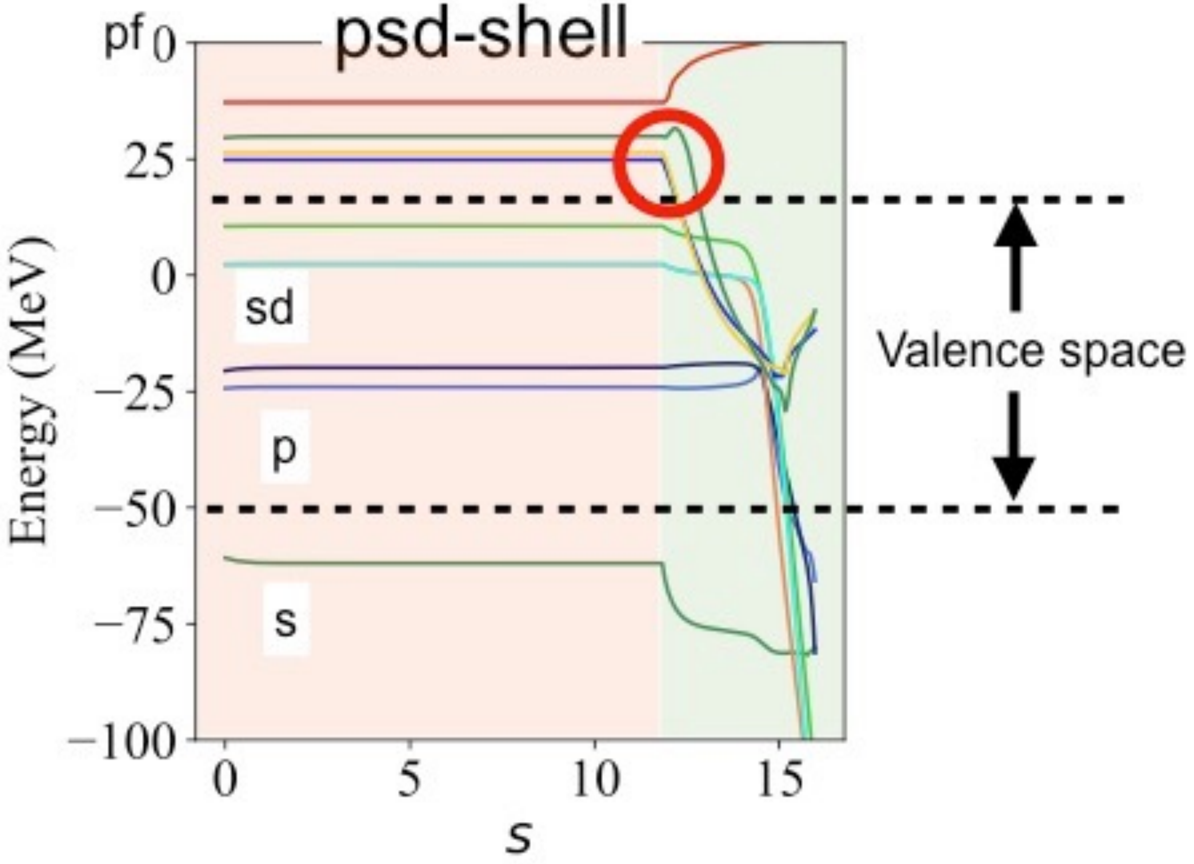
Standard VS-IMSRG typically fails!

- Flow of single-particle energies



Typical IMSRG Failure

- Flow of single-particle energies
  - At the very beginning of valence-decoupling flow, some of pf-shell orbits come down.
  - Intuitively, we expect that P- and Q-space single particle energies do not mix.
  - At the beginning of the flow, the slope of single-particle energies (df/ds) seems to be crucial.



Proposed Fix: Modified Generator

Proposed fix: modify generator to give constant shift to energy denominator

Never have negative energy denominators if on order of hw…

K. Suzuki, Prog. Theor. Phys. **58**, 1064 (1977).

N. Tsunoda, K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C **89**, 024313 (2014).

$$\begin{aligned}\eta_{12} &= \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212}} \\ \eta_{1234} &= \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}} \\ A_{1234} &= \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}\end{aligned}$$

$$\Longrightarrow$$

$$\begin{aligned}\eta_{12} &= \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta} \\ \eta_{1234} &= \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta} \\ A_{1234} &= \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}\end{aligned}$$

Miyagi et al., PRC (2020)

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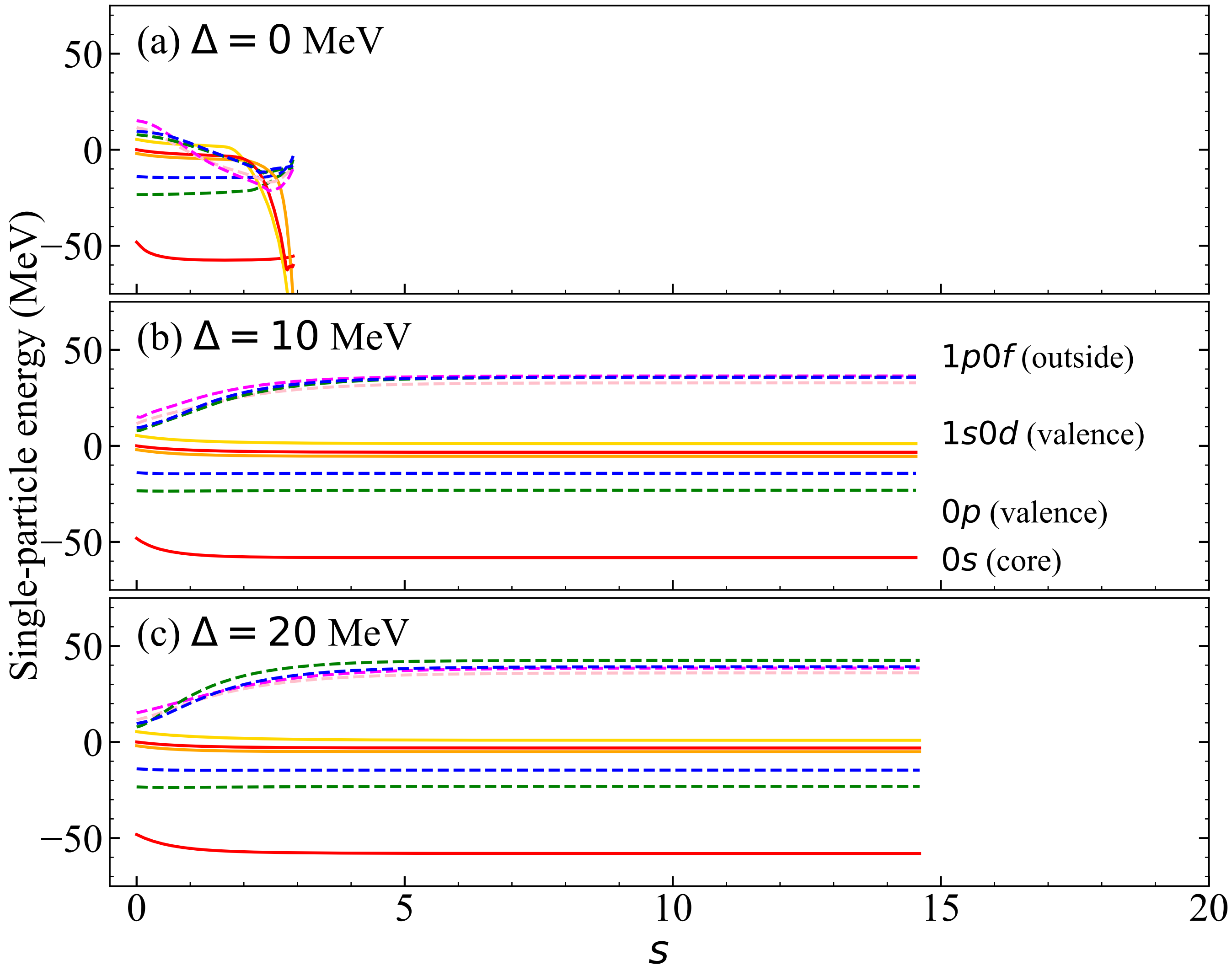


Miyagi et al., PRC (2020)

Longstanding Shell Model Issue: Center of Mass

Centre of mass: long-standing issue in the shell-model universe

So far: add CoM at the shell-model calculation stage

$$H \longrightarrow H_{\mathrm{VS}} + \beta H_{\mathrm{cm}} \longrightarrow \text{energies}$$

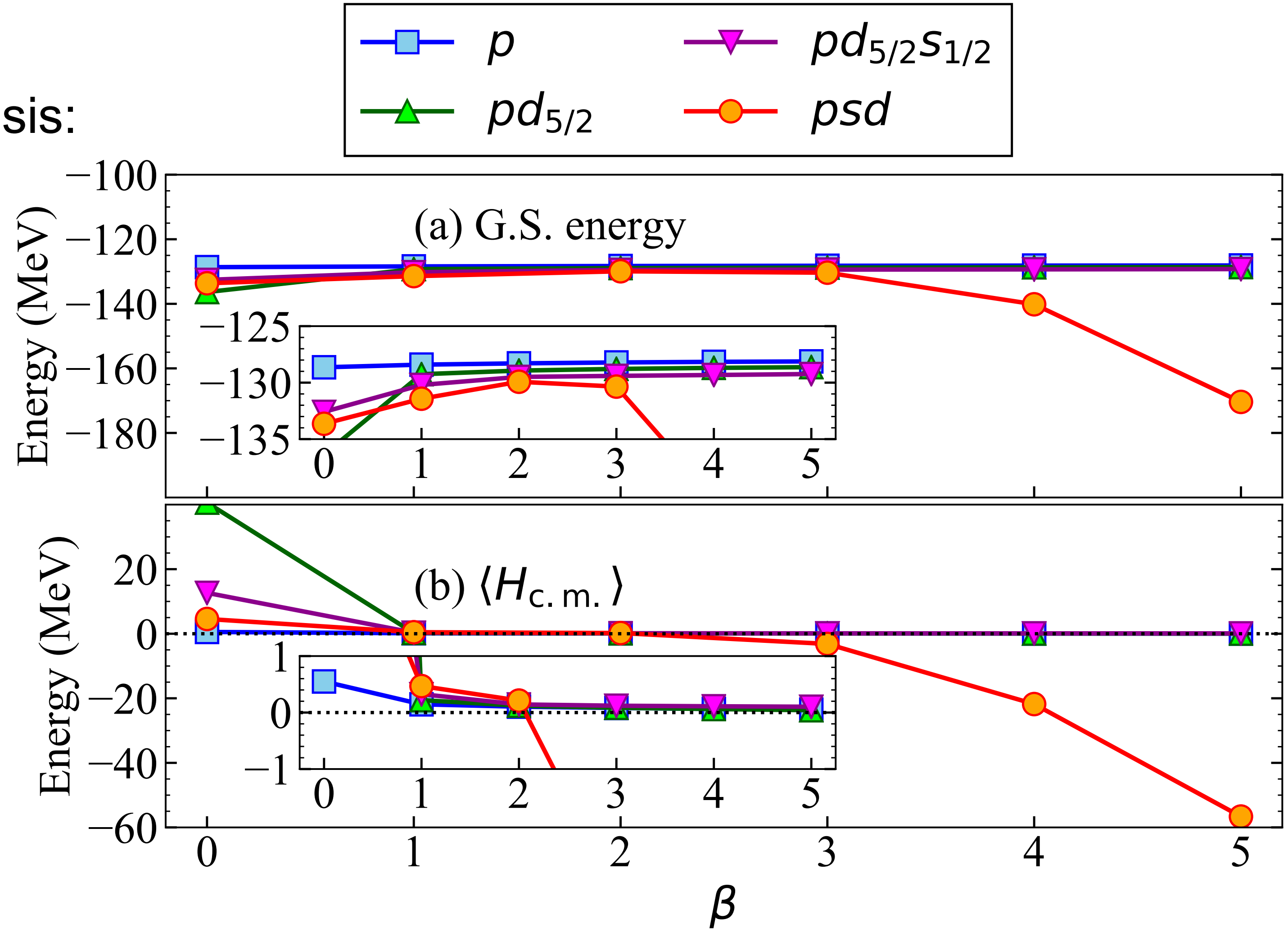
BUT H_{VS} is no longer represented in HO basis:

Add from beginning instead

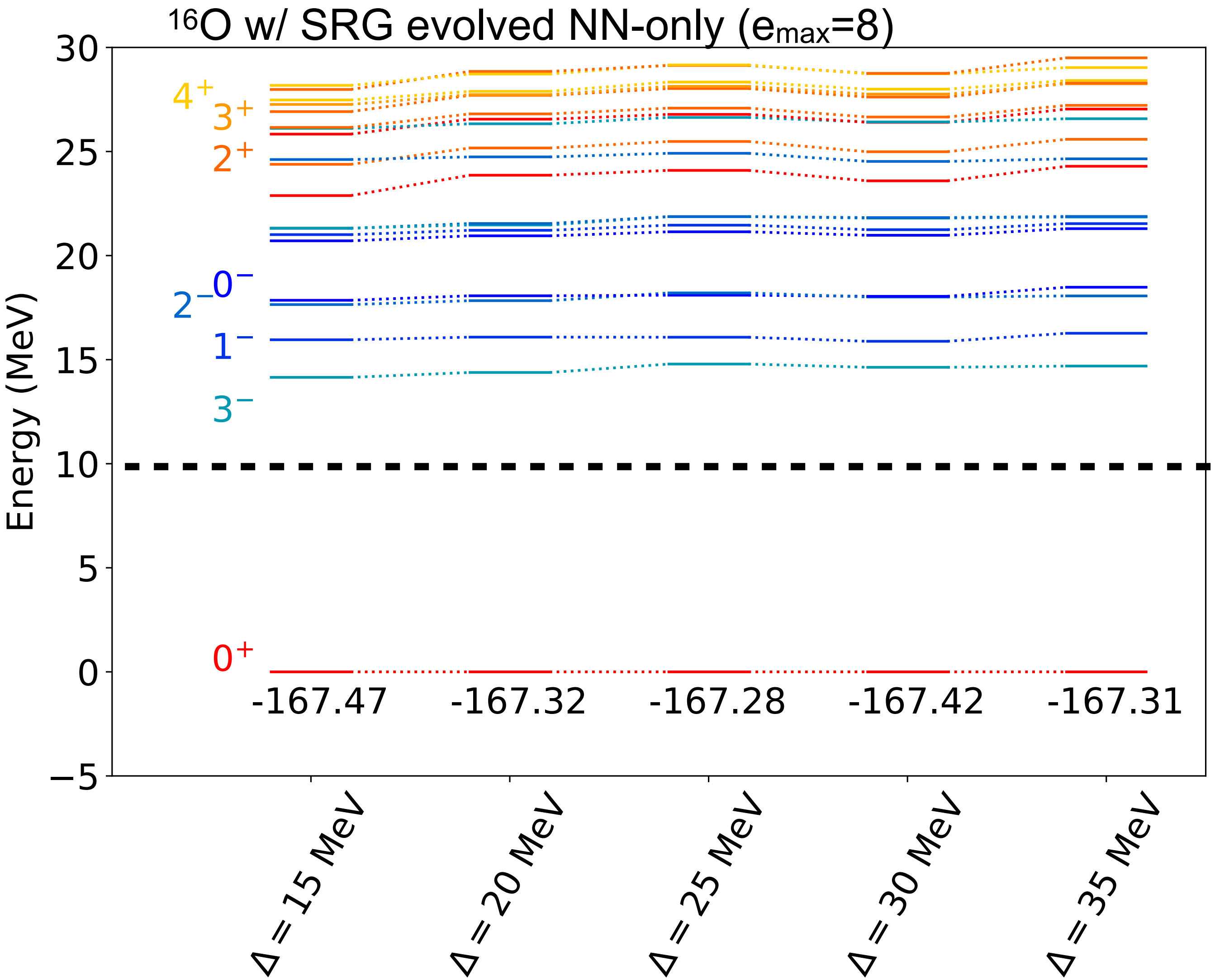
$$H + \beta H_{\mathrm{cm}} \longrightarrow H_{\mathrm{VS}} \longrightarrow \text{energies}$$

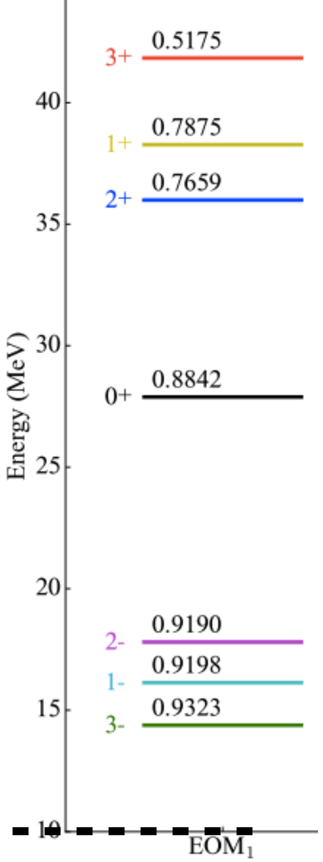
Full two-shell suffers from H_{cm} dep.

Removing $d_{3/2}$ solves problem!



Comparison with EOM method





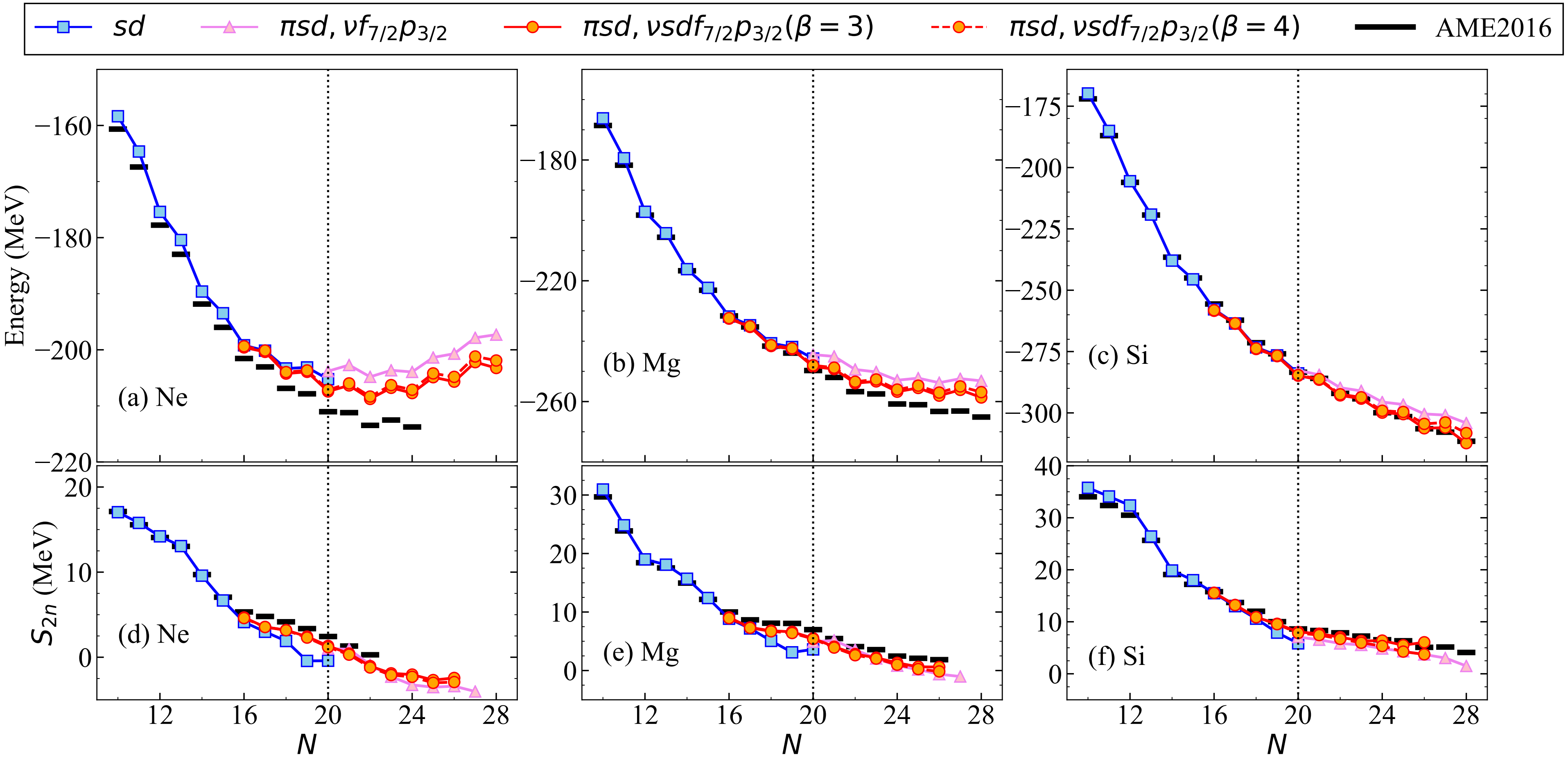
1p1h dominant lowest 3^-, 1^-, 2^- agree well with the EOM-IMSRG results.

EOM-IMSRG results are take from N. M. Parzuchowski, T. D. Morris, and S. K. Bogner, Phys. Rev. C **95**, 044304 (2017).

Island of Inversion: sd-Shell Ground States

Ground-state energies of Ne, Mg, Si isotopes: 1.8/2.0(EM)

Multi-shell space improves IoI physics



Miyagi et al., PRC (2020)

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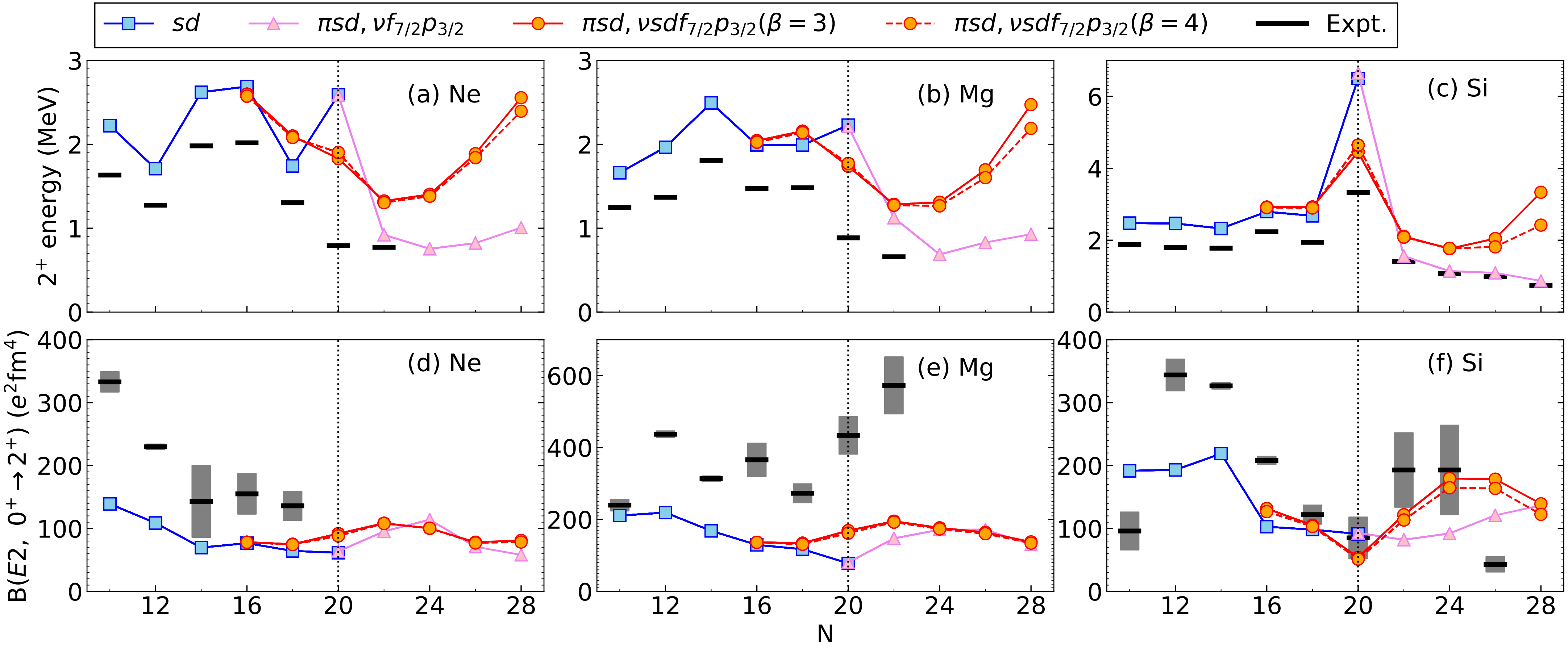
Island of Inversion: sd-Shell Excited States

Excited-state properties of Ne, Mg, Si isotopes: 1.8/2.0(EM)

Multi-shell improves IoI physics… not enough to fix completely

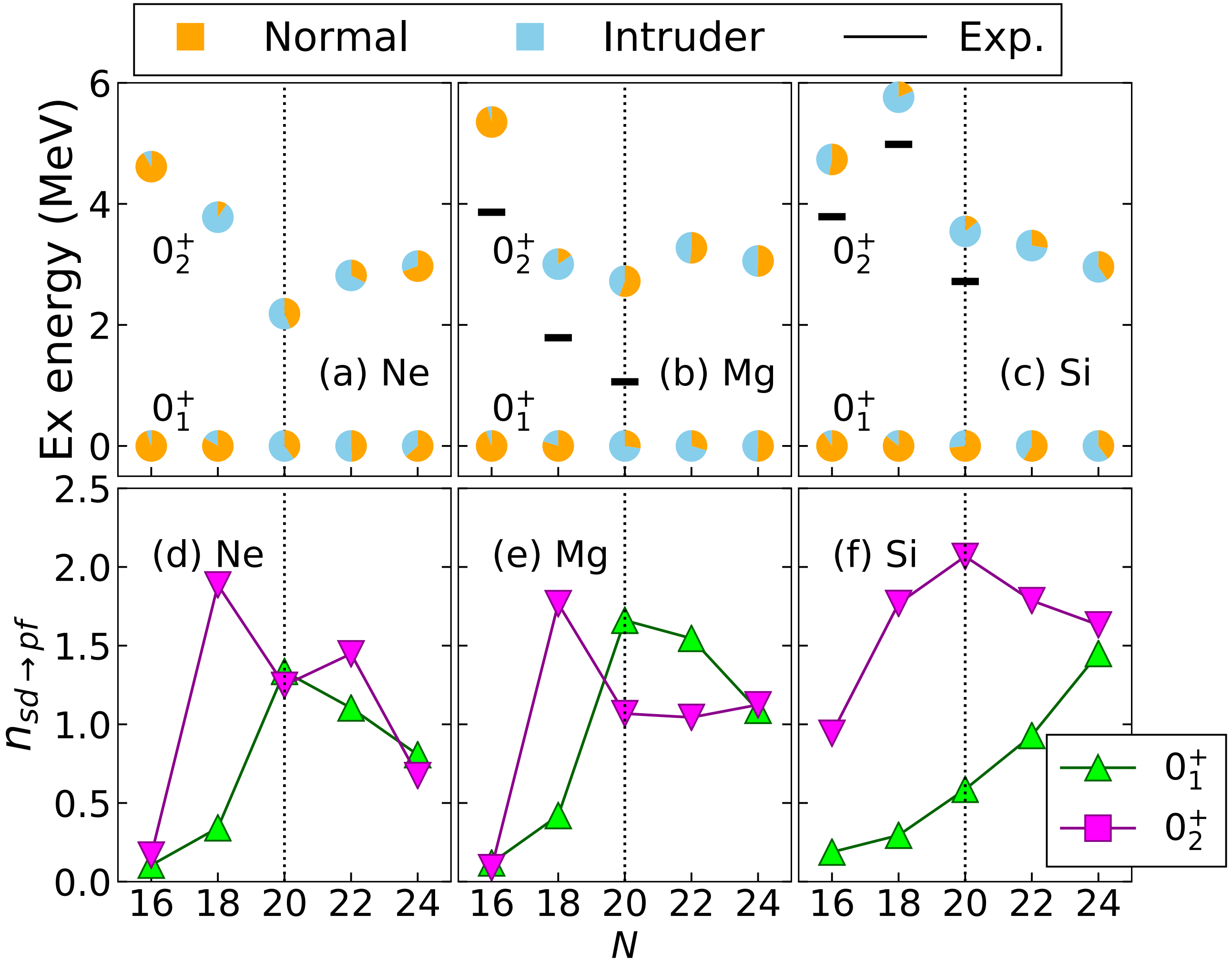


Miyagi et al., PRC (2020)

Island of Inversion: sd-Shell Intruder Configurations

Explore intruder configurations in 0+ states

Multi shell space dramatically improves IoI physics



Editors' Suggestion

Ab initio multishell valence-space Hamiltonians and the island of inversion

T. Miyagi, S. R. Stroberg, J. D. Holt, and N. Shimizu
Phys. Rev. C **102**, 034320 – Published 16 September 2020

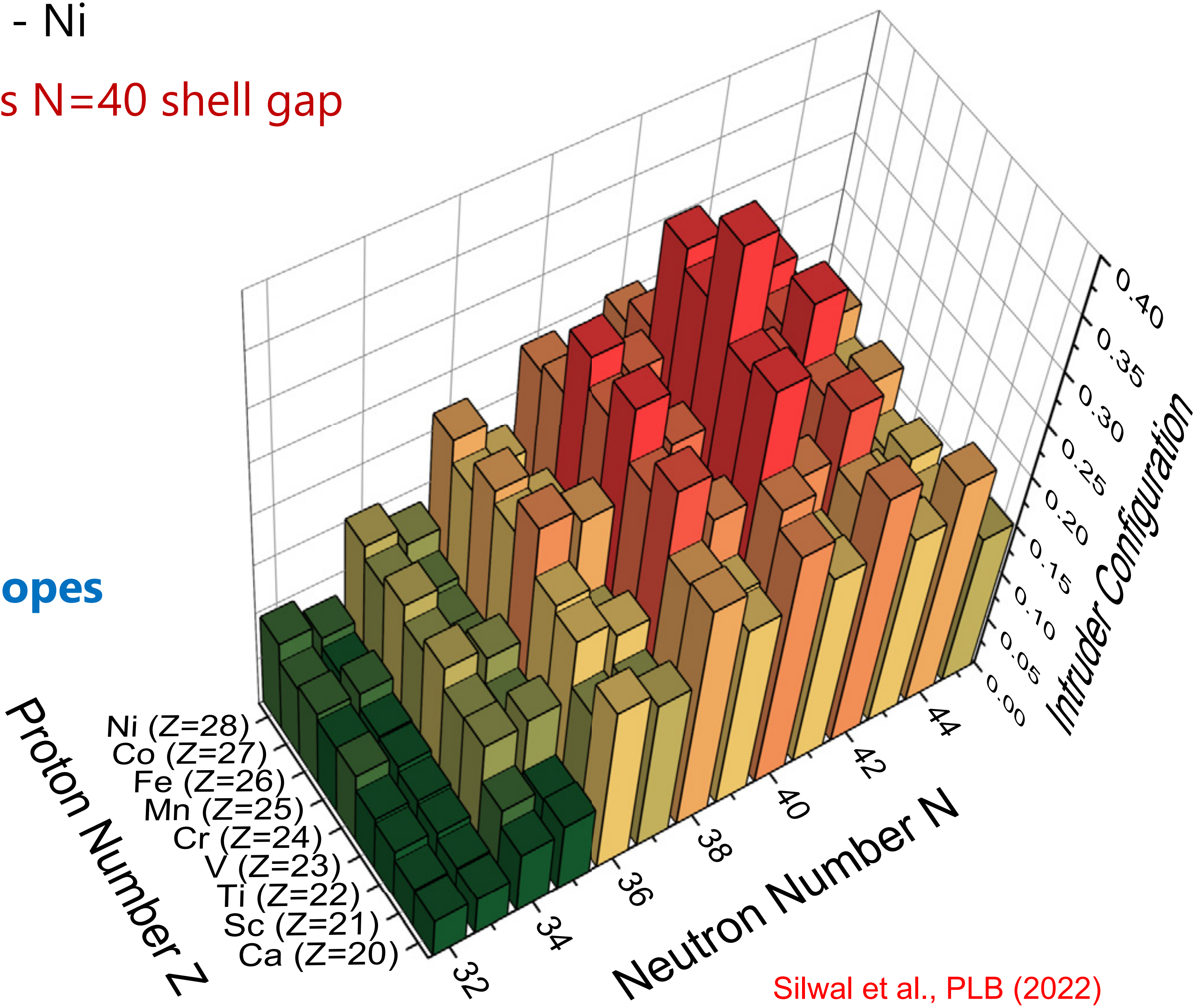
Island of Inversion: pf-Shell

Explore Intruder configurations from Ca - Ni

Already important for Ca isotopes across N=40 shell gap

^{60}Ca unlikely doubly magic

Strong increase at Ti, **summit at Cr isotopes**

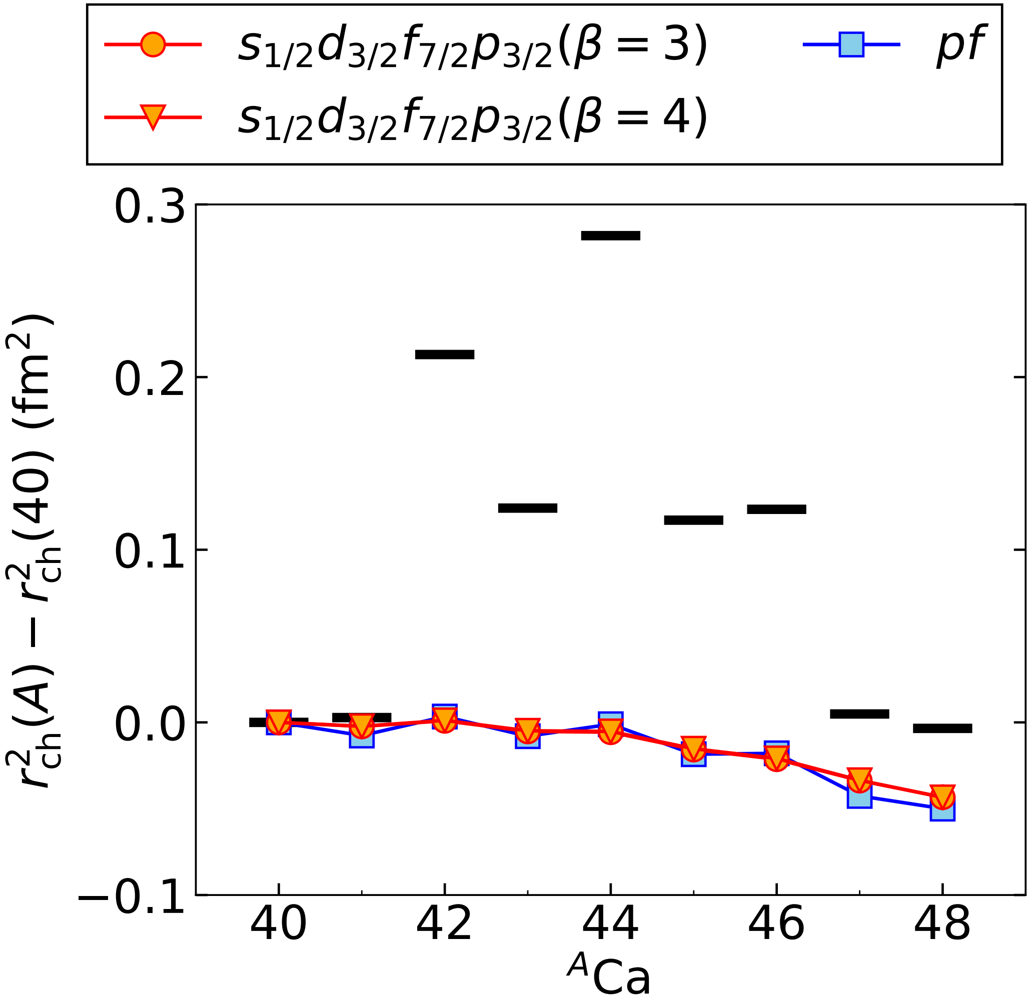


Silwal et al., PLB (2022)

Charge Radii: Ca Isotopes

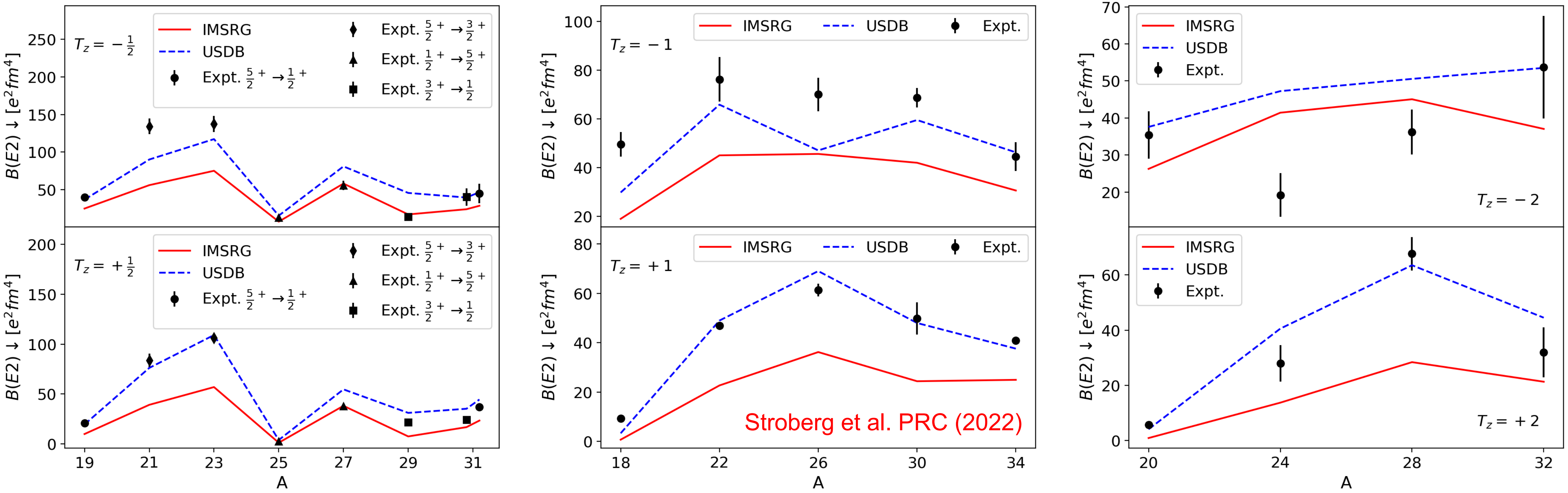
Calculate charge radii in Ca isotopes – parabolic behavior, long-standing problem

Previous SM studies identified cross-shell excitations as origin



Global Trends in Absolute B(E2): sd Shell

Study E2 transitions across sd-shell



Stroberg et al. PRC (2022)

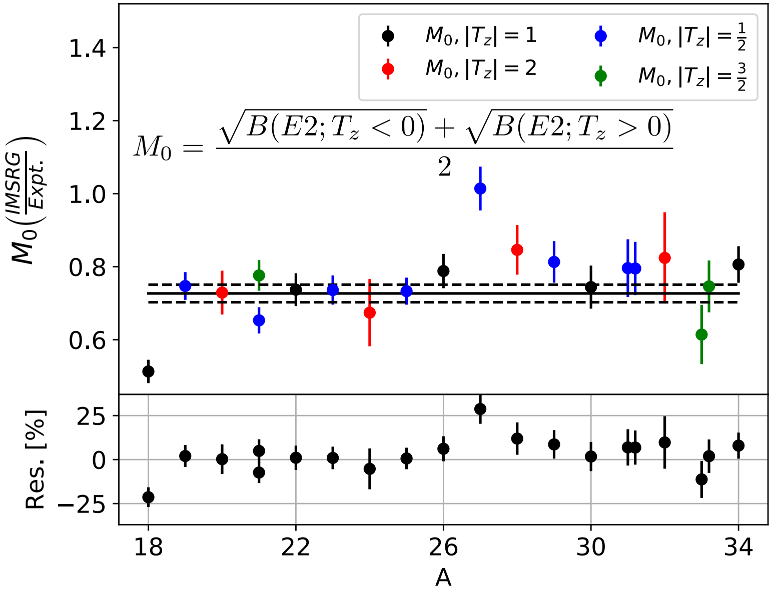
USDB with effective charges typically reproduces absolute values well

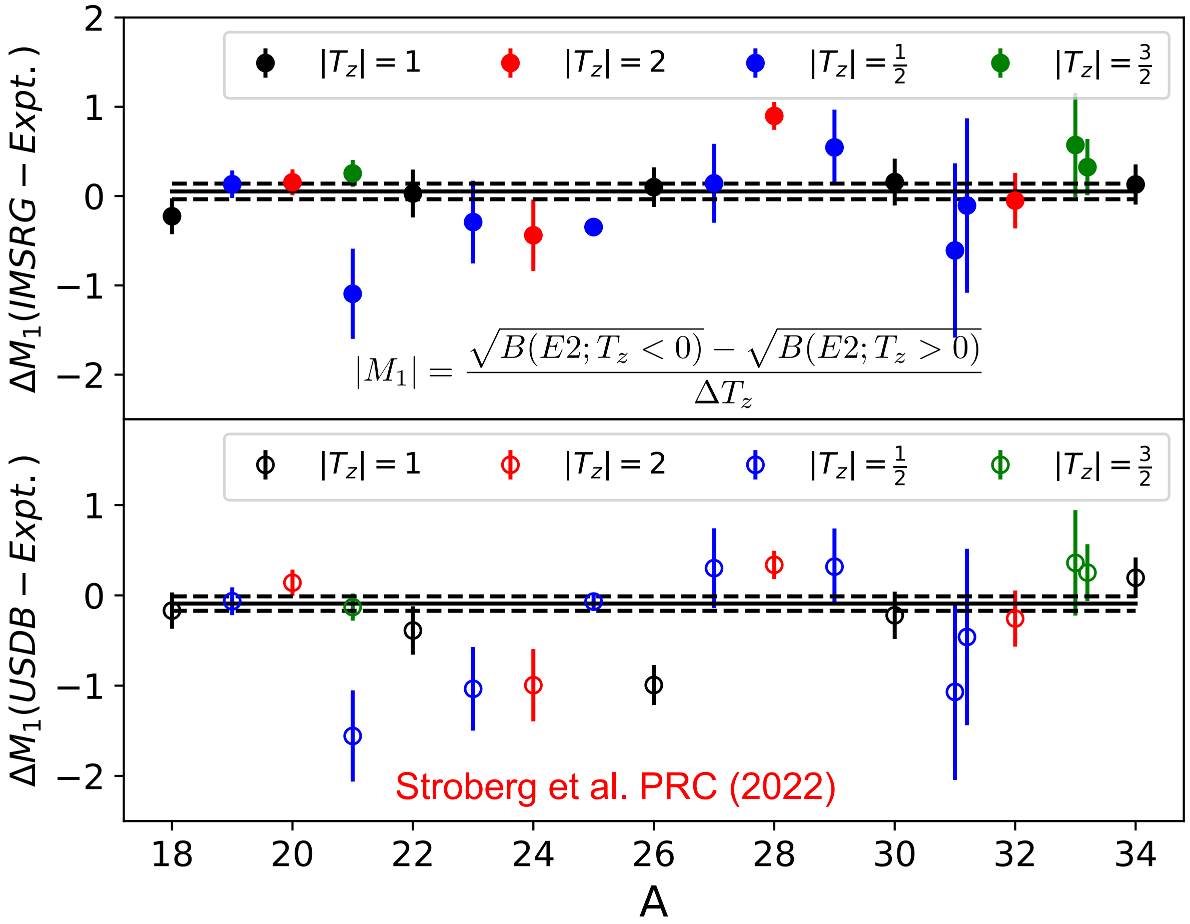
VS-IMSRG (**no effective charges**) typically under-predicts experiment

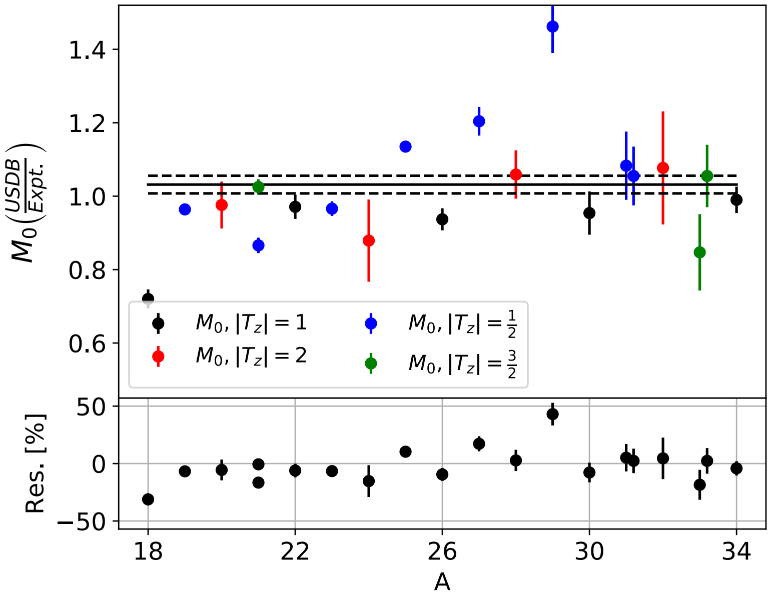
Trends well reproduced in all cases

Global Trends in B(E2): IS/IV Components

Study charge E2 transitions across sd-shell: IS (M_0) and IV (M_1)







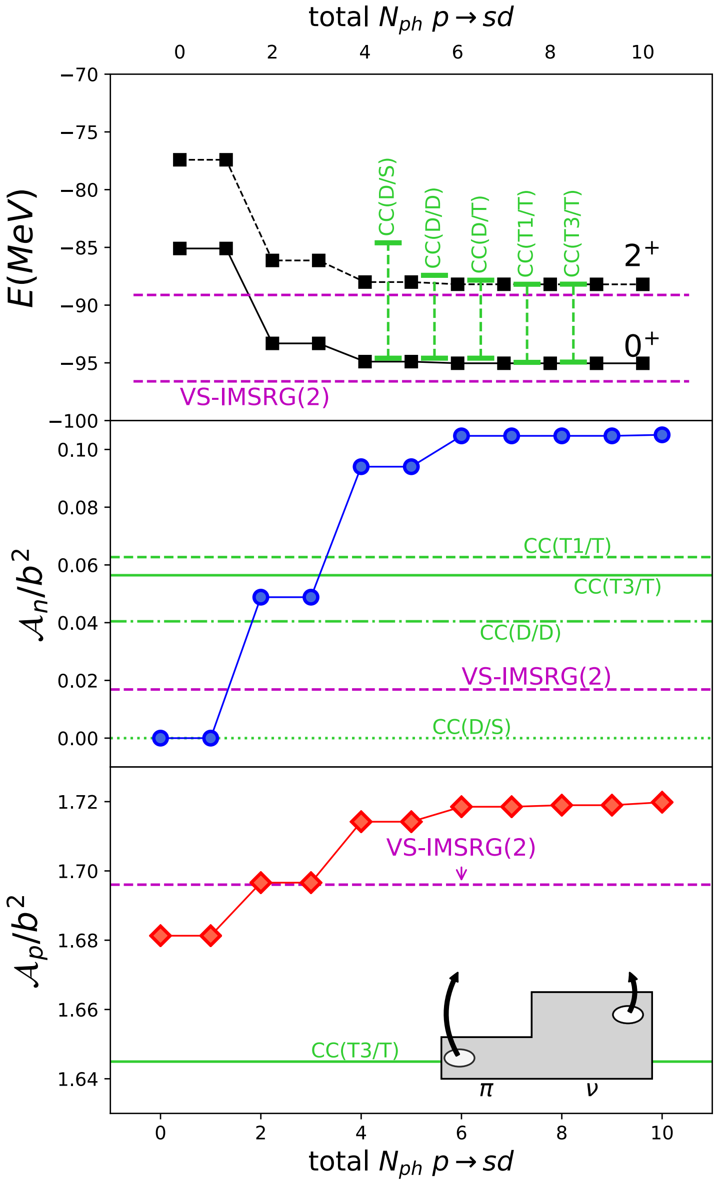
IS: USDB good agreement, VS-IMSRG systematically small

IV: Both agree well

Deficiencies in IS only

Origin of E2 Puzzle: ^{14}C in p-sd Shell

Perform CC and VS-IMSRG calculations of ^{14}C in toy p-sd space with phenomenological potential



Energies well converged all around

p/n amplitudes increase with p/h ex.

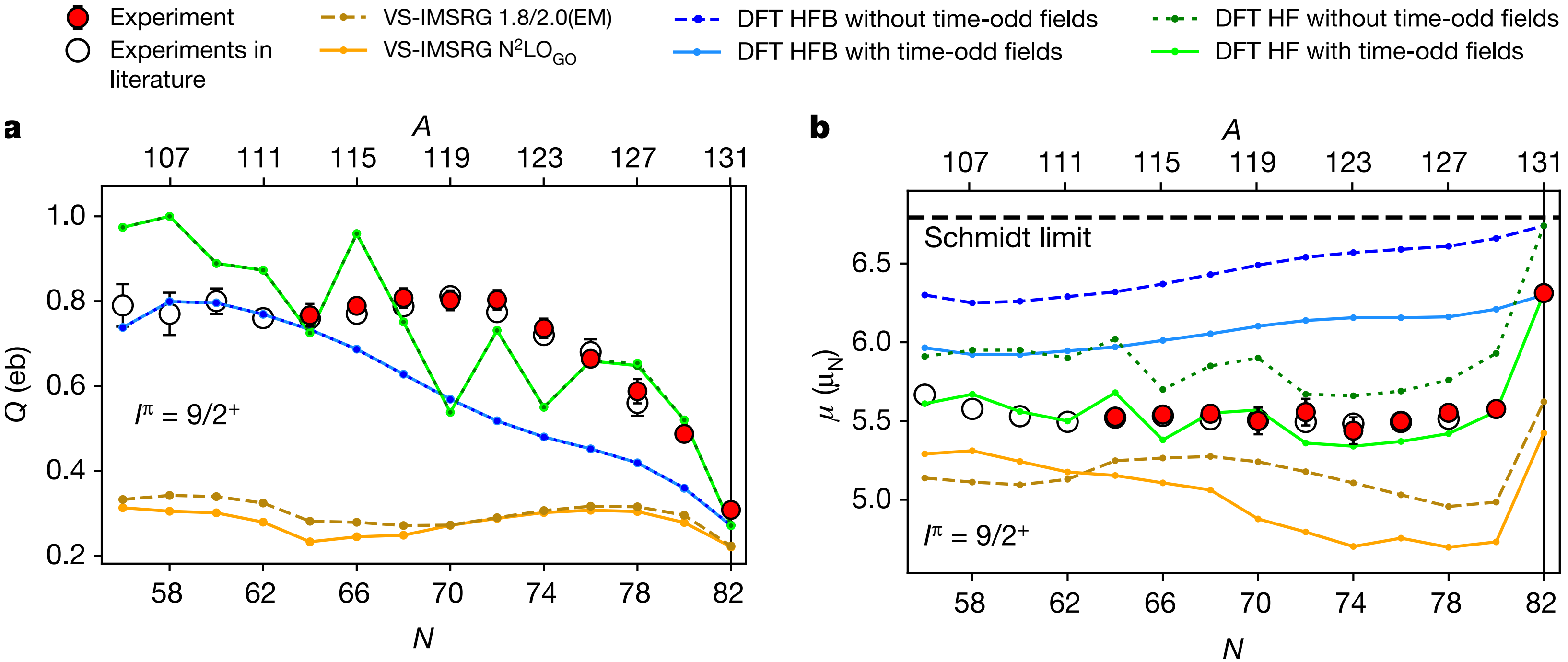
Only converged at ~6 Nph

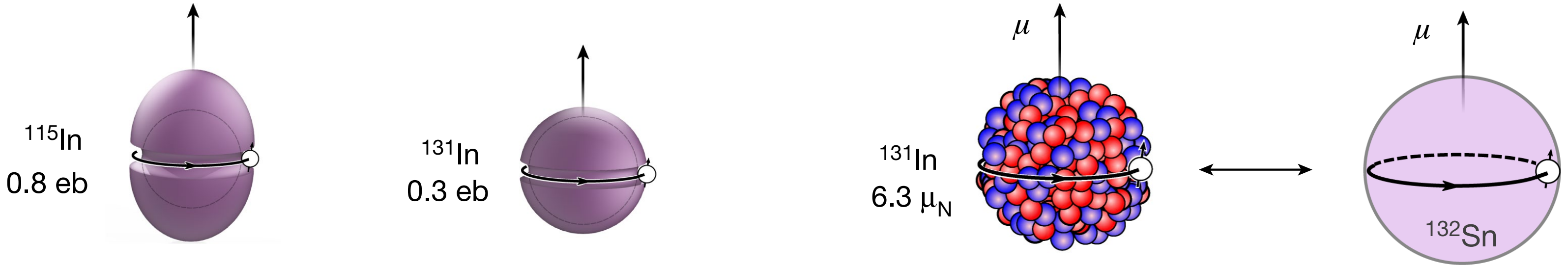
Not possible to capture fully in spherical CC or IMSRG

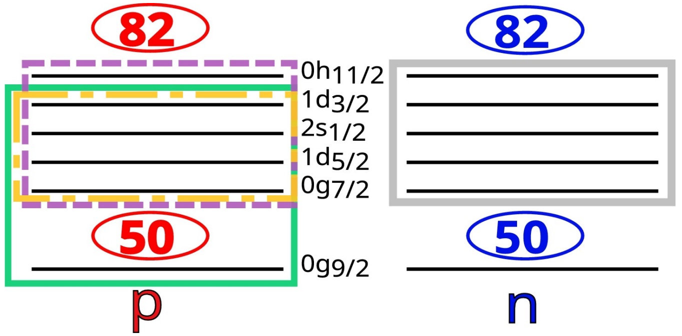
Stroberg et al. PRC (2022)

Systematic studies in Sn region: In Isotopes

Comparisons with EDF (hit and miss): overall consistent picture of single-particle nature

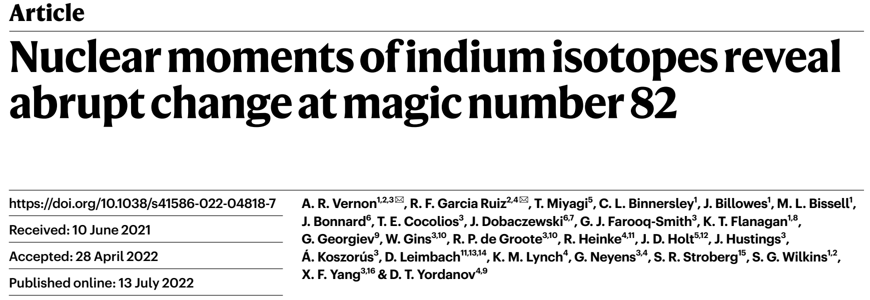






Ab initio reproduces trends of new measurements

Q missing correlations, μ missing physics?


Article

Nuclear moments of indium isotopes reveal abrupt change at magic number 82

https://doi.org/10.1038/s41586-022-04818-7

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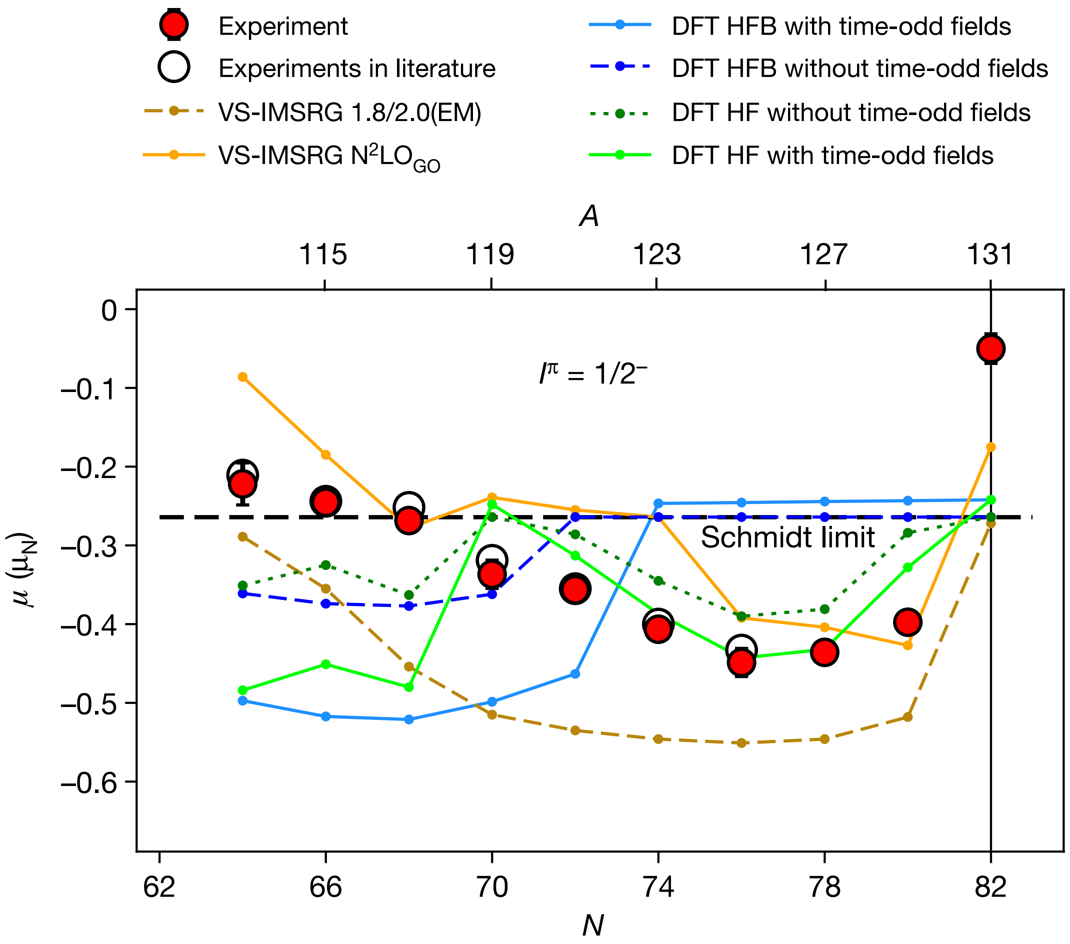
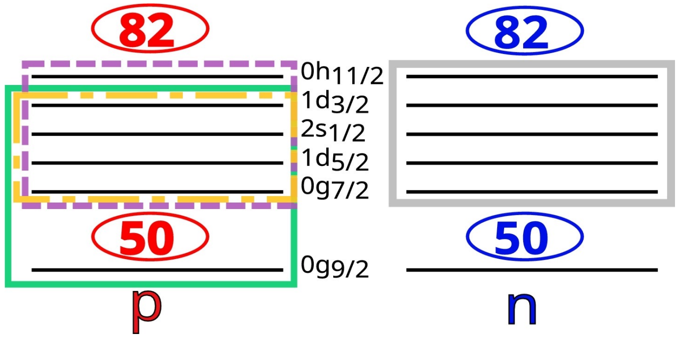
A. R. Vernon[1,2,3]✉, R. F. Garcia Ruiz[2,4]✉, T. Miyagi[5], C. L. Binnersley[1], J. Billowes[1], M. L. Bissell[1], J. Bonnard[6], T. E. Cocolios[3], J. Dobaczewski[6,7], G. J. Farooq-Smith[3], K. T. Flanagan[1,8], G. Georgiev[9], W. Gins[3,10], R. P. de Groote[3,10], R. Heinke[4,11], J. D. Holt[5,12], J. Hustings[3], Á. Koszorús[3], D. Leimbach[11,13,14], K. M. Lynch[4], G. Neyens[3,4], S. R. Stroberg[15], S. G. Wilkins[1,2], X. F. Yang[3,16] & D. T. Yordanov[4,9]

Systematic studies in Sn region: In Isotopes

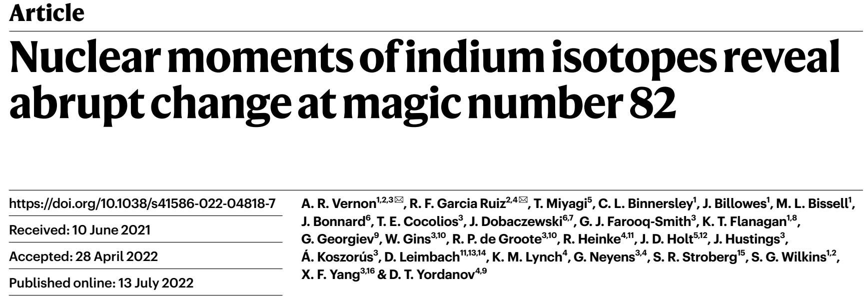
Comparisons with EDF (hit and miss): only VS-IMSRG reproduces trend for 1/2$^-$ isomer





Strong coupling of 9/2+ to 5- state from $nh_{11/2}$-$ps_{1/2}$

Q missing correlations, μ missing physics?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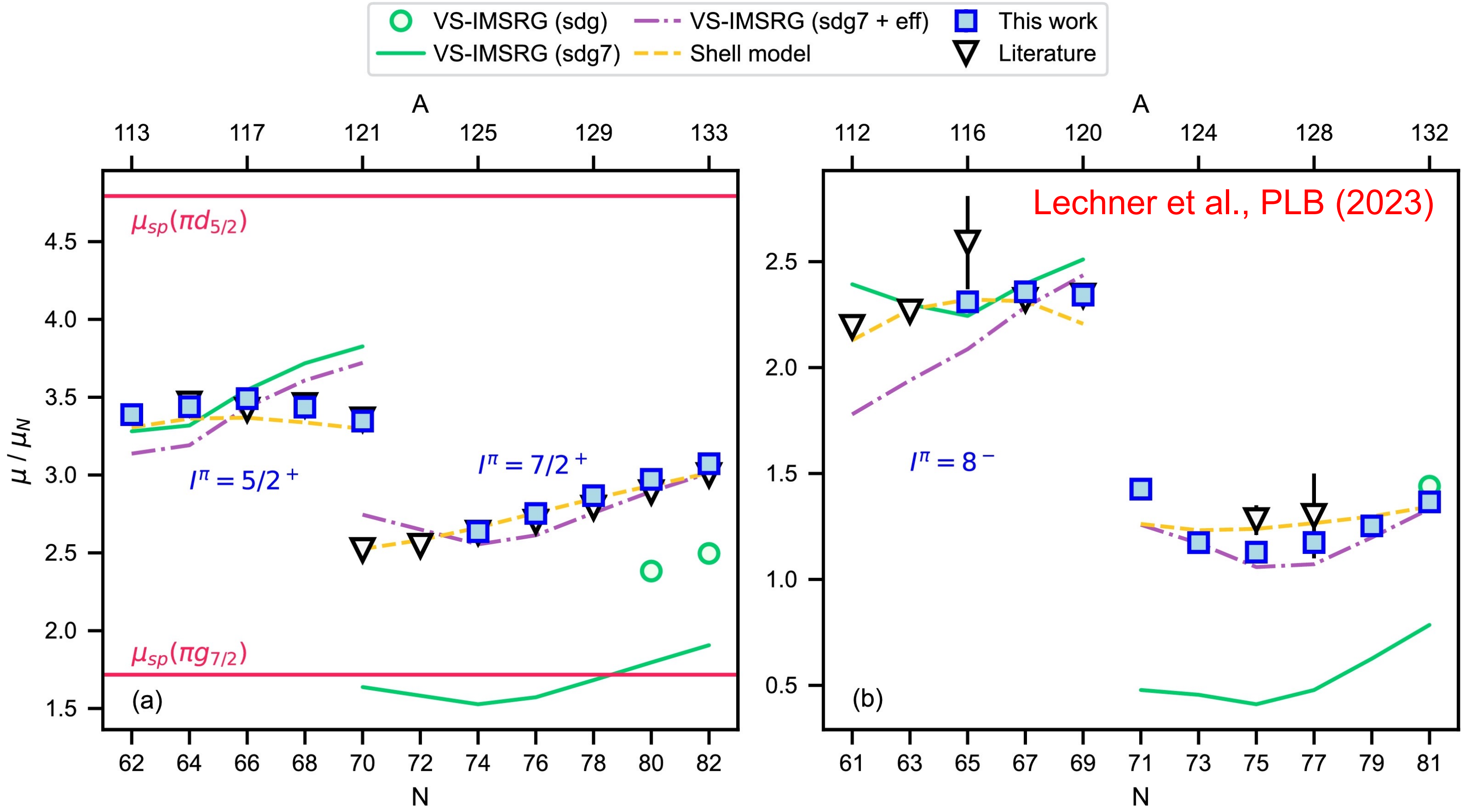
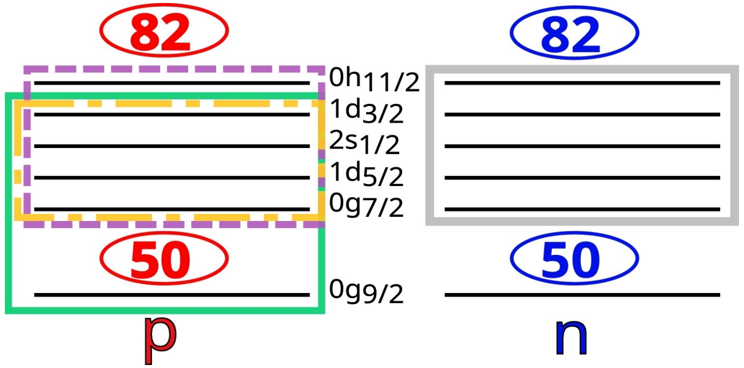
Systematic studies in Sn region: Sb Isotopes

Magnetic moments of even/odd Sb isotopes compared with nuclear shell model

Inclusion of $g_{9/2}$ orbit significantly improves results





VS-IMSRG with effective g-factors of SM agrees with data – (1.8/2.0 as good as phen)

Missing physics in M1 operator – MEC?

A Tale of Two Analyses: $B(M1{:}1^+\longrightarrow 0^+)$ in ^{48}Ca

Three different experimental measurements yield different results

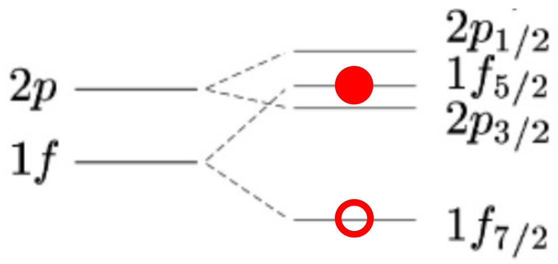
Papenbrock (Talk @ PAINT2024)

(e, e') scattering: $B(M1) = 4.0 \pm 0.3\ \mu_N^2$ [Steffen et al 1980; 1983]

$(\gamma, n\ )$ scattering: $B(M1) = 6.8 \pm 0.5\ \mu_N^2$ [Tompkin et al 2011]

(p, p') scattering: $B(M1) = 3.85(32) - 4.63(38)\ \mu_N^2$ [Birkhan et al 2016]

Extreme s.p. model: $B(M1) = 12\ \mu_N^2$ $\mu_{1\mathrm{B}} = \mu_N \sum_i \left(g_i^l l_{i,z} + g_i^s \sigma_{i,z}\right)$



Theory 1980-2000: 7-8 μ^2_N

A Tale of Two Analyses: $B(M1:1^+ \rightarrow 0^+)$ in ^{48}Ca

Three different experimental measurements yield different results

Papenbrock (Talk @ PAINT2024)

(e,e') scattering:	$B(M1) = 4.0 \pm 0.3\ \mu_N^2$	[Steffen et al 1980; 1983]
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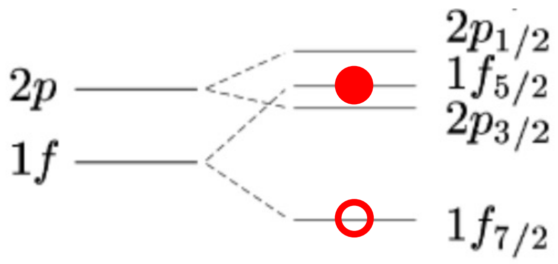
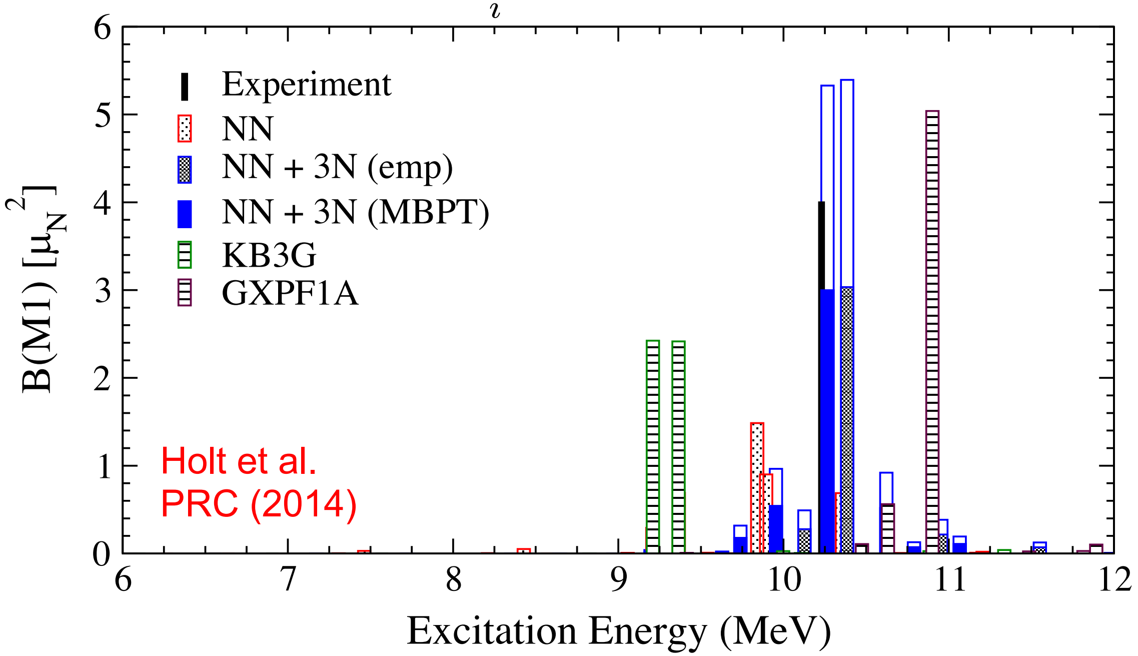


Theory 1980-2000: 7-8 μ^2_N

VS-MBPT with NN+3N

~Agrees if quenched



Holt et al.
PRC (2014)

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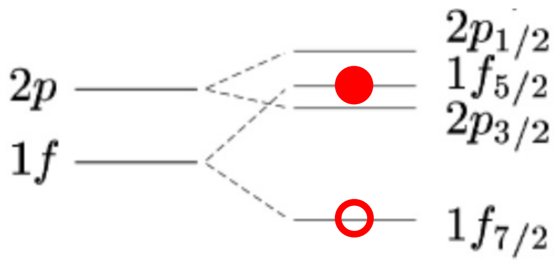
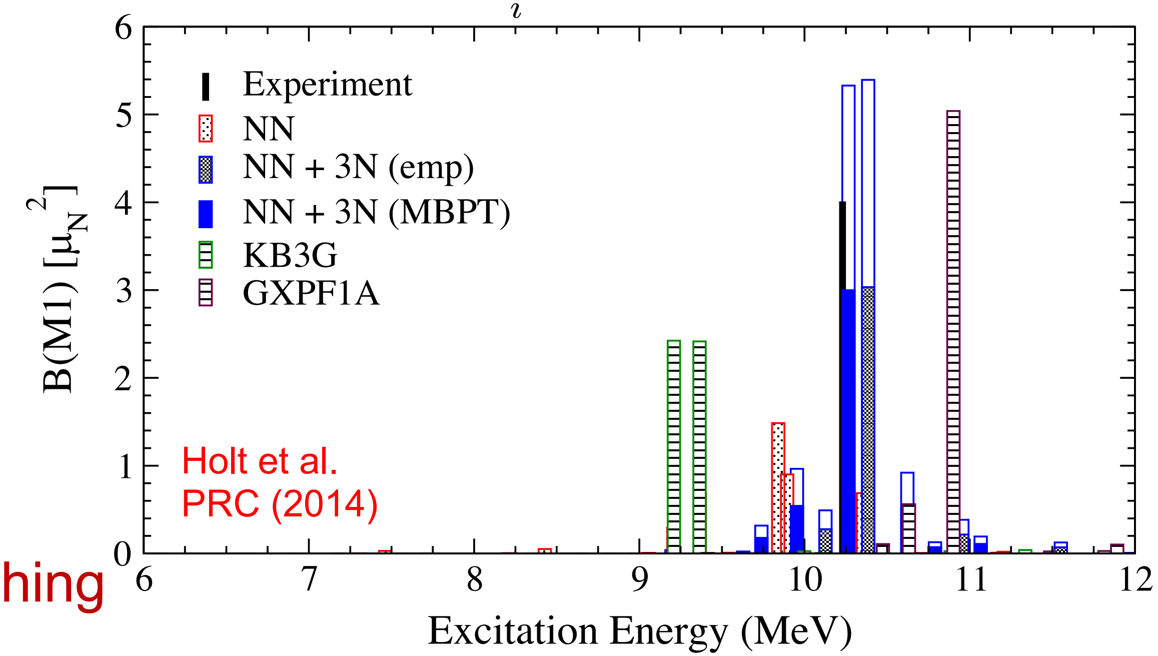


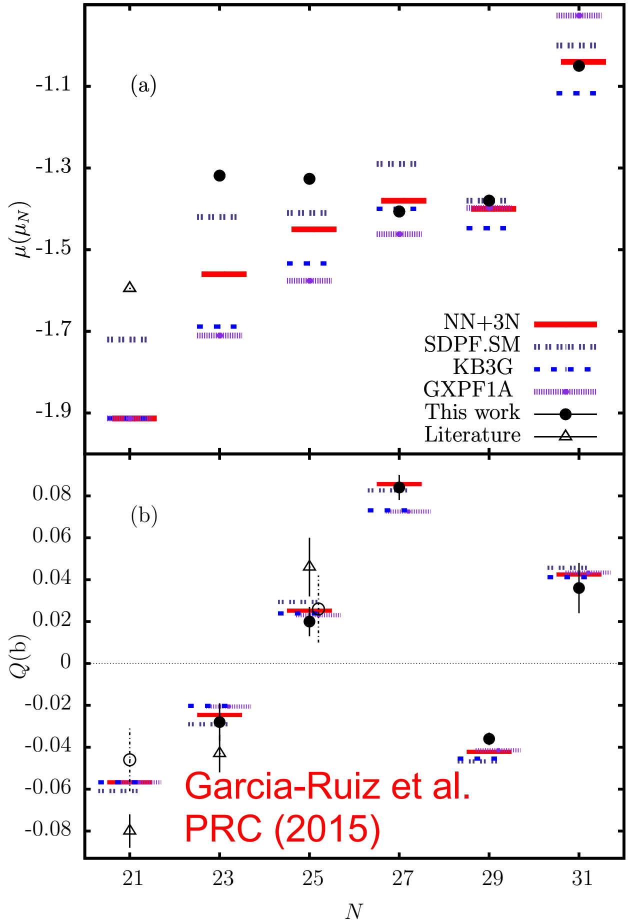
Theory 1980-2000: 7-8 μ^2_N

VS-MBPT with NN+3N

- ~Agrees if quenched
- Moments ok w/o quenching



Holt et al. PRC (2014)



Garcia-Ruiz et al. PRC (2015)

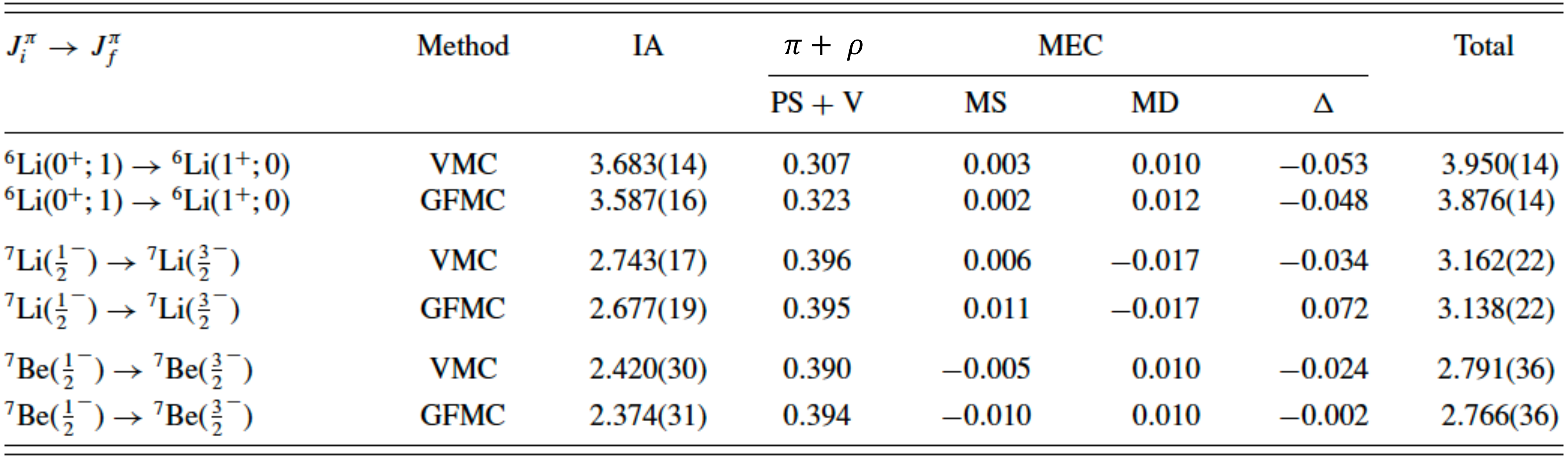
What's going on/missing?

- Continuum: $E(1^+) \sim 10$MeV, above threshold
- Meson-exchange currents

A Tale of Two Analyses: B(M1:$1^+ \longrightarrow 0^+$) in ^{48}Ca

Monte Carlo calculations in light nuclei showed two-body currents do not quench

Papenbrock (Talk @ PAINT2024)



$J_i^\pi \to J_f^\pi$	Method	IA	$\pi + \rho$	MEC			Total
			PS + V	MS	MD	Δ	
^{6}Li(0^+; 1) → ^{6}Li(1^+; 0)	VMC	3.683(14)	0.307	0.003	0.010	−0.053	3.950(14)
^{6}Li(0^+; 1) → ^{6}Li(1^+; 0)	GFMC	3.587(16)	0.323	0.002	0.012	−0.048	3.876(14)
^{7}Li($\frac{1}{2}^-$) → ^{7}Li($\frac{3}{2}^-$)	VMC	2.743(17)	0.396	0.006	−0.017	−0.034	3.162(22)
^{7}Li($\frac{1}{2}^-$) → ^{7}Li($\frac{3}{2}^-$)	GFMC	2.677(19)	0.395	0.011	−0.017	0.072	3.138(22)
^{7}Be($\frac{1}{2}^-$) → ^{7}Be($\frac{3}{2}^-$)	VMC	2.420(30)	0.390	−0.005	0.010	−0.024	2.791(36)
^{7}Be($\frac{1}{2}^-$) → ^{7}Be($\frac{3}{2}^-$)	GFMC	2.374(31)	0.394	−0.010	0.010	−0.002	2.766(36)

Marcucci, Muslema Pervin, Pieper, Schiavilla, Wiringa, Phys Rev C 78, 065501 (2008)

This is similar to what we will use

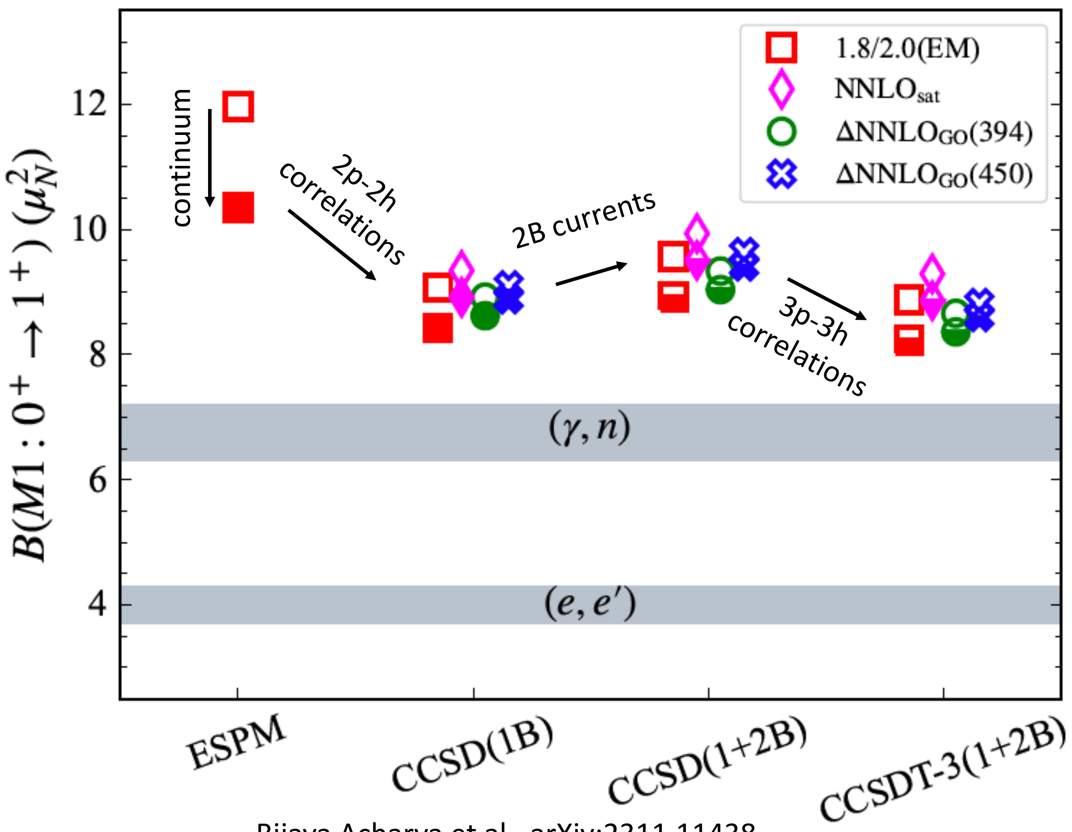
This is perhaps similar to what people used in the 1980s

TRIUMF

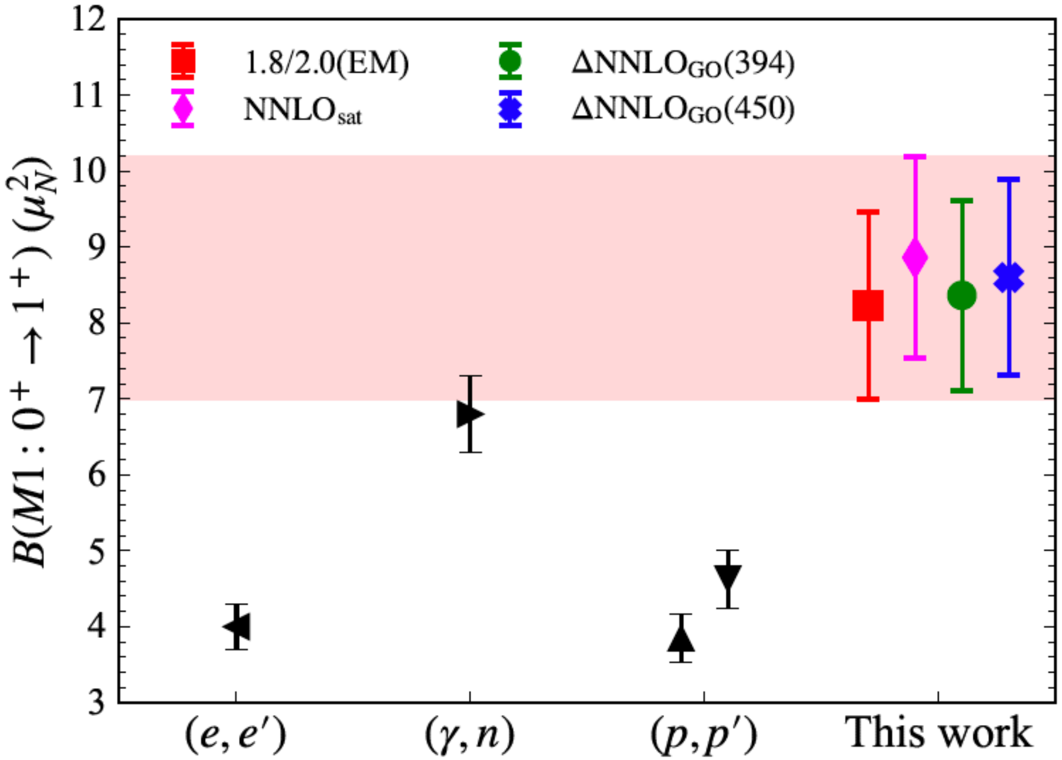
A Tale of Two Analyses: B(M1:$1^+\rightarrow 0^+$) in ^{48}Ca

Coupled-cluster calculations including all relevant physics

Papenbrock (Talk @ PAINT2024)



Bijaya Acharya et al., arXiv:2311.11438



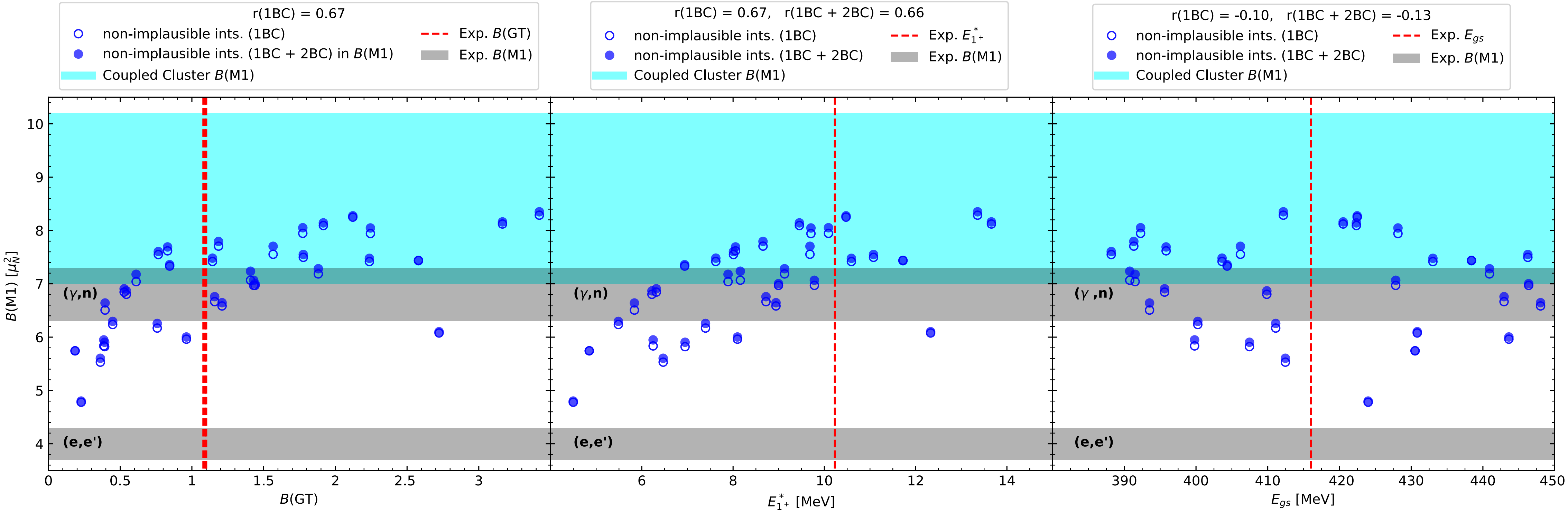
Bijaya Acharya et al., arXiv:2311.11438

Significant decrease from continuum and correlations

2BC do not quench - final results higher than experiment

A Tale of Two Analyses: $B(M1{:}1^+\longrightarrow 0^+)$ in ^{48}Ca

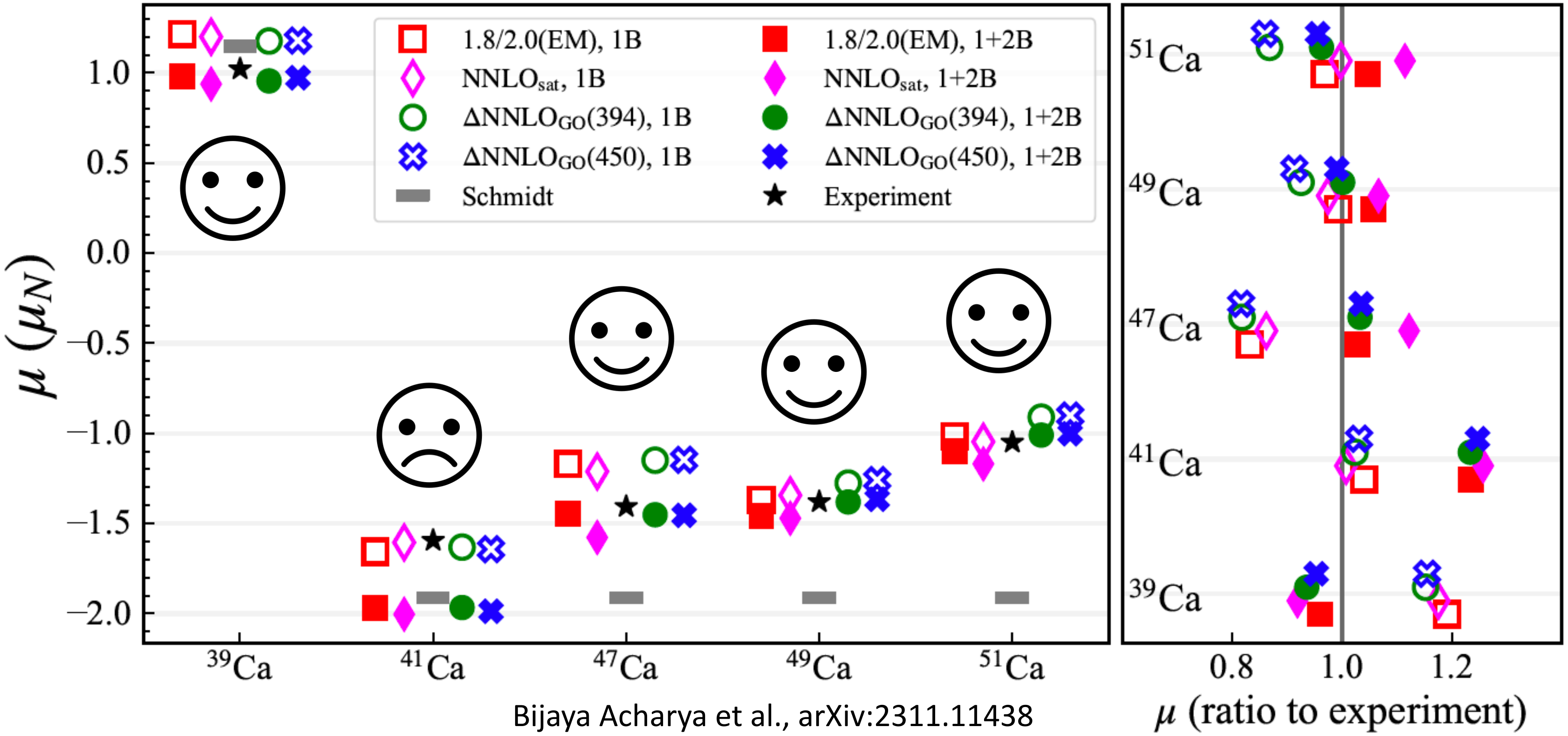
IMSRG Calculations with 34 non-implausible interactions



non-implausible interactions favor $B(M1)$ from $(\gamma,\mathbf{n})$ exp. and
show partial overlap with Coupled Cluster calculation

A Tale of Two Analyses: Magnetic Moments in Ca

Coupled-cluster calculations including all relevant physics for moments



Bijaya Acharya et al., arXiv:2311.11438

Generally good agreement with data w/o quenching

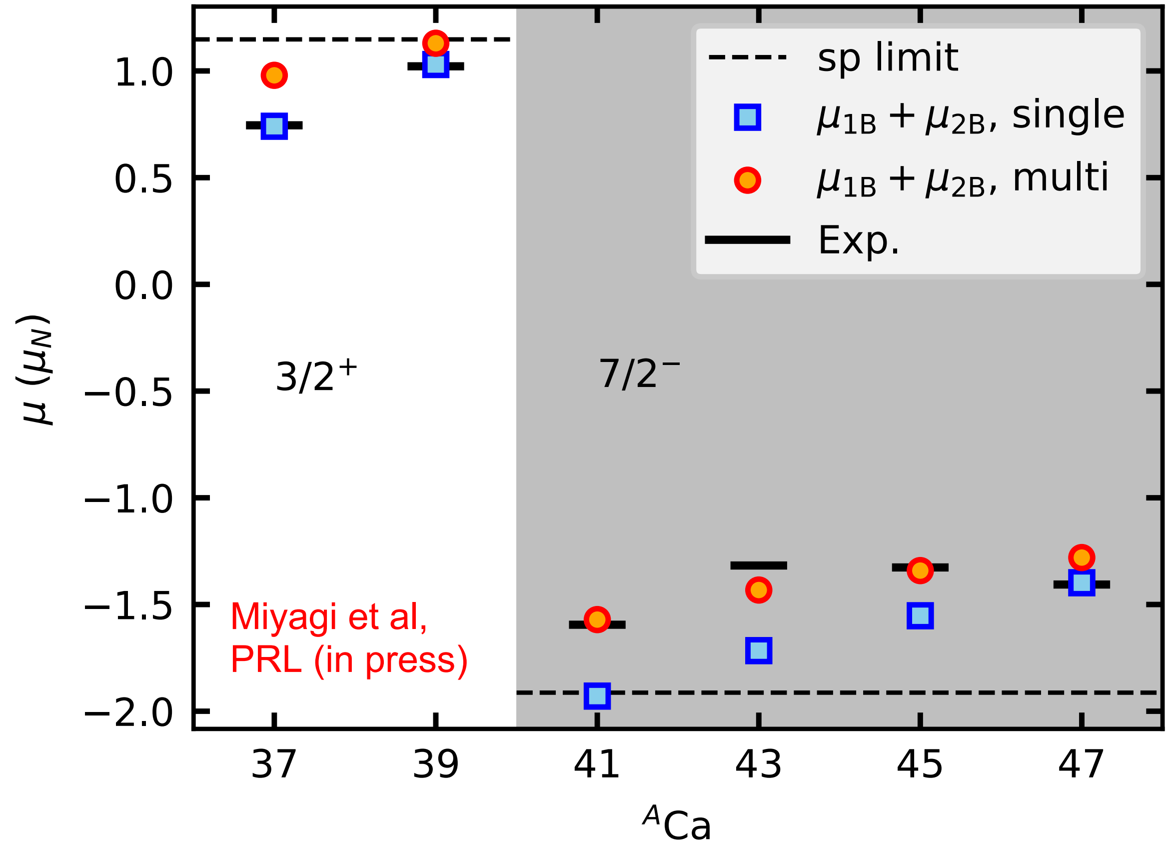
Issue in ^{41}Ca related to cross-shell excitations?

TRIUMF

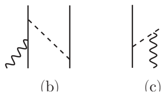
VS-IMSRG μ Moments: O → Pb

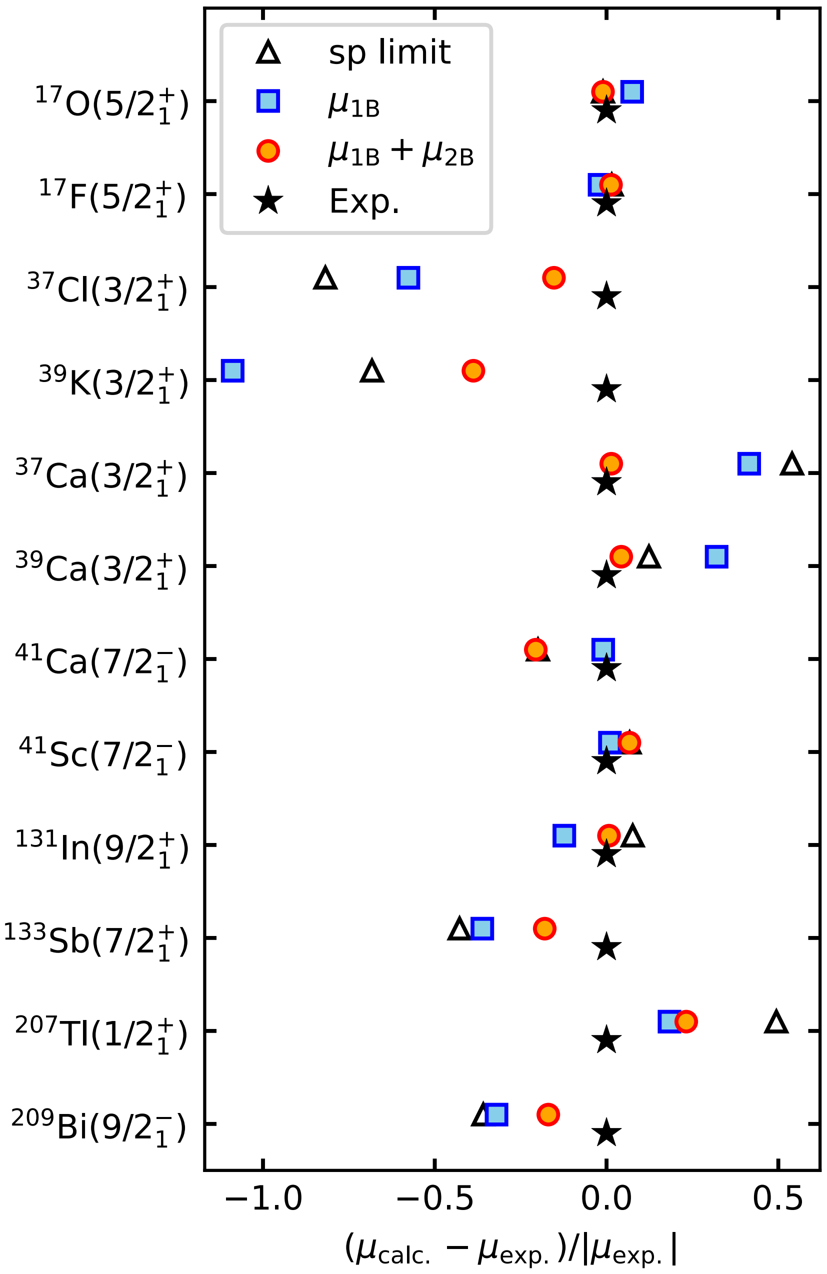
Ab initio calculations throughout the nuclear chart w/ 2BC

Ca discrepancies solved with multi-shell approach



Miyagi et al, PRL (in press)



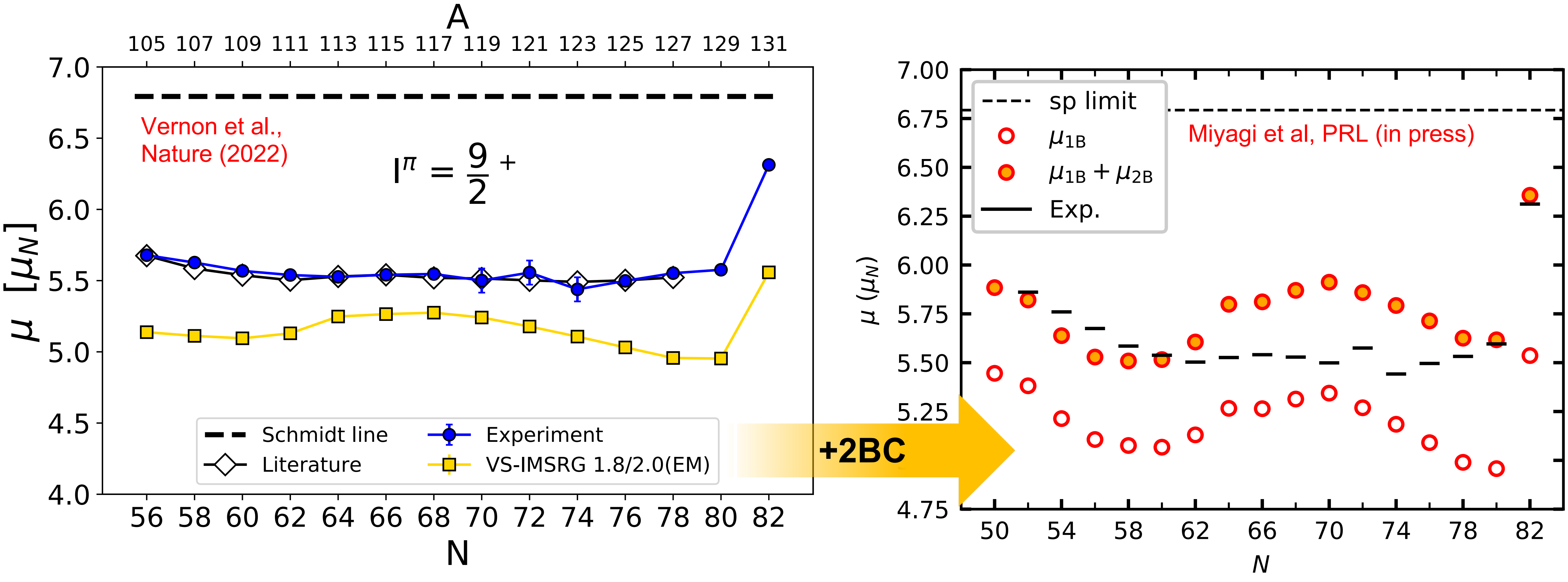


Magnetic moments significantly improved across chart!

VS-IMSRG μ Moments: In Isotopes

Revisit discrepancies in In isotopes with addition of 2BC

Systematic agreement with experiment except in mid-shell region (deformation)



Vernon et al., Nature (2022)

Miyagi et al, PRL (in press)

Next Step: Improve with IMSRG(3f)

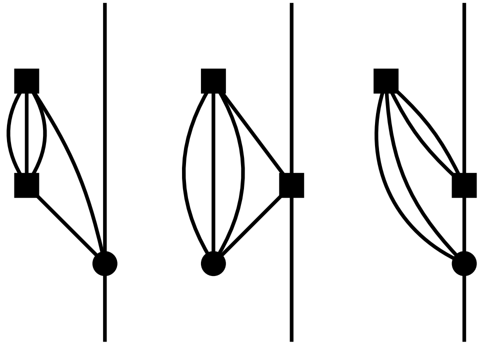
Full IMSRG(3) improves results, but contributions scale $N^7 - N^9$

Explore contractions of 3b structures that can be factorized to 1b and 2b: IMSRG(3f)

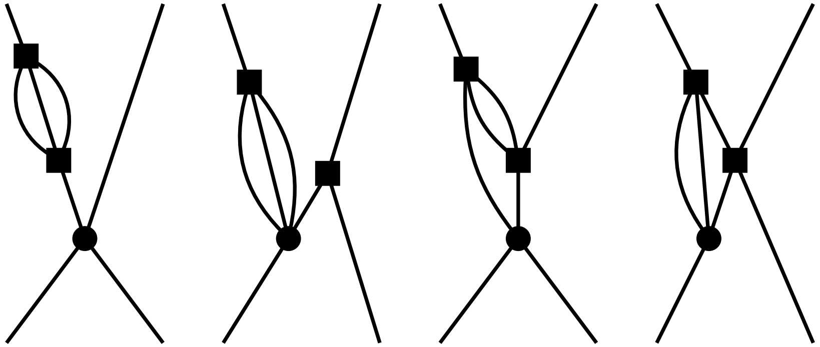
$$\Delta^{(2)}_{\Omega H} = [\Omega_{2\mathrm{b}}\ , [\Omega_{2\mathrm{b}}\ , H_{2\mathrm{b}}]_{3\mathrm{b}}]_{1\mathrm{b},2\mathrm{b}}$$

$$\Delta^{(2)}_{\Omega H,1\mathrm{b}} = f^{\mathrm{I}} + f^{\mathrm{II}} + f^{\mathrm{III}}$$

$$\Delta^{(2)}_{\Omega H,2\mathrm{b}} = \Gamma^{\mathrm{I}} + \Gamma^{\mathrm{II}} + \Gamma^{\mathrm{III}} + \Gamma^{\mathrm{IV}}$$



(a) f^{I} (b) f^{II} (c) f^{III}



(d) Γ^{I} (e) Γ^{II} (f) Γ^{III} (g) Γ^{IV}

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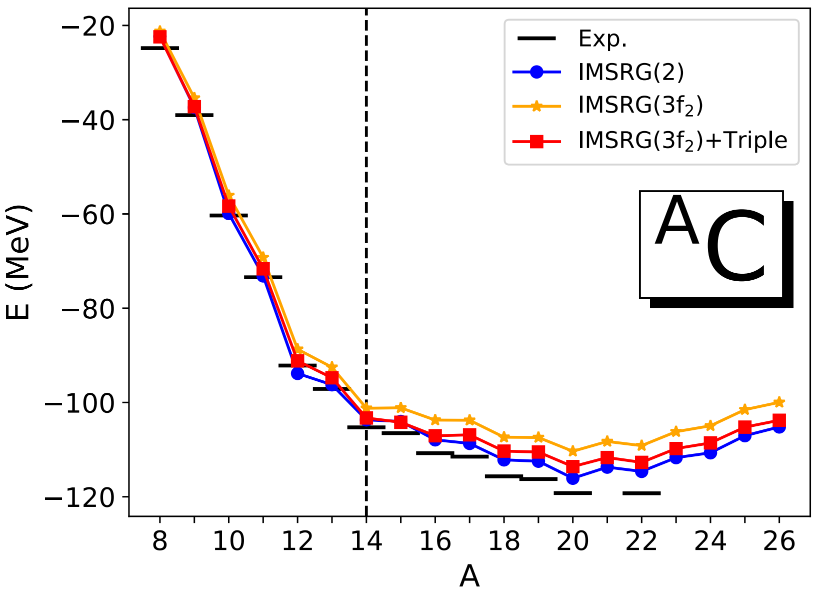

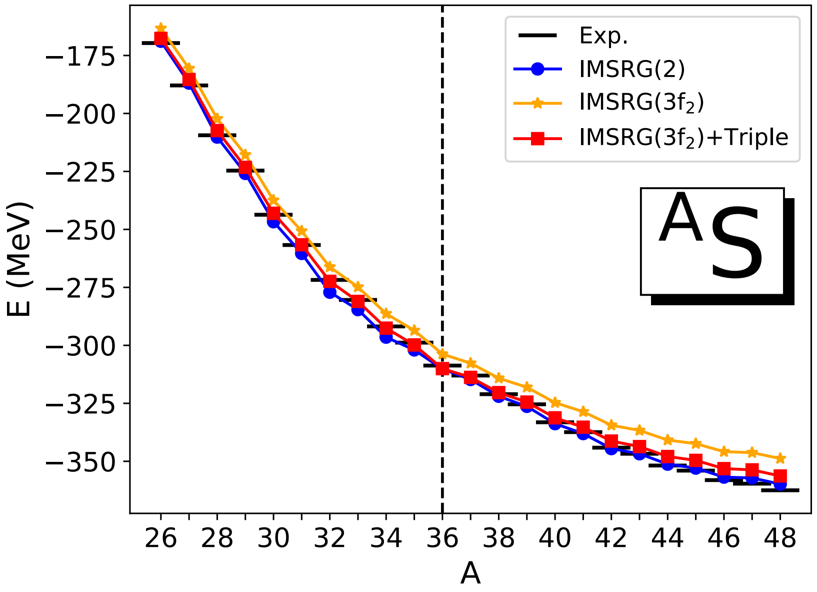

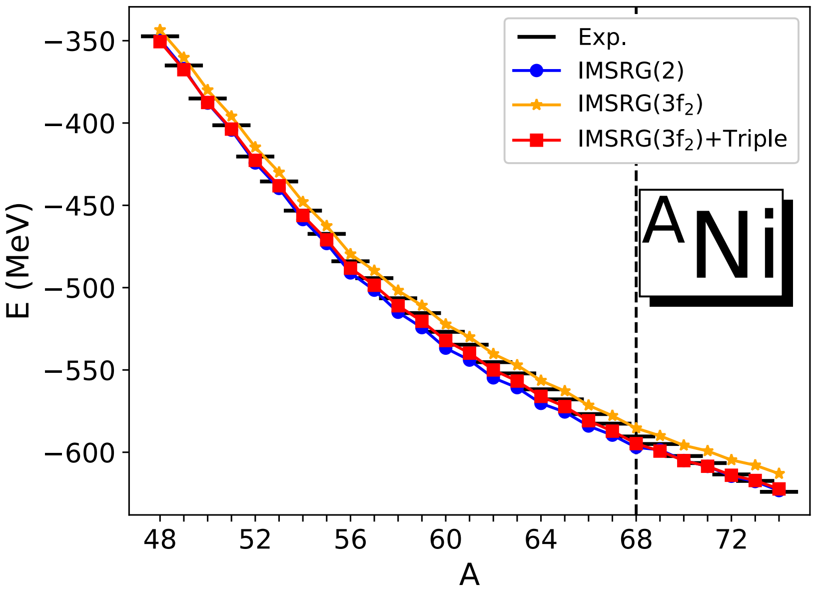

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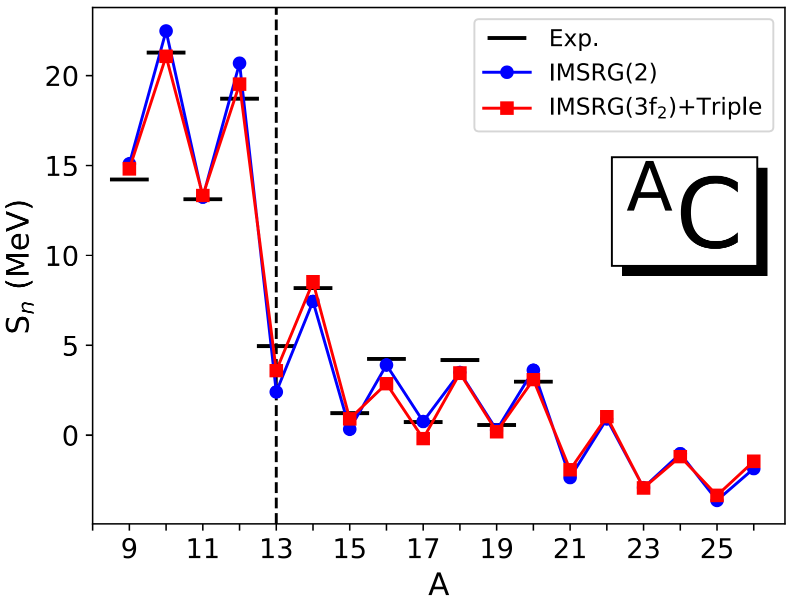

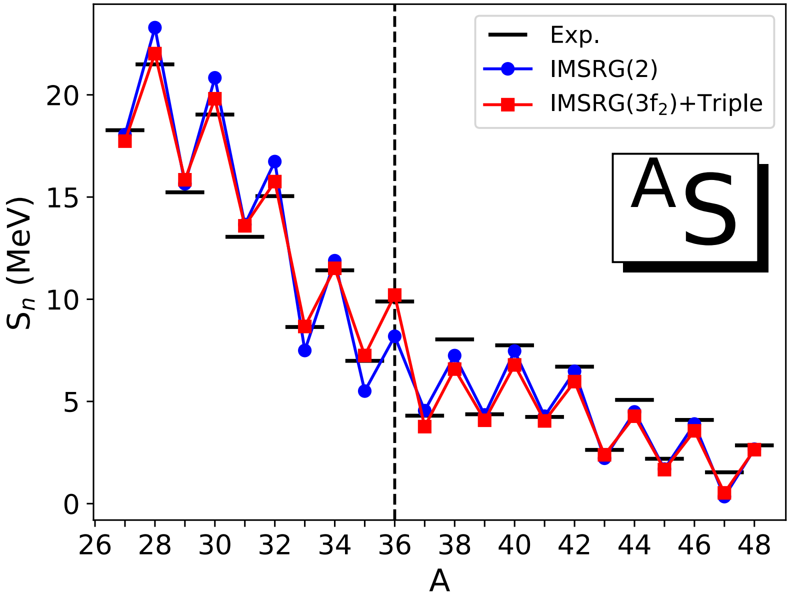

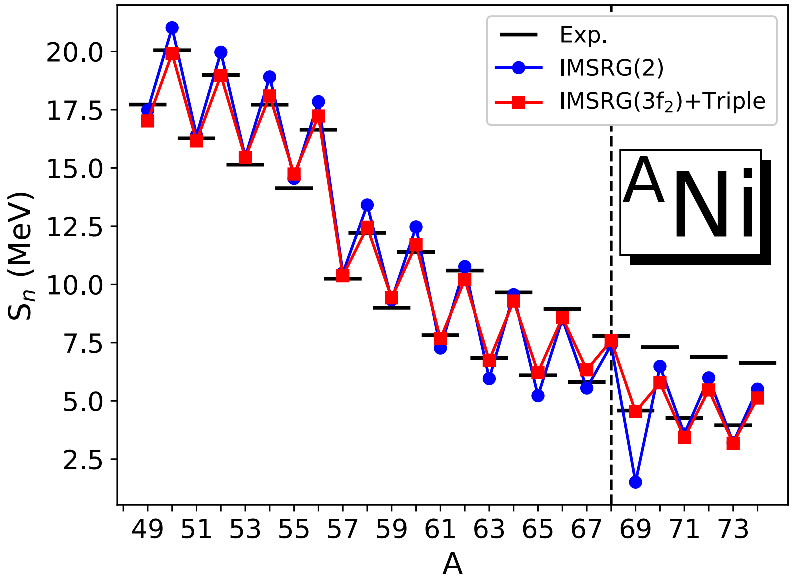

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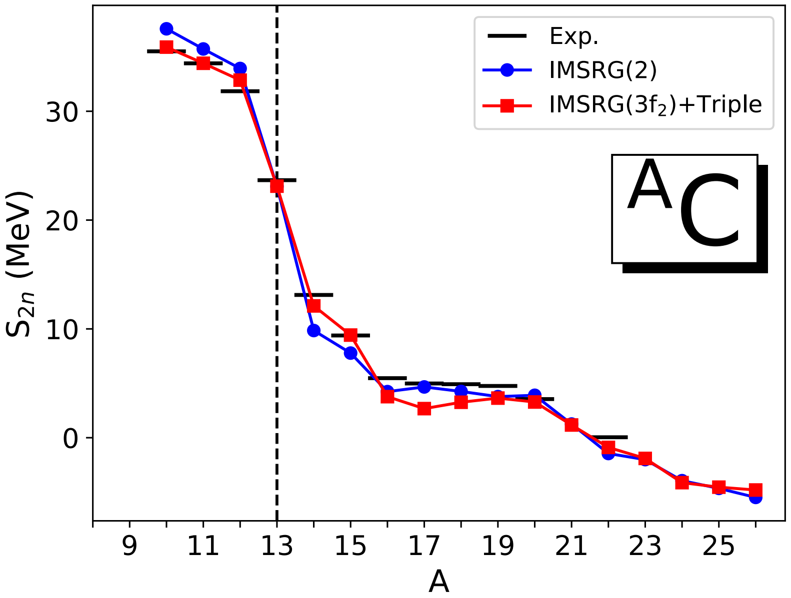

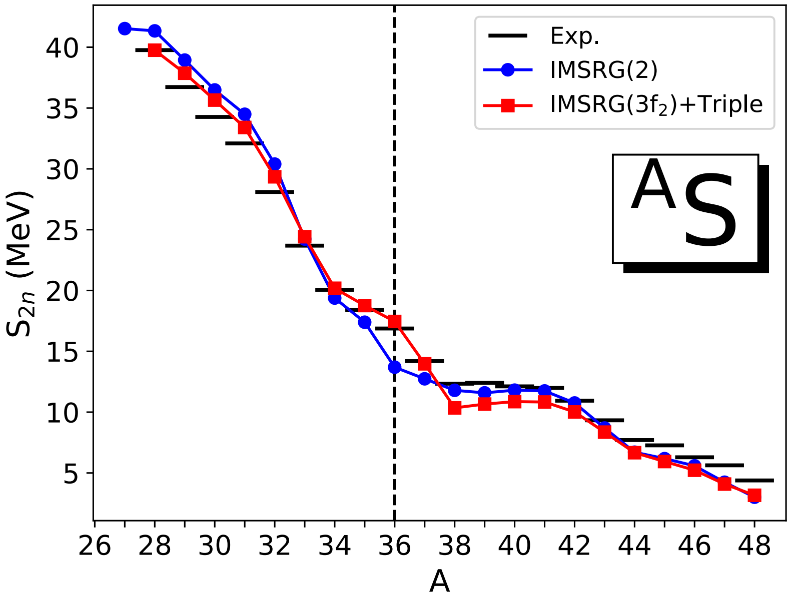

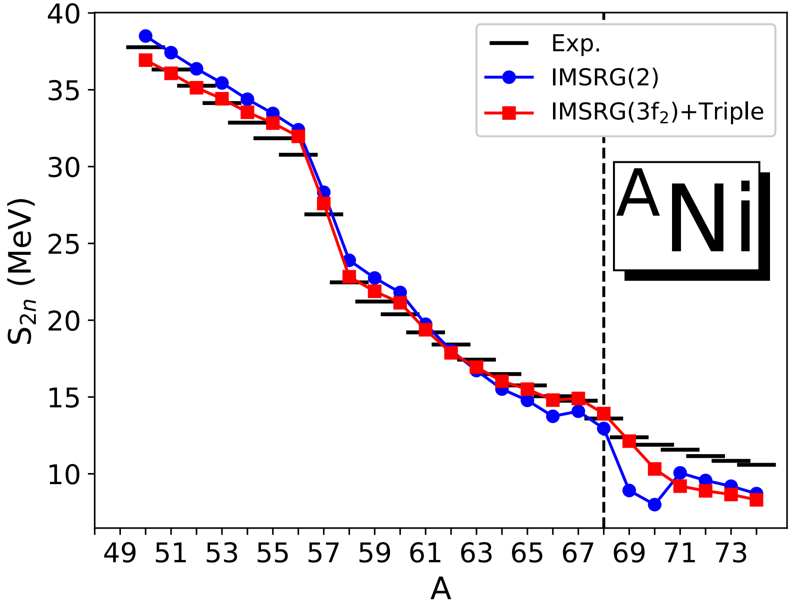

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