TRIUMF McGill UNIVERSITY nEXO

Neutrinoless double-beta decay from an ab initio (and machine learning) perspective

Jason D. Holt
TRIUMF, Theory Department

INT Program: New Physics Searches

‘May 19, 2023

NSERC CRSNG

Arthur B. McDonald Canadian Astroparticle Physics Research Institute

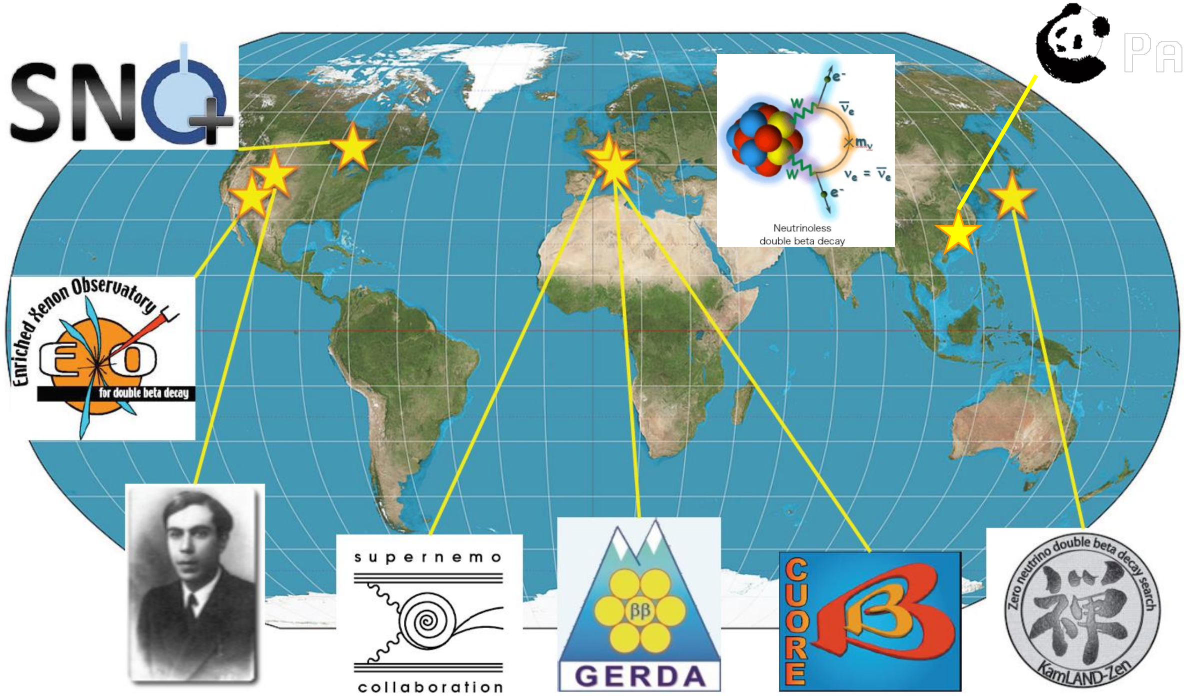
NRC·CNRC

Discovery, accelerated

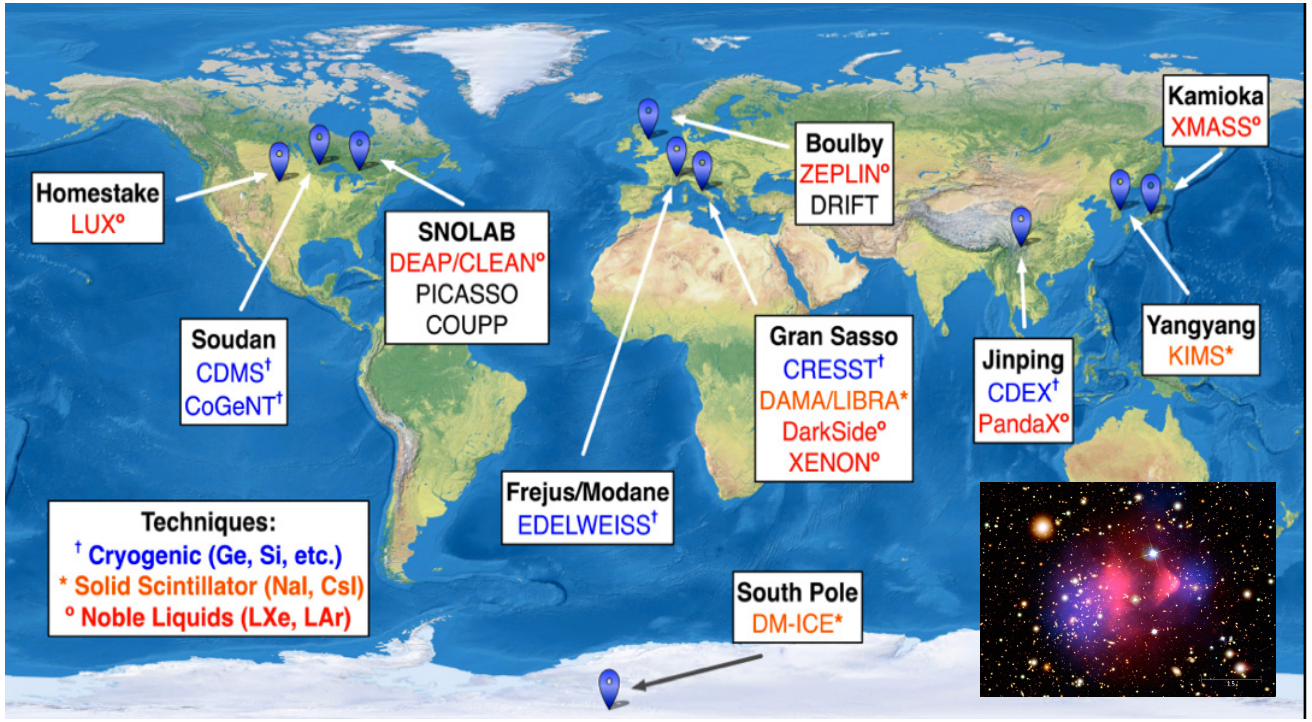
Major Underground Facilities Worldwide

Worldwide searches for BSM physics involving neutrinos and dark matter

0νββ Decay



Dark Matter Direct Detection



Billions invested worldwide

Theory essential for: strategic planning for discovery (**motivation**) + **interpretation**

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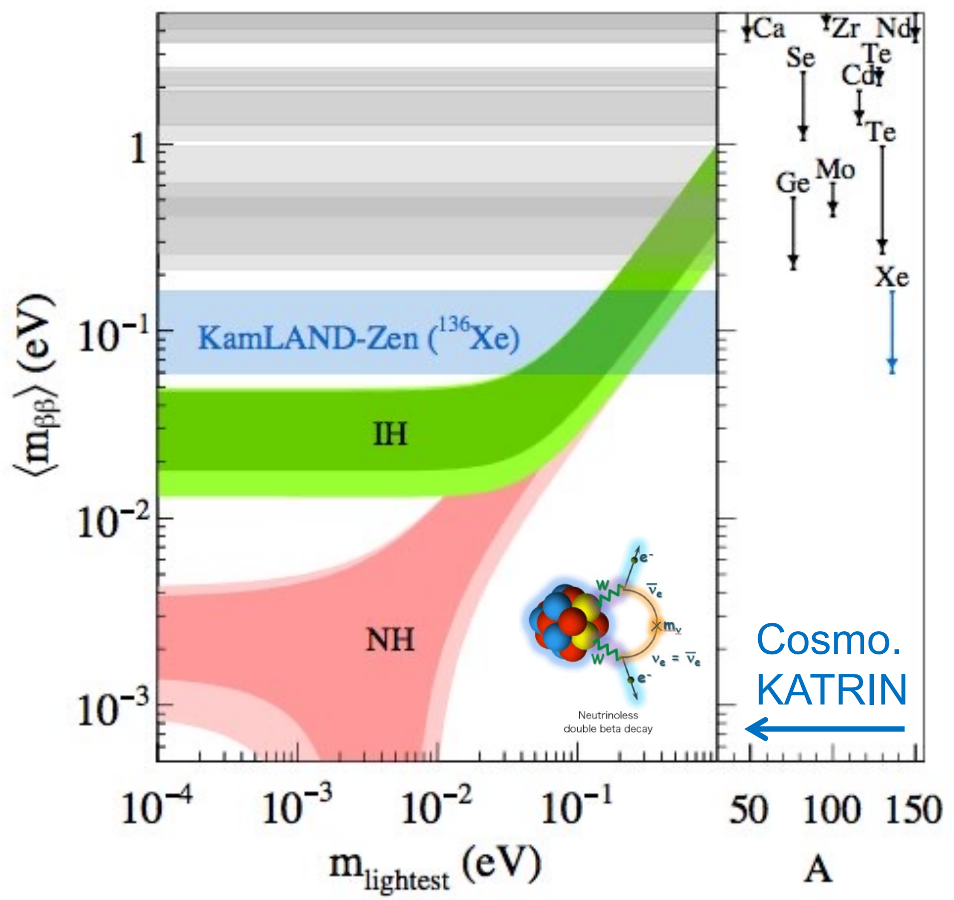
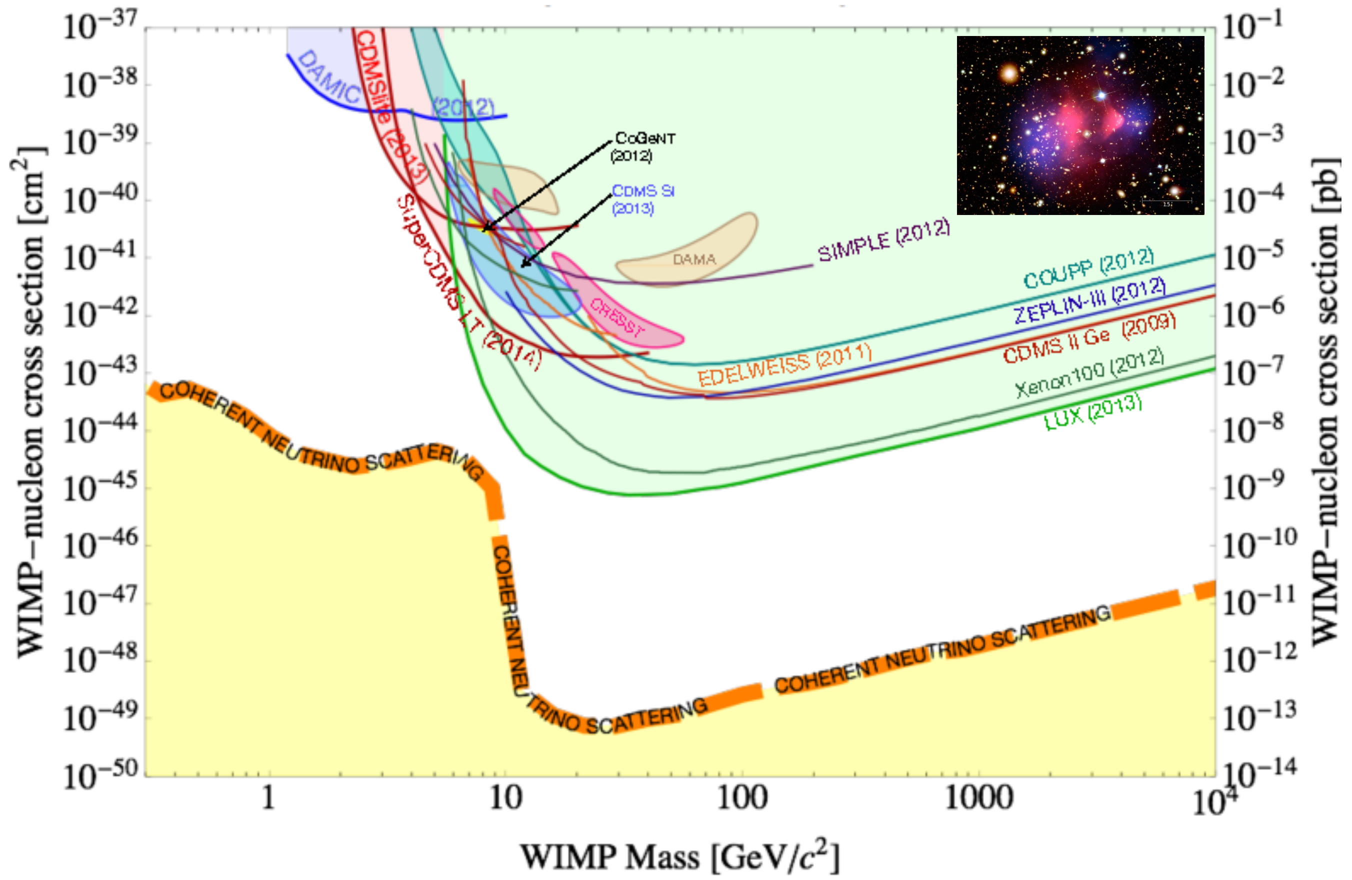
Nuclear Theory for BSM Searches

Exclusion plots for 0νββ decay + WIMP/ν scattering require nuclear theory



$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu}\left|M^{0\nu}\right|^2 \langle m_{\beta\beta}\rangle^2$$



$$\frac{d\sigma}{dq^2} = \frac{8G_F^2}{(2J+1)v^2} S_A(\mathbf{q}^2)$$

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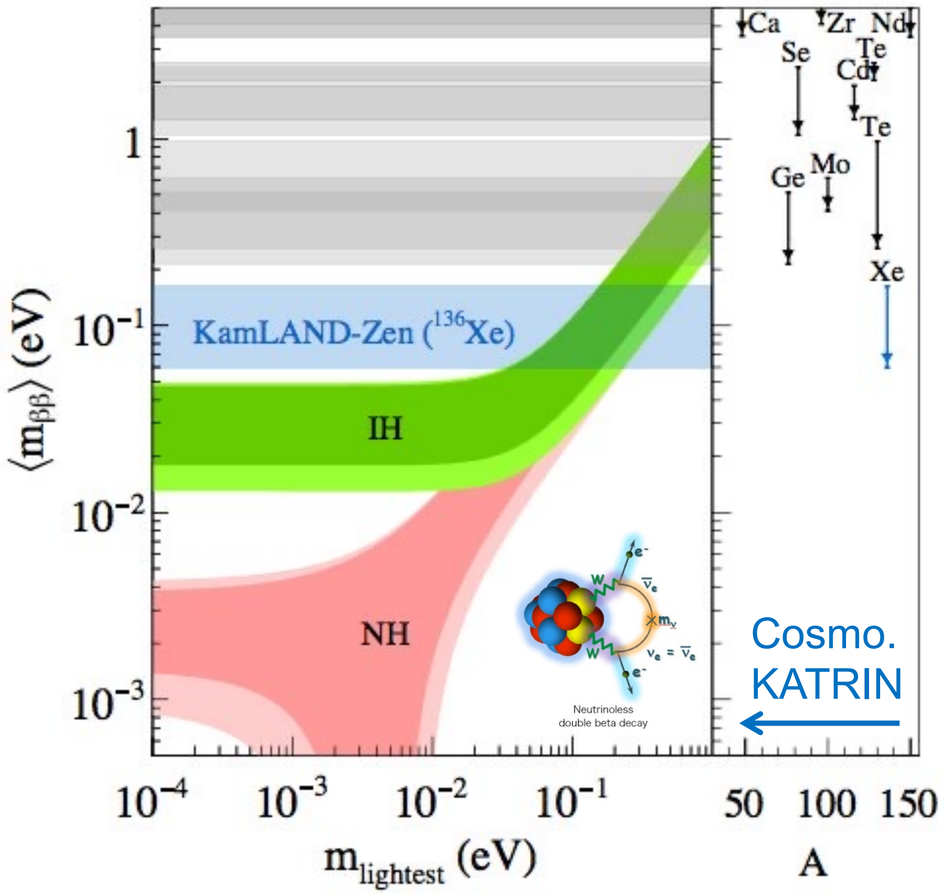

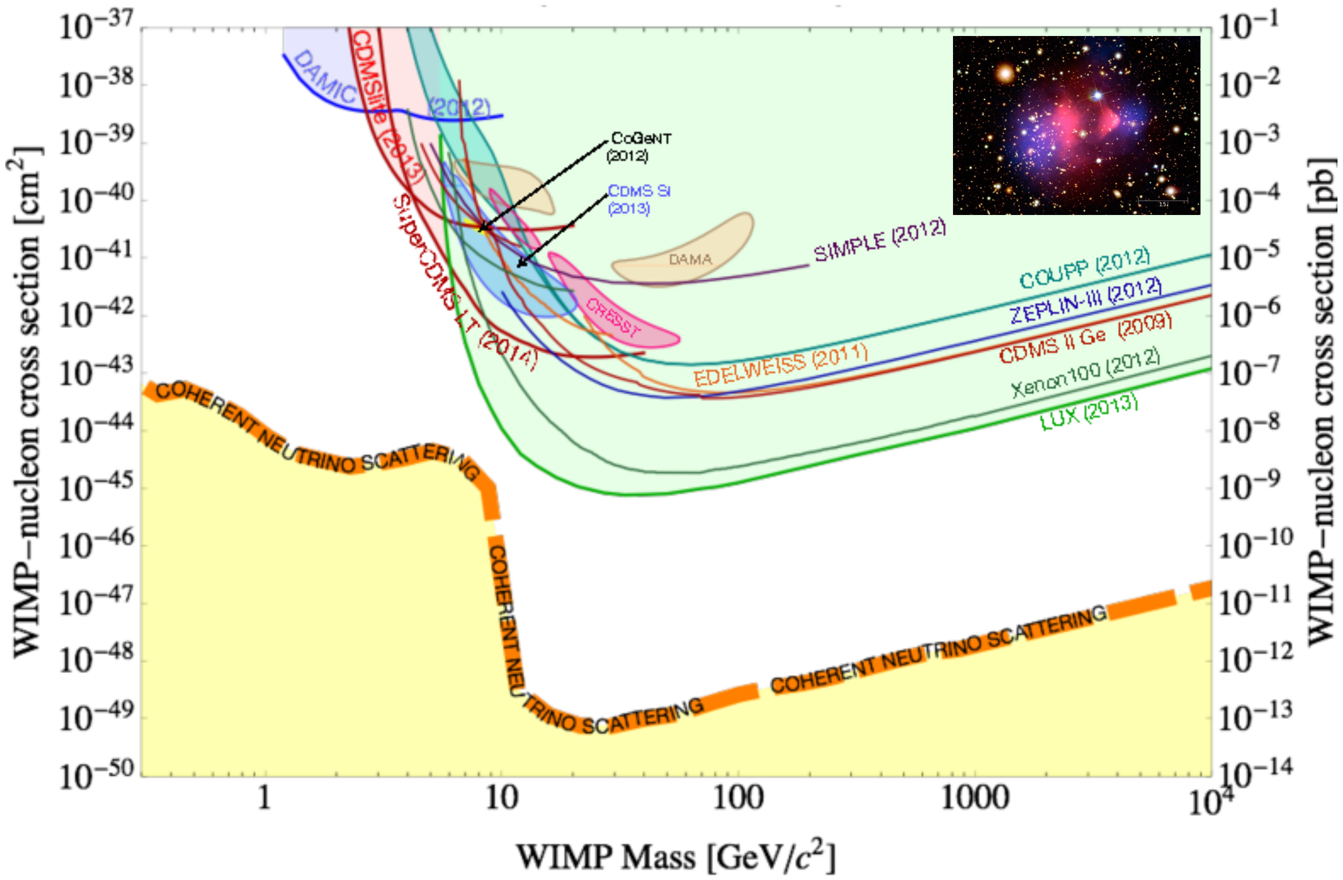

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Nuclear matrix element: rate of decay

Structure functions for WIMP/ν scattering

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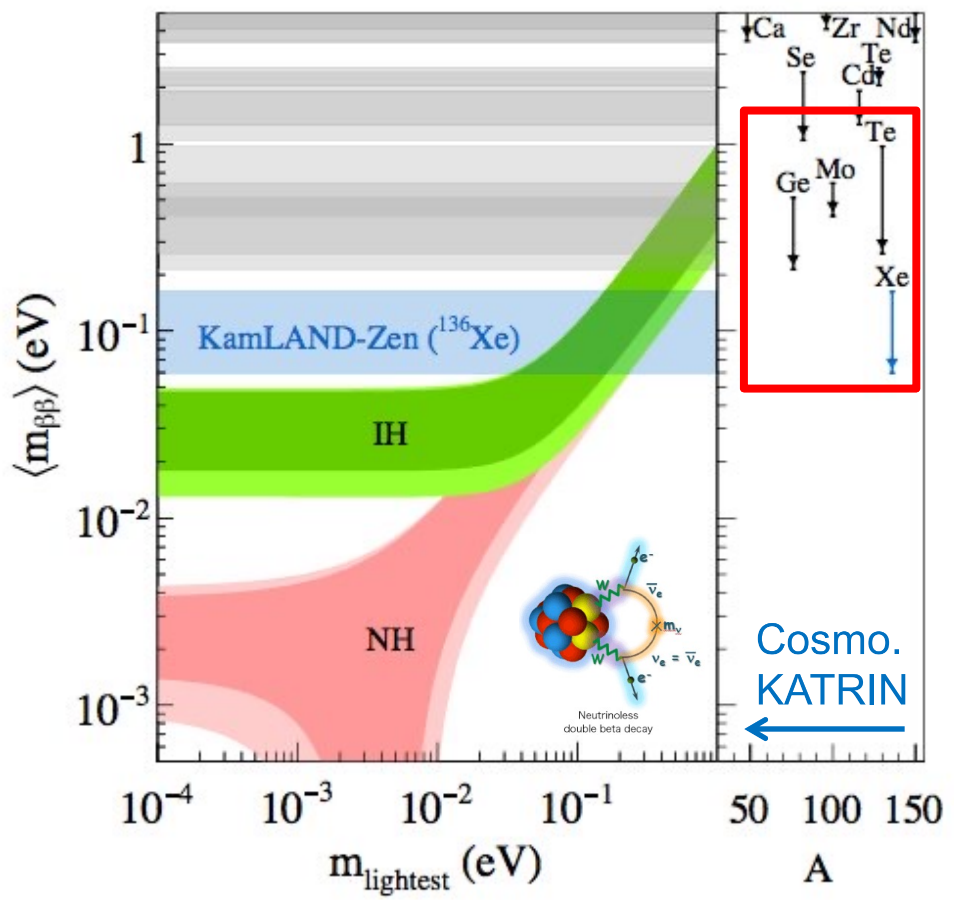
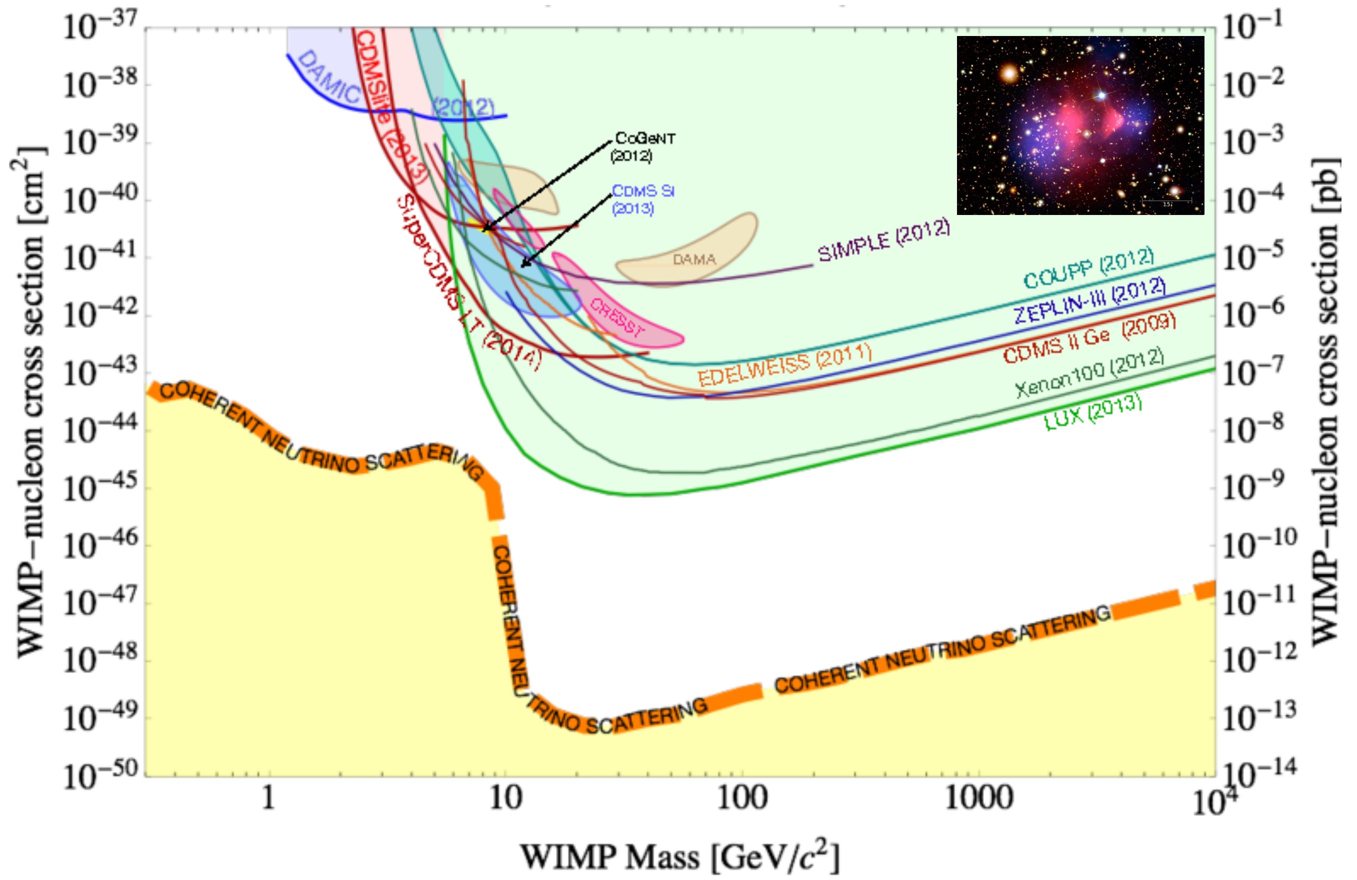
Nuclear Theory for BSM Searches

Exclusion plots for $0\nu\beta\beta$ decay + WIMP/ν scattering require nuclear theory





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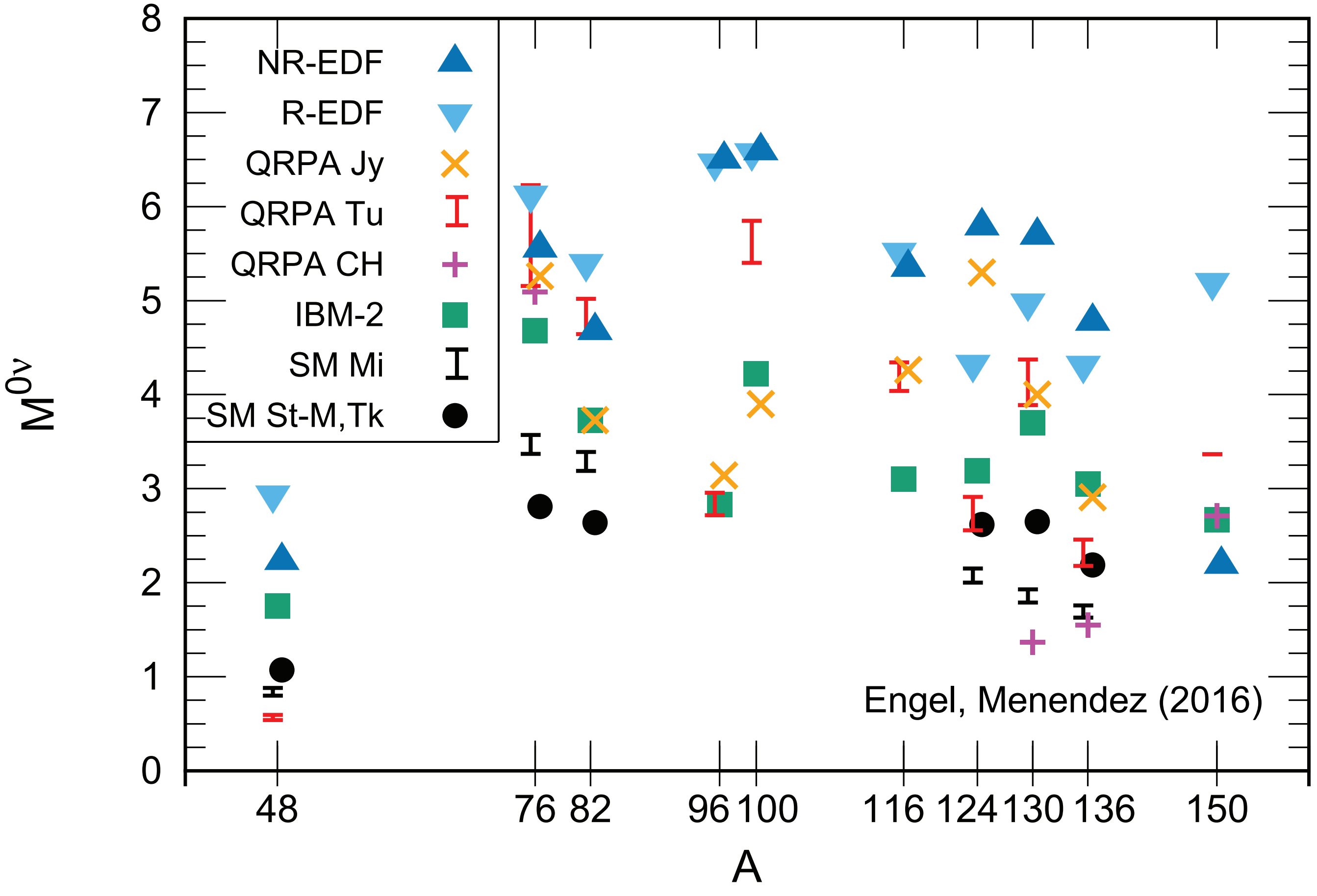
Status of 0νββ-Decay Matrix Elements

All calculations to date from **extrapolated** phenomenological models; large spread in results



All models missing essential physics: correlations, single-particle levels, two-body currents

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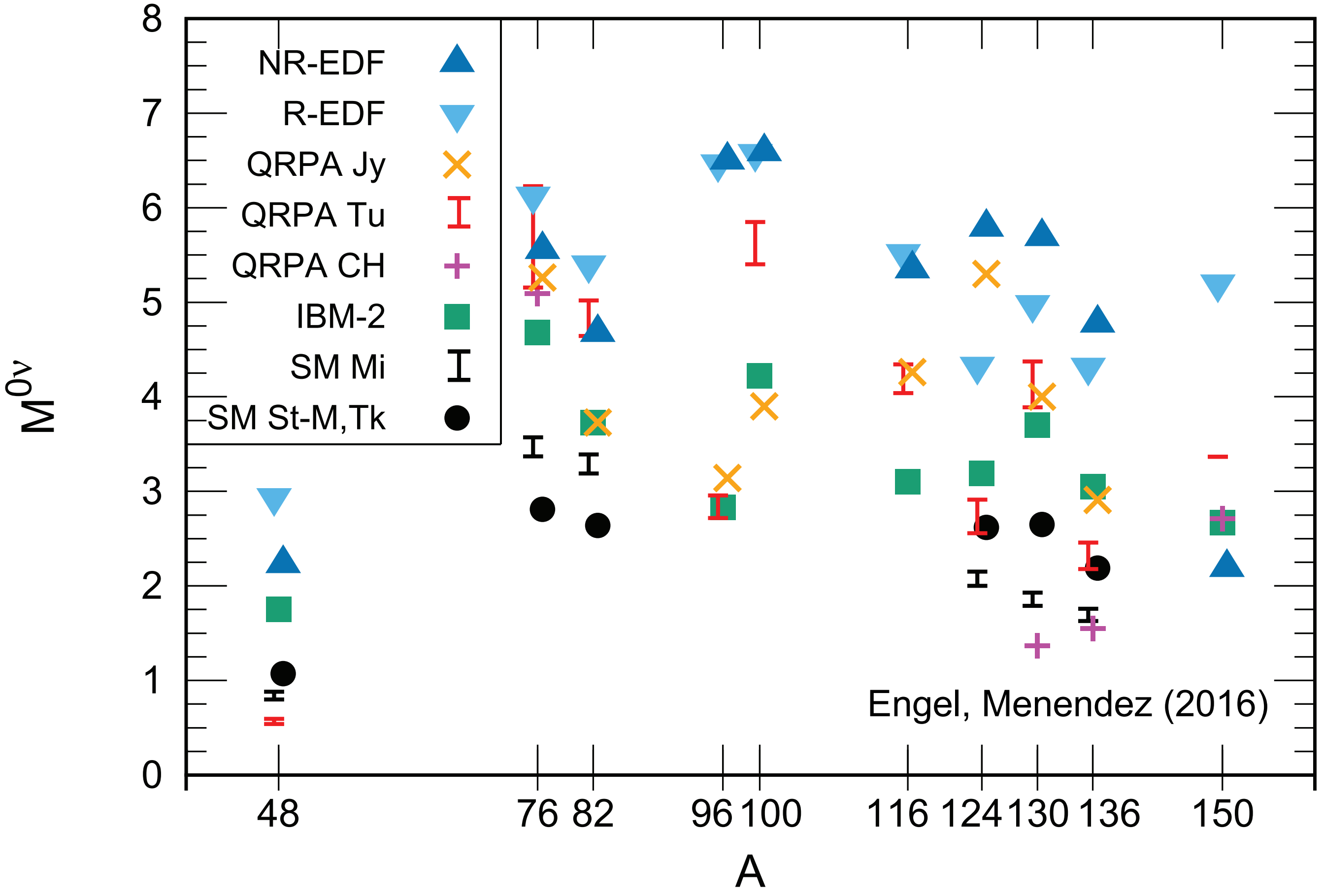
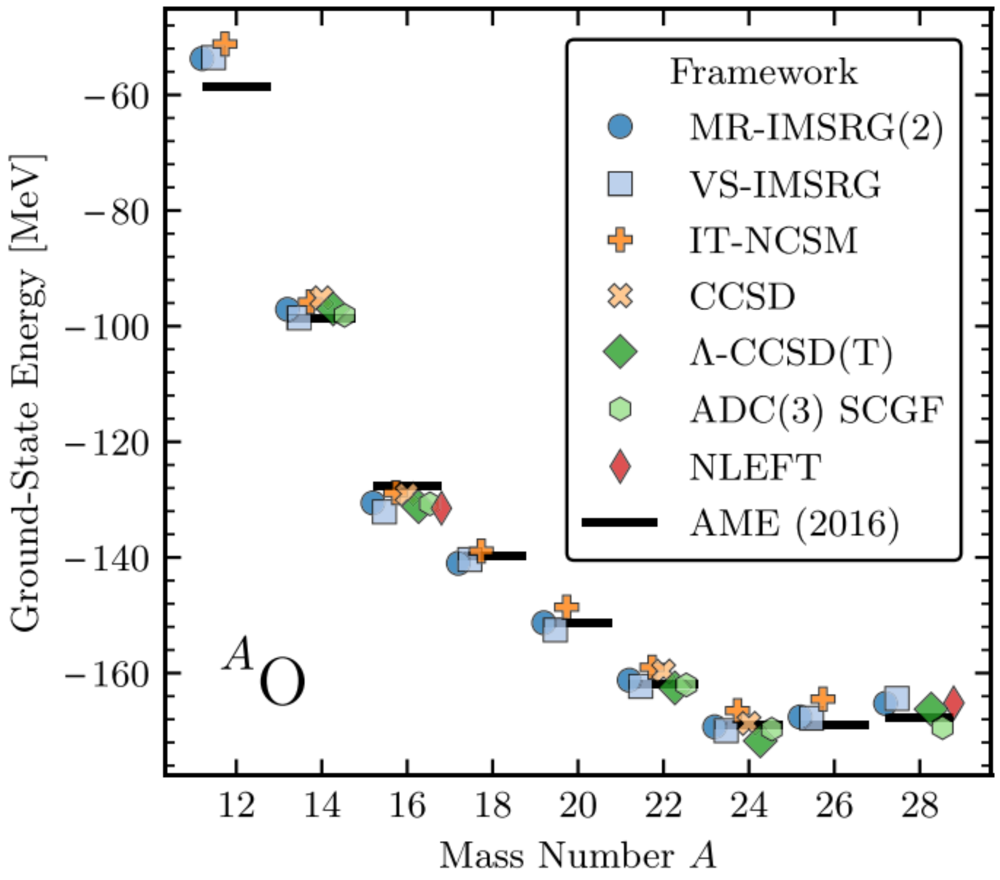




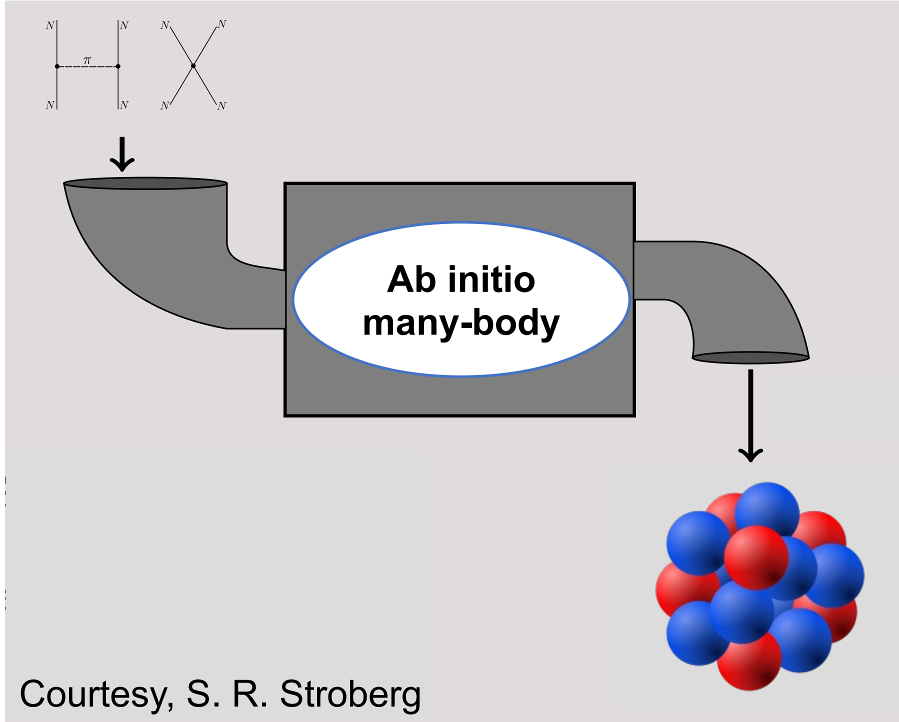
Rethink approach to NME calculations: **ab initio theory** consistent when extrapolated

Ab Initio Approach to Nuclear Structure

Aim of modern nuclear theory: develop unified *first-principles* picture of structure and reactions

(Approximately) solve nonrelativistic Schrödinger equation

$$H\psi_n = E_n\psi_n$$



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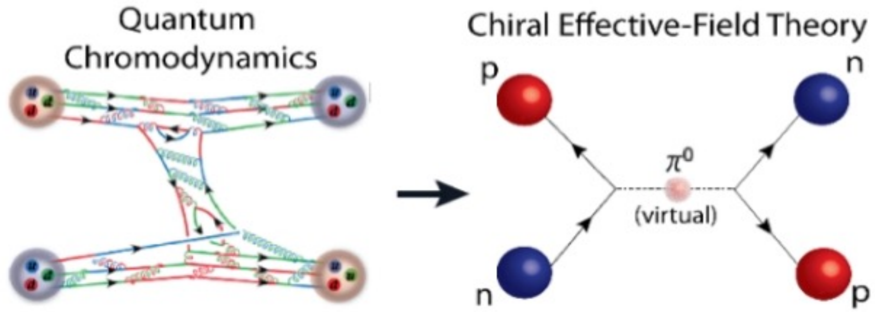
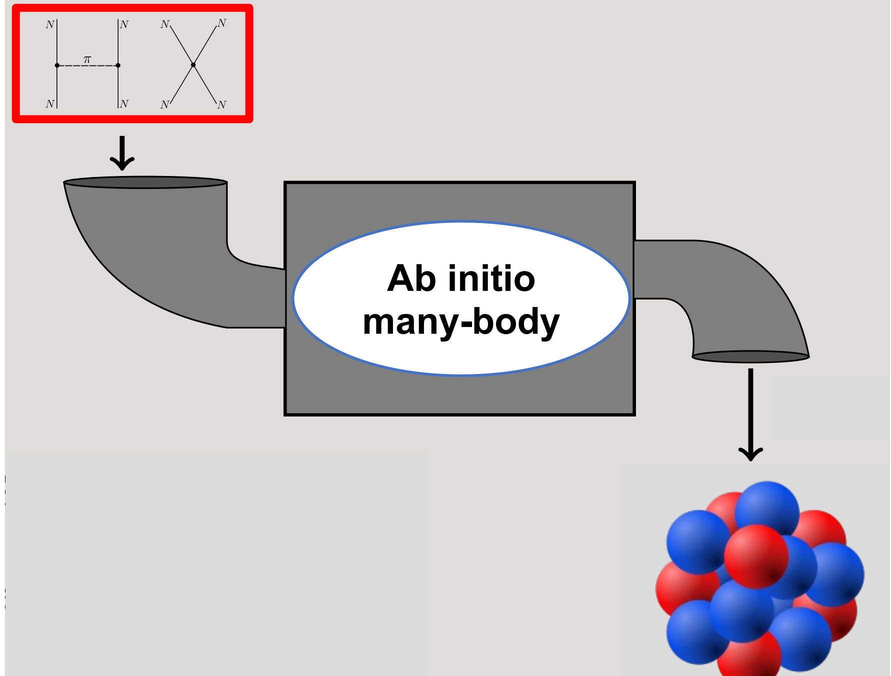




Courtesy, S. R. Stroberg

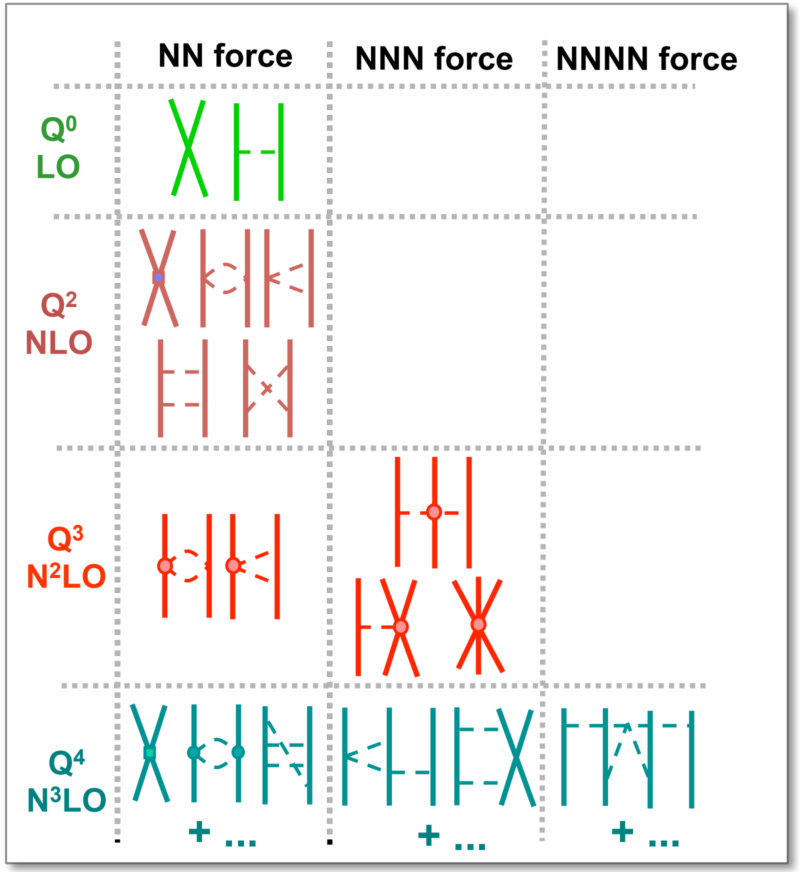
Chiral Effective Field Theory

Consistent treatment of
- 2N, 3N, 4N, … forces
- Electroweak physics

Quantifiable uncertainties

Interactions

1.8/2.0, N2LO$_{GO}$, N3LO$_{LNL}$
(2.0/2.0, N4LO$_{LNL}$)
34 non-implausible



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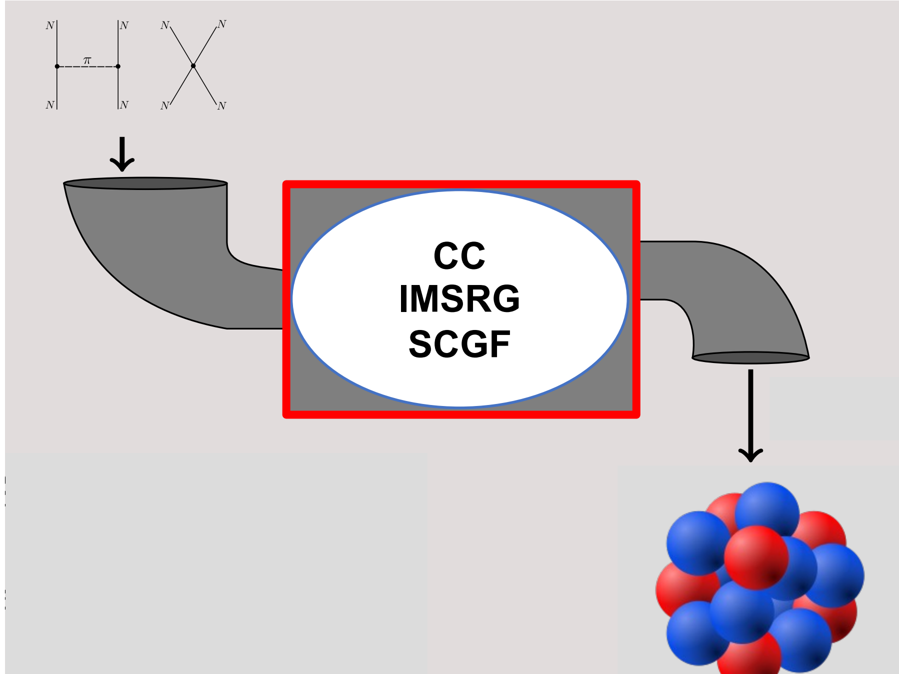

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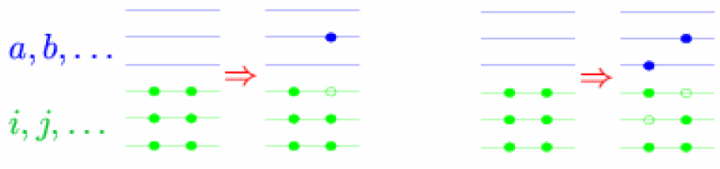
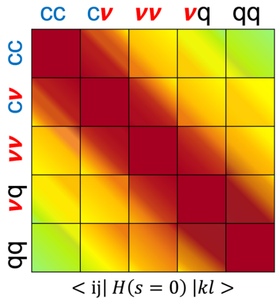
Ab Initio Cheat Sheet (polynomial scaling methods)

CC: Coupled cluster theory

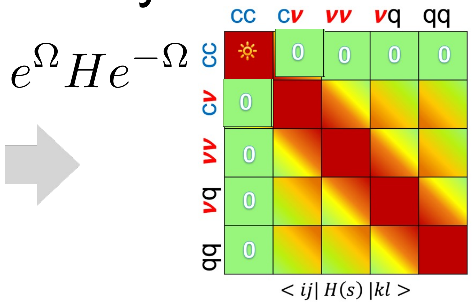


$$\begin{aligned} E &= \langle\Phi|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\ \overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c \end{aligned}$$

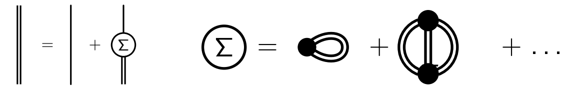
IMSRG: In-medium similarity renormalization group



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



SCGF: Self-consistent Green's function



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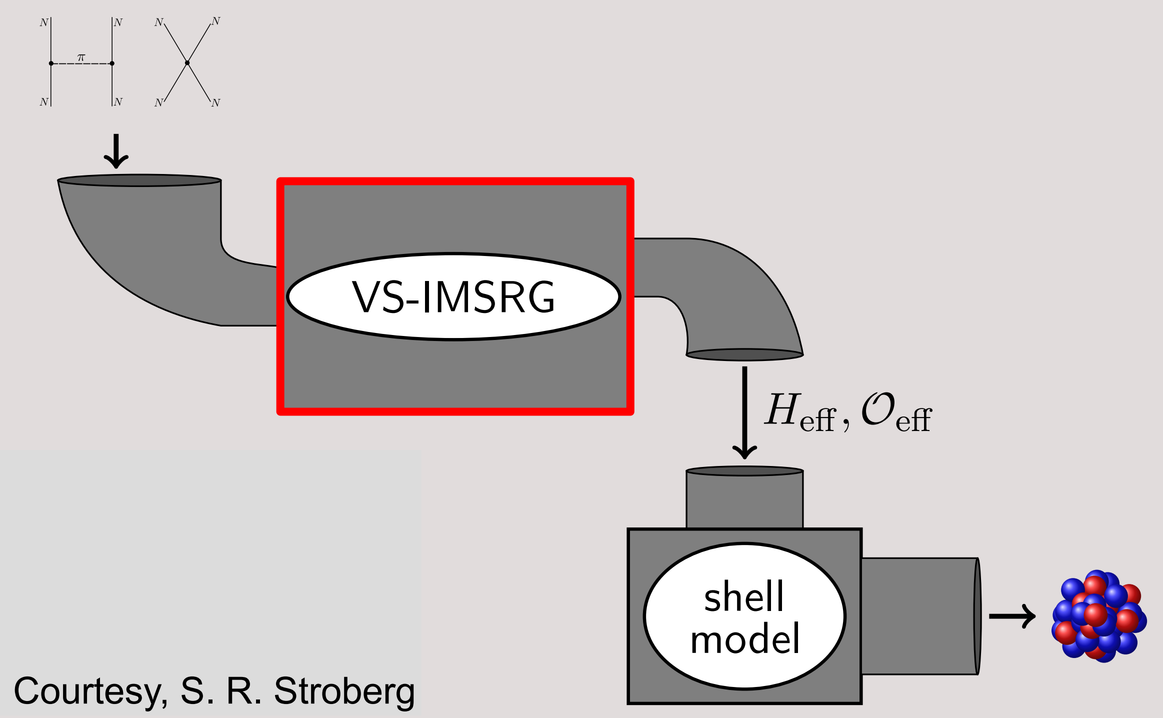
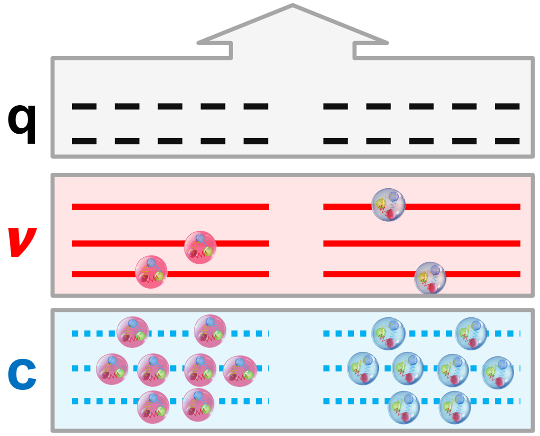


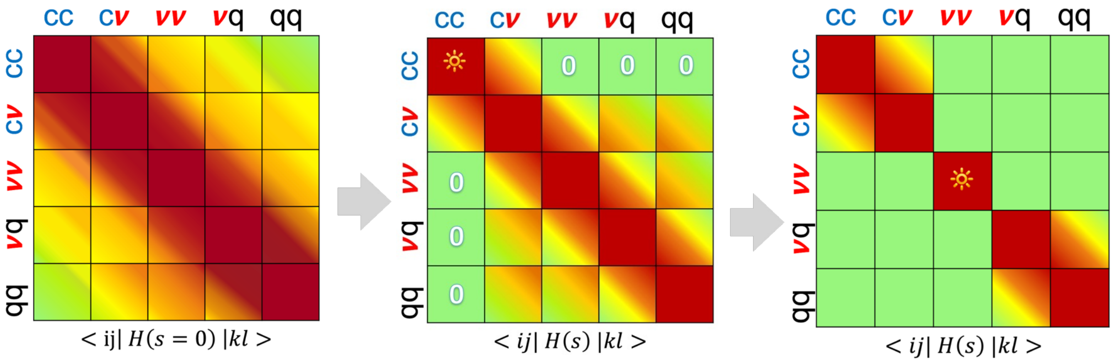
Courtesy, S. R. Stroberg



Valence-space approach for open-shell nuclei

Decoupled Valence-space Hamiltonian

Decoupled core



Extends ab initio to scope of traditional nuclear shell model

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Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

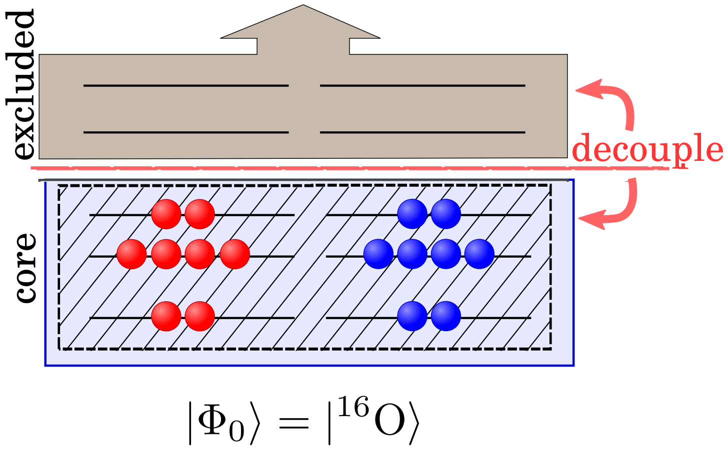
$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \qquad \eta = \frac{1}{2}\arctan\left(\frac{2H_{\rm od}}{\Delta}\right) - {\rm h.c.}$$

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

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



Can we achieve accuracy of large-space methods?

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

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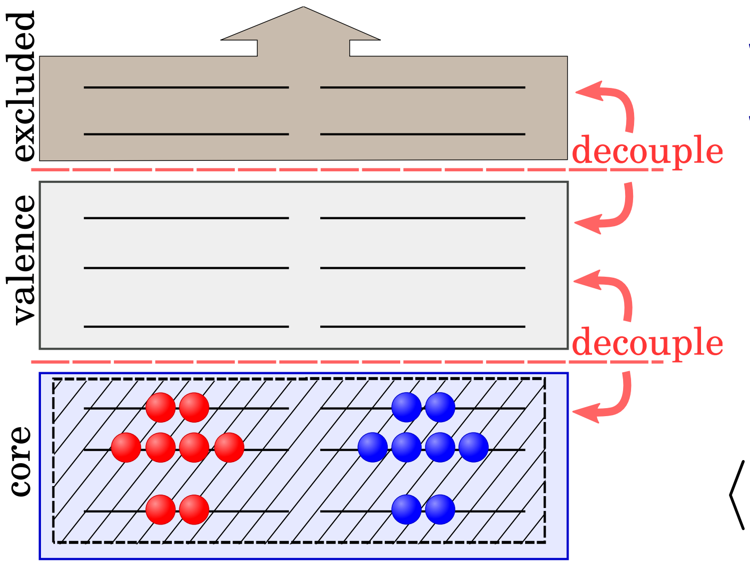

$|\Phi_0\rangle = |^{16}\text{O}\rangle$

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Step 2: Decouple valence space

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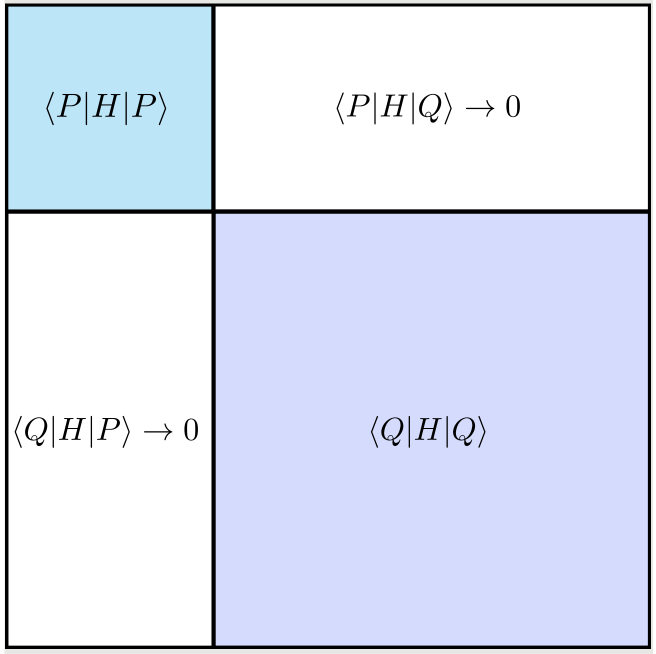

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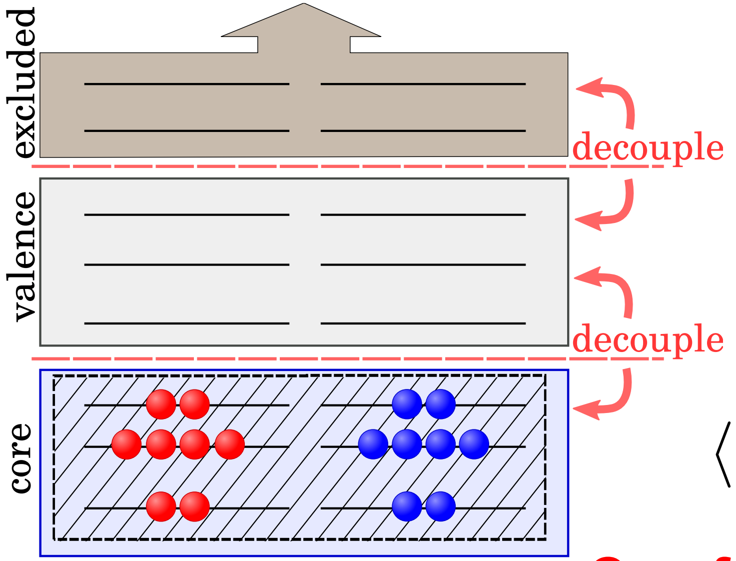
$$\tilde{\mathcal{O}} = e^{\Omega} \mathcal{O} e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2}[\Omega,[\Omega,\mathcal{O}]] + \cdots$$



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

Step 1: Decouple core

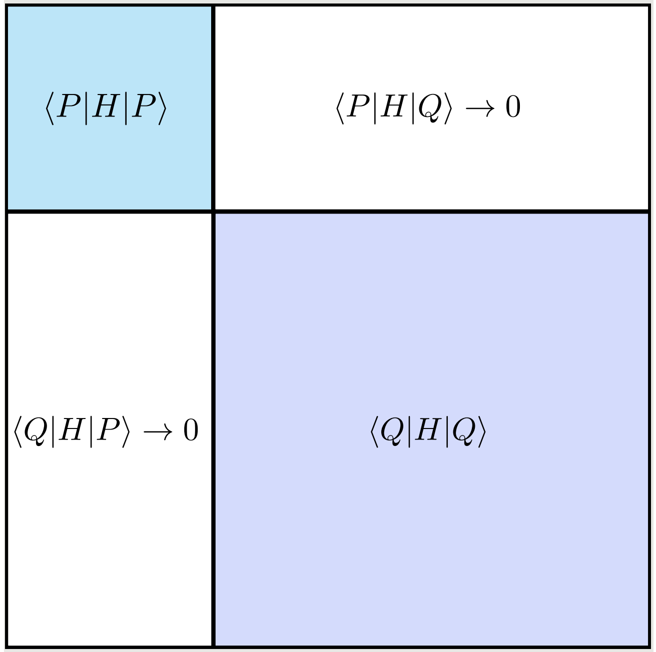
Step 2: Decouple valence space

Step 3: Decouple additional operators

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

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

Careful benchmarking essential



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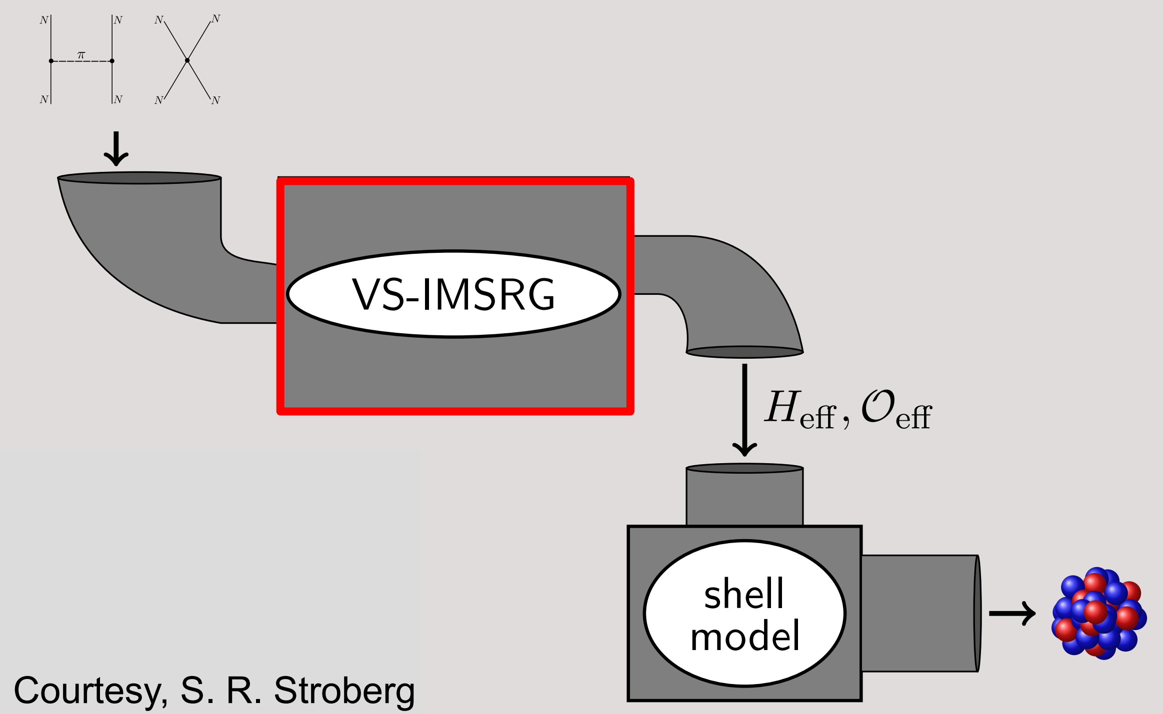


Courtesy, S. R. Stroberg

Methods Exact up to Truncations

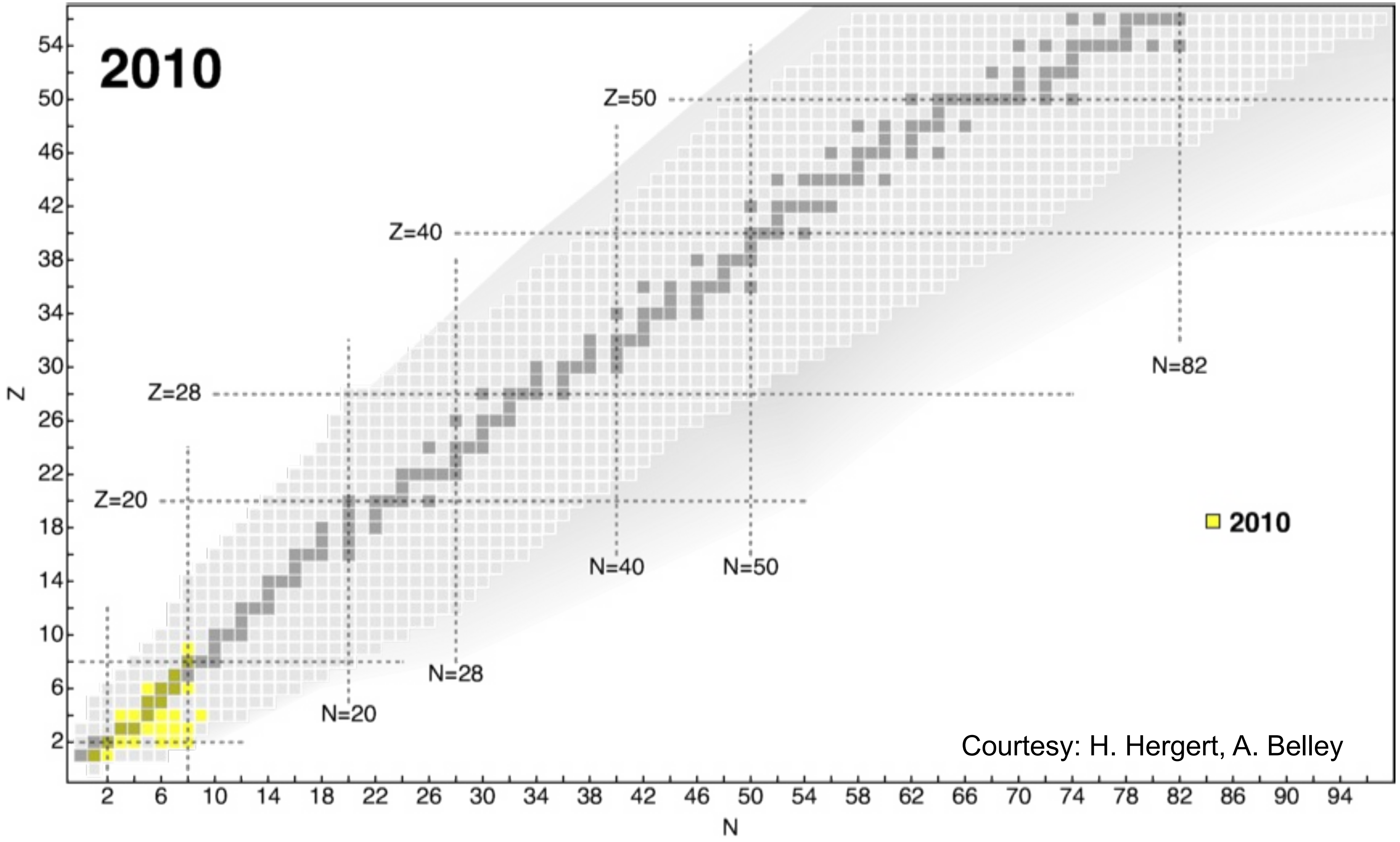
✅ **Single-particle basis** $e_{\rm max} = 2n + l$

✅ **Storage limits of 3N forces** $e_1 + e_2 + e_3 \leq E_{\rm 3max}$

🤷‍♂️ **Many-body operators: e.g., CCSD(T), IMSRG(2)**

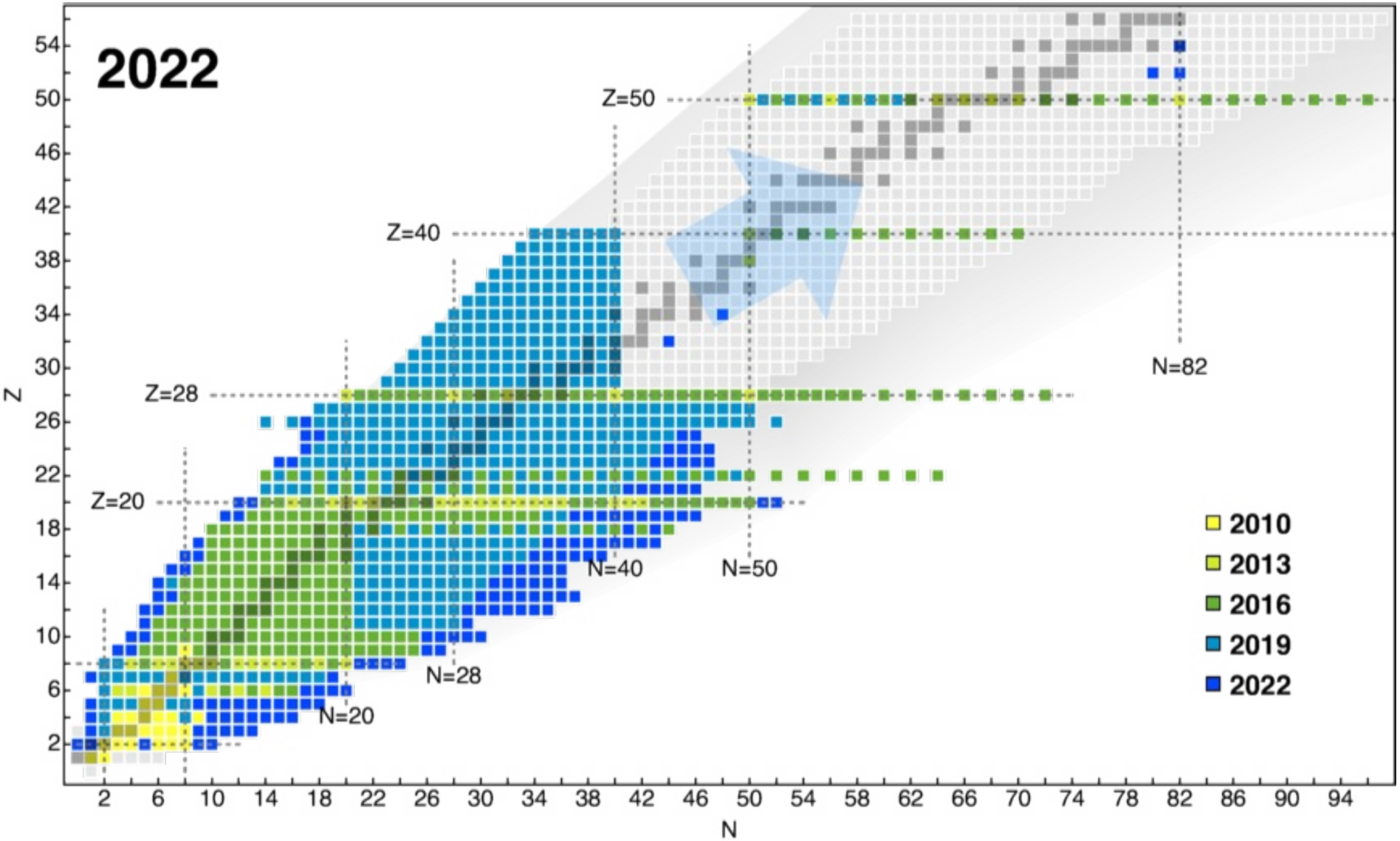
Progress of Ab Initio Theory Since 2010

2010: Limited capabilities for 3N forces; ^{16}O heaviest



Ab Initio Progress: How Heavy Can We Go?

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



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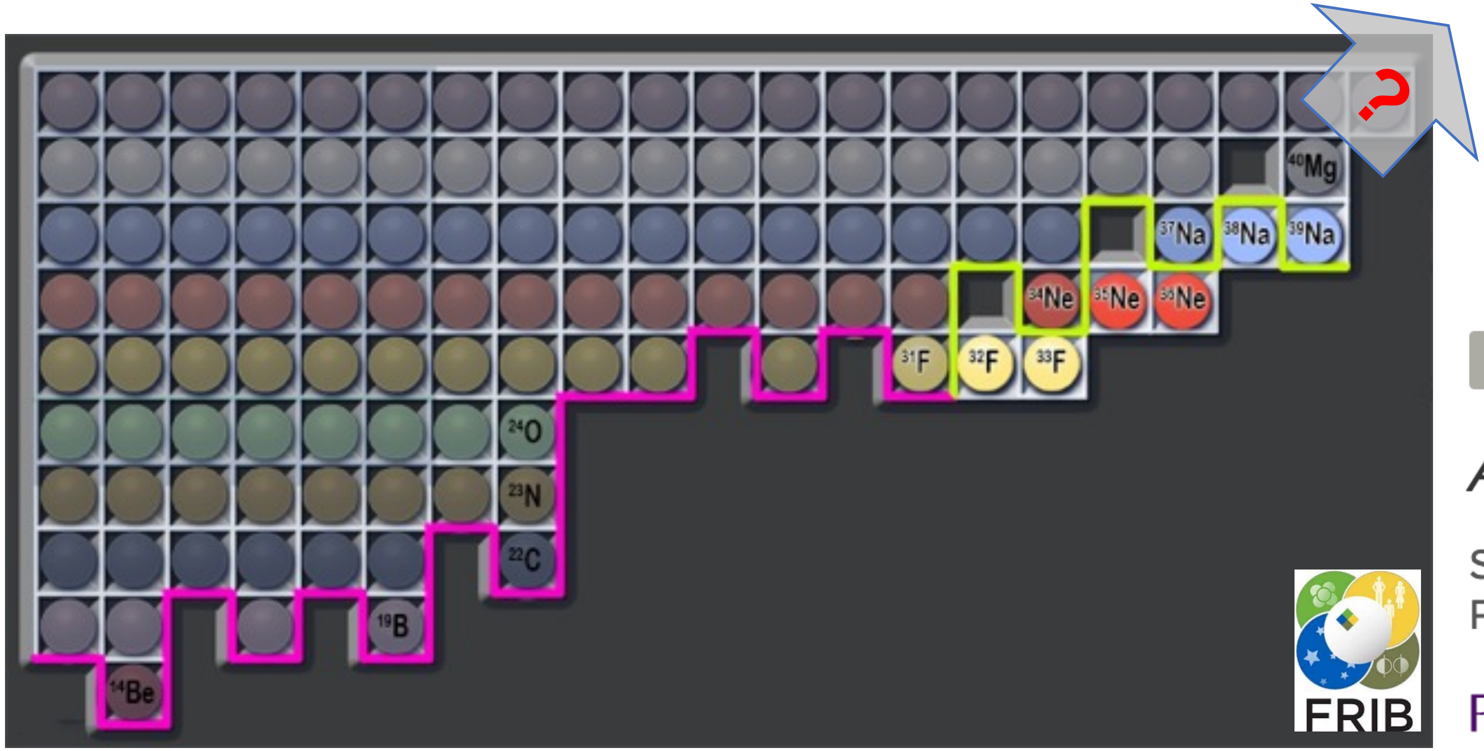
Global Ab Initio Calculations: Proton/Neutron Driplines



Featured in Physics | Editors' Suggestion

Ab Initio Limits of Atomic Nuclei

S. R. Stroberg, J. D. Holt, A. Schwenk, and J. Simonis

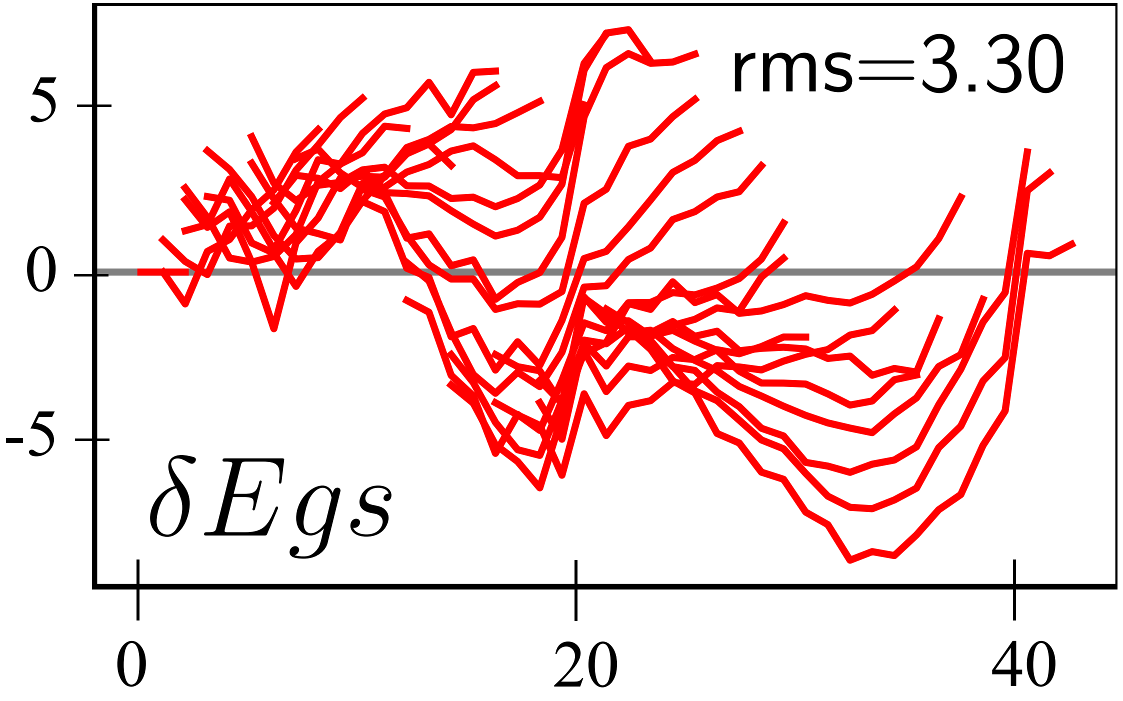
Phys. Rev. Lett. **126**, 022501 – Published 12 January 2021

Physics See synopsis: Predicting the Limits of Atomic Nuclei

Ab Initio Goes Global!

Long considered the domain of DFT or shell model

Ab initio calculations of ~700 nuclei from He to Fe!



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

B-W Mass formula: ~3.5MeV (Z<28)

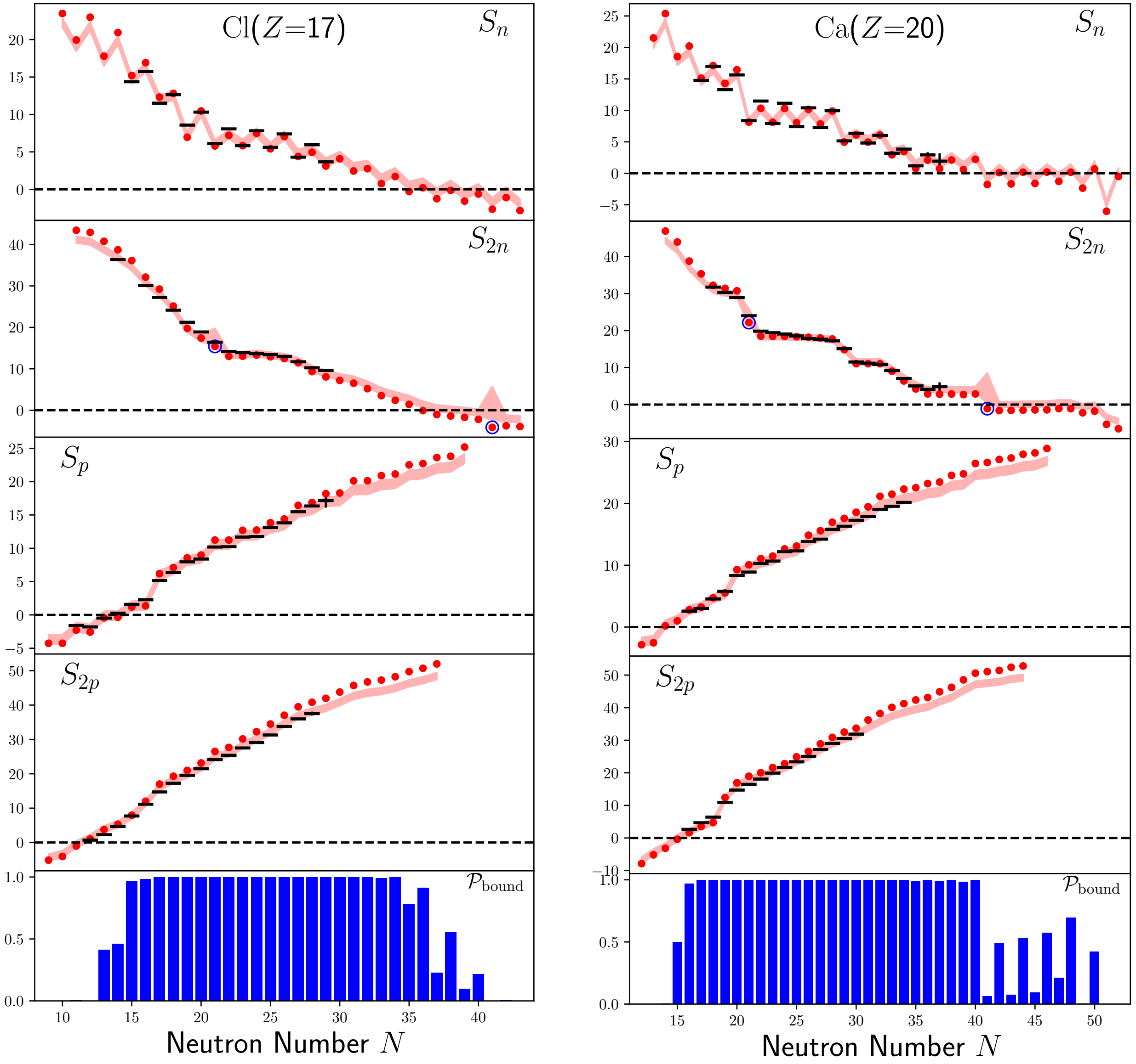
DFT: 0.6-2.0 MeV

Input Hamiltonians fit to A=2,3,4 – **not biased towards known data**

Apply to proton/neutron driplines separation energies?

Estimating Separation Energy Uncertainties

rms deviation from experiment → model for theoretical uncertainties



rms = 0.7-1.4MeV

Obtain PPD for separation energies

$$p(\tilde{S}^{\rm exp}|\tilde{S}^{\rm th}, S^{\rm th}, S^{\rm exp})$$

Total probability to be bound

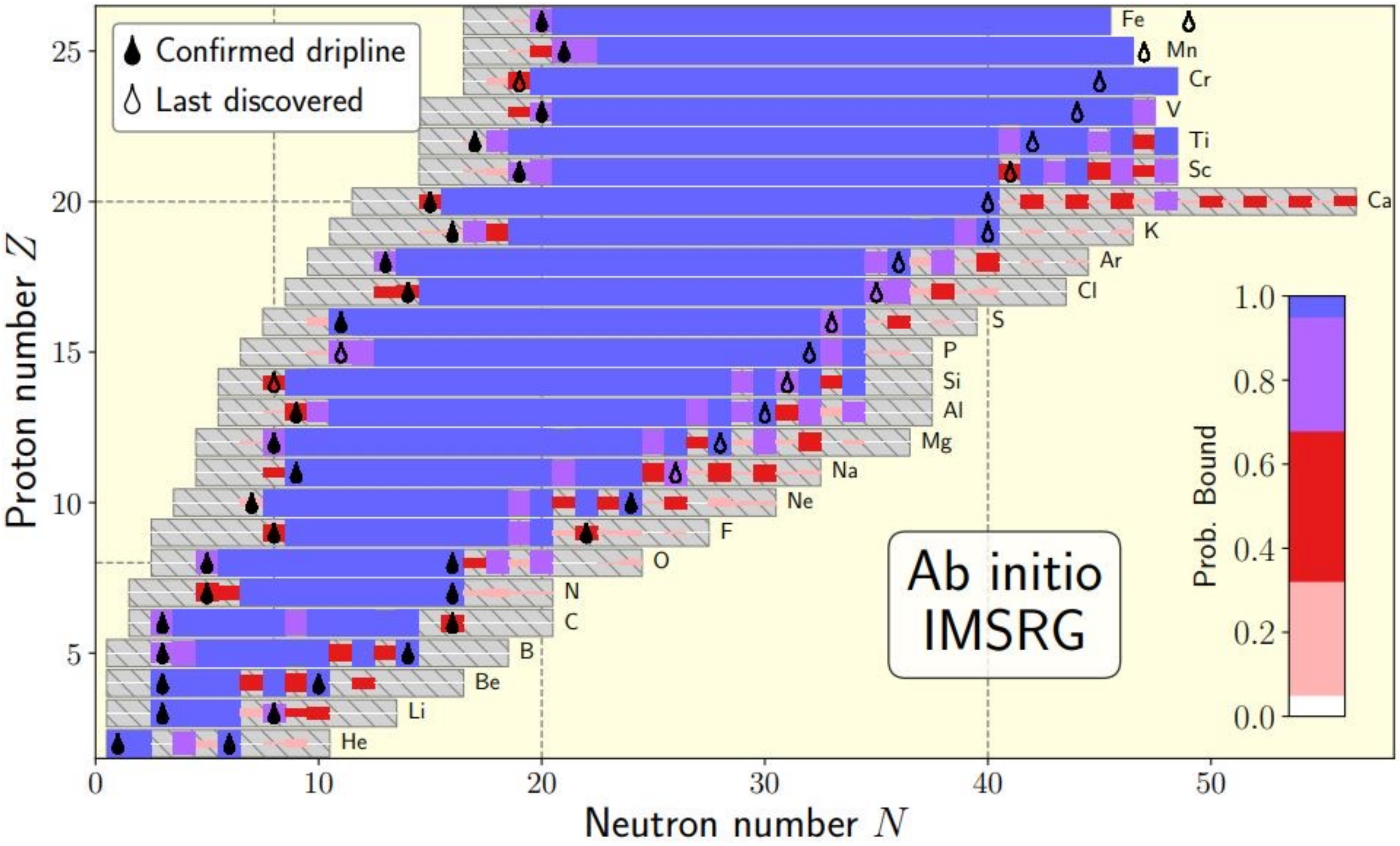
$$\mathcal{P}_{\rm bound} = \prod_{\alpha} \int_0^{\infty} d\tilde{S}_{\alpha}^{\rm exp} p(\tilde{S}_{\alpha}^{\rm exp}|\tilde{S}^{\rm th}, S^{\rm th}, S^{\rm exp})$$

$$\alpha \in \{n, p, 2n, 2p\}$$

Determine probabilities for each nucleus

Dripline Predictions to Medium Mass Region

Predictions of proton and neutron driplines from first principles



Known drip lines predicted within uncertainties (artifacts at shell closures)

Ab initio guide for neutron-rich driplines

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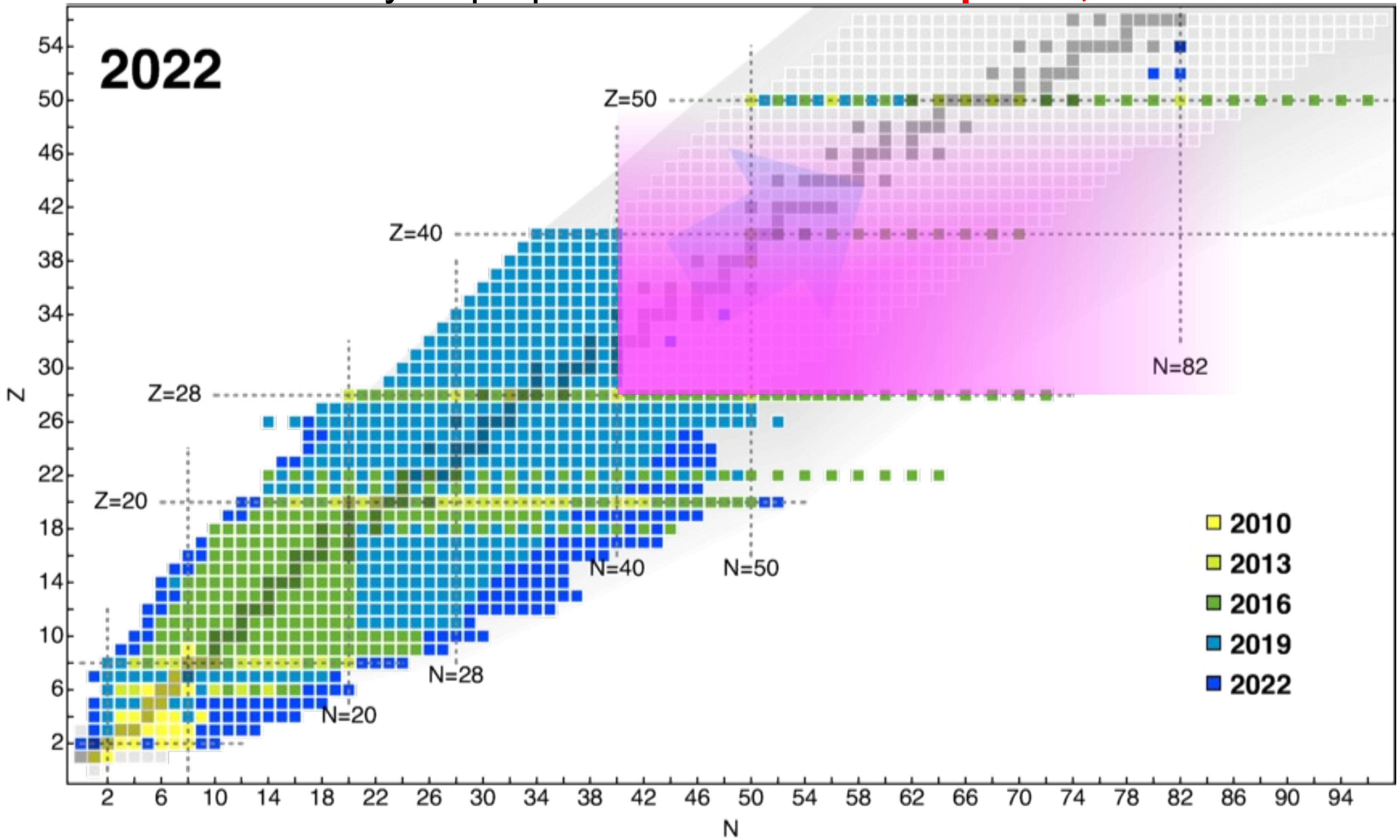
Ab Initio Progress: How Heavy Can We Go?

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

Calculate essentially all properties all of nuclei… **up to N, Z ~ 50**



Key Limitation

3NF matrix element storage

$$e_1 + e_2 + e_3 \leq E_{3\max}$$

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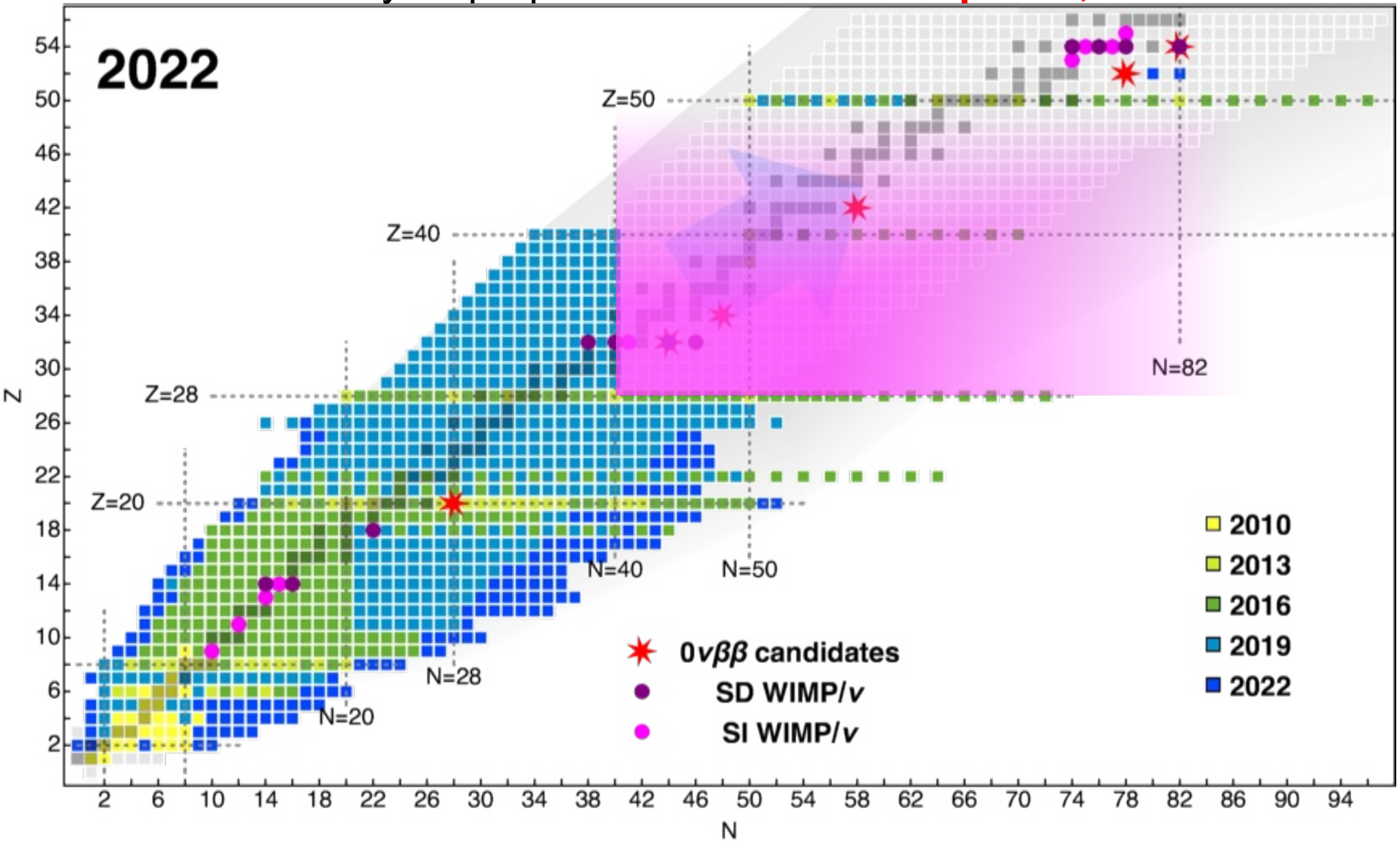

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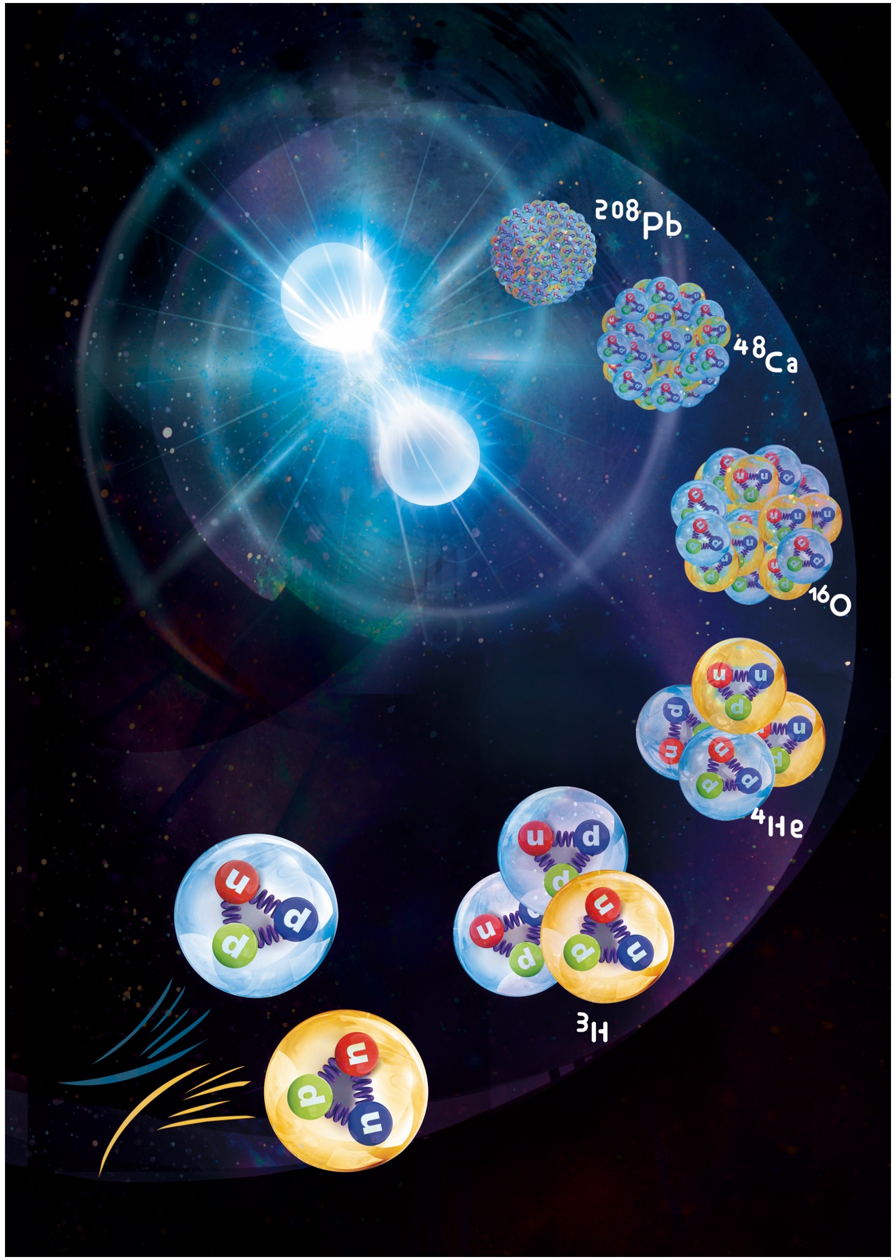
Converged Calculations in Heavy Nuclei



Converged *ab initio* calculations of heavy nuclei

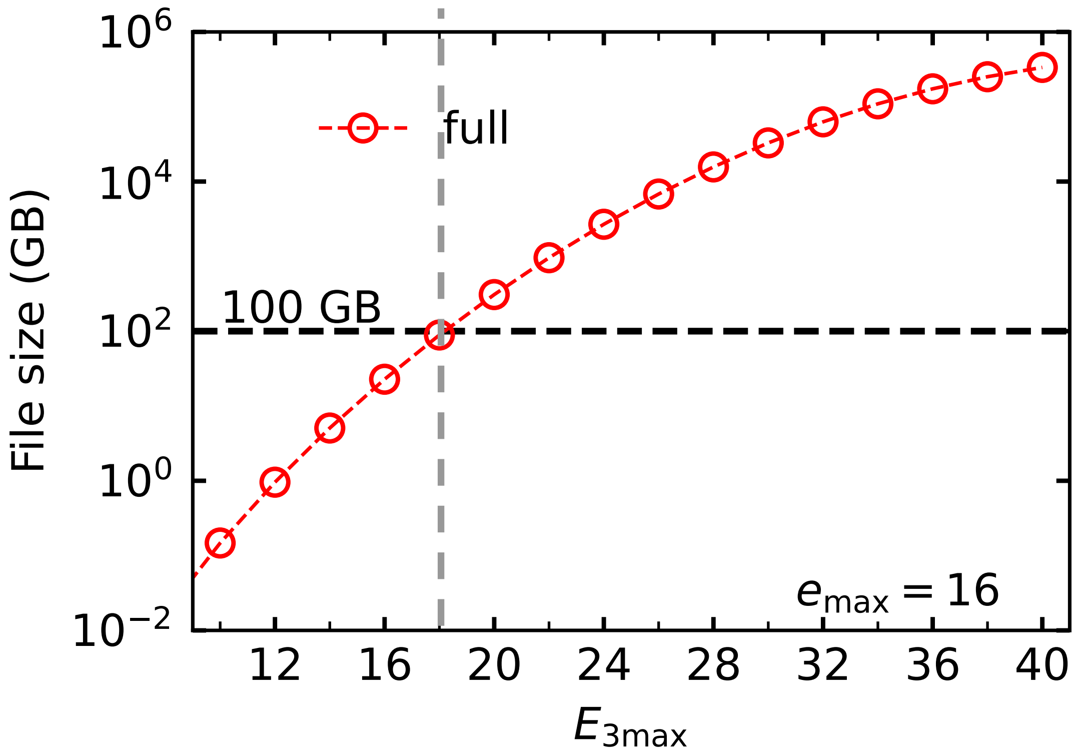
T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt

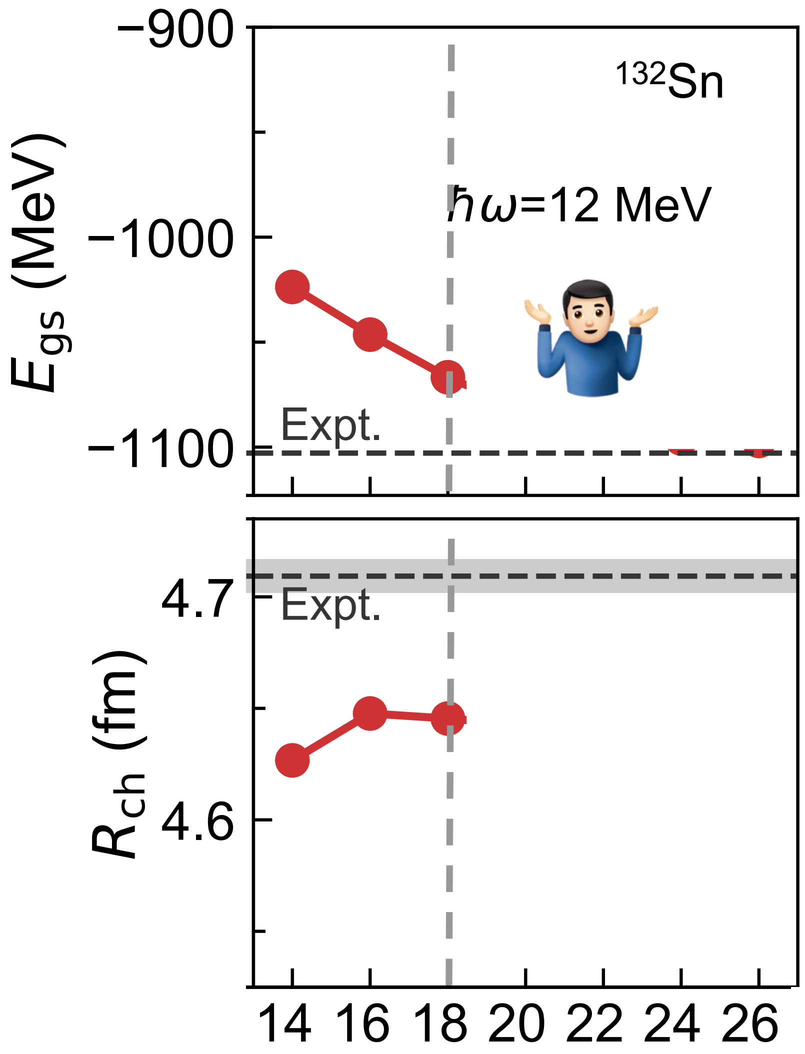
Phys. Rev. C **105**, 014302 – Published 3 January 2022

Ab Initio Calculations of Heavy Nuclei

Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3\max} = 18$

No sign of convergence in ^{132}Sn - E_{gs} or R_{ch}

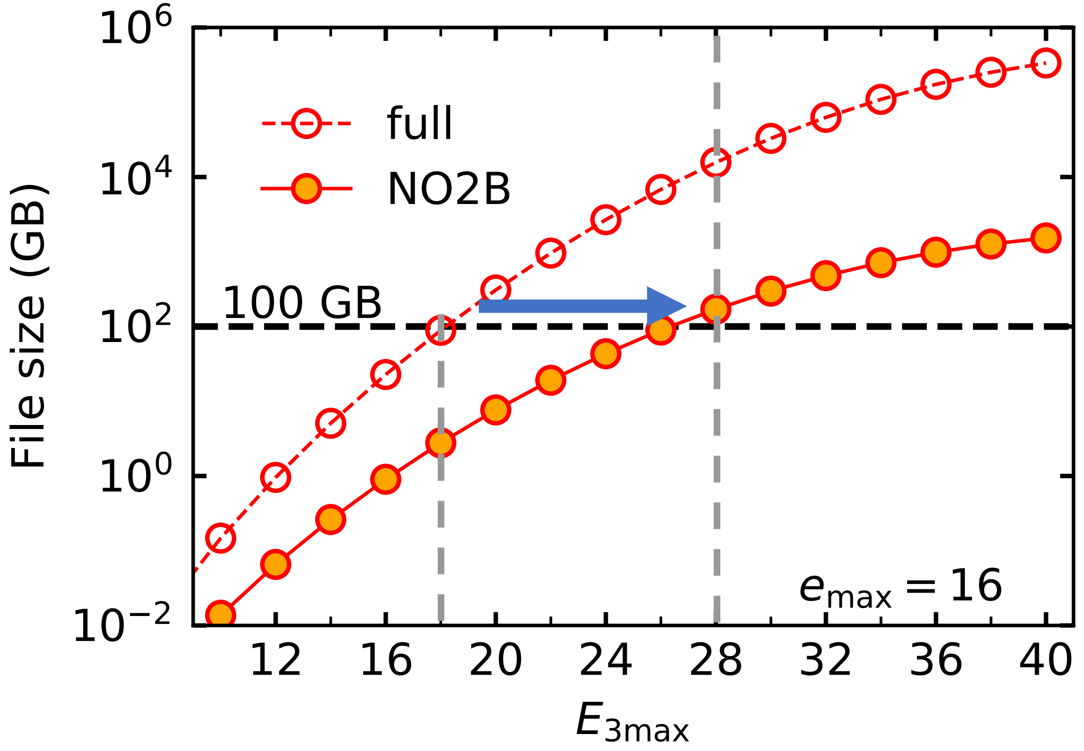


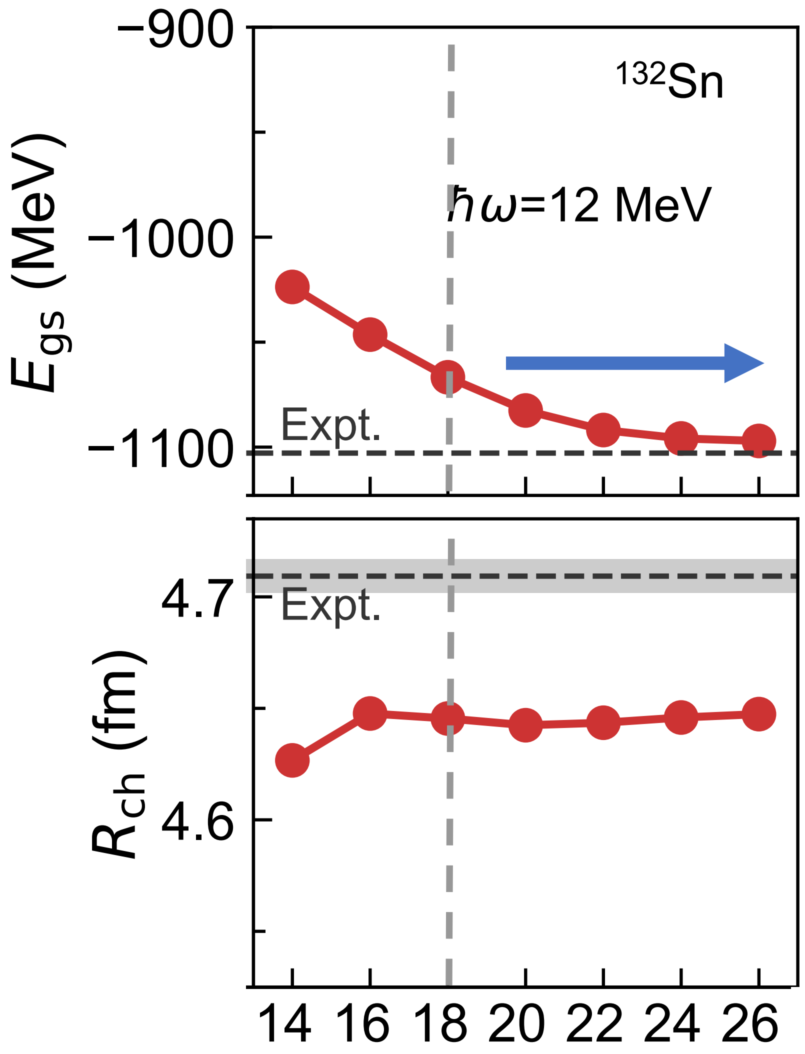


Ab Initio Calculations of Heavy Nuclei

Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3\text{max}} = 18$

Clever storage reduces needs by factor of 100!





First converged ground-state properties of ^{132}Sn!

Opens heavy region to ab initio…

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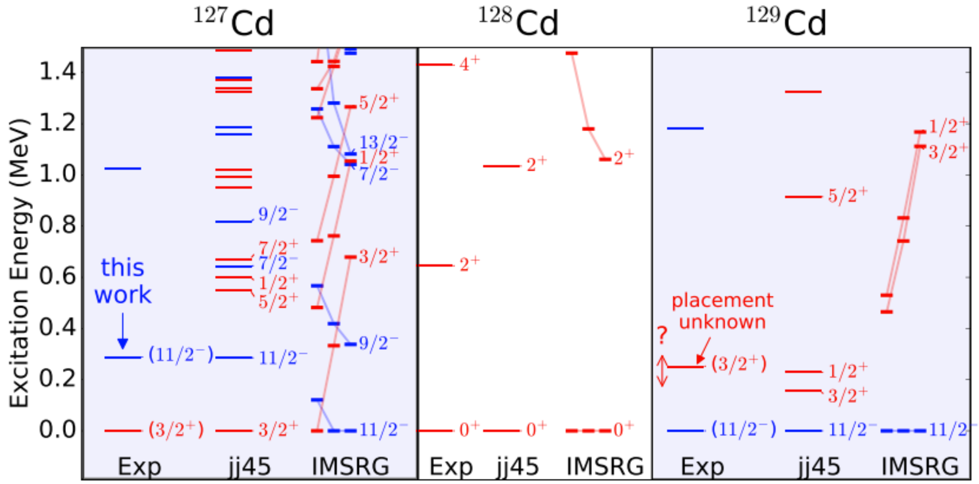
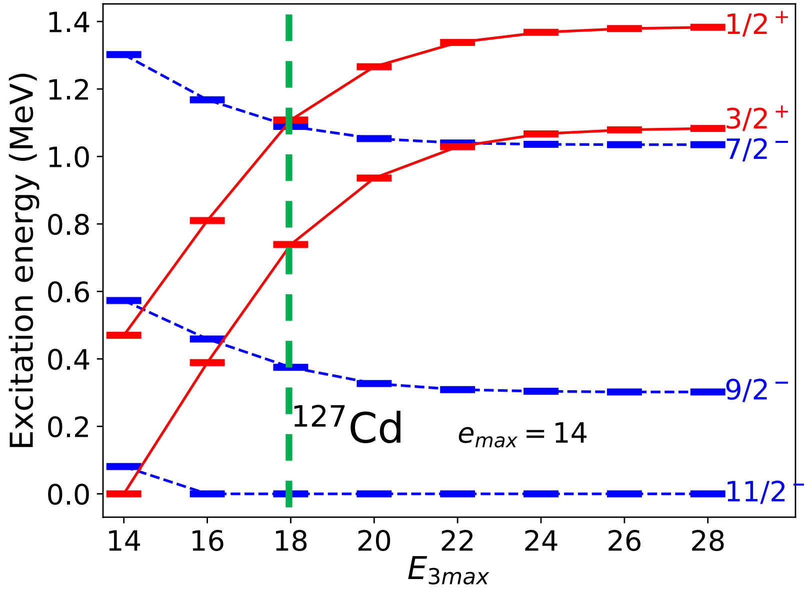
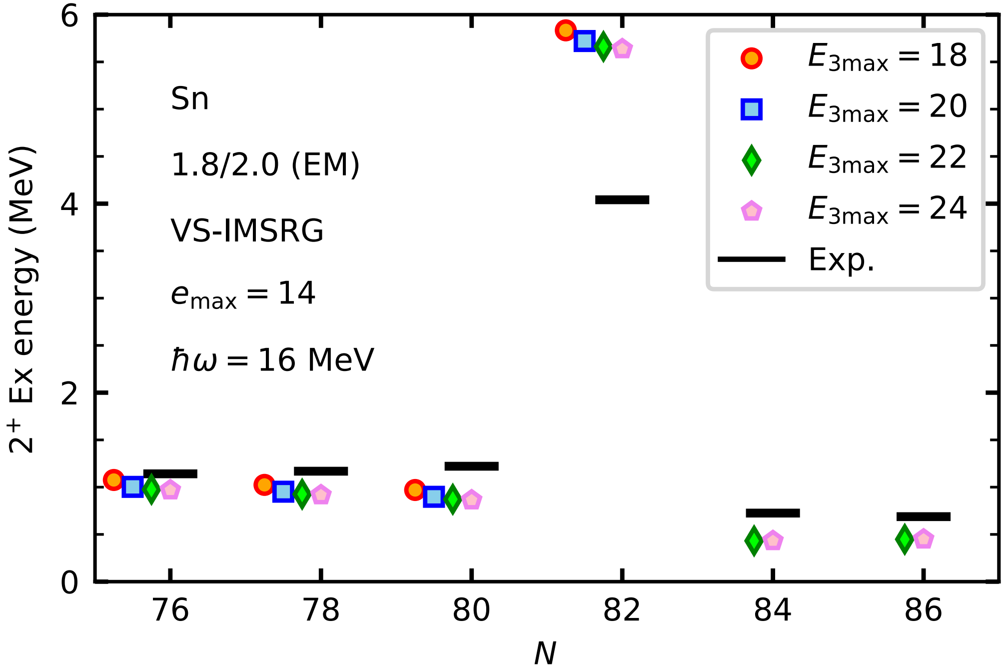
Convergence of N=82 Gap

Size of N=70 gap **well** converged at E_{3max}=28 for neutron-rich Sn, In, Cd!







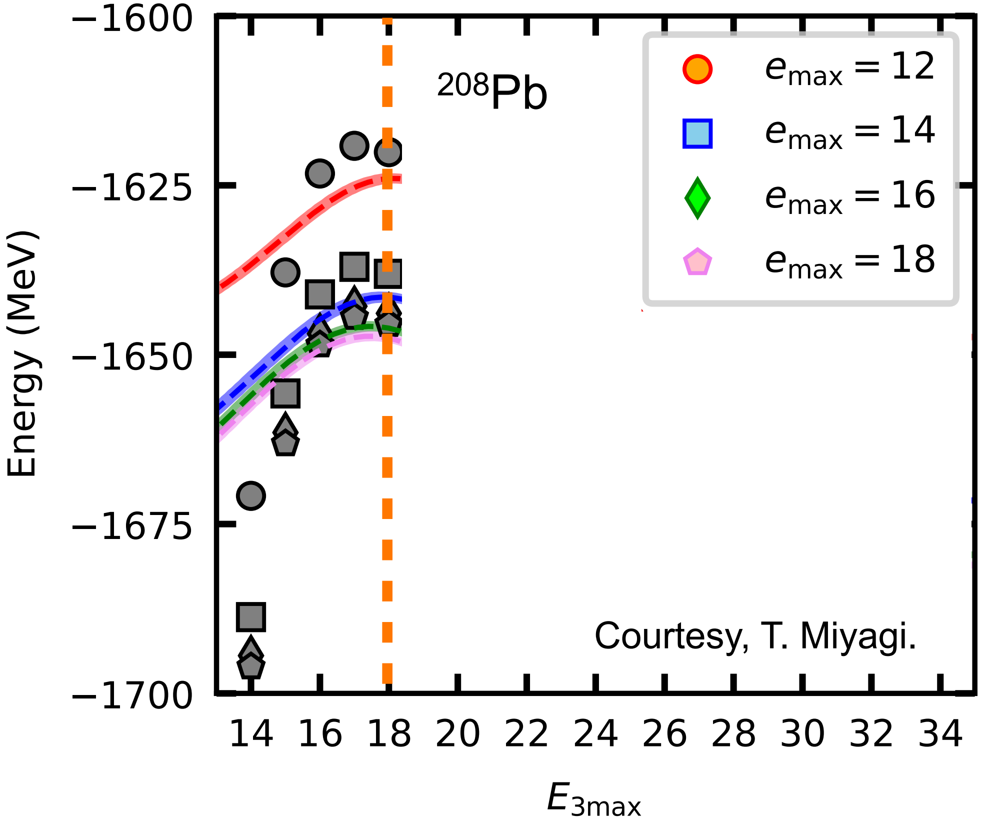
New capabilities: converged spectra in N=82 region

Converged (overpredicted) doubly magic ^{132}Sn

Can we go heavier?

Convergence in Heavy Nuclei: ^{208}Pb

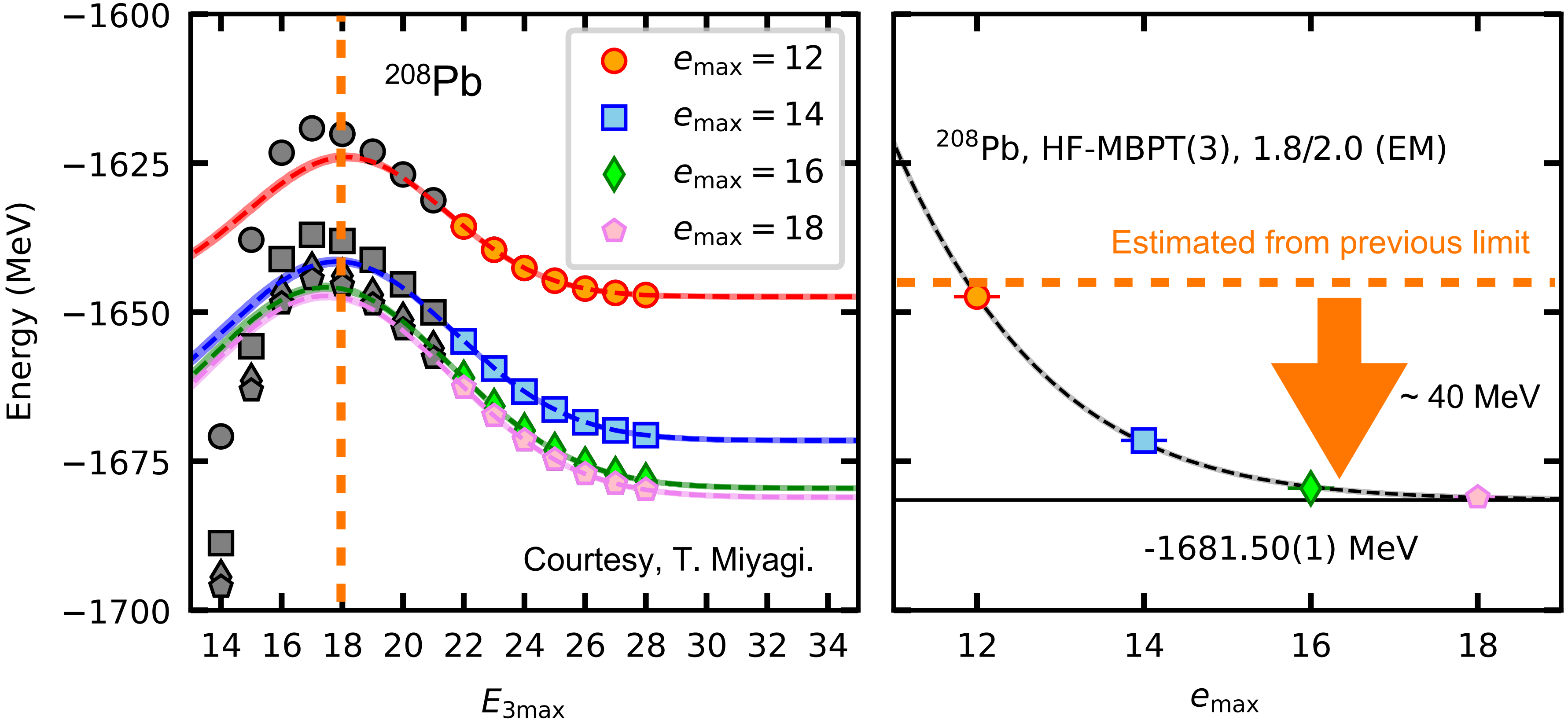
Previous limit, no hope of convergence in ^{208}Pb g.s. energy…



Convergence in Heavy Nuclei: ^{208}Pb

Previous limit, no hope of convergence in ^{208}Pb g.s. energy

Improved $E_{3\text{max}} = 18 \to 28$ clear convergence



First converged ab initio calculation of ^{208}Pb!

TRIUMF

Ab Initio Analysis: Neutron Skin of ^{208}Pb Linked with neutron star properties

nature physics

ARTICLES

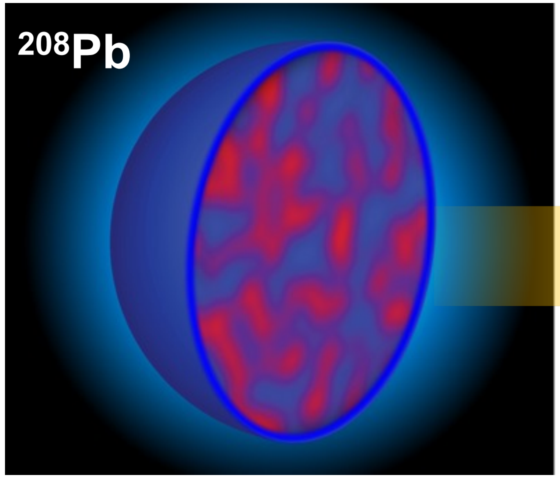
https://doi.org/10.1038/s41567-022-01715-8

Check for updates

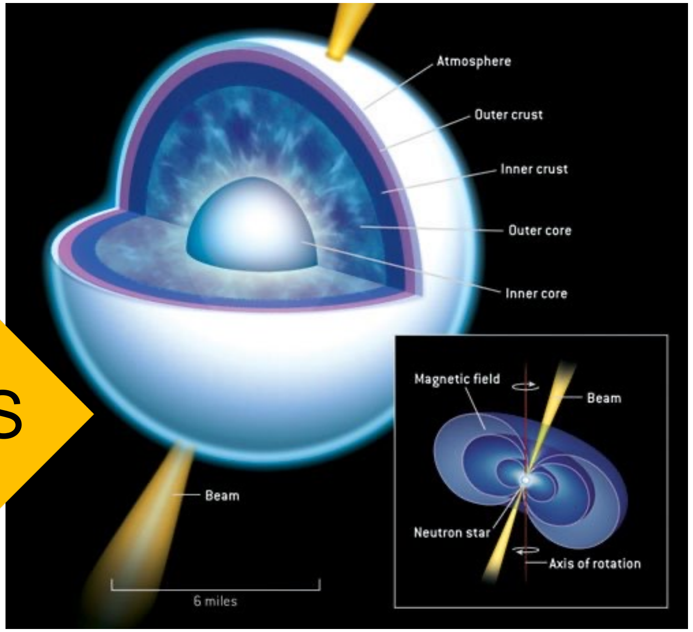
OPEN

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2]✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]



Nuclear EOS



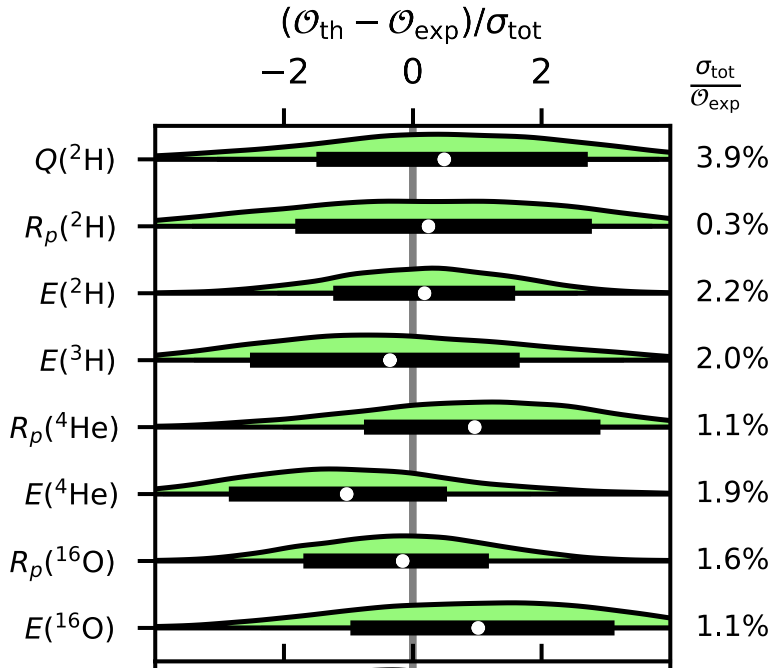
Neutron Skin of ^{208}Pb

Combine TRIUMF/ORNL/Chalmers advances!

I: History Matching confronted with A=2,3,4 data + ^{16}O

10^9 calculations spanning EFT parameter space at N^{2}LO

34 non-implausible interactions



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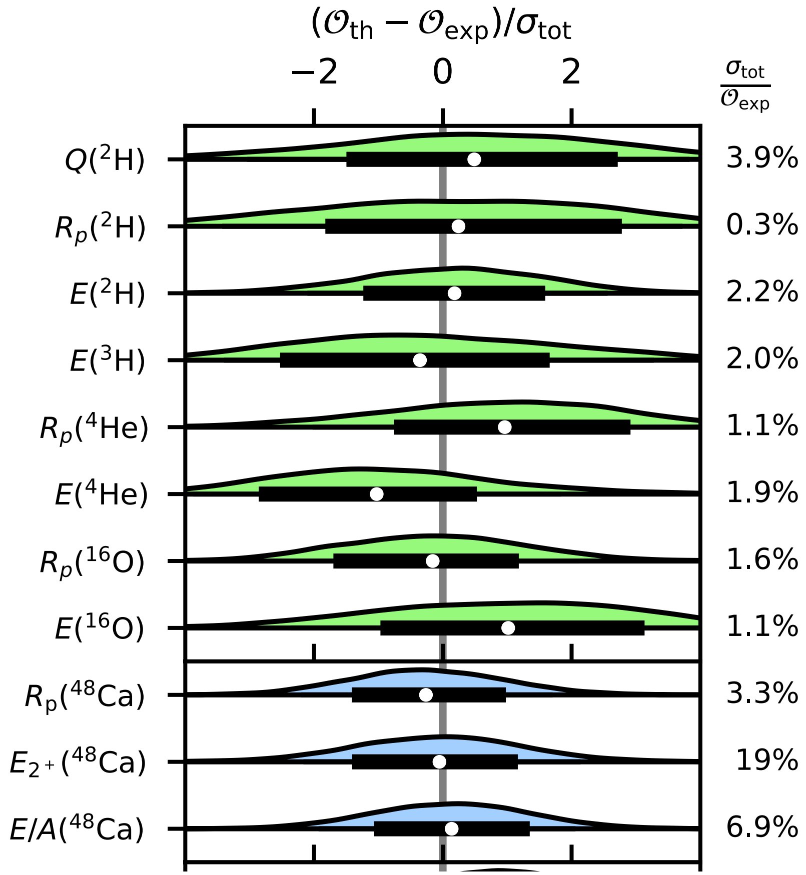
II: Calibration use ^{48}Ca E/A, E(2$^+$), R_p, dipole polarizability

Importance resampling – statistically weight interactions



Neutron Skin of ^{208}Pb

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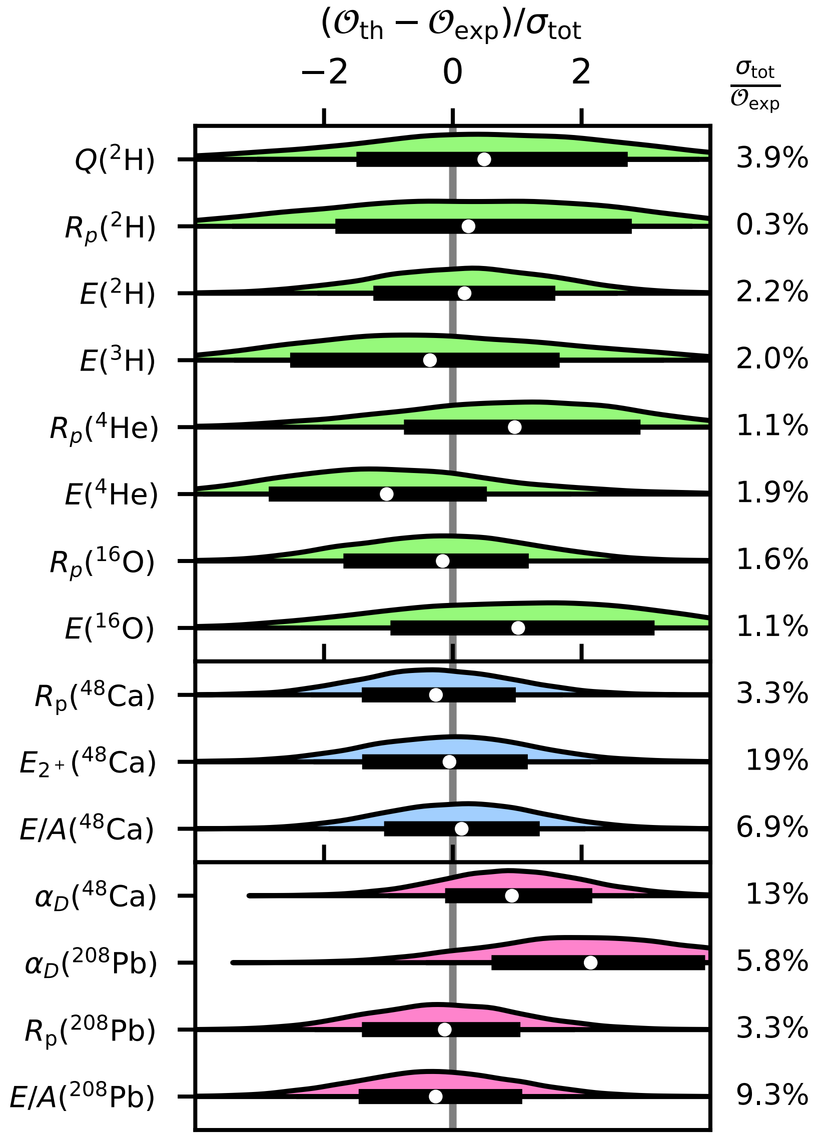
III: Validation ^{208}Pb E/A, R_p + ^{48}Ca/^{208}Pb DP from ab initio

Clear quality description of data



TRIUMF

Neutron Skin of ^{208}Pb

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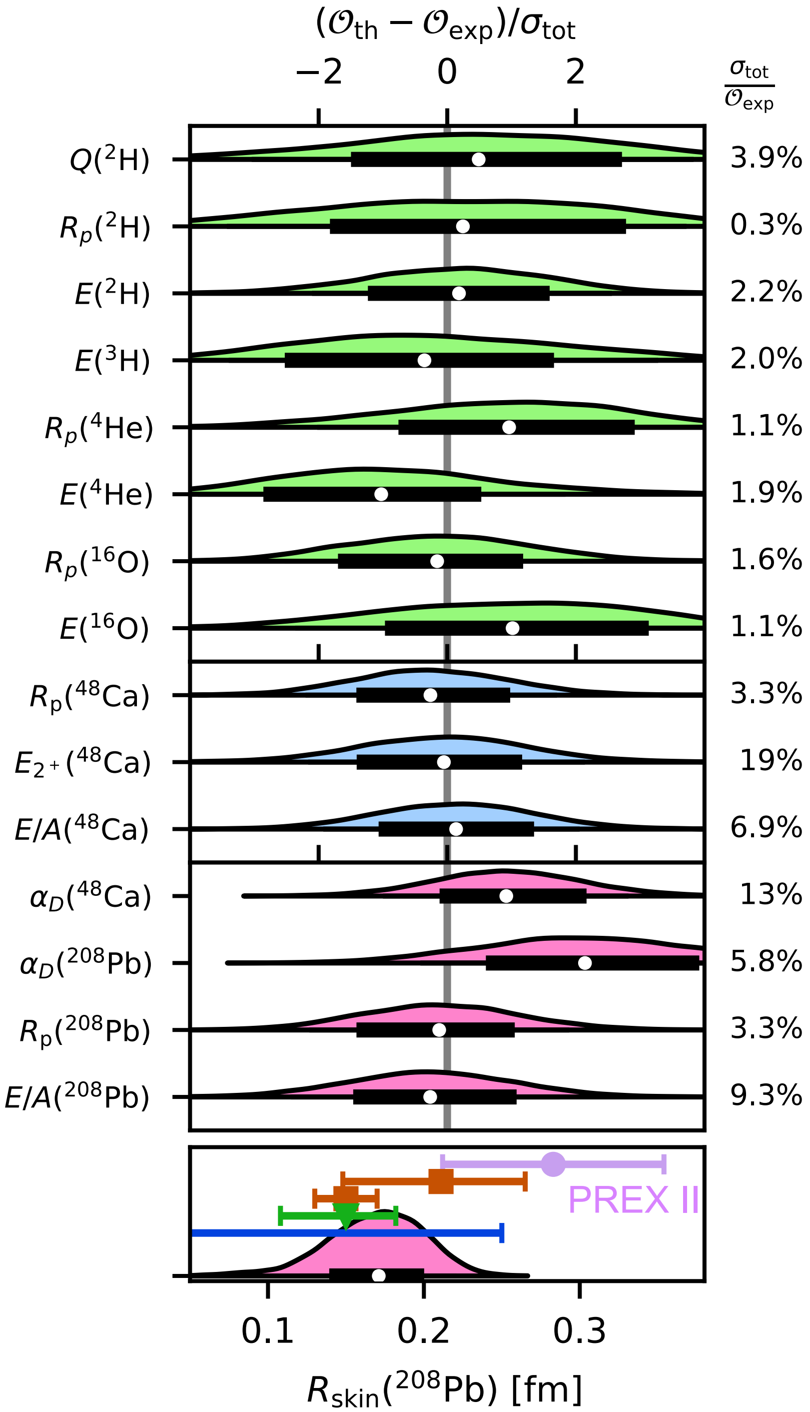
III: Validation ^{208}Pb E/A, R_p + ^{48}Ca/^{208}Pb DP from ab initio

Clear quality description of data

IV: Prediction - posterior predictive distribution for neutron skin

R_{skin}(^{208}Pb)= 0.14-0.20fm (68% credible level)

Consistent(ish) with extracted **PREXII result**



Infinite Matter Equation of State

Explore correlations between finite nuclei and nuclear EOS

Use same 34 non-implausible interactions

Reveals correlation as seen in mean field models

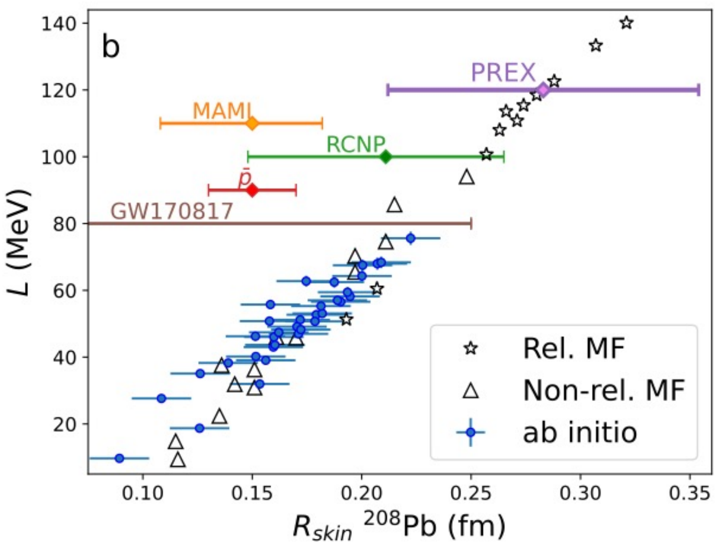
L = 37-63 MeV

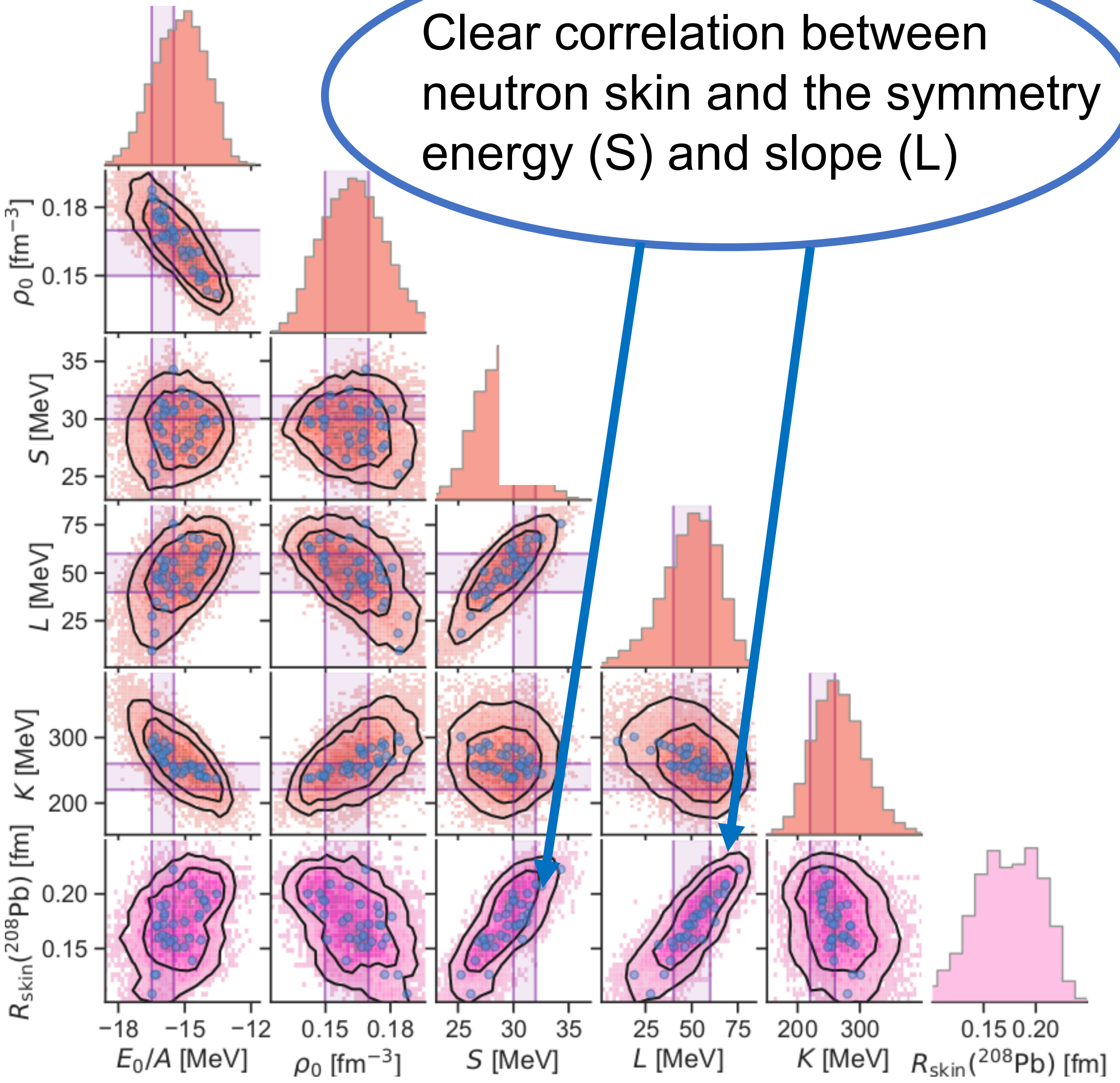
Constrain forces potentially from:

Neutron star radii/mergers

Mean field accommodates large range of skins

Tighter range from
ab initio calculations





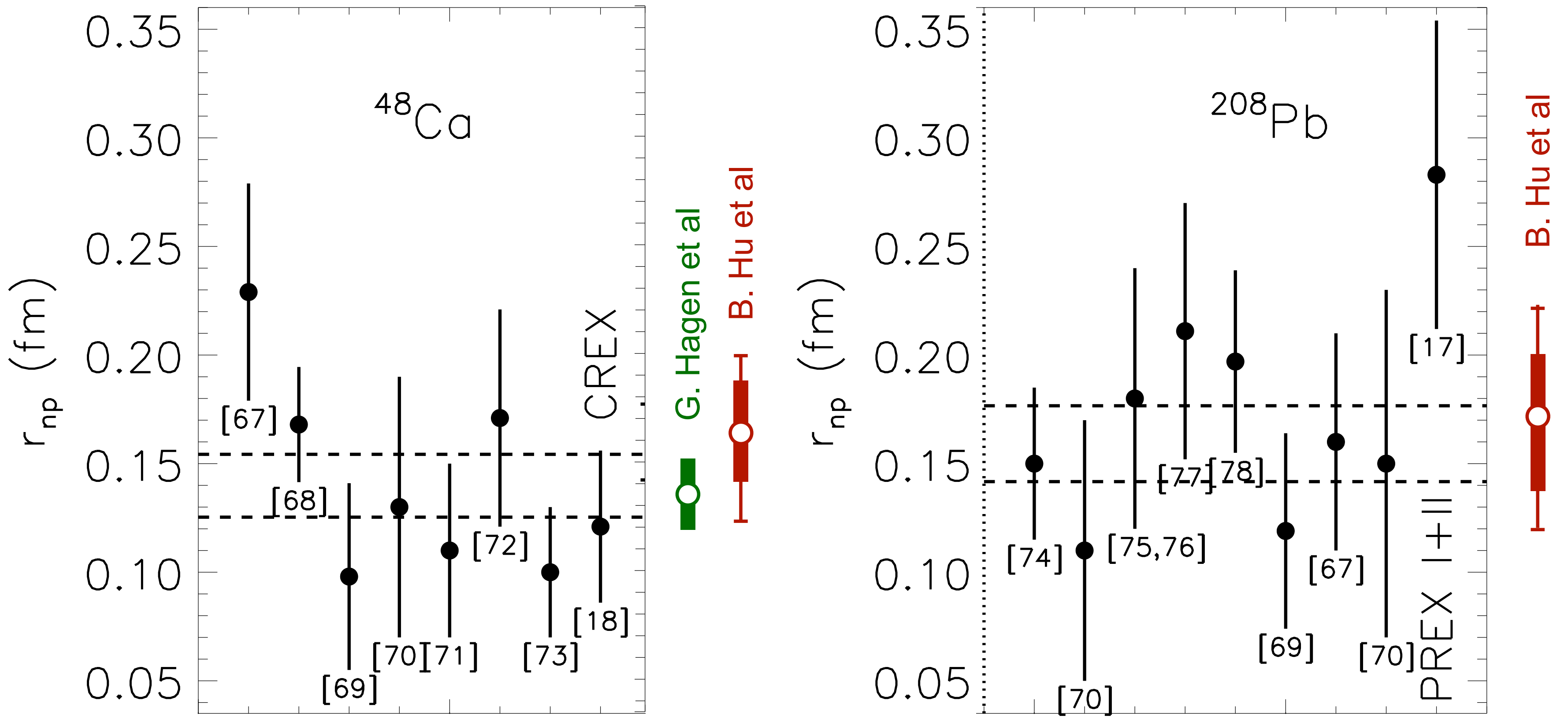
Clear correlation between neutron skin and the symmetry energy (S) and slope (L)

Confrontation with R_{skin} of ^{48}Ca

Newly extracted neutron skin in ^{48}Ca

Use same 34 interactions – predictions in good agreement with CREX result

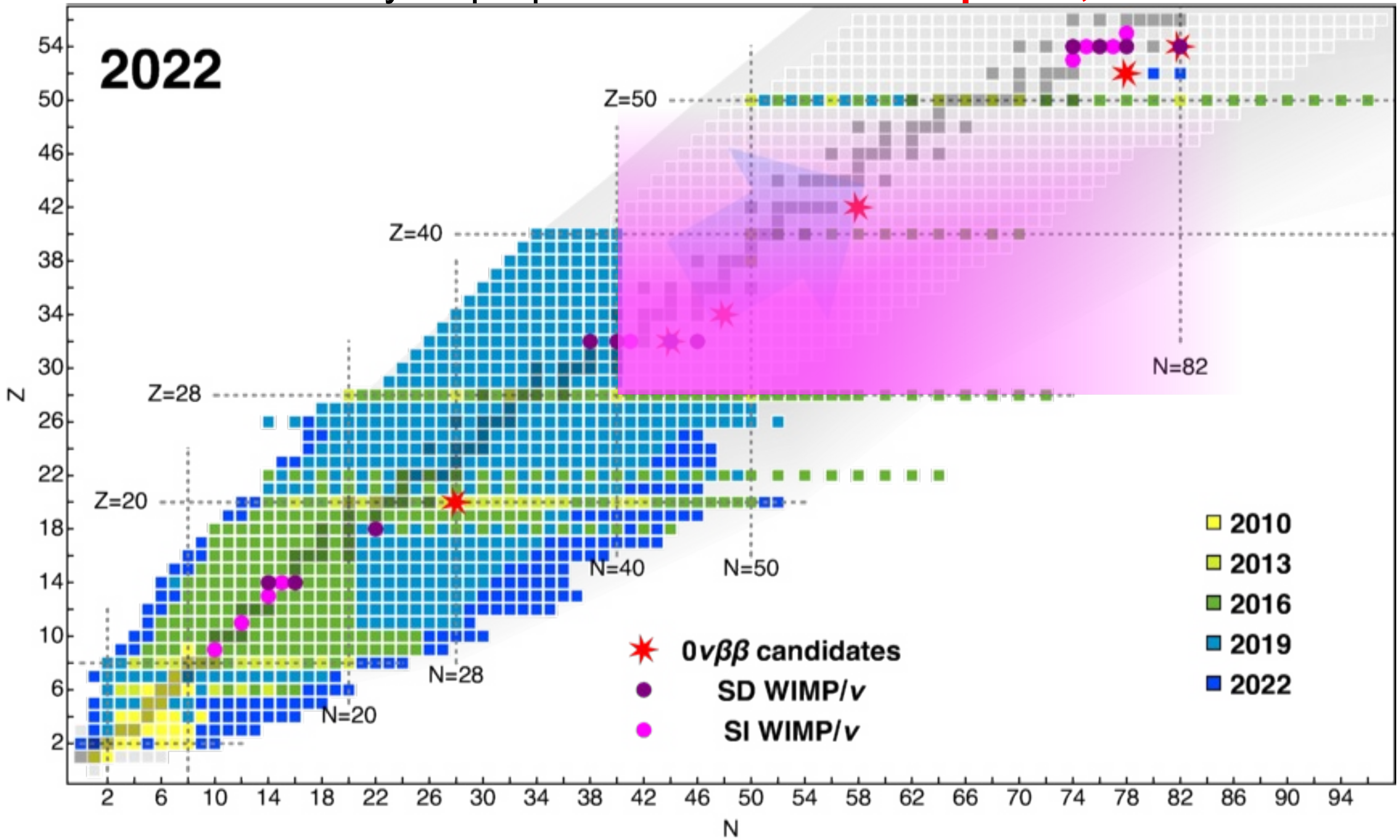
Constraints on Nuclear Symmetry Energy Parameters
J. Lattimer (2023)



Ab Initio Progress: How Heavy Can We Go?

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

Calculate essentially all properties all of nuclei… **up to N, Z ~ 50**



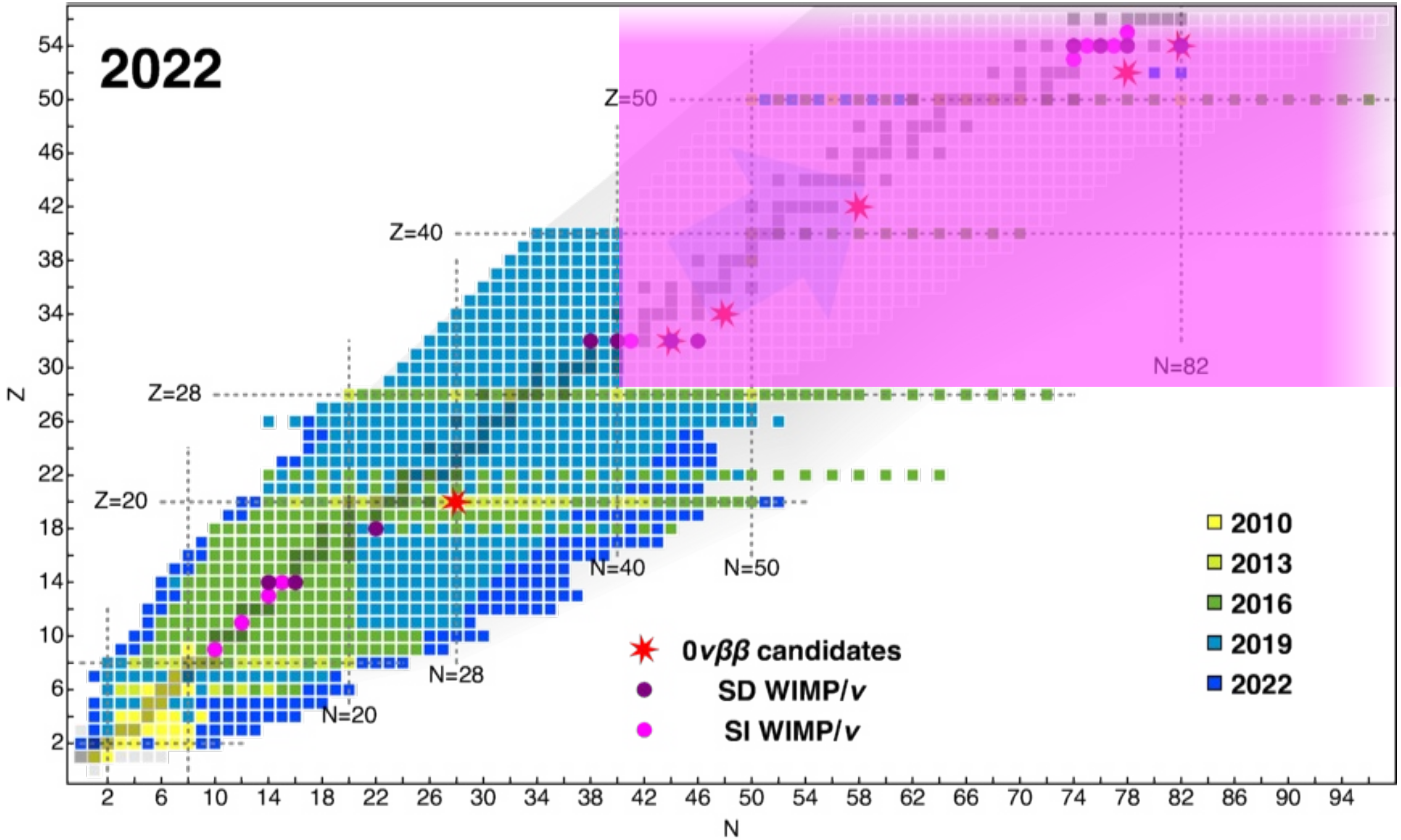
Key Limitation

3NF matrix element storage

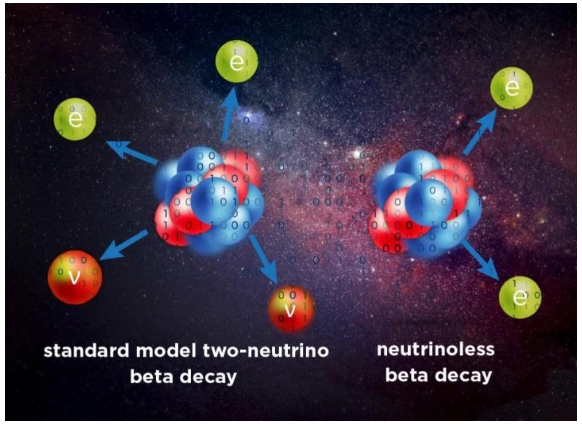
$$e_1 + e_2 + e_3 \leq E_{3\mathrm{max}}$$

Recalibrating Ab Initio Progress

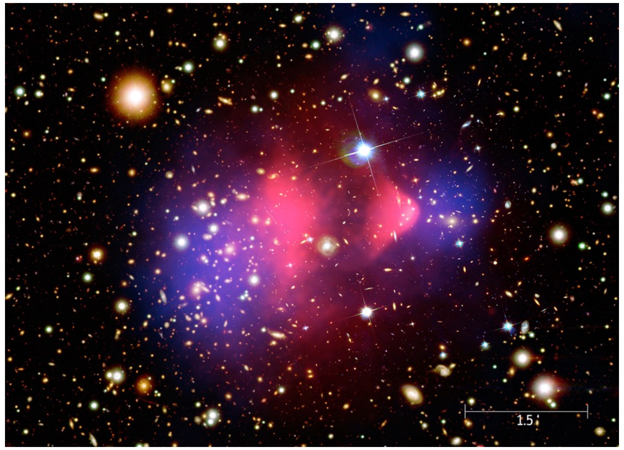
Rapid progress in ab initio reach, due to valence-space approach… up to...



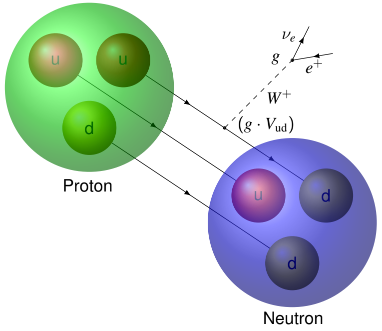
Searches for BSM Physics



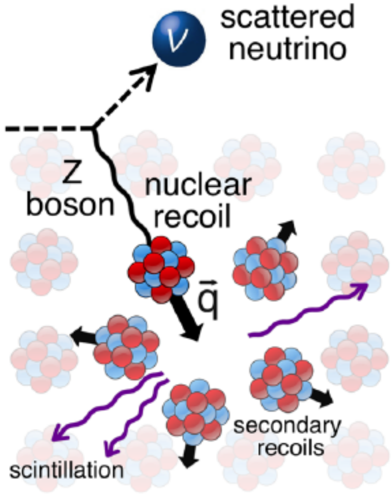
Neutrinoless double beta decay



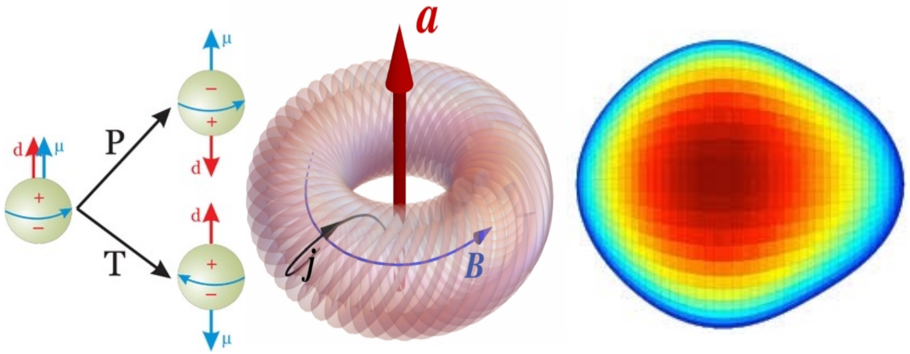
Dark matter direct detection



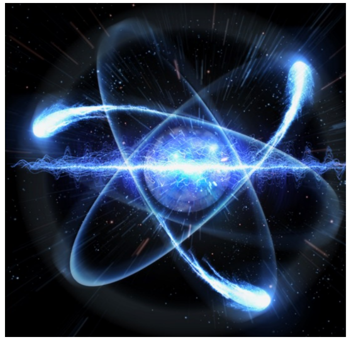
Superallowed Fermi transitions



Neutrino scattering

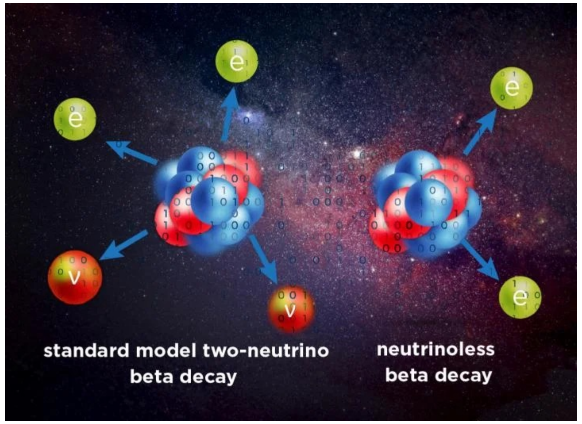


Symmetry-violating moments

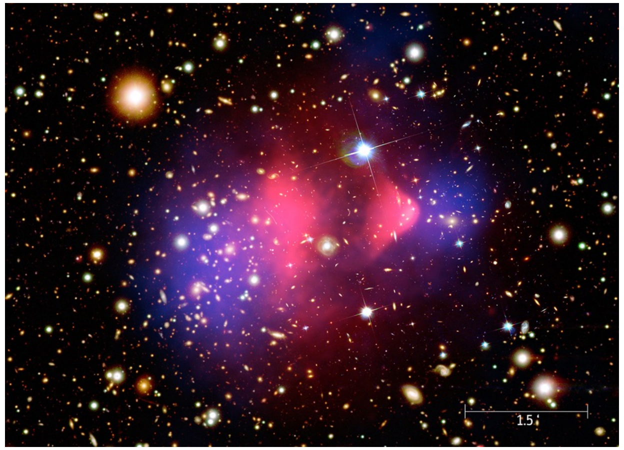


Atomic theory

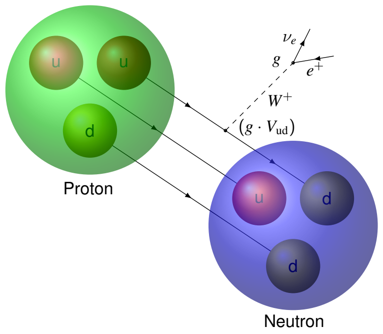
Searches for BSM Physics



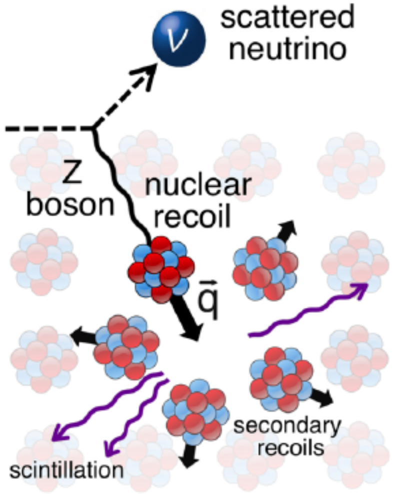
Neutrinoless double beta decay



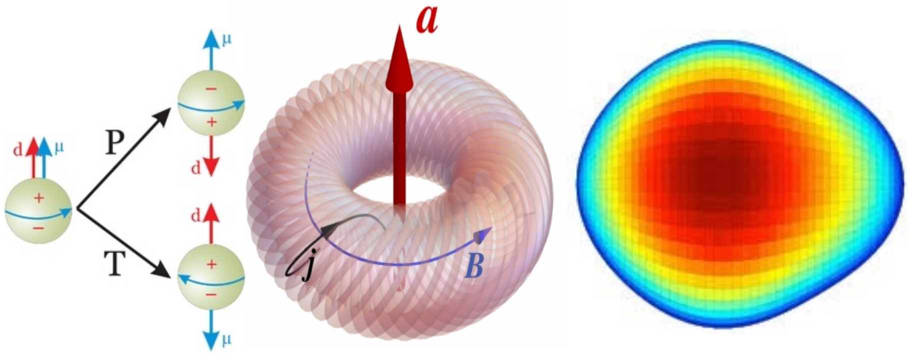
Dark matter direct detection



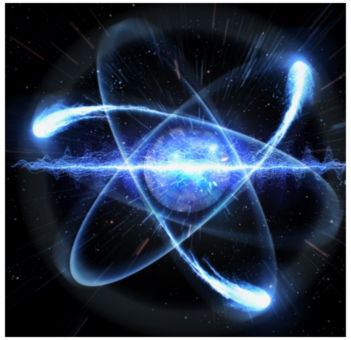
Superallowed Fermi transitions



Neutrino scattering



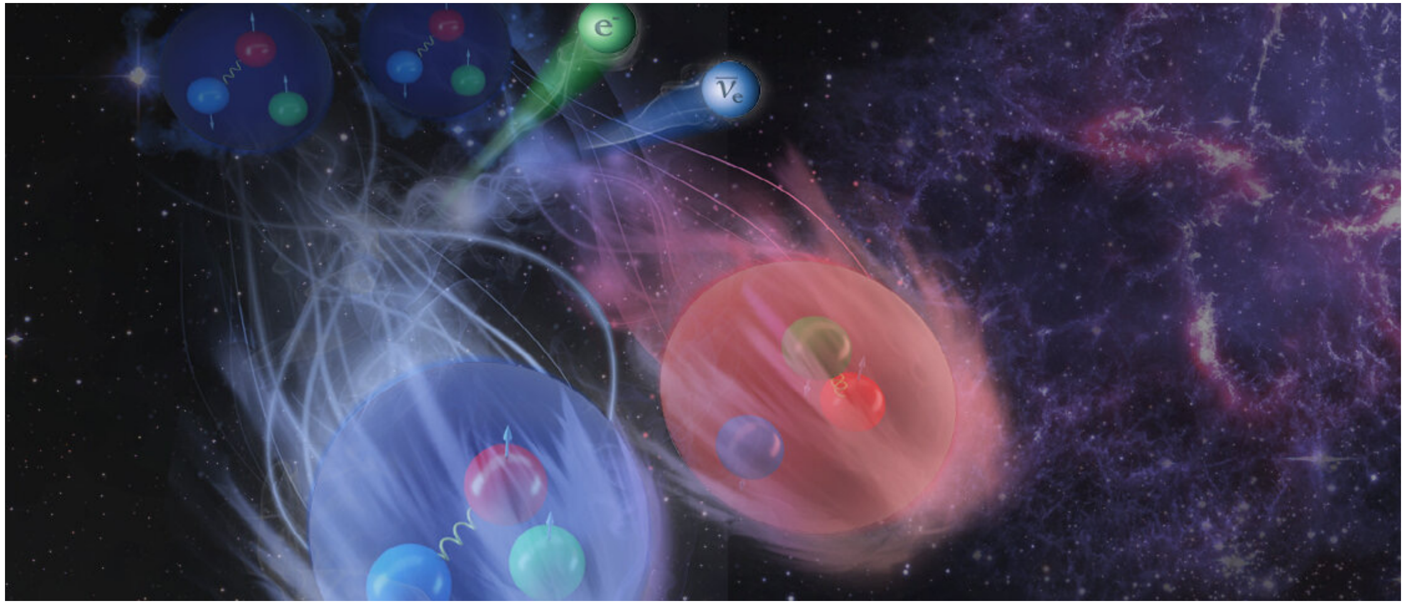
Symmetry-violating moments



Atomic theory

TRIUMF

Two-Body Currents for Gamow-Teller Transitions and g_A Quenching



LETTERS
https://doi.org/10.1038/s41567-019-0450-7
nature physics

Discrepancy between experimental and theoretical β-decay rates resolved from first principles

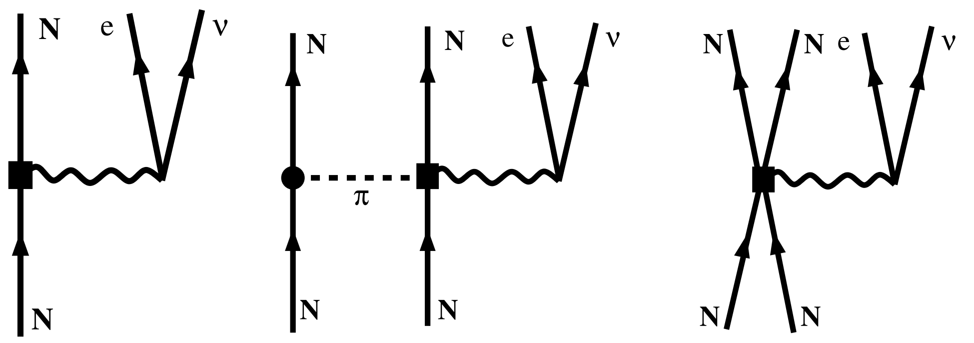
P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

TRIUMF

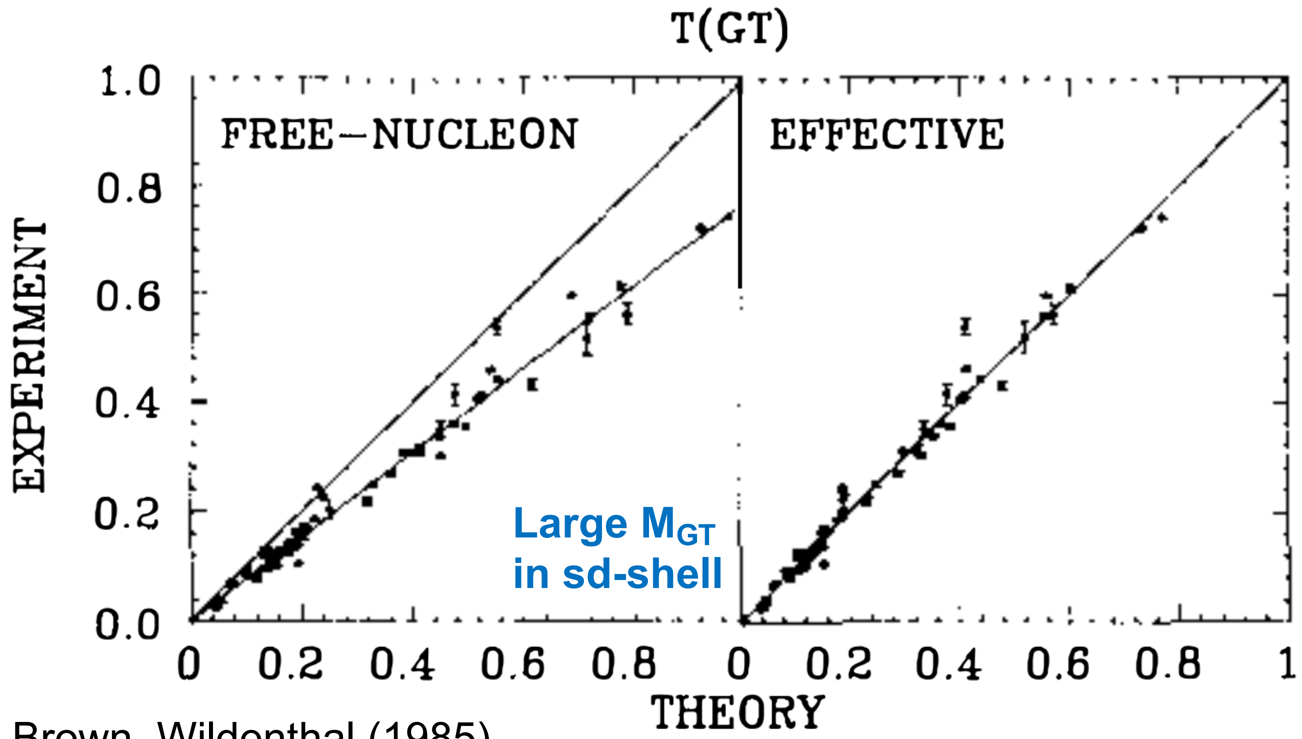
Beta-Decay "Puzzle": Quenching of g_A

Long-standing problem in weak decays: experimental values systematically smaller than theory

$$M_{\rm GT} = g_A \langle f | \mathcal{O}_{\rm GT} | i \rangle \quad \mathcal{O}_{\rm GT} = \mathcal{O}^{\rm 1b}_{\sigma\tau} + \mathcal{O}^{\rm 2b}_{2BC}$$



Using $g_A^{\rm eff} \approx 0.77 \times g_A^{\rm free}$ agrees with data



Brown, Wildenthal (1985)

- Missing wavefunction correlations
- Renormalized VS operator?
- Neglected two-body currents?
- Model-space truncations?

Explore in ab initio framework

Large-Scale Efforts for Ab Initio GT Transitions

Calculate **large GT matrix elements**

$$M_{\mathrm{GT}} = g_A \langle f | \mathcal{O}_{\mathrm{GT}} | i \rangle$$

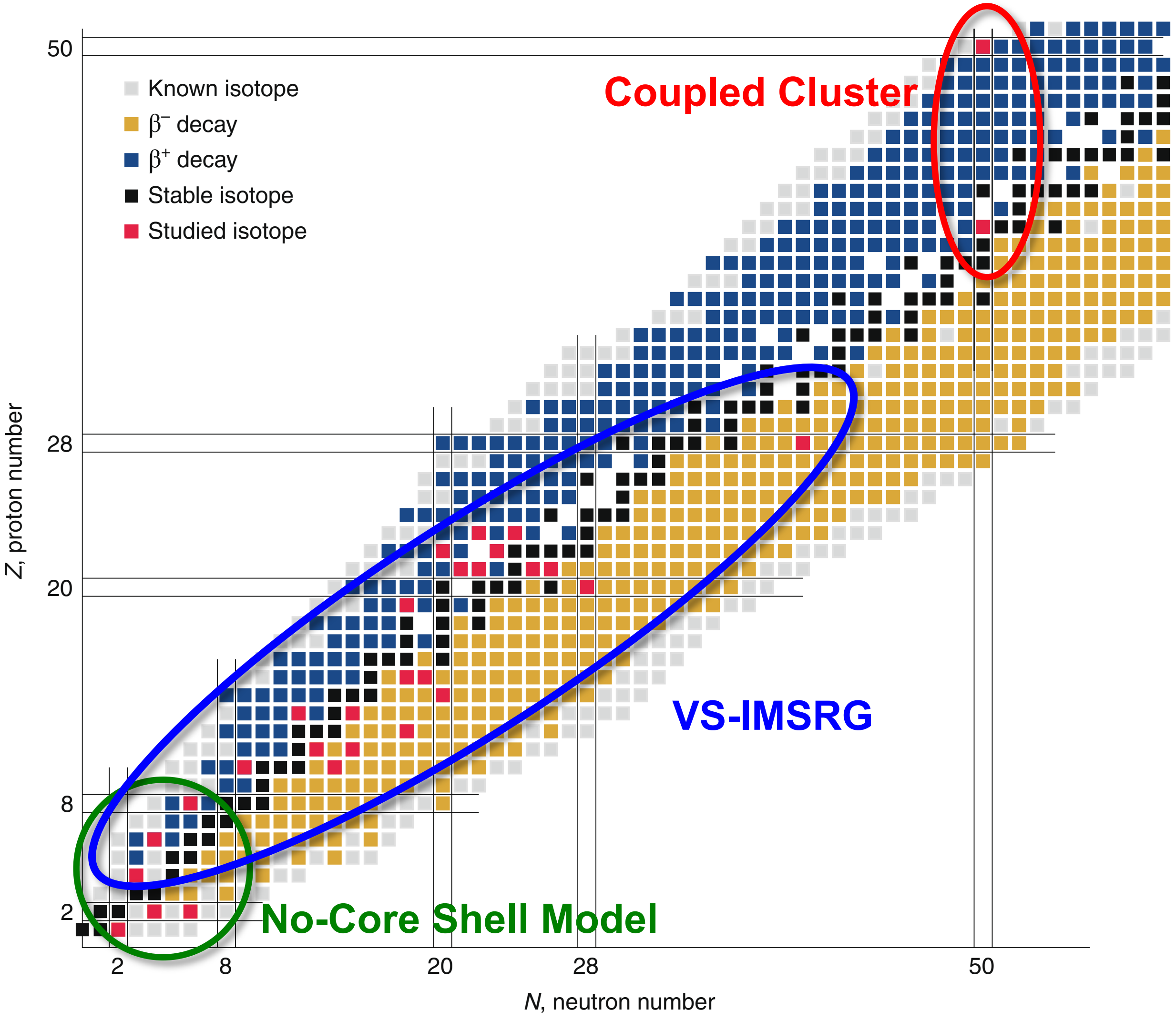
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

- Light, medium, and heavy regions
- Benchmark different ab initio methods
- Range of NN+3N forces
- Consistent inclusion of 2BC

NUCLEAR PHYSICS

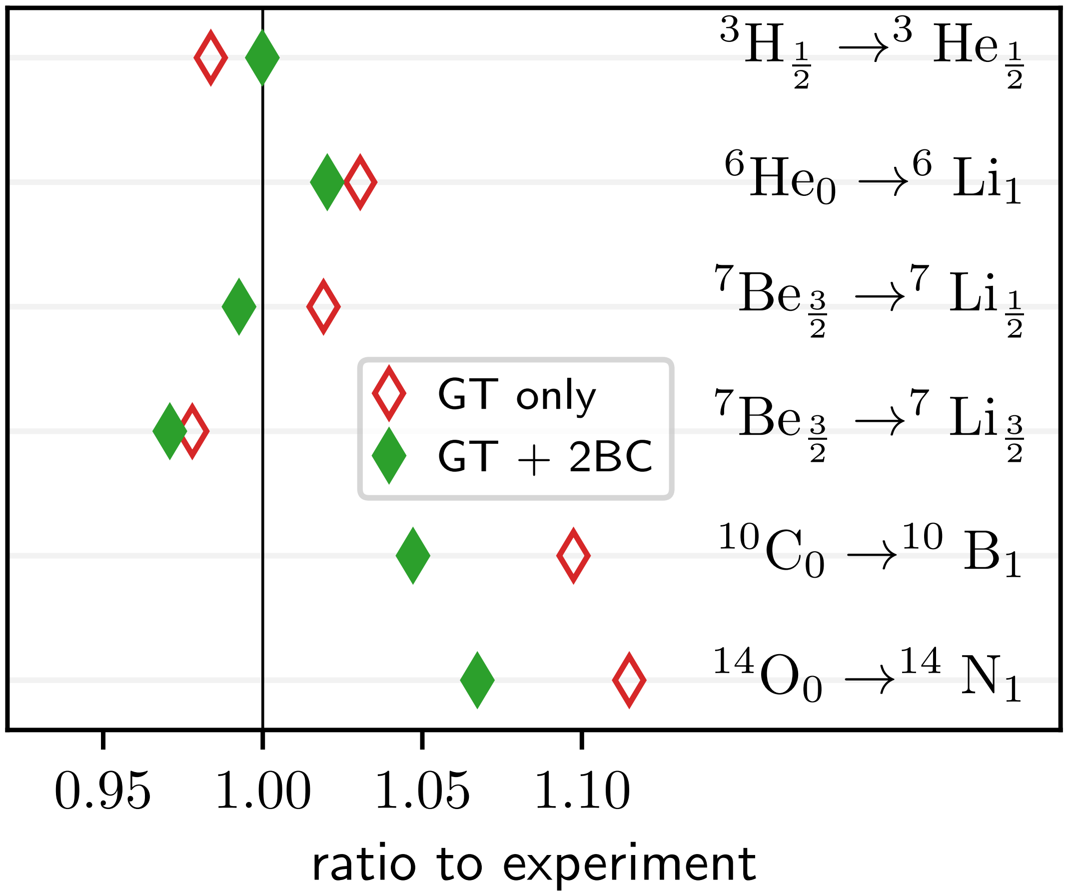
Beta decay gets the ab initio treatment

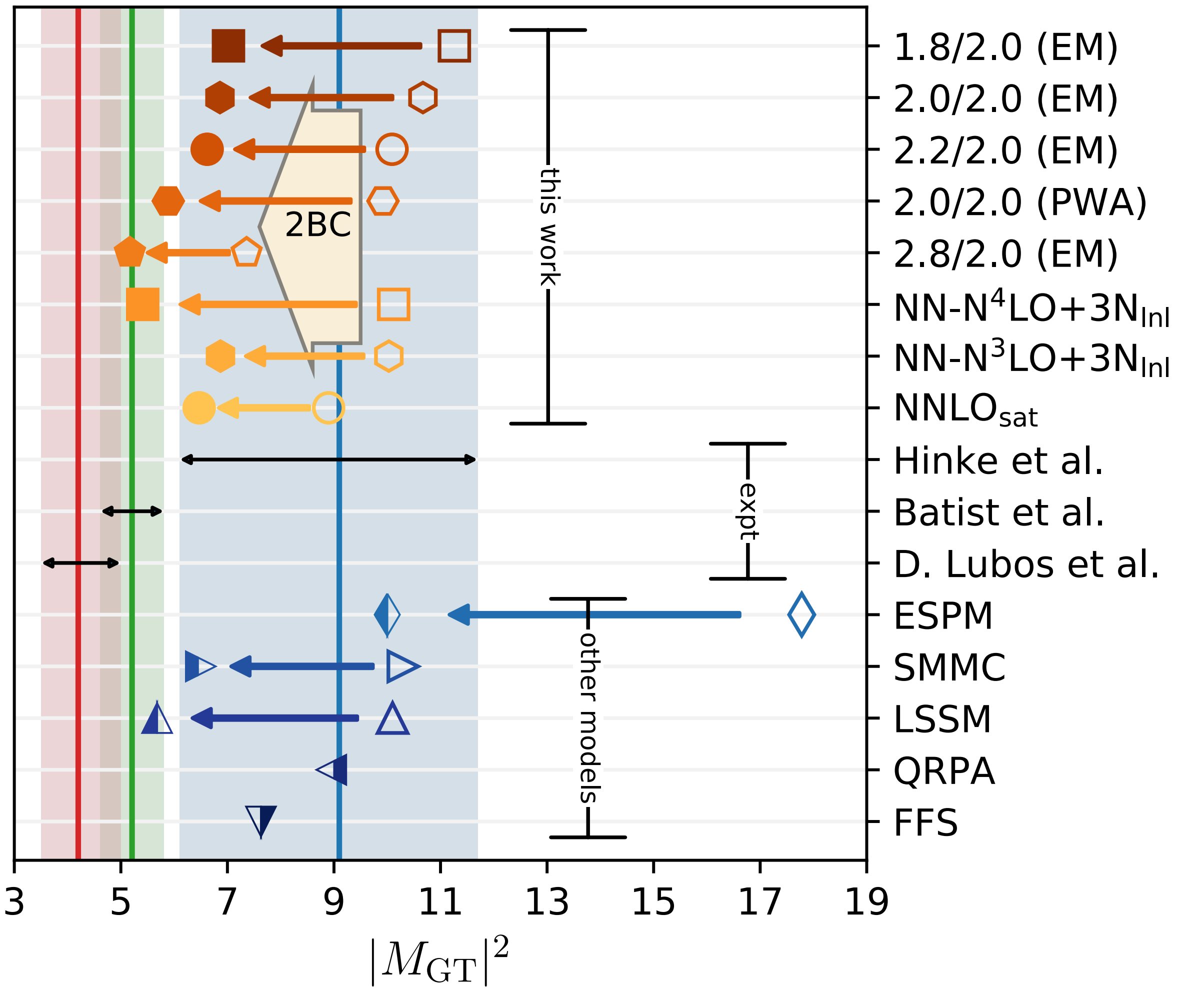
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.



GT Transitions in Light Nuclei + ^{100}Sn

NCSM in light nuclei, **CC** calculations of GT transition in ^{100}Sn from different forces





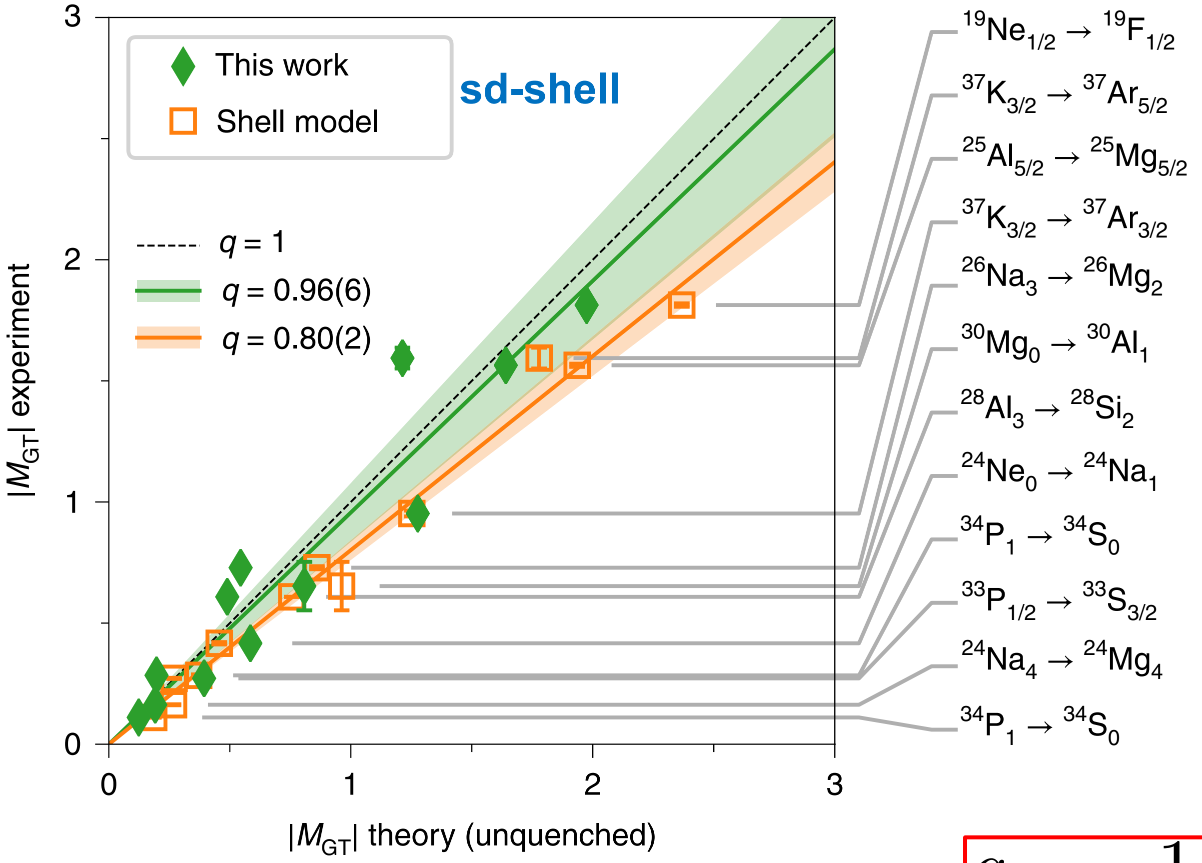
Large quenching from correlations in ^{100}Sn

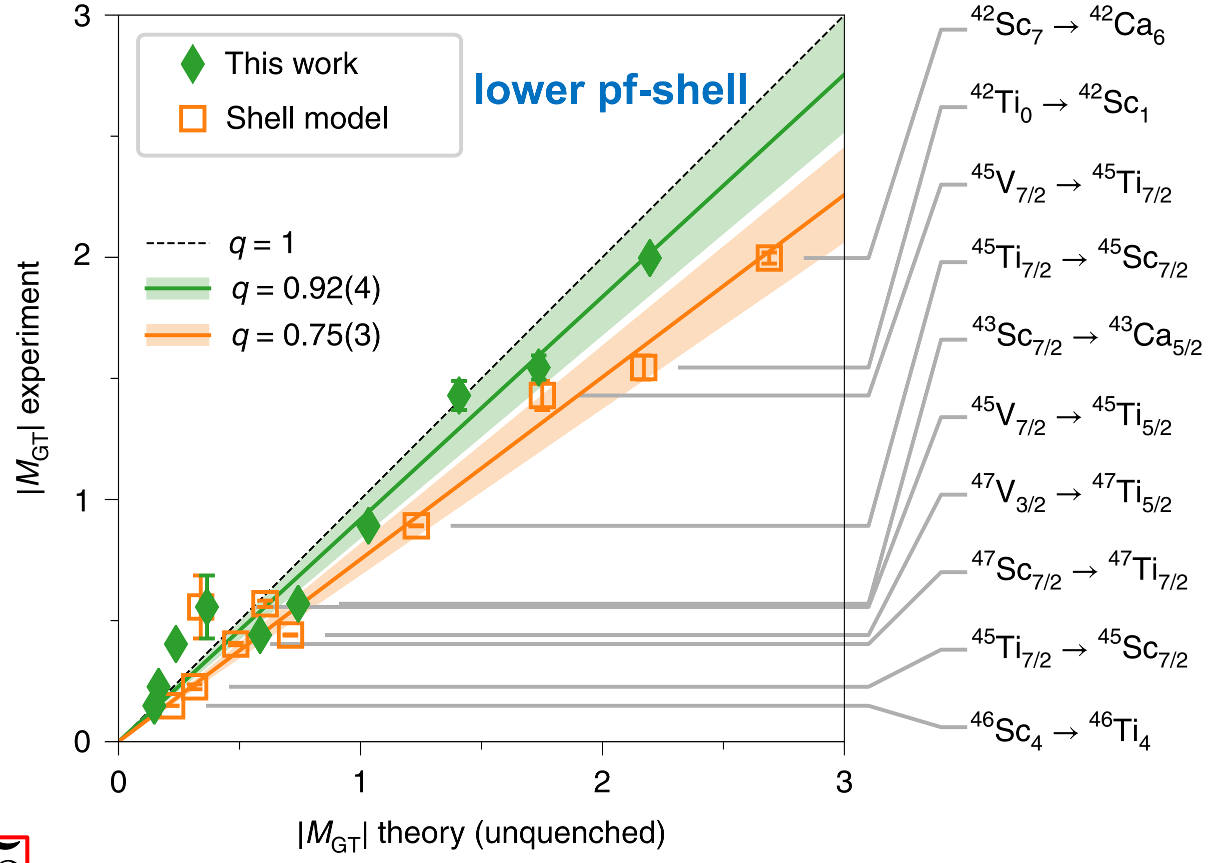
Addition of 2BC further quenches; reduces spread in results

TRIUMF

Solution to g_A-Quenching Problem

VS-IMSRG calculations throughout sd and pf shells





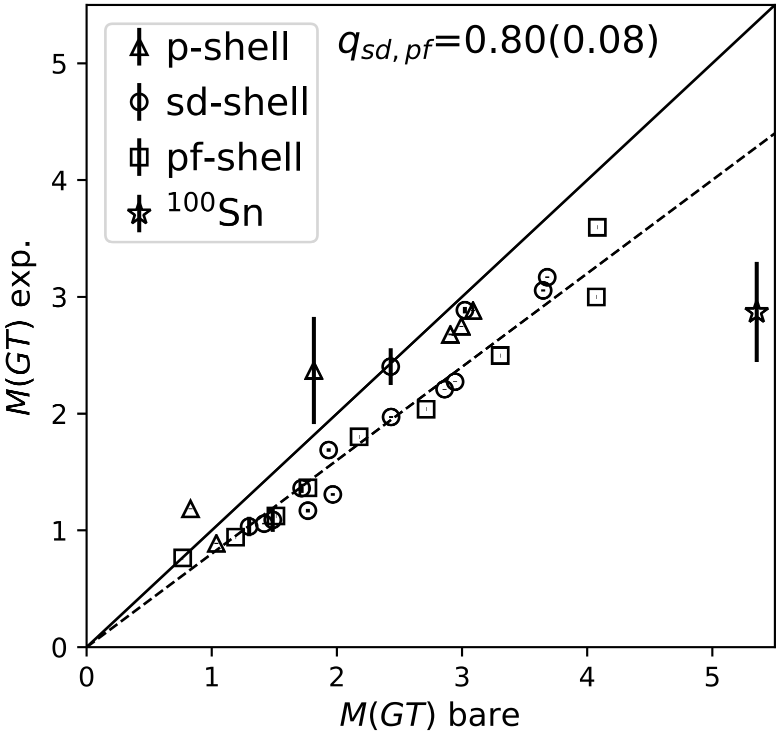
$$g_A = 1.25$$

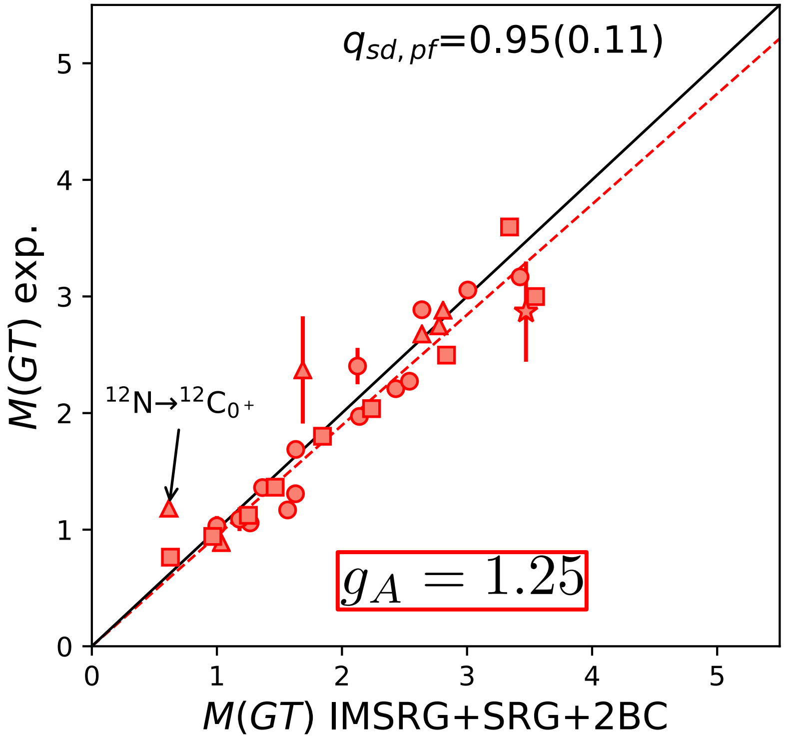
Ab initio calculations across the chart explain data with unquenched g_A

Refine results: improvements in forces and many-body methods

Complete GT Picture: Light to ^{100}Sn

Ab initio calculations throughout sd and pf shells





Stroberg (2021)

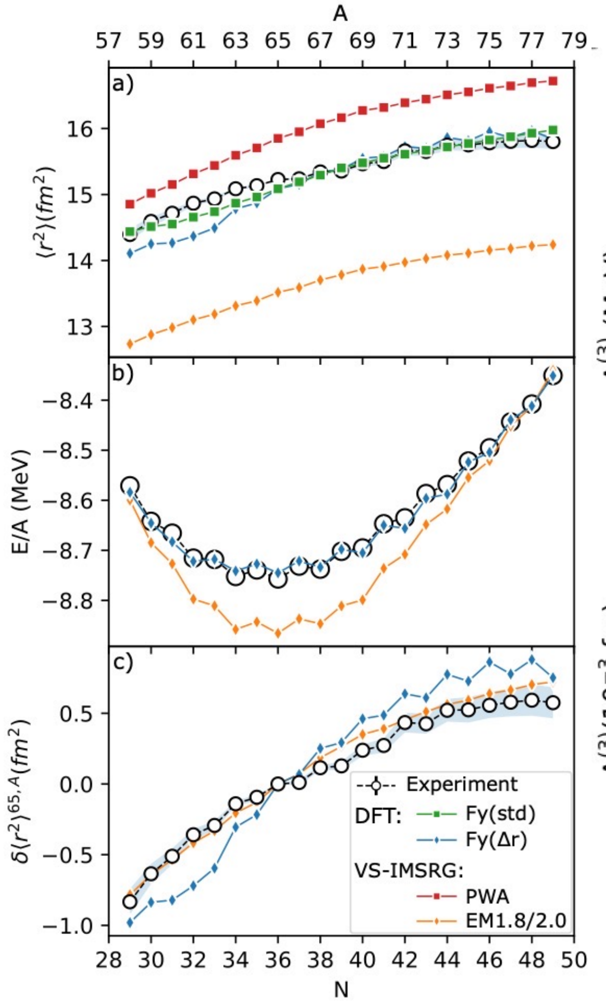
Ab initio calculations across the chart explain data with unquenched g_A

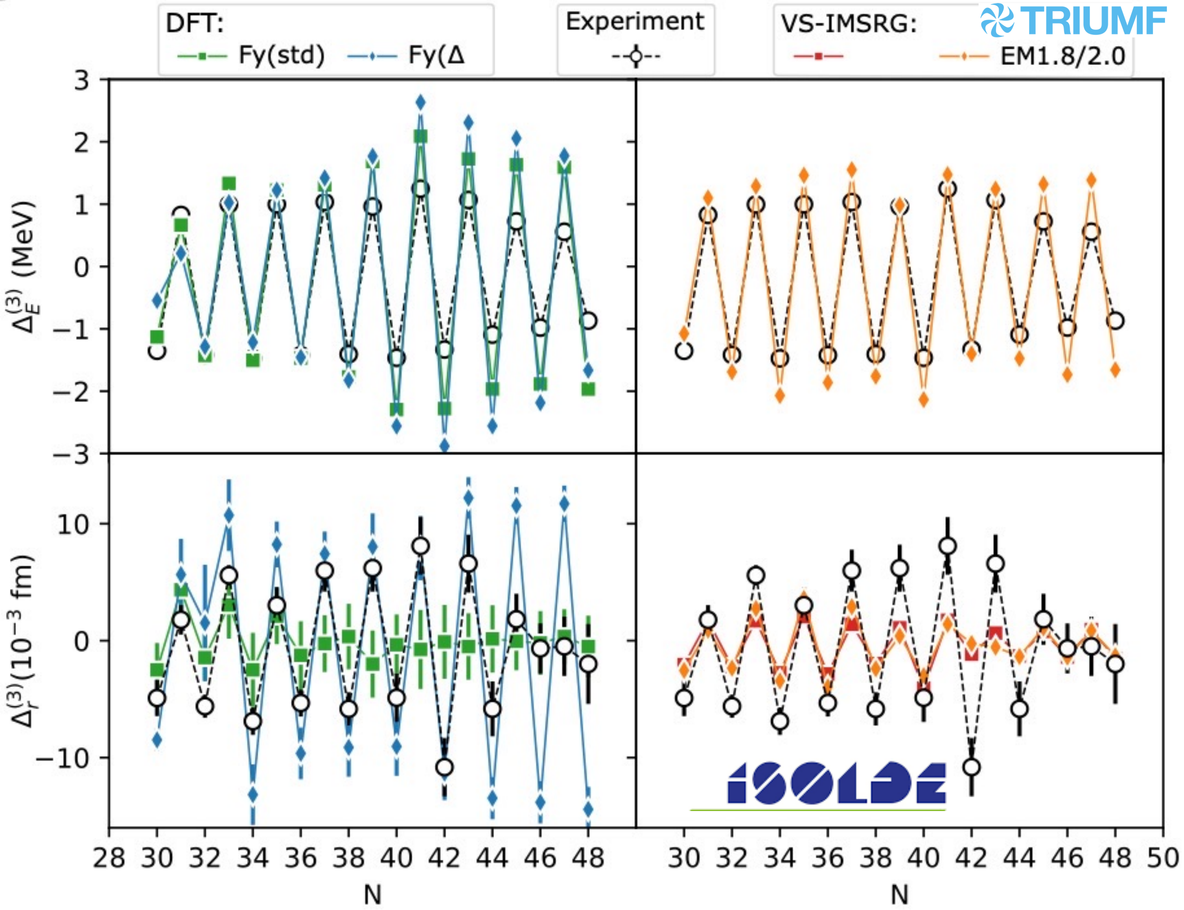
Including p-shell: q=0.99(21)

Laser Spectroscopy: Charge Radii of Cu Isotopes

TRIUMF

Odd-even staggering of charge radii across Cu chain





LETTERS

https://doi.org/10.1038/s41567-020-0868-y

nature physics

Check for updates

OPEN

Measurement and microscopic description of odd–even staggering of charge radii of exotic copper isotopes

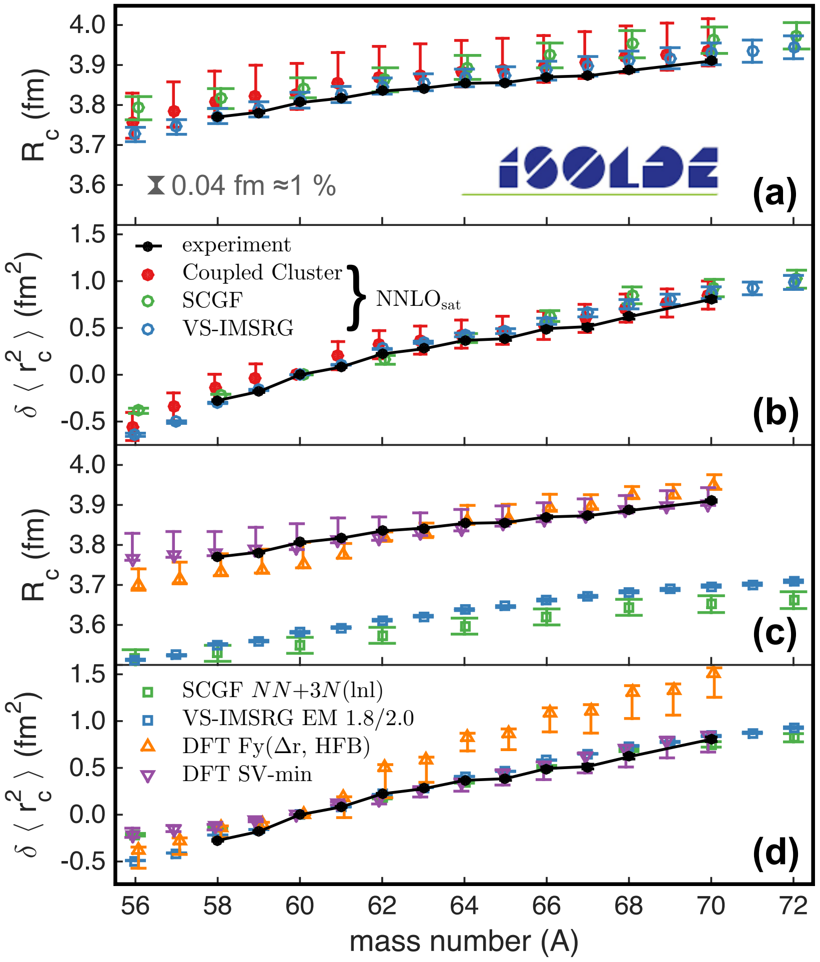
R. P. de Groote[1,2], J. Billowes[3], C. L. Binnersley[3], M. L. Bissell[3], T. E. Cocolios[1], T. Day Goodacre[4,5], G. J. Farooq-Smith[1], D. V. Fedorov[6], K. T. Flanagan[3], S. Franchoo[7], R. F. Garcia Ruiz[3,8,9], W. Gins[1,2], J. D. Holt[5,10], Á. Koszorús[1], K. M. Lynch[9], T. Miyagi[5], W. Nazarewicz[11], G. Neyens[1,9], P.-G. Reinhard[12], S. Rothe[3,4], H. H. Stroke[13], A. R. Vernon[1,3], K. D. A. Wendt[14], S. G. Wilkins[3,4], Z. Y. Xu[1] and X. F. Yang[1,15]

Cu isotopes, odd-even staggering well reproduced

Ab initio competitive with DFT (fit to reproduce odd-even staggering)

Laser Spectroscopy: Charge Radii of Ni Isotopes

Study charge radii systematics across Ni isotopic chain



Nuclear Charge Radii of the Nickel Isotopes $^{58-68,70}$Ni

S. Malbrunot-Ettenauer *et al.*
Phys. Rev. Lett. **128**, 022502 – Published 14 January 2022

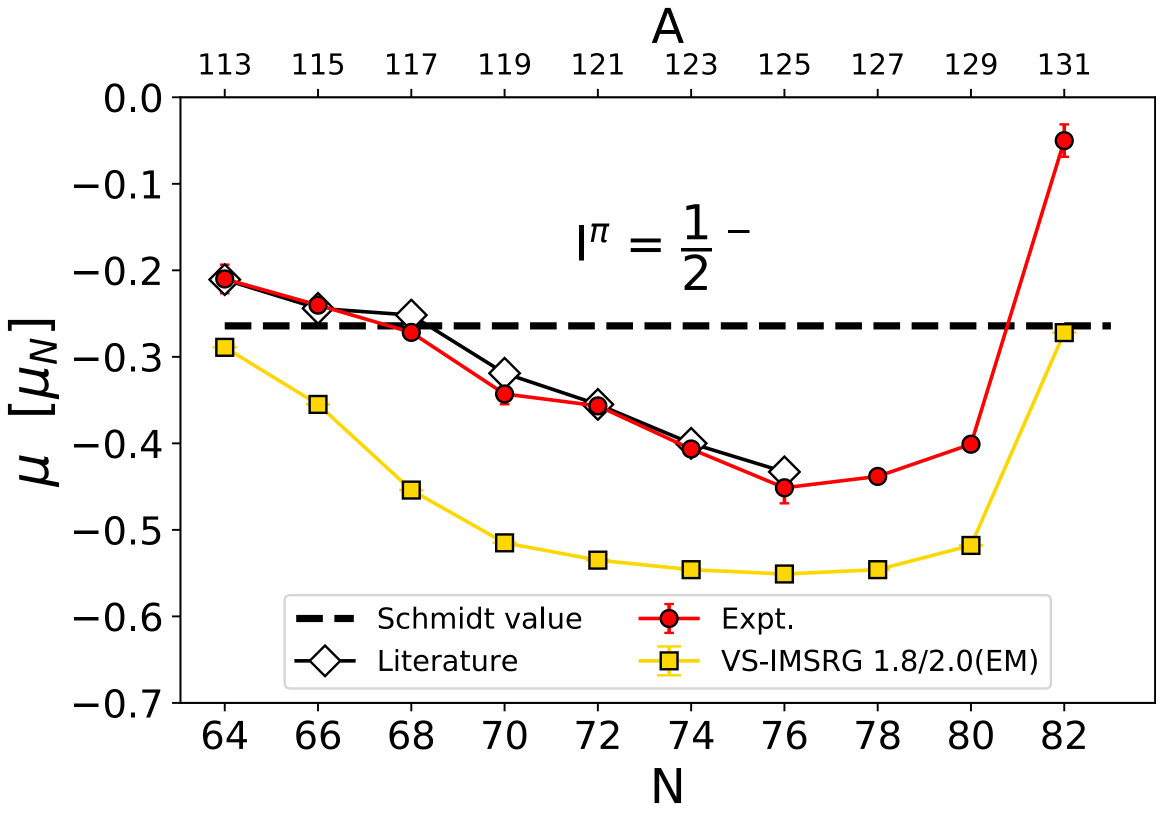
Multiple ab-initio methods largely agree within uncertainties

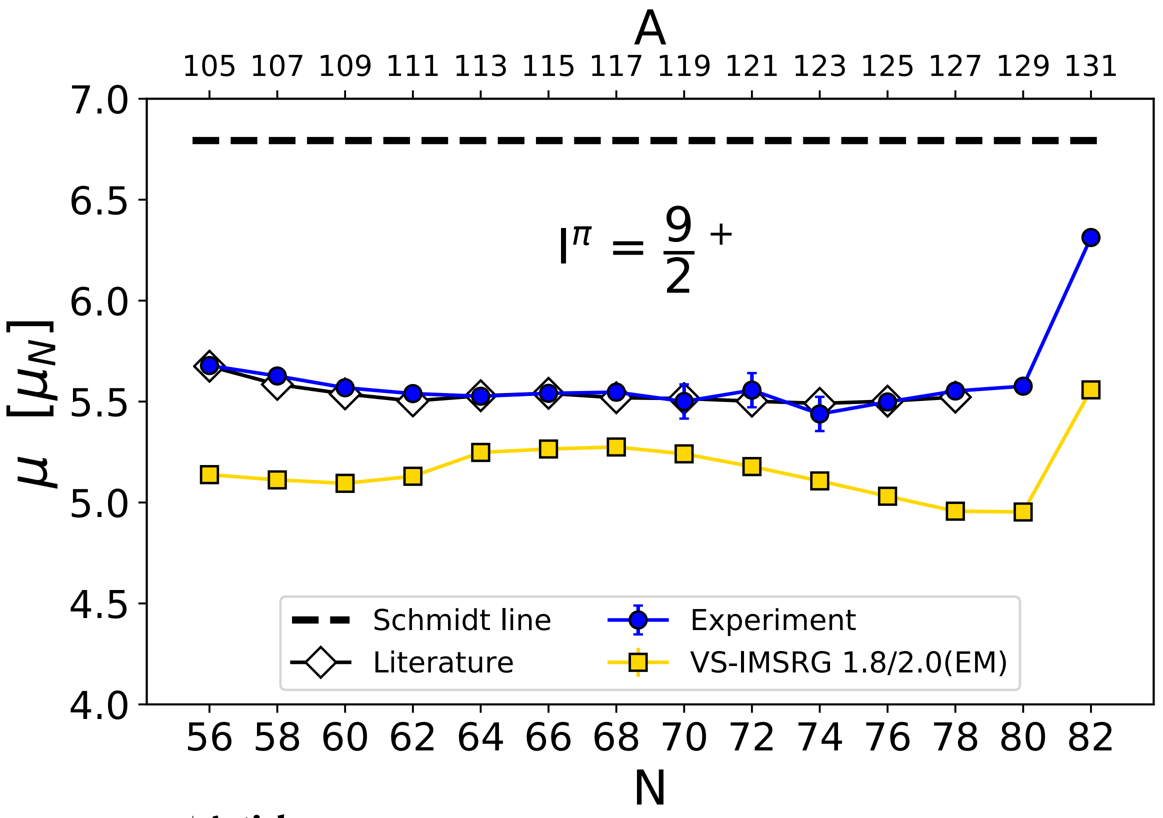
Ab initio (again) competitive with DFT

TRIUMF

EM Moments in Neutron-Rich In Isotopes

Electromagnetic moments of entire In chain – sharp increase at N=82





Ab initio reproduces trends of new measurements

Neglected physics: two-body meson-exchange currents

Article

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

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

Received: 10 June 2021

Accepted: 28 April 2022

Published online: 13 July 2022

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]

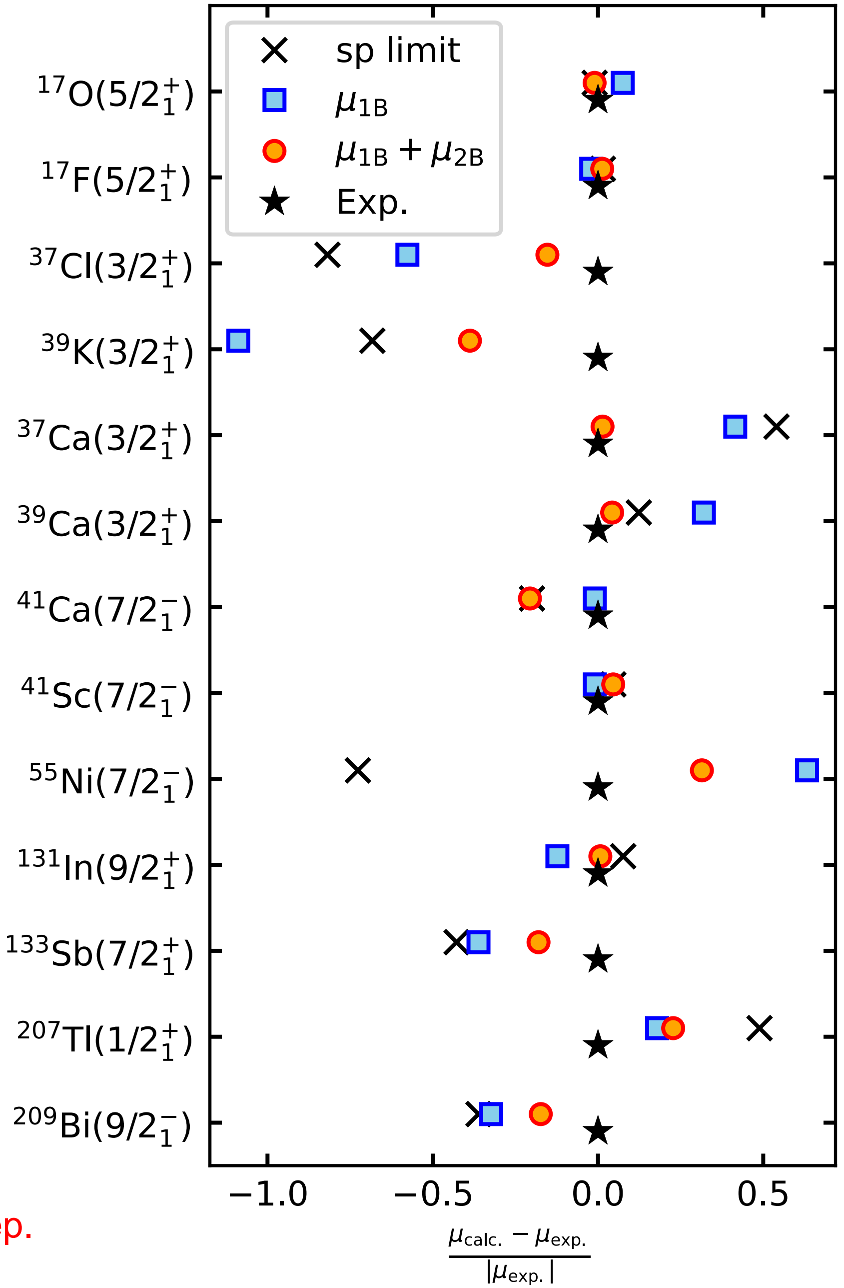
TRIUMF

Impact of Two-Body M1 Currents

Ab initio calculations throughout the nuclear chart

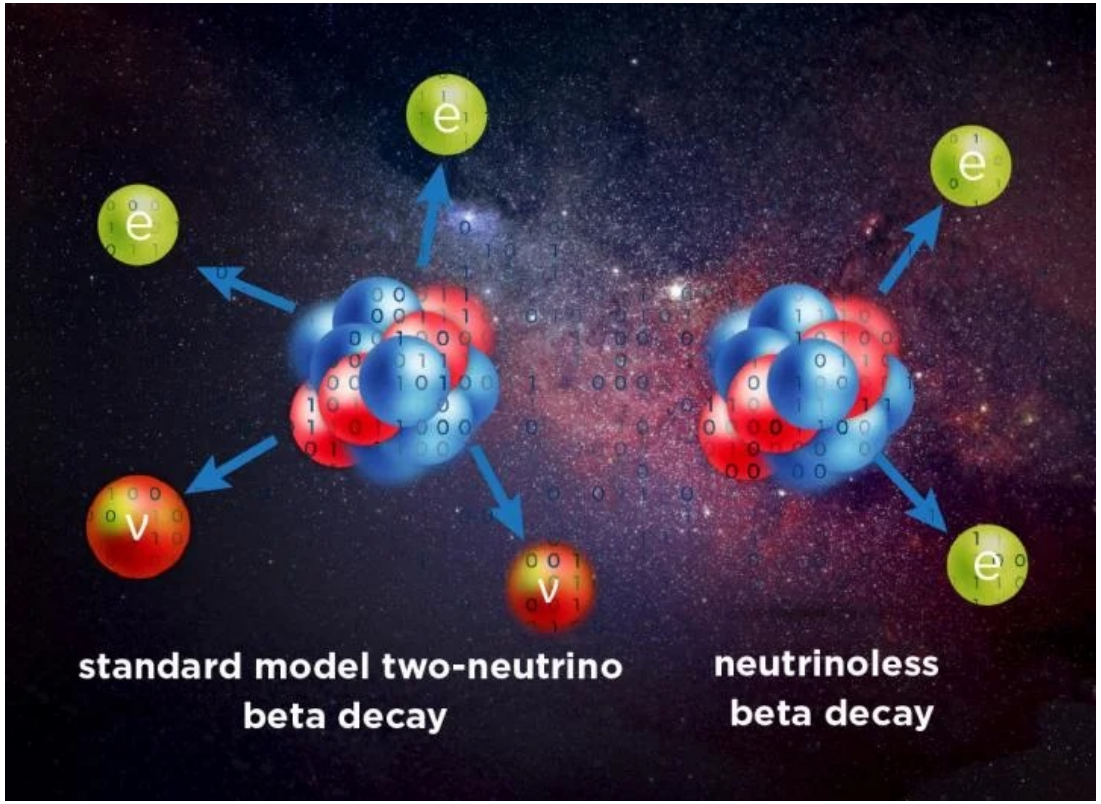
Including 2bc consistent with input forces

Magnetic moments significantly improved



T. Miyagi et al, in prep.

Neutrinoless Double Beta Decay NMEs for Major Players: ^{76}Ge, (^{100}Mo), ^{130}Te, ^{136}Xe



Ab Initio Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca

J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, and H. Hergert
Phys. Rev. Lett. **124**, 232501 – Published 11 June 2020

Ab Initio Neutrinoless Double-Beta Decay Matrix Elements for ^{48}Ca, ^{76}Ge, and ^{82}Se

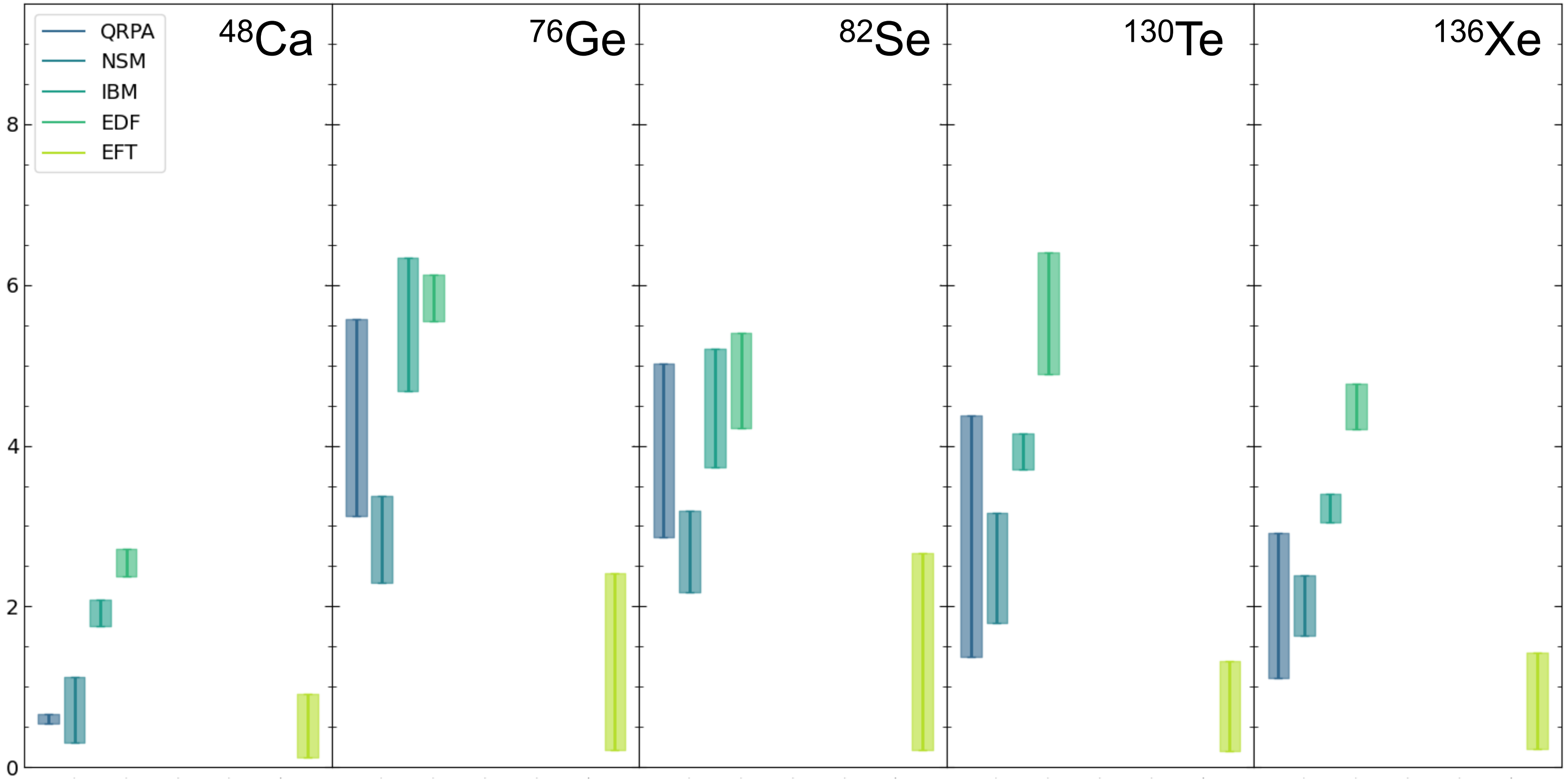
A. Belley, C. G. Payne, S. R. Stroberg, T. Miyagi, and J. D. Holt
Phys. Rev. Lett. **126**, 042502 – Published 29 January 2021

Coupled-Cluster Calculations of Neutrinoless Double-β Decay in ^{48}Ca

S. Novario, P. Gysbers, J. Engel, G. Hagen, G. R. Jansen, T. D. Morris, P. Navrátil, T. Papenbrock, and S. Quaglioni
Phys. Rev. Lett. **126**, 182502 – Published 7 May 2021

Current Status of NMEs

Calculations to date from phenomenological models; large spread in results



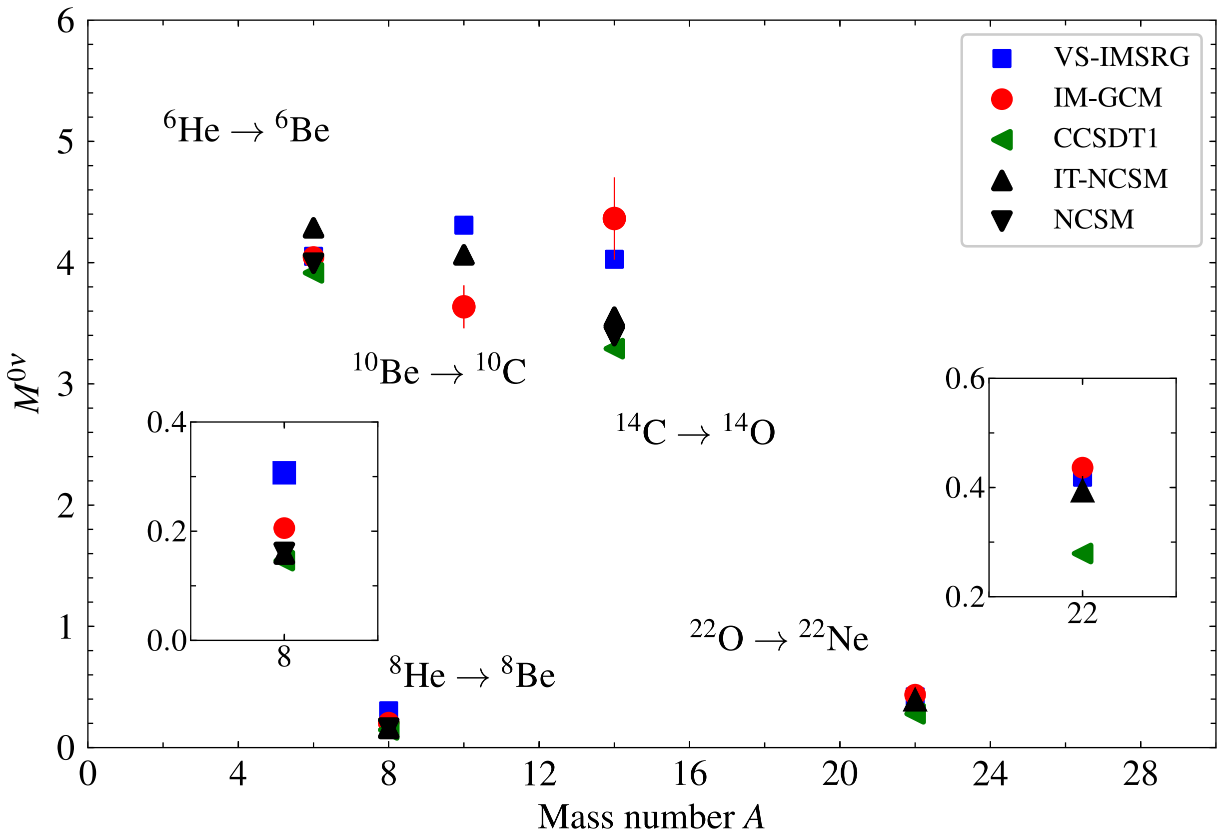
Compiled values from: Engel and Menéndez (2017); Brase et al, PRC (2022)

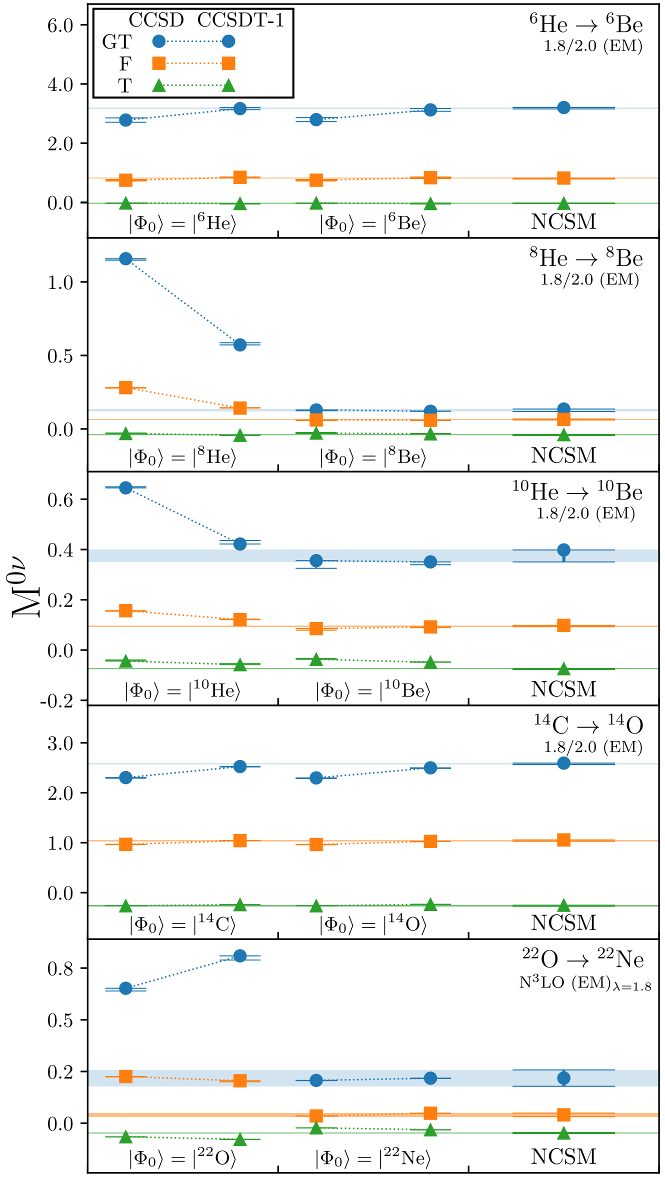
All models missing essential physics: correlations, single-particle levels, two-body currents

Address with ab initio theory

Strategy I: Benchmark NMEs in Light Nuclei

Benchmark with quasi-exact NCSM, IT-NCSM, IM-GCM, and CC in light systems: A=6-22





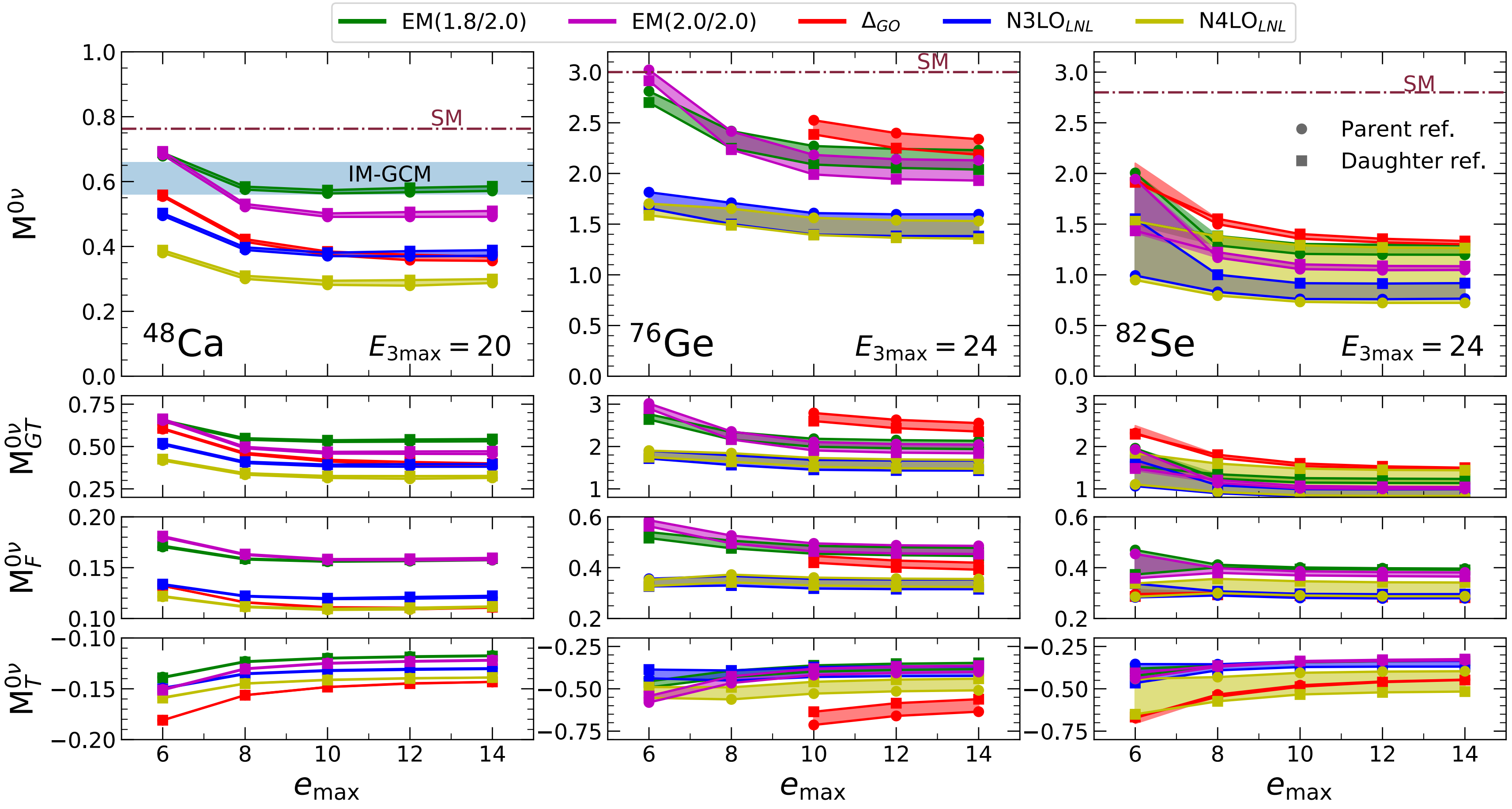
Reasonable to good agreement in all cases

Pursue true double-beta decay candidates!

Strategy II: "Uncertainties" from Input Forces

"Uncertainty" bands from input NN+3N forces with **5 chiral Hamiltonians**

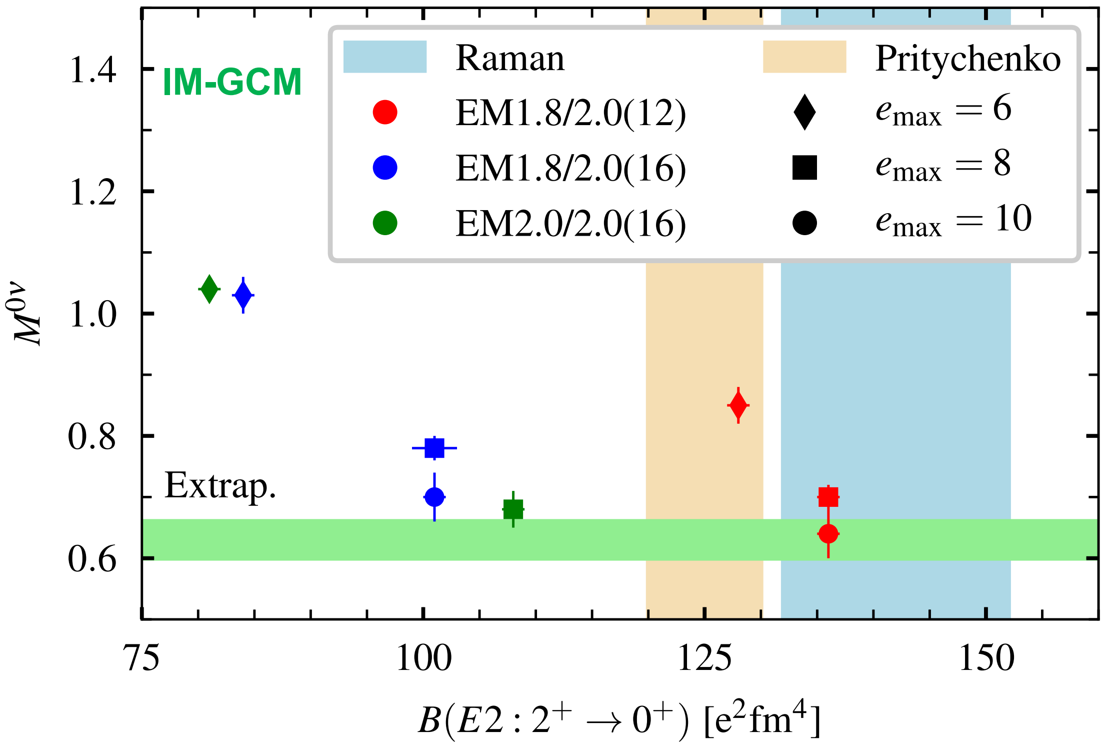
VS-IMSRG: clear convergence for ^{48}Ca, ^{76}Ge, ^{82}Se

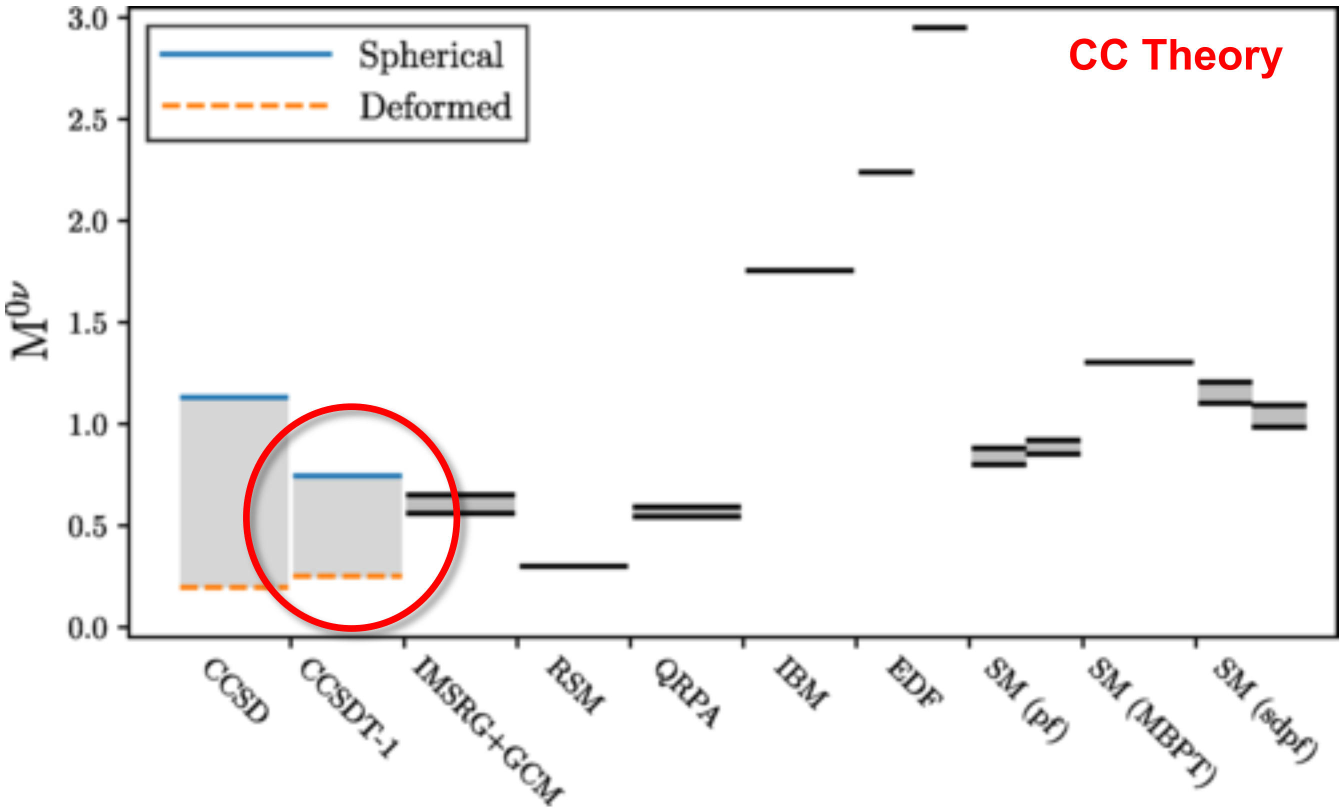


TRIUMF Strategy II: "Uncertainties" from Many-Body Methods

Calculations in ^{48}Ca from IM-GCM and CC theory using same interactions

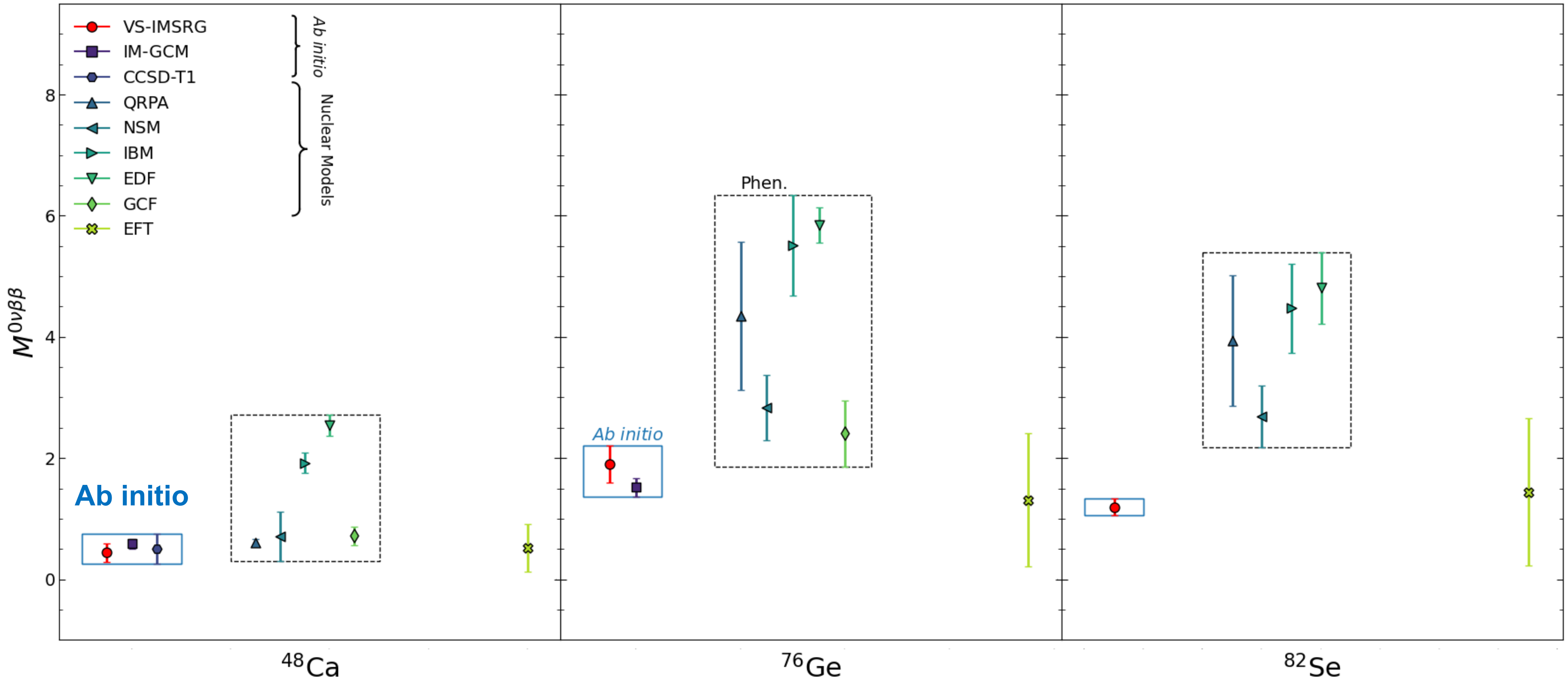
Key development: **treatment of deformation** in CC and IMSRG





First Ab Initio Results

Ab initio NMEs generally smaller than phenomenology; less spread from uncertainties



Ab initio results agree within uncertainties!

Promising results, but…

TRIUMF

The Year(s) We Lost Hope: Leading-Order Contact

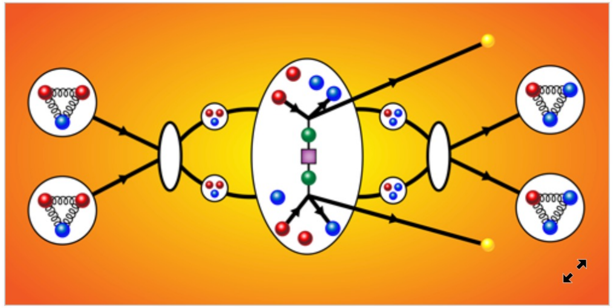
Proper renormalization requires short-range contact term at leading order

Physics — SYNOPSIS

A Missing Piece in the Neutrinoless Beta-Decay Puzzle

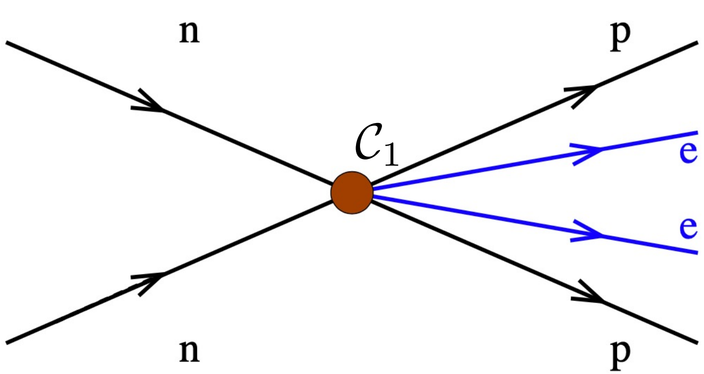
May 16, 2018 • *Physics* 11, s58

The inclusion of short-range interactions in models of neutrinoless double-beta decay could impact the interpretation of experimental searches for the elusive decay.



J. de Vries/Nikhef; adapted by APS/Alan Stonebraker

Cirigliano et al. PRL (2018)



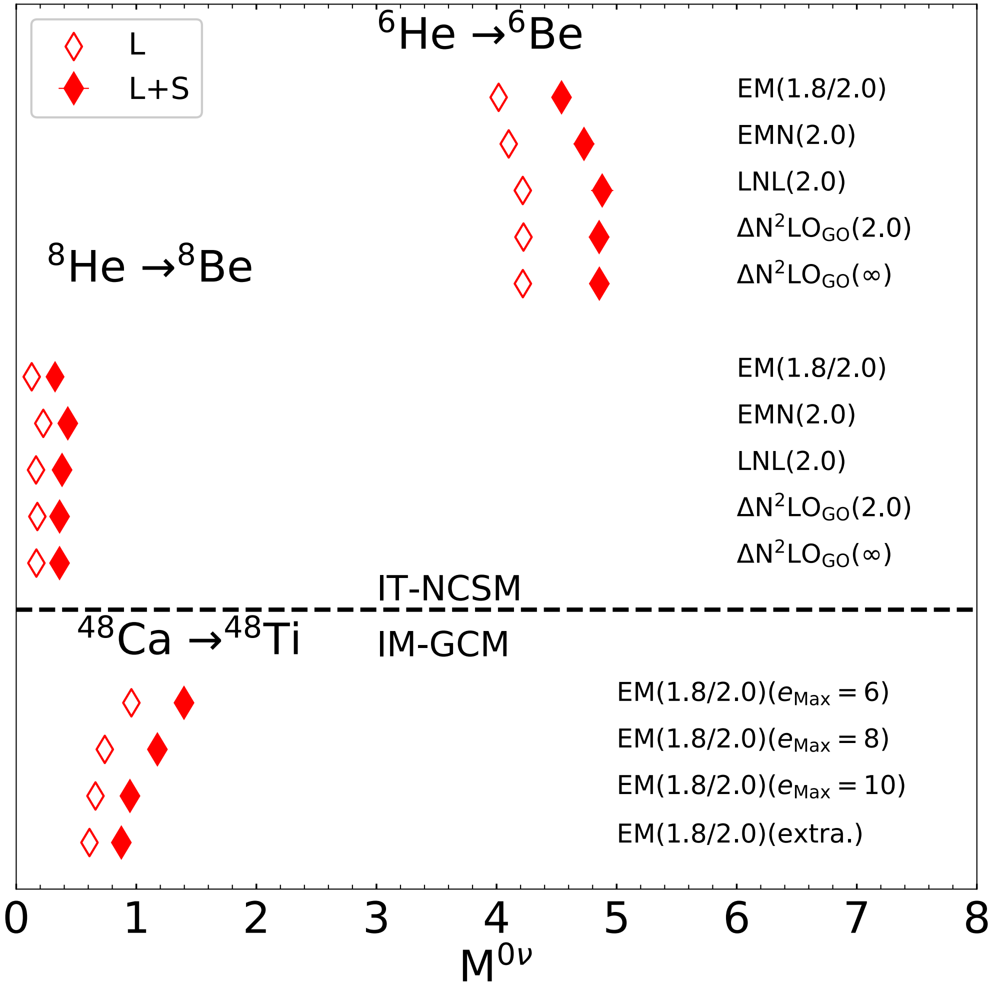
New physics inside blob:
High-energy ν exchange

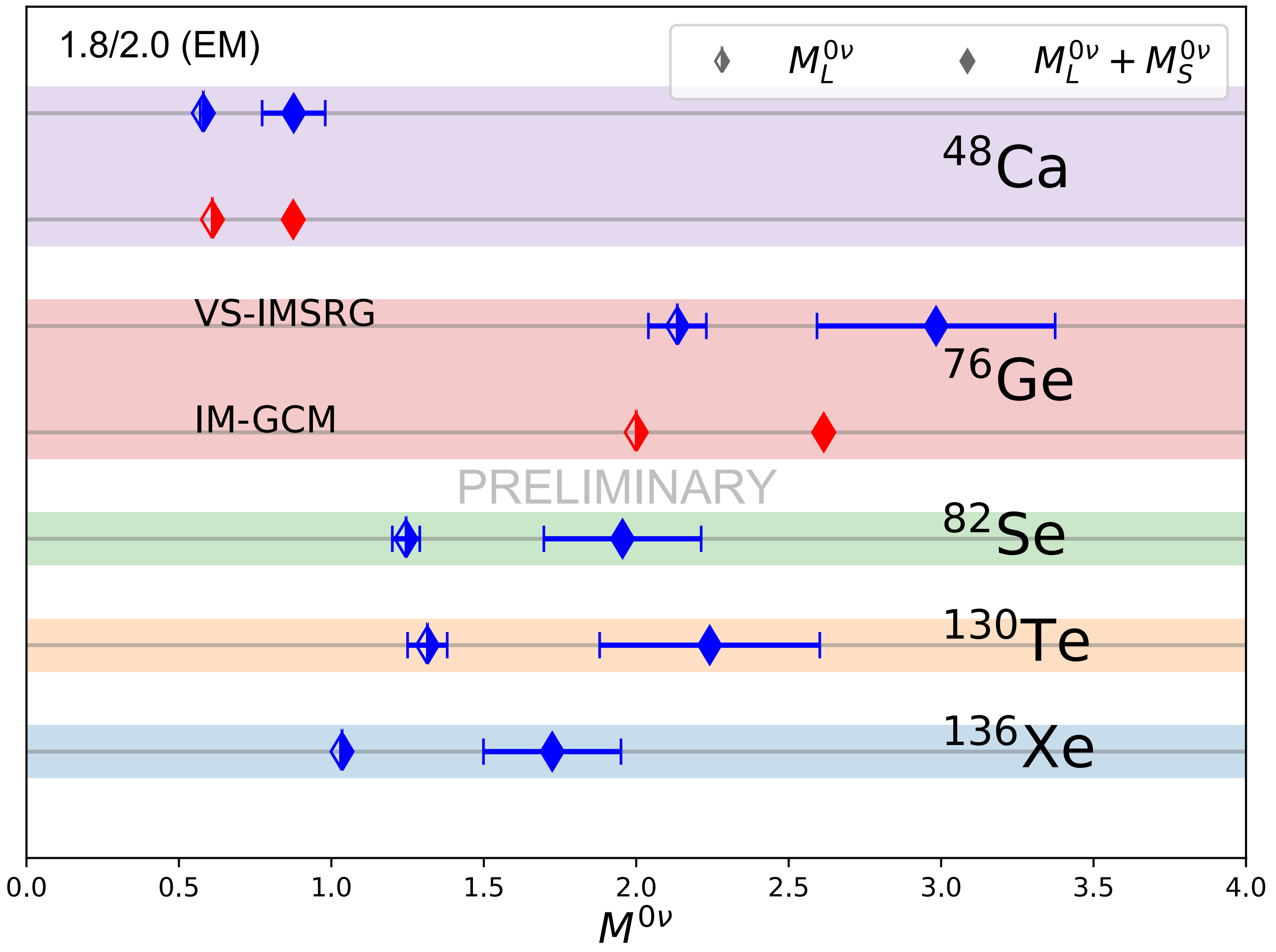
New paradigm for 0νββ decay: include long- and short-range terms

$$M^{0\nu} \to M_L + M_S = M_{\rm GT} + \frac{M_{\rm F}}{g_A^2} + M_{\rm T} + M_{\rm CT}$$

The Year We Regained Hope: Coupling Constant Fit

Match nn → pp+ee amplitude from approximate QCD methods: estimate contact term to 30%

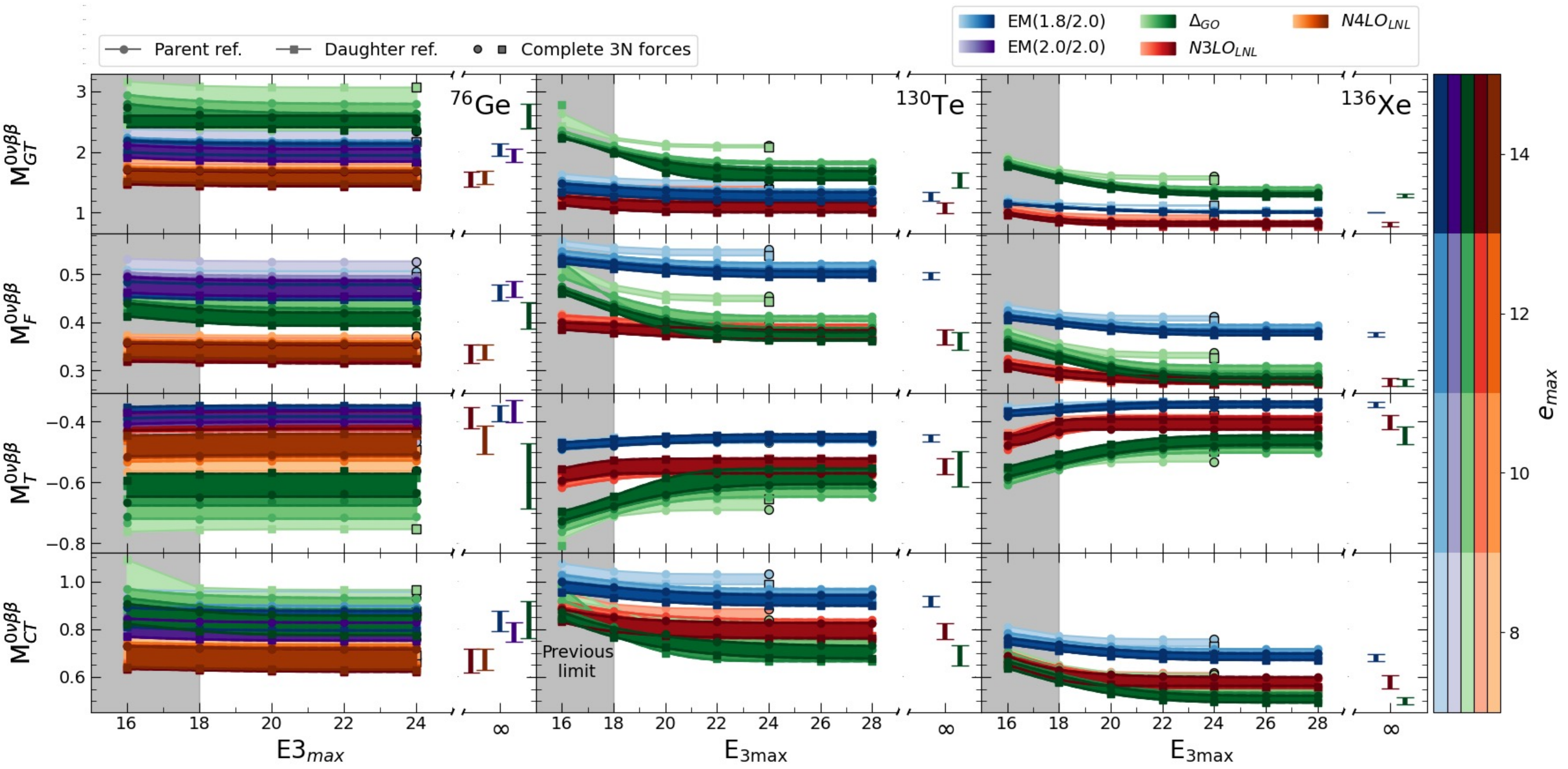




Increase of 40% (^{76}Ge) to 60% (^{130}Te/^{136}Xe)

Ab Initio Predictions in Heavy Nuclei

Converged NMEs for major players in global searches: ^{76}Ge, ^{130}Te, ^{136}Xe

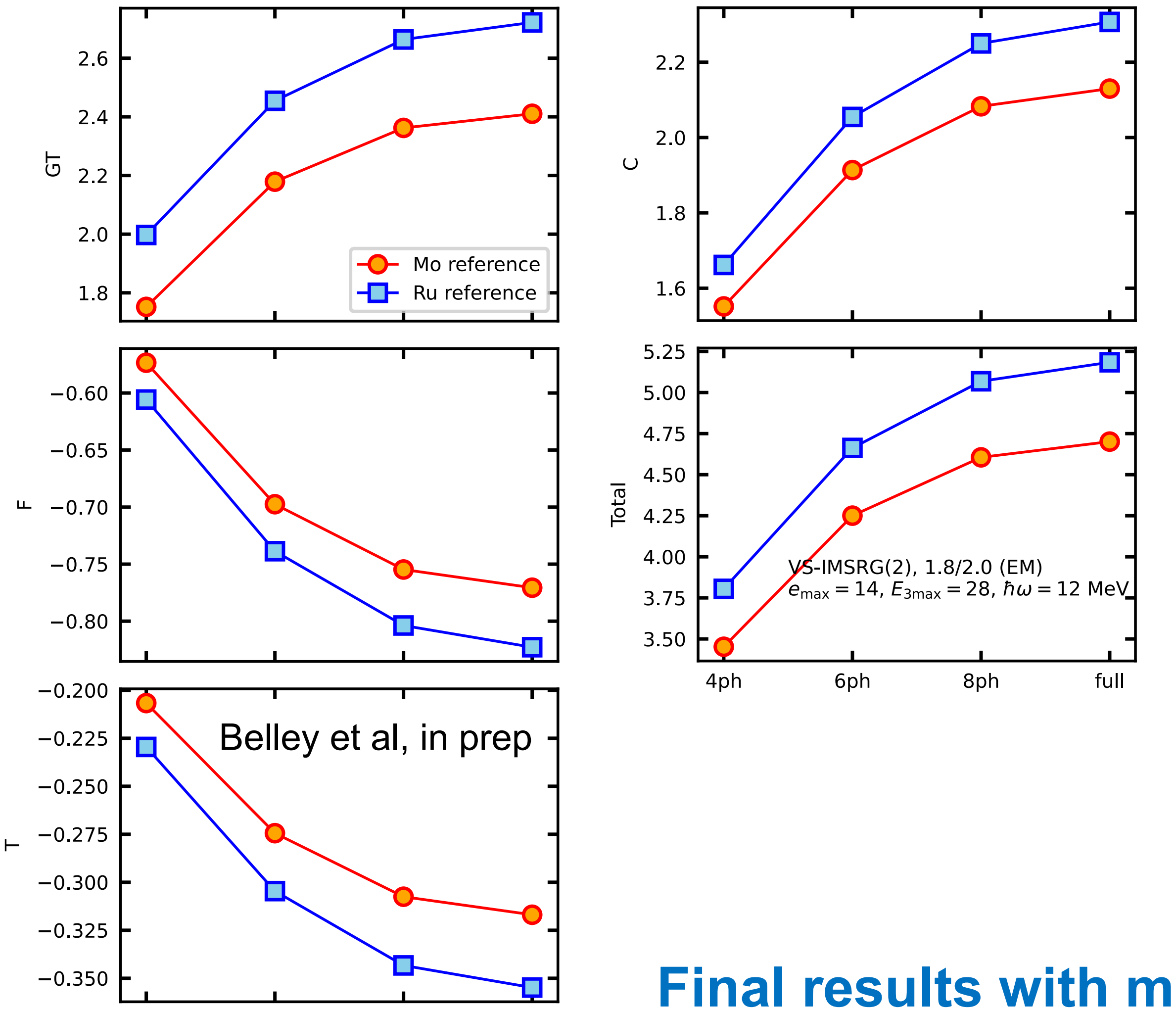


Belley et al, in prep

Towards Ab Initio Calculation of ^{100}Mo

Final competitive candidate in worldwide searches: AMoRE, NEMO 3, CUORE…

Highly mid-shell, difficult for SM - access with p-h truncations in KSHELL

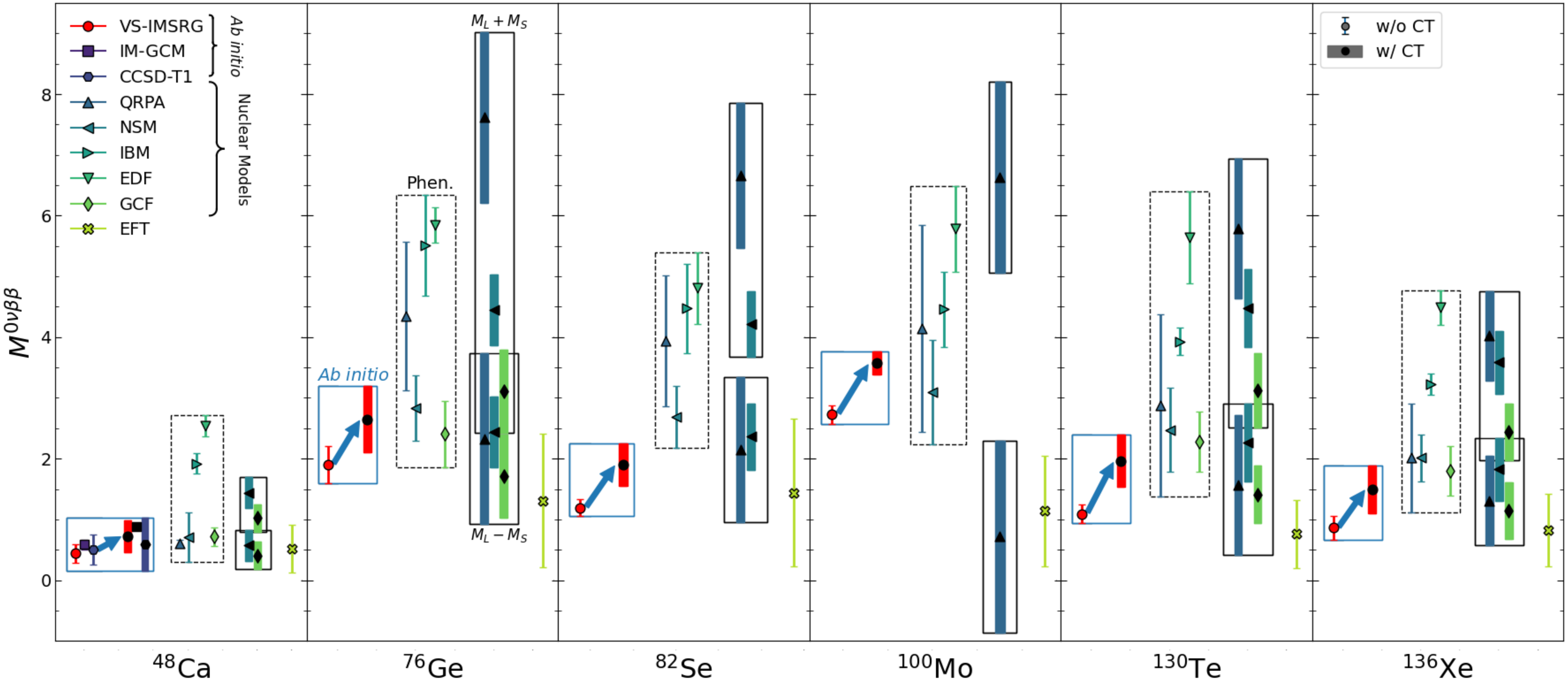


Final results with multiple NN+3N forces coming soon!

Ab Initio Predictions in Heavy Nuclei

Converged NMEs for major players in global searches: ^{76}Ge, ^{100}Mo ^{130}Te, ^{136}Xe

Ab initio results: differences from models; **large NMEs strongly disfavored**

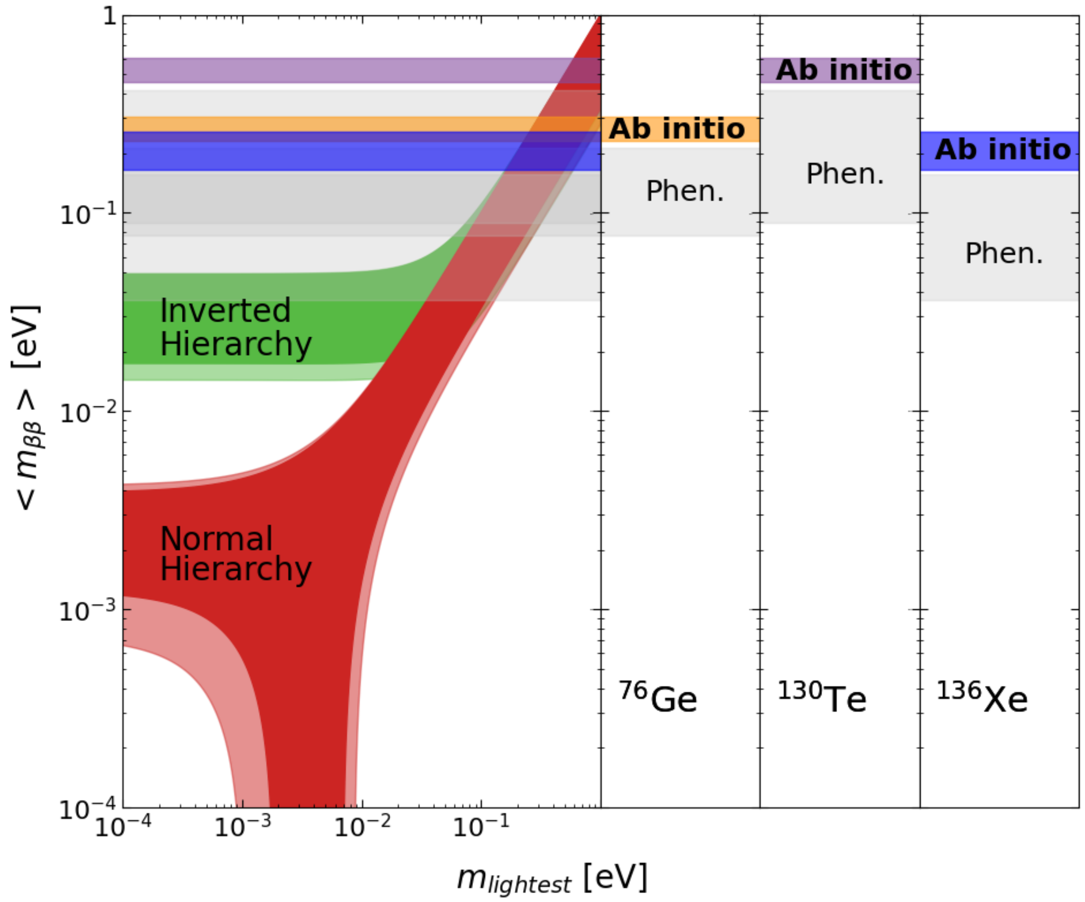


Belley et al, in prep

Impact of Ab Initio NMEs on Worldwide Searches

Impact for next-generation searches: Large matrix elements disfavored, lowers expected rates

Current experimental reach – more than an order of magnitude diminished

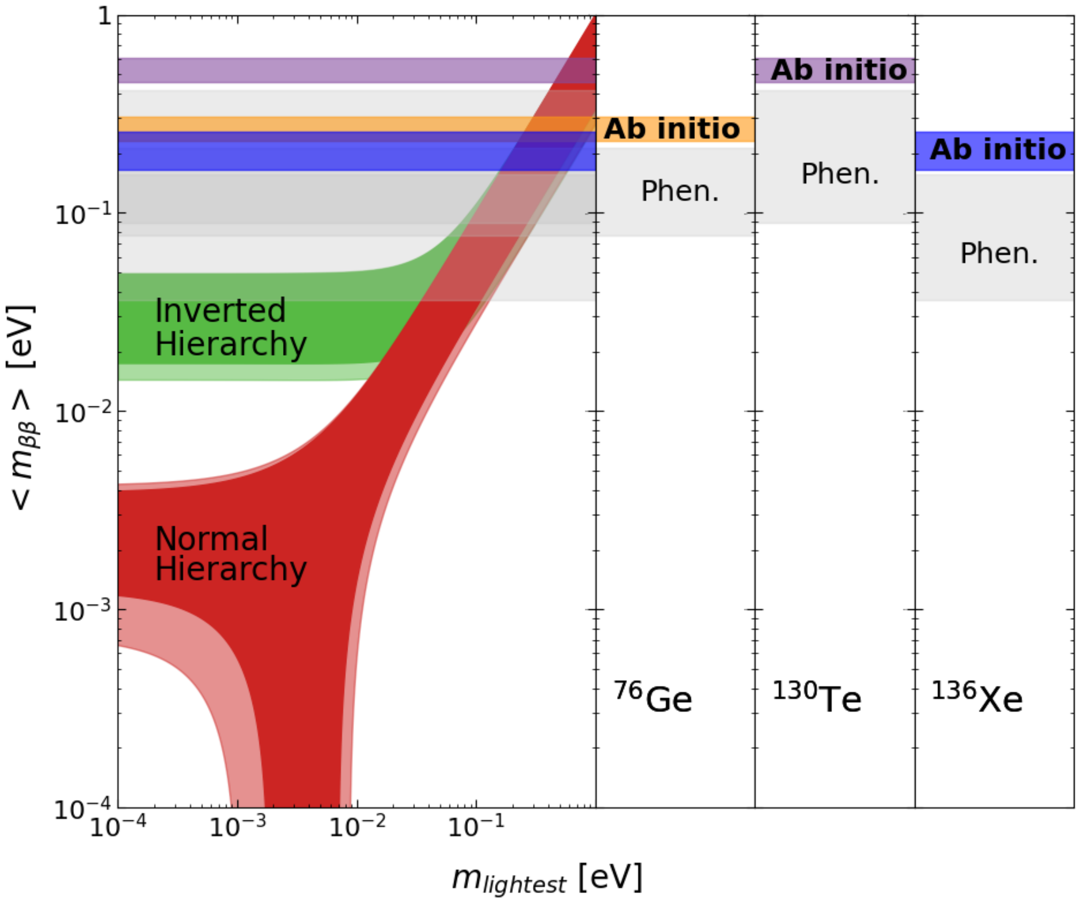


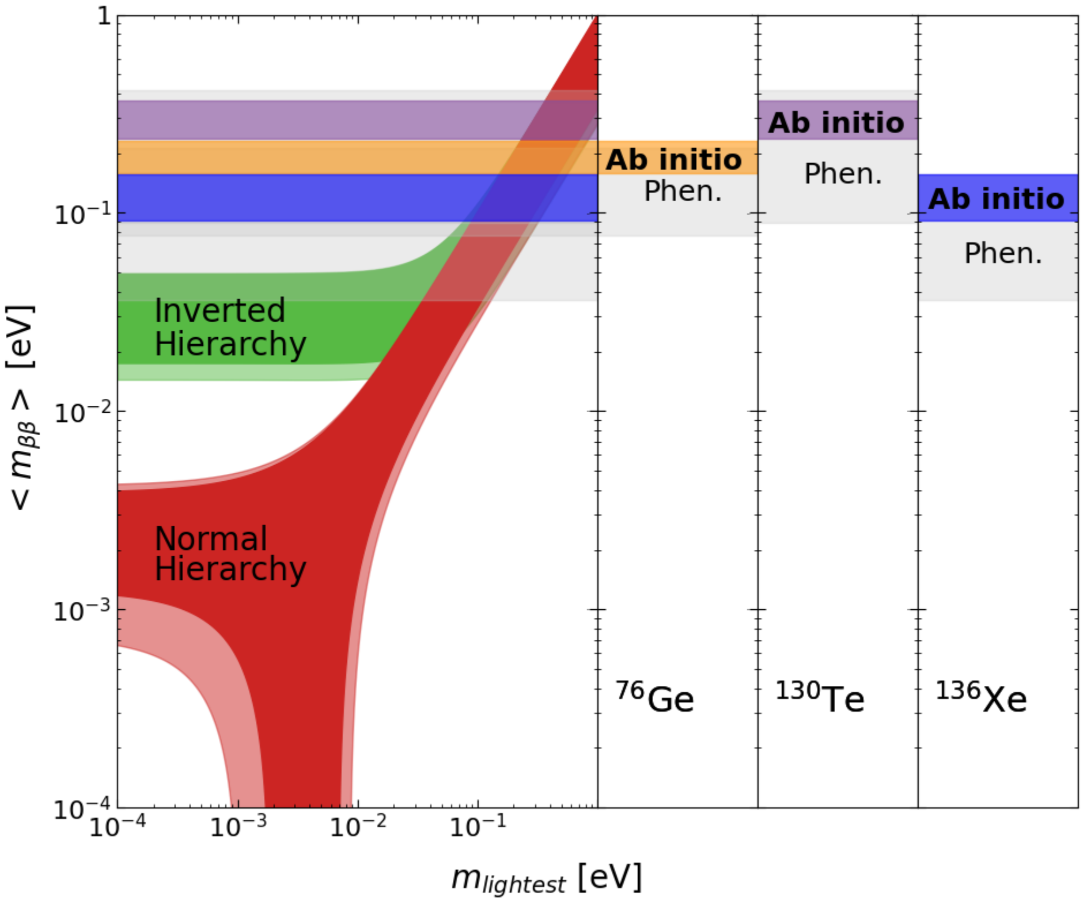
Belley et al, in prep

Impact of Ab Initio NMEs on Worldwide Searches

Impact for next-generation searches: Large matrix elements disfavored, lowers expected rates

Current experimental reach – improved with effects of contact term,





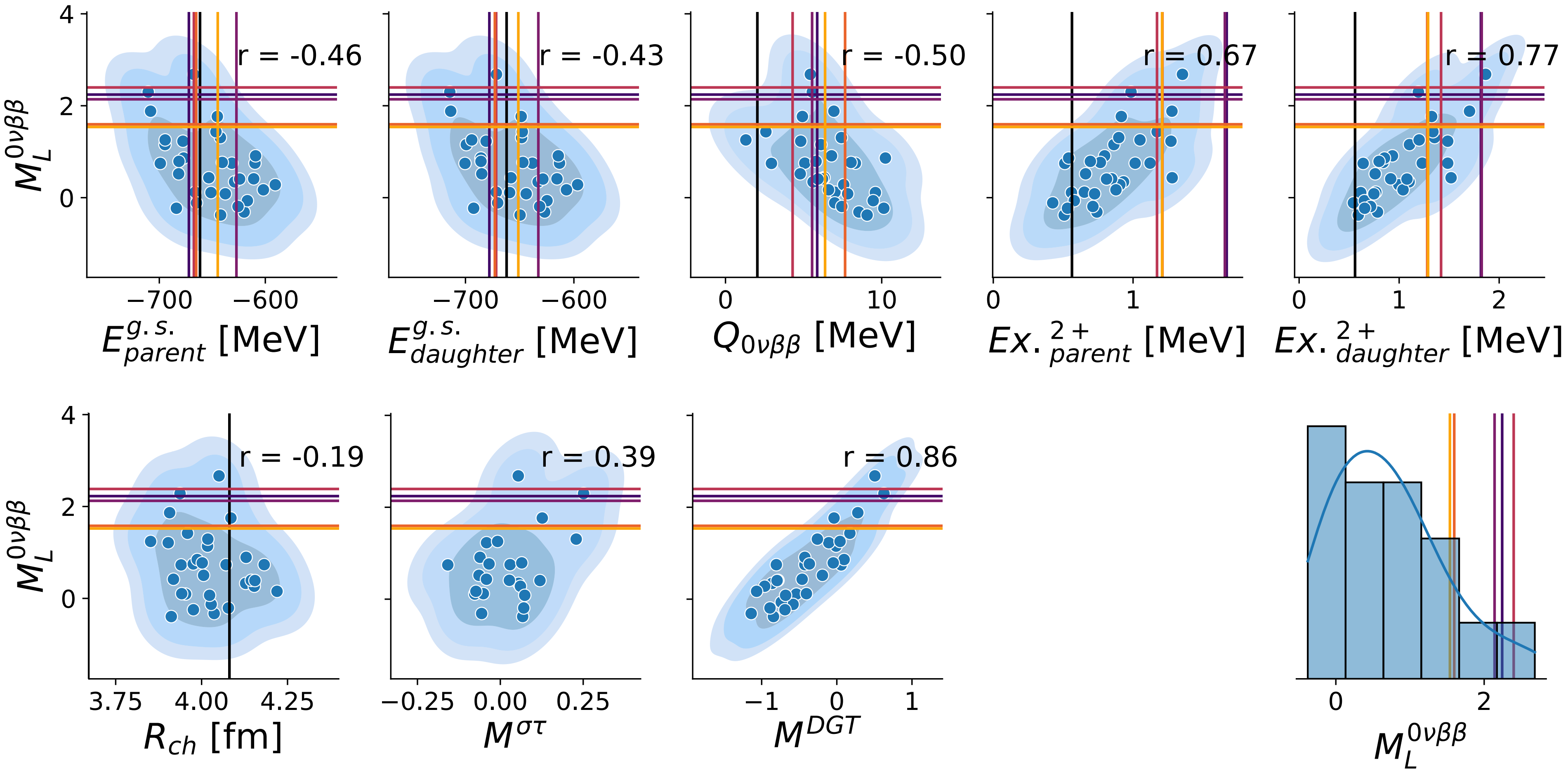
Not the end of the story: estimate three-body corrections + two-body currents

Belley et al, in prep

Strategy III: Correlation with Structure Observables

^{76}Ge: Explore correlations with other observables from systematic analysis (34 interactions)

Few clear correlations, except DGT



Belley et al., arXiV:2210.05809
Belley et al., in preparation

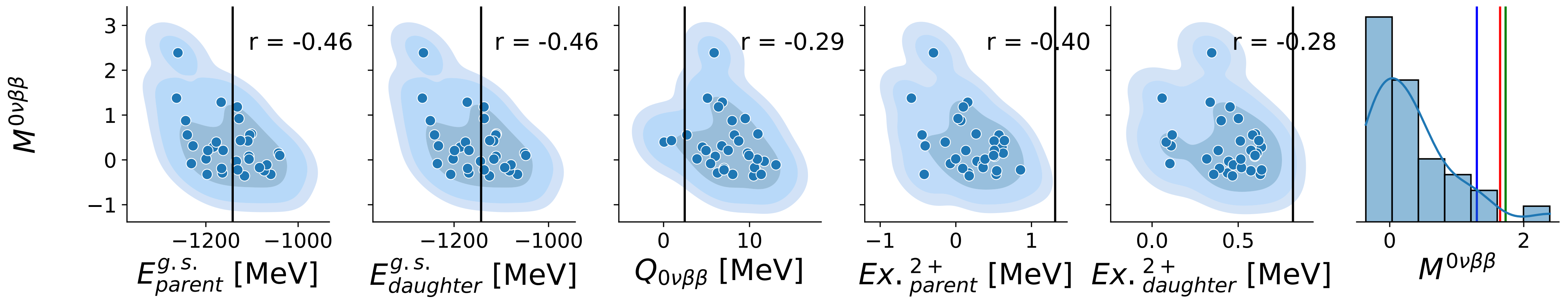
Maybe with first excited 2⁺ states?

Strategy III: Correlation with Structure Observables

Explore correlations with other observables from systematic analysis (34 interactions)

Few clear correlations, except DGT

Similar picture in ^{136}Xe… BUT no correlation with 2^+



TRIUMF

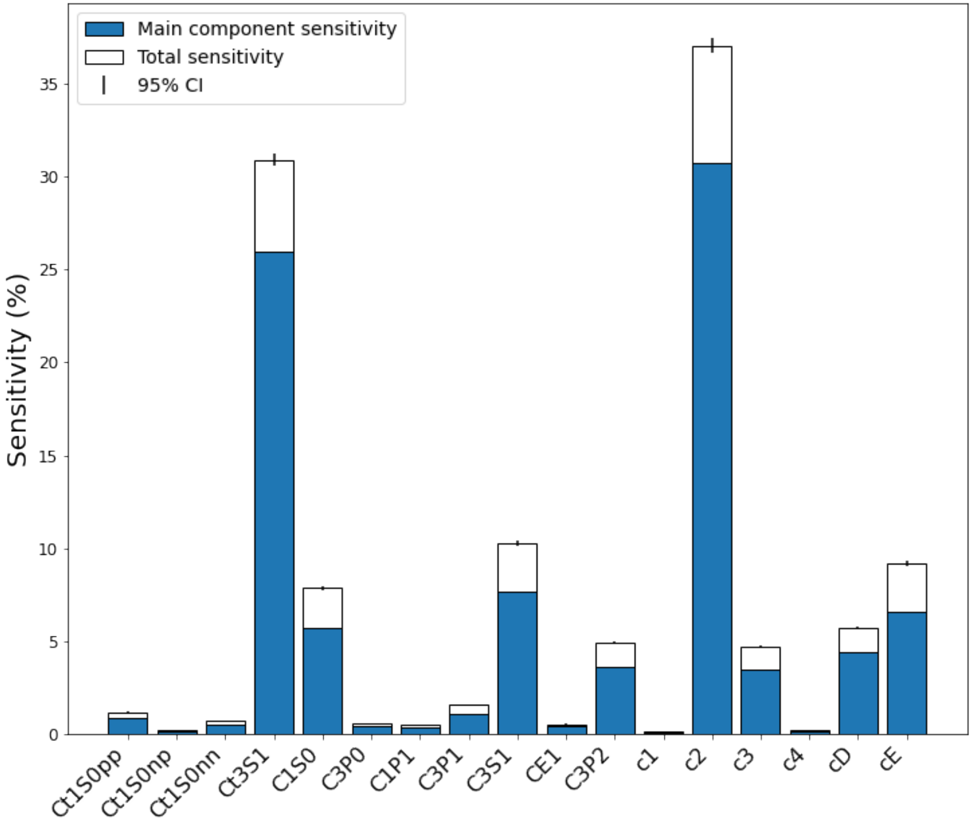
MM-DGP Emulator: Sensitivity Analysis

Explore correlations with other observables from systematic analysis (34 interactions)

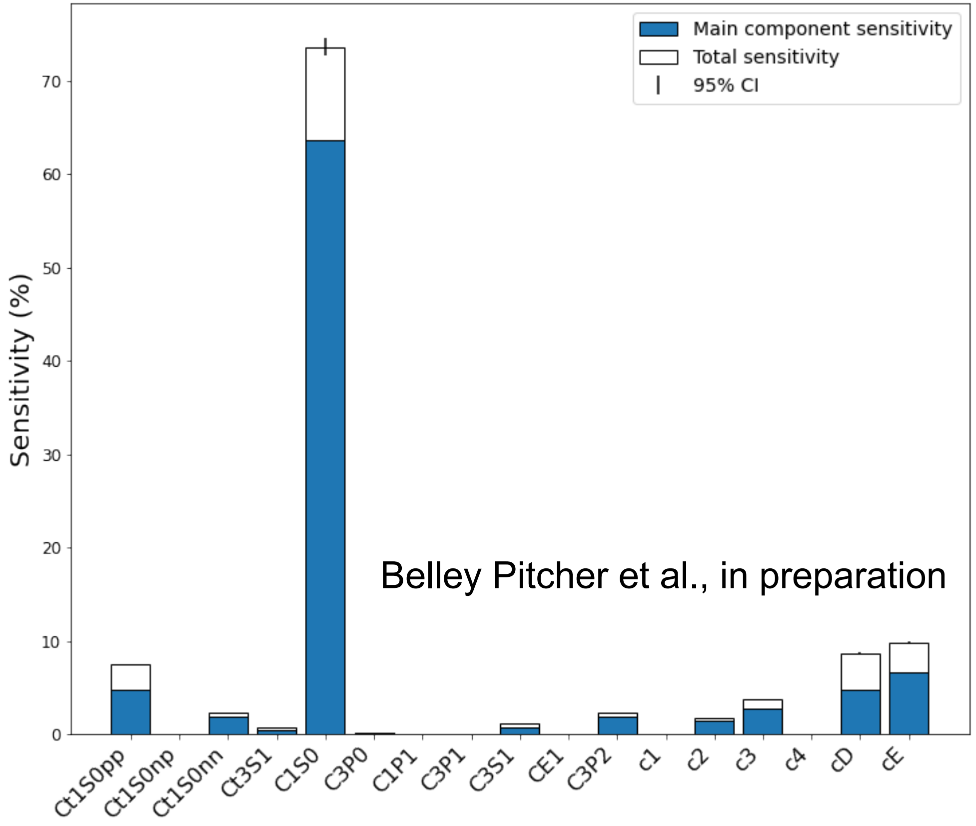
Similar sensitivity as found in ^{208}Pb study!

26

Ground state energies



$M_L^{0\nu}$

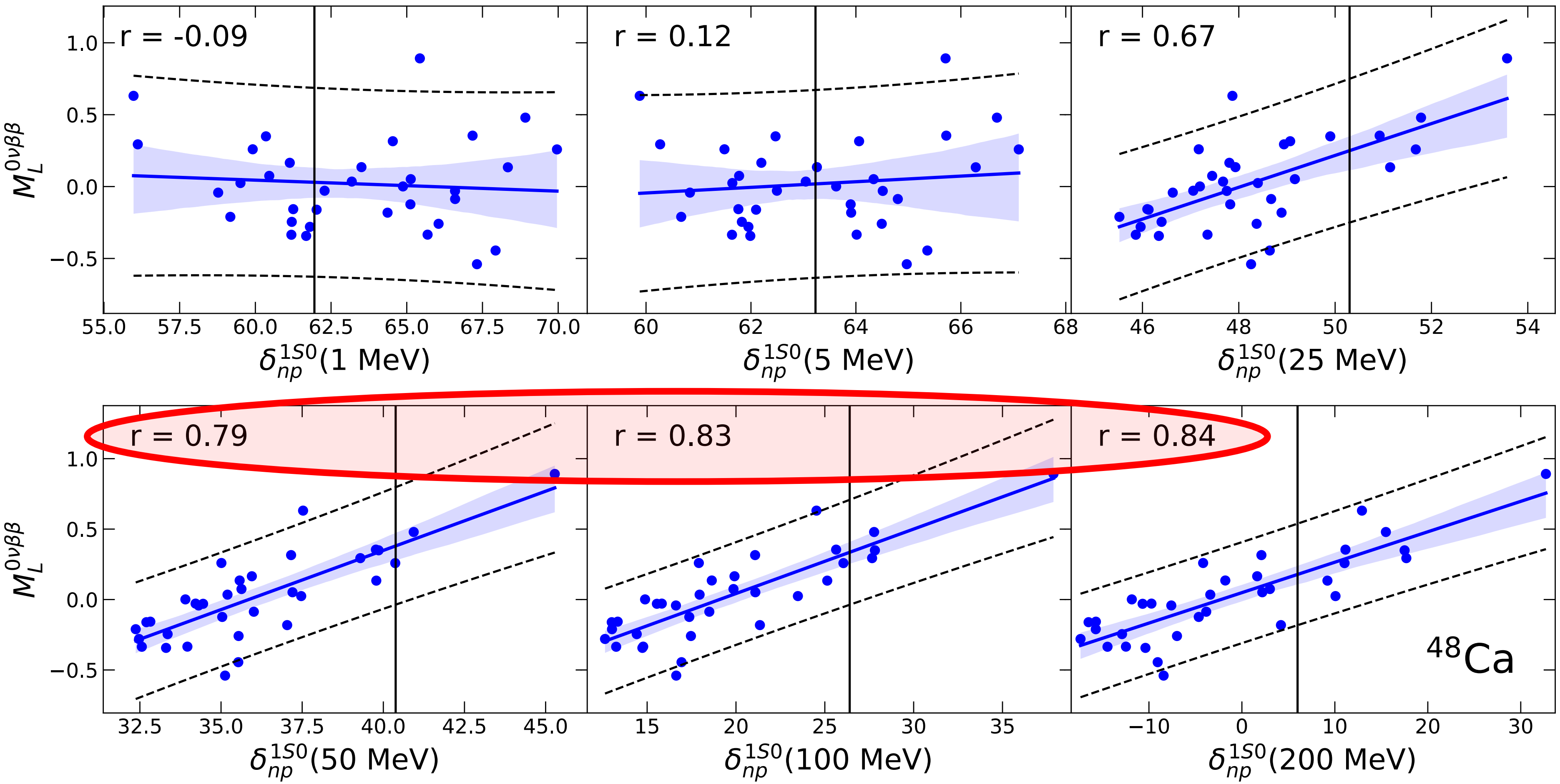


Highly sensitive to C1S0 – possible correlation with $^1S_0$ phase shift (observable!)

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca

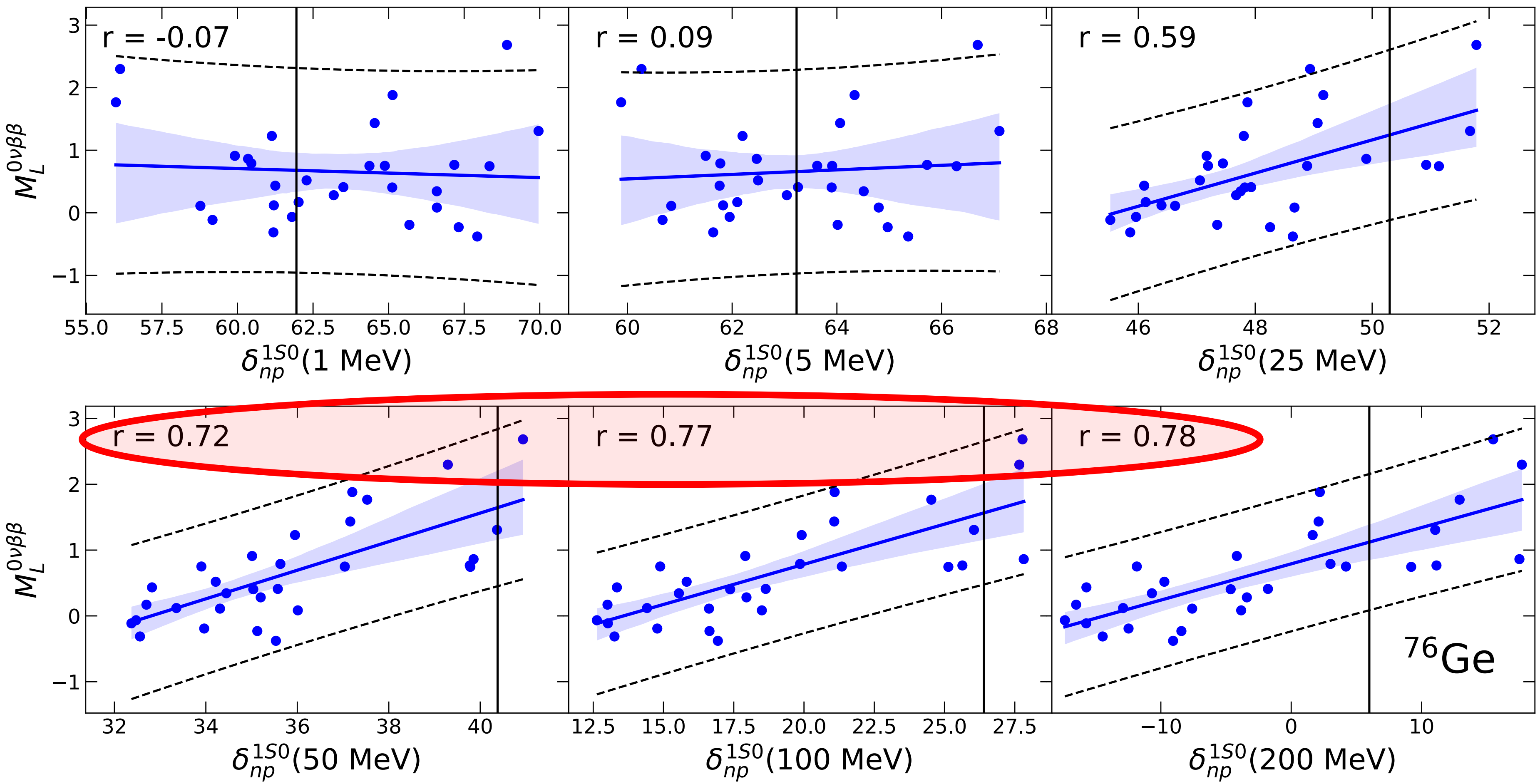


Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca, ^{76}Ge



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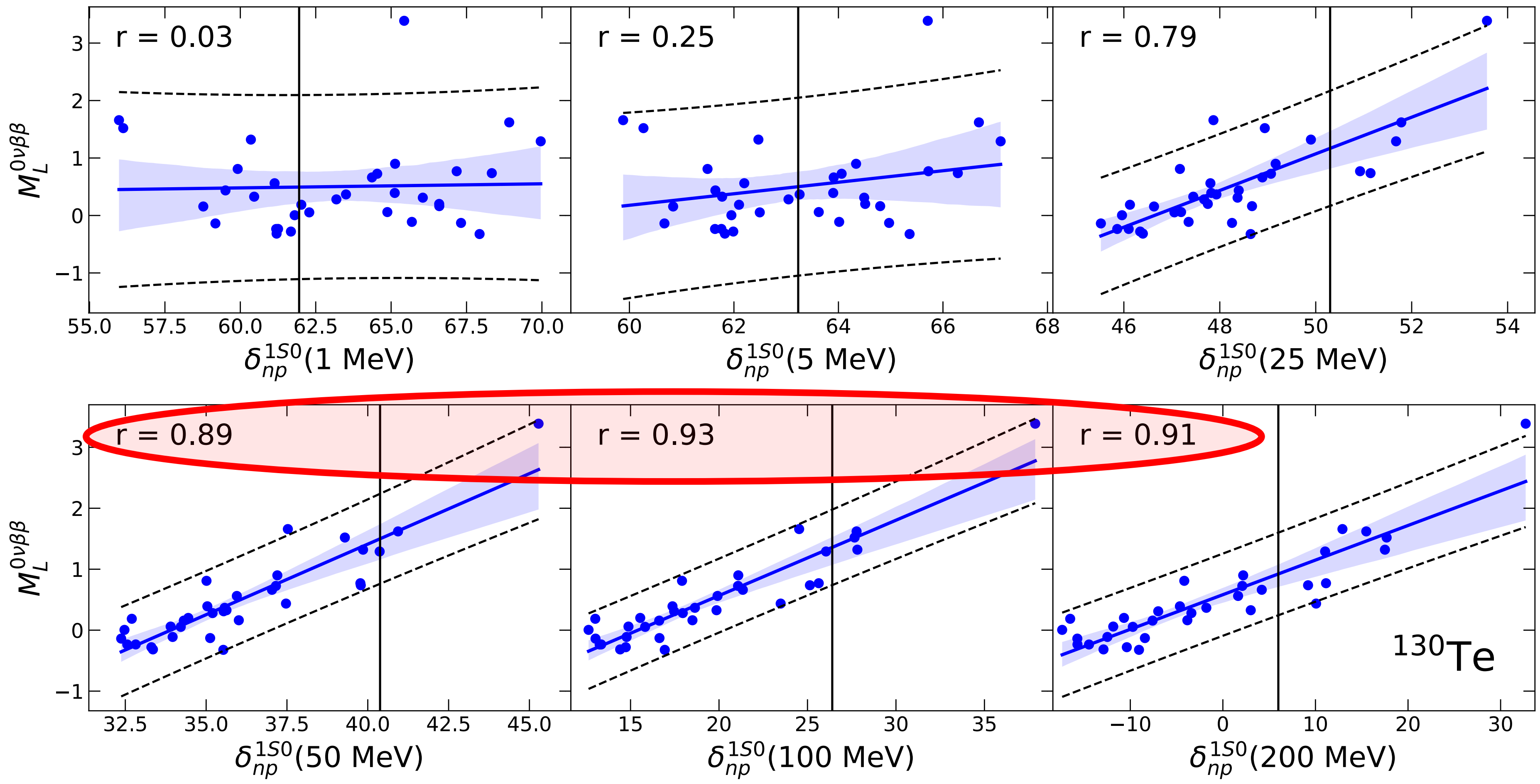
MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

TRIUMF

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca, ^{76}Ge, ^{130}Te



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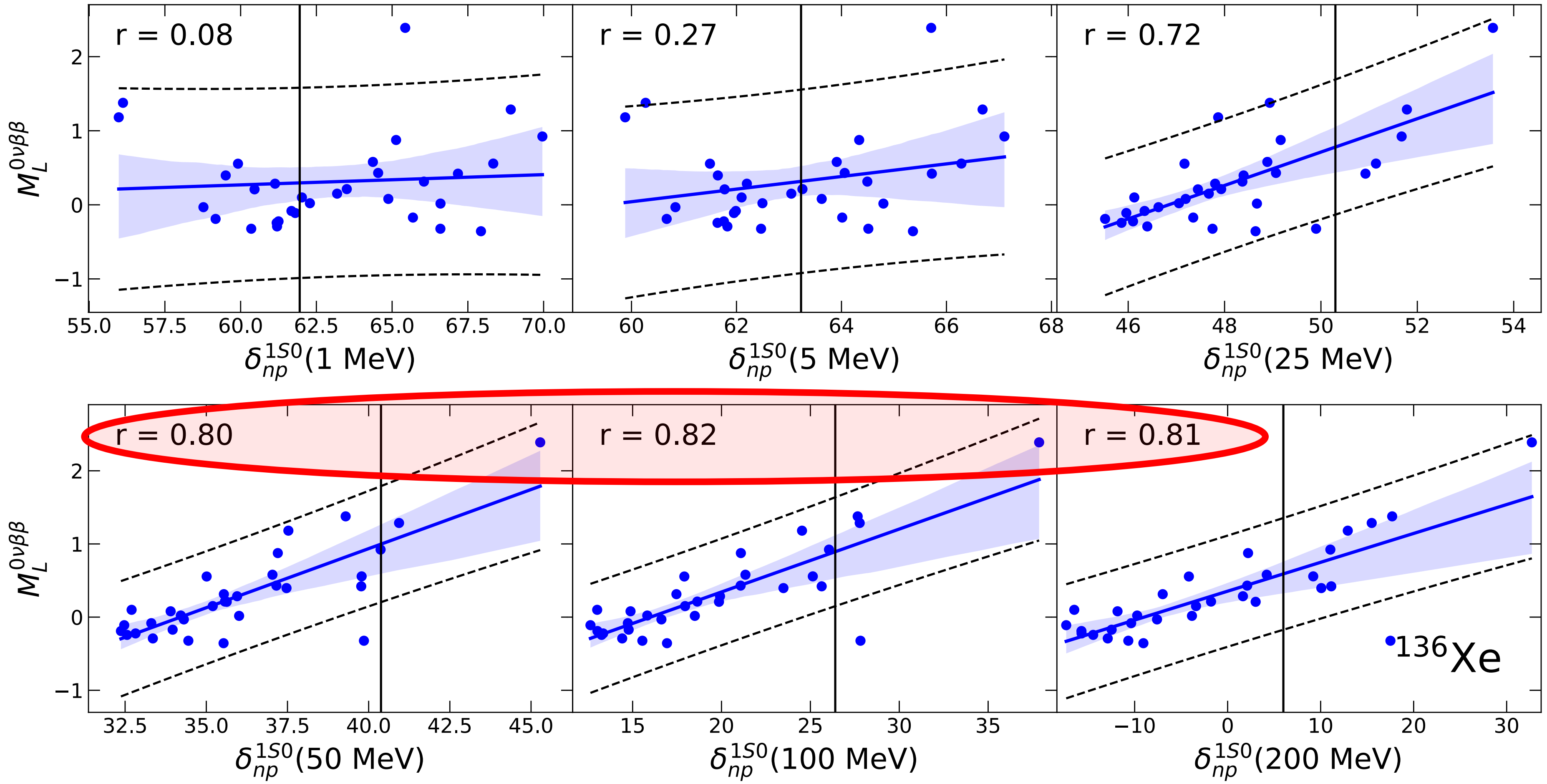

Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

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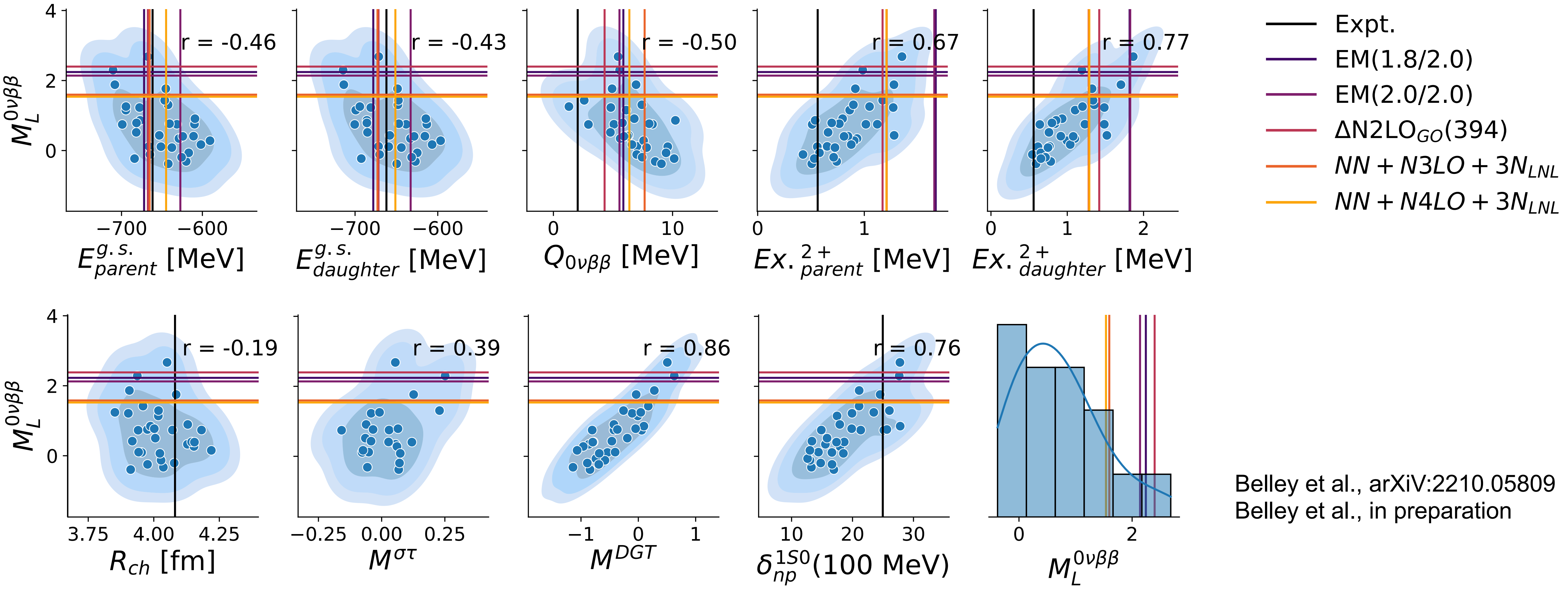

Belley et al., arXiV:2210.05809
Belley et al., in preparation

Now clear correlation with **measured** $^1S_0$ phase shift!

Strategy III: Correlation with Structure Observables

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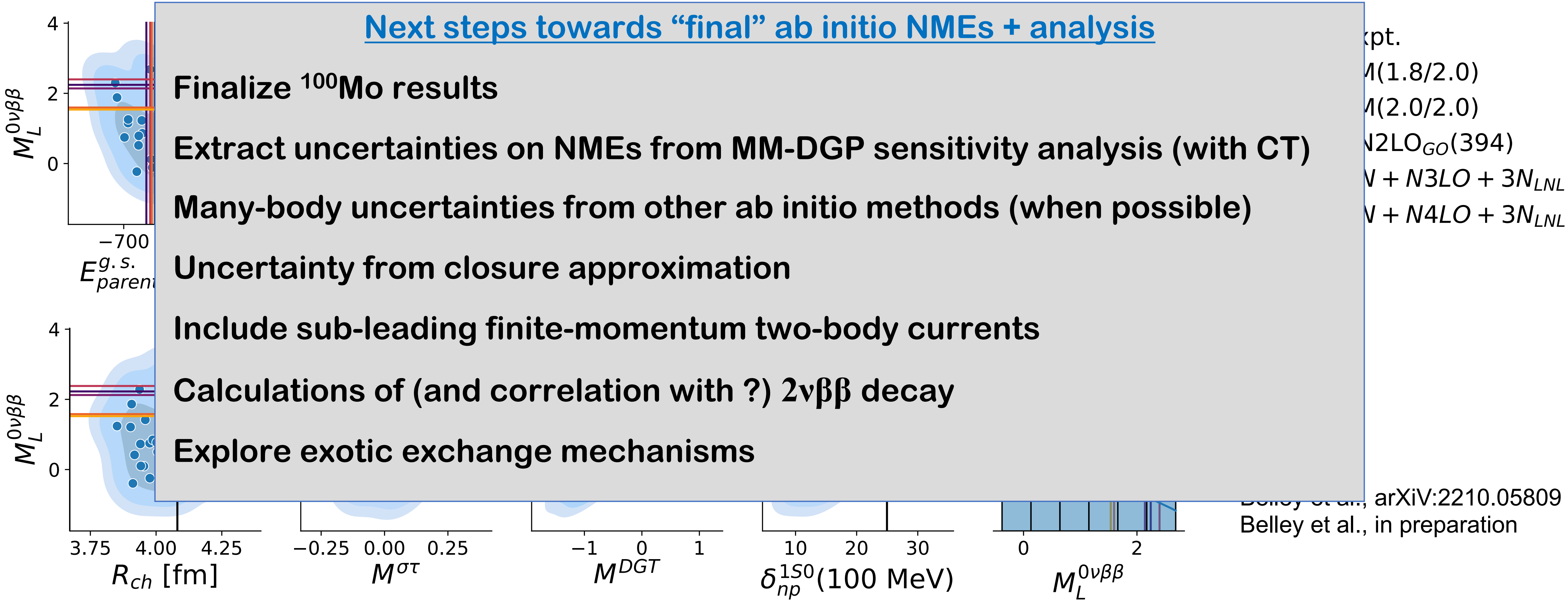
Few clear correlations, except DGT in ^{76}Ge



Next steps towards "final" ab initio NMEs + analysis

Finalize ^{100}Mo results

Extract uncertainties on NMEs from MM-DGP sensitivity analysis (with CT)

Many-body uncertainties from other ab initio methods (when possible)

Uncertainty from closure approximation

Include sub-leading finite-momentum two-body currents

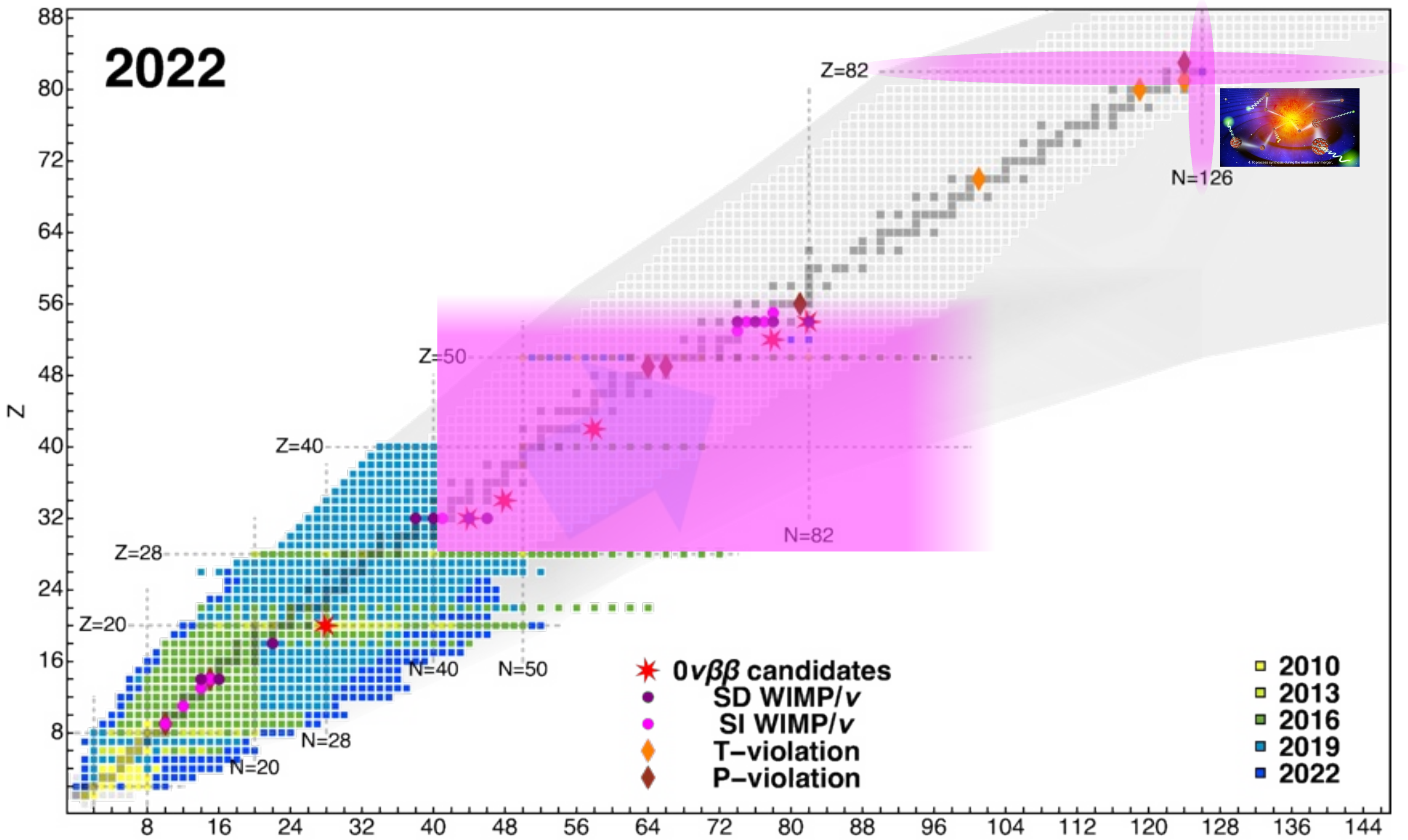
Calculations of (and correlation with ?) $2\nu\beta\beta$ decay

Explore exotic exchange mechanisms

Now clear correlation with **measured** $^1S_0$ phase shift!

New Scope of Ab Initio Theory

Possible to access most nuclei relevant for BSM searches!



TRIUMF

Present and Future for Ab Initio Theory

Nuclear Structure/Astrophysics

Development of forces and currents
Ab initio to ^{208}Pb: neutron skin, r-process
Dripline predictions to medium-masses
Evolution of magic numbers:
masses, radii, spectra, EM transitions
Multi-shell theory:
Islands of inversion, forbidden decays
Nuclear EOS/Neutron star properties
Atomic systems

Fundamental Symmetries/BSM Physics

EW operators: GT quenching, muon capture
$0\nu\beta\beta$ decay matrix elements + DGT/ECEC/Dg
WIMP-Nucleus scattering for dark matter detection
Coherent elastic neutrino-nucleus scattering
Superallowed Fermi transitions
Symmetry-violating moments: EDM, anapole…

Work in progress

Higher-order many-body physics: IMSRG(3)
Monte Carlo shell model diagonalization
Extension to superheavy nuclei

TRIUMF
THE UNIVERSITY OF BRITISH COLUMBIA
McGill UNIVERSITY

T. Miyagi, B. S. Hu, L. Jokiniemi
A. Belley, I. Ginnett, C. G. Payne
M. Bruneault, J. Padua
S. Leutheusser
E. Love
K. Evidence, D. Kush
G. Tenkila, H. Patel, V. Chand
B. Wong, X. Cao
S. R. Stroberg N. Vassh

TECHNISCHE UNIVERSITÄT DARMSTADT — A. Schwenk
THE UNIVERSITY of TENNESSEE UT KNOXVILLE — G. Hagen, T. Papenbrock
MICHIGAN STATE UNIVERSITY — J.M. Yao, H. Hergert
COLORADO SCHOOL OF MINES — M. Martin, K. G. Leach
Massachusetts Institute of Technology — R. F. Garcia-Ruiz
UNIVERSITAT DE BARCELONA — J. Menéndez
THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL — J. Engel
TEXAS A&M UNIVERSITY — J. W. Holt

Strategy IIIb: Sensitivity Analysis

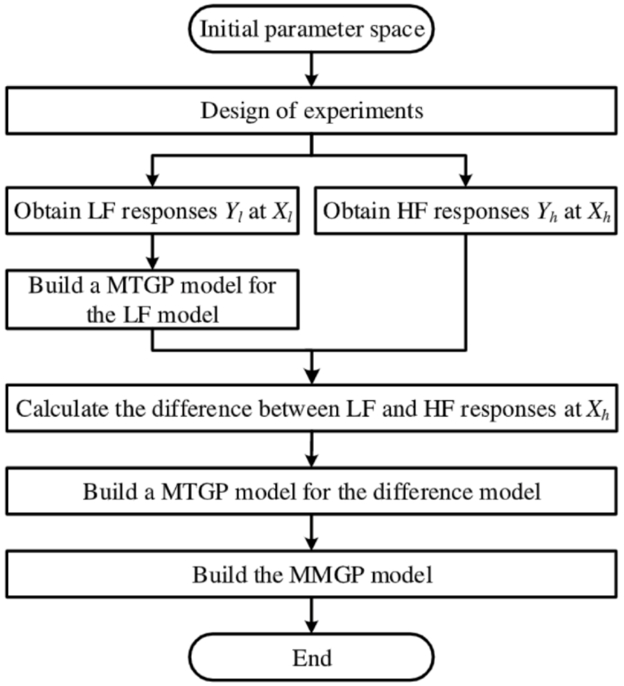
Explore dependence on chiral EFT LECs: requires many samples (as in ^{208}Pb)

Use gaussian processes as an emulator

Multi-Fidelity Gaussian Process: connects few (complicated) high-fidelity data points (eg, full IMSRG) w/ many low-fidelity data points (HF, low e_{max}, etc)

Difference function fit with Gaussian process: predict HF from LF

When relation between LF and HF is complicated, MFGP fails



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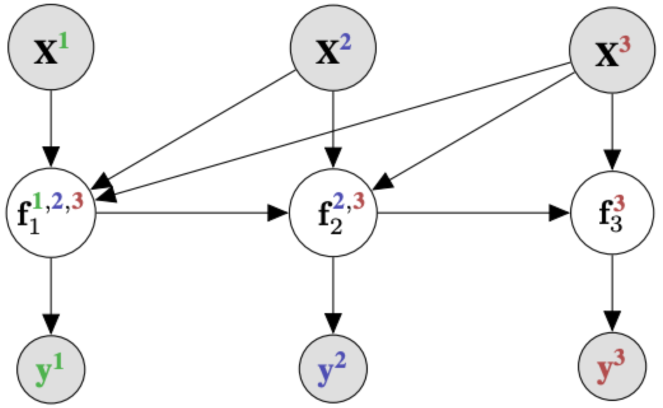
Deep Gaussian Process: Neural network links multiple GP



Include outputs of previous fidelity as new HF point:
- Improves modeling of difference between LF and HF

Adapted for multi output:
Multi-Output Multi-Fidelity Deep Gaussian Process (MM-DGP)

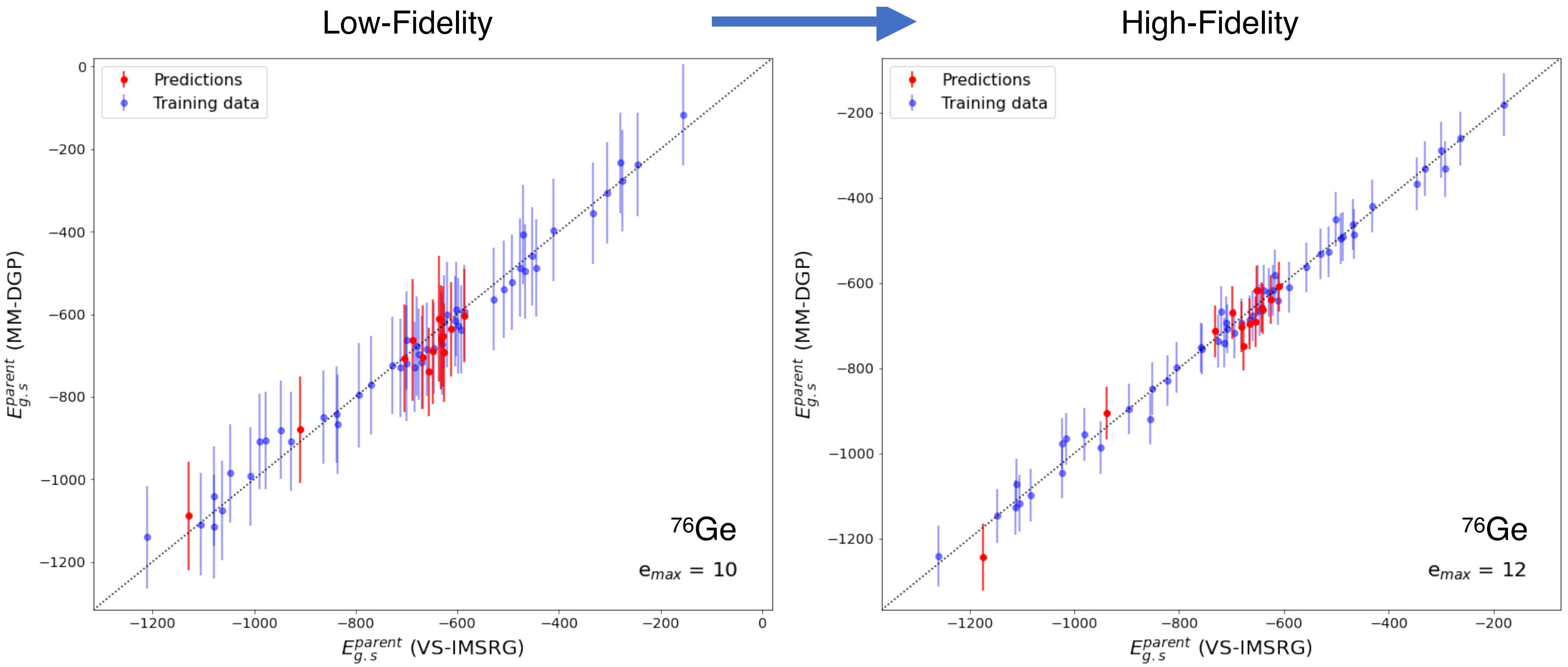
Belley Pitcher et al., in preparation

TRIUMF

MM-DGP Emulator: Ground-State Energies

Testing MM-DGP: use delta-full chiral EFT at N2LO

Improved energy predictions with high-fidelity training points



Belley, Pitcher et al. in prep.

MM-DGP Emulator: $0\nu\beta\beta$-Decay

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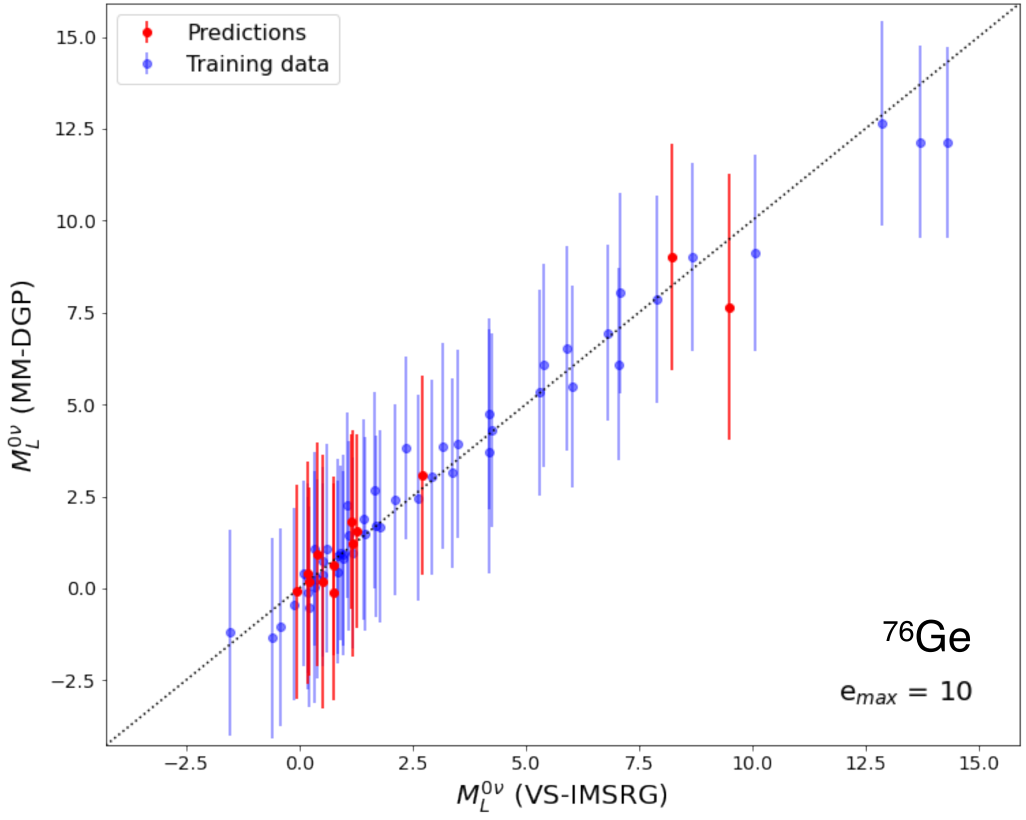
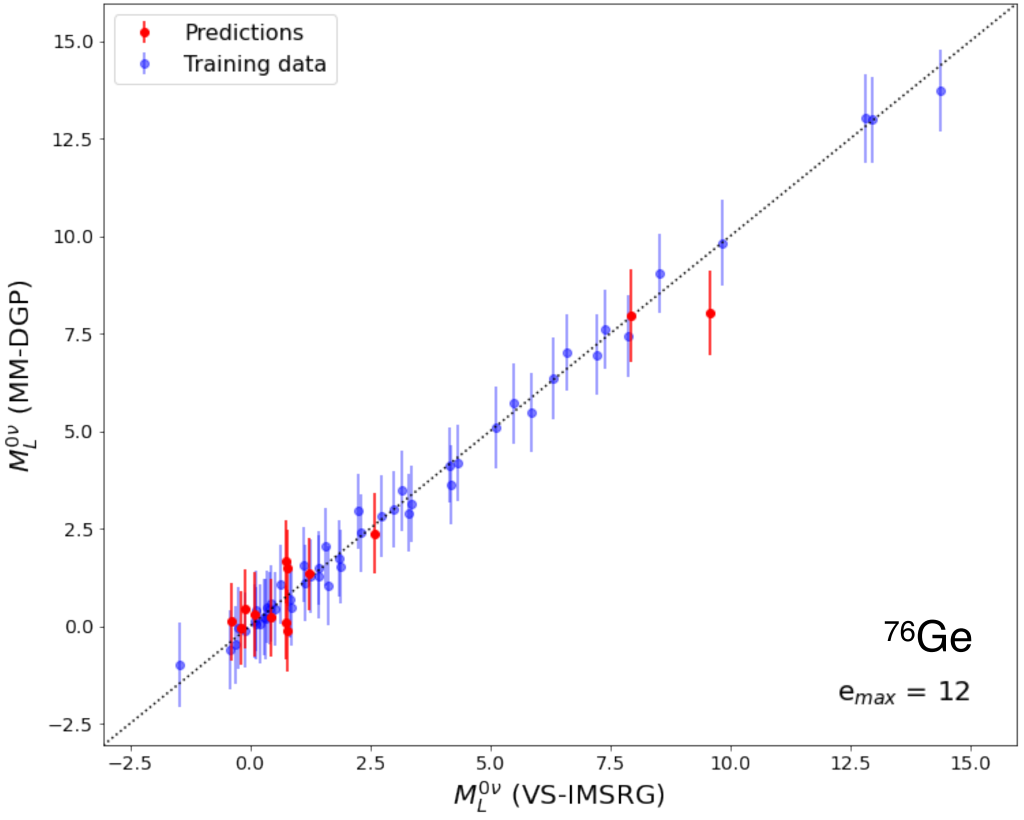
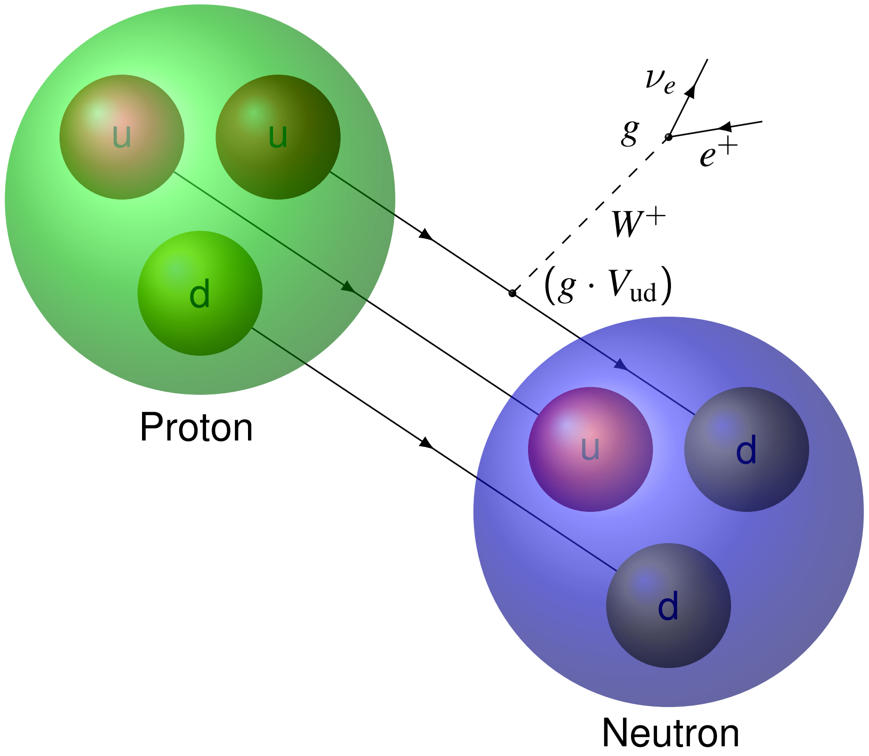
Low-Fidelity → High-Fidelity





Belley, Pitcher et al. in prep.

Ab Initio Approach to ISB and Superallowed $0^+ \rightarrow 0^+$



Editors' Suggestion

Testing isospin symmetry breaking in *ab initio* nuclear theory

M. S. Martin, S. R. Stroberg, J. D. Holt, and K. G. Leach

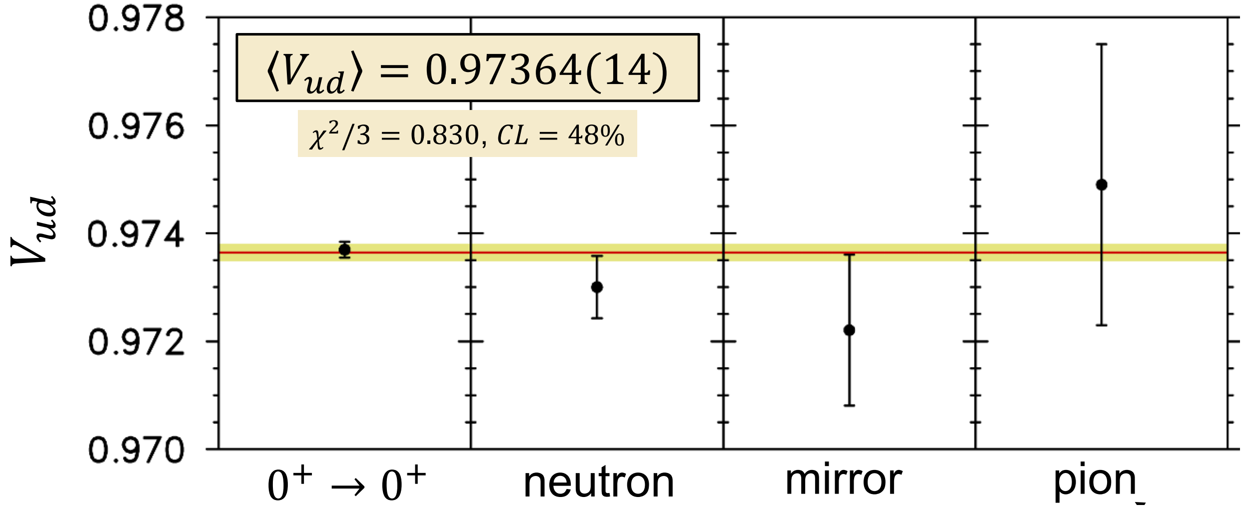
Phys. Rev. C **104**, 014324 – Published 30 July 2021

Superallowed Fermi Transitions

$0^+ \rightarrow 0^+$ transitions: most stringent constraint on V_{ud} from corrected (parameterized) lifetime

$$G_V = G_F V_{ud}, \text{ where } ft = \frac{K}{2G_V^2} \quad \text{(isospin limit)}$$

$$\mathcal{F}t = ft(1+\delta'_R[1-(\delta_C-\delta_{NS})] = \frac{K/G_F^2}{2V_{ud}^2(1+\Delta_R^V)}$$



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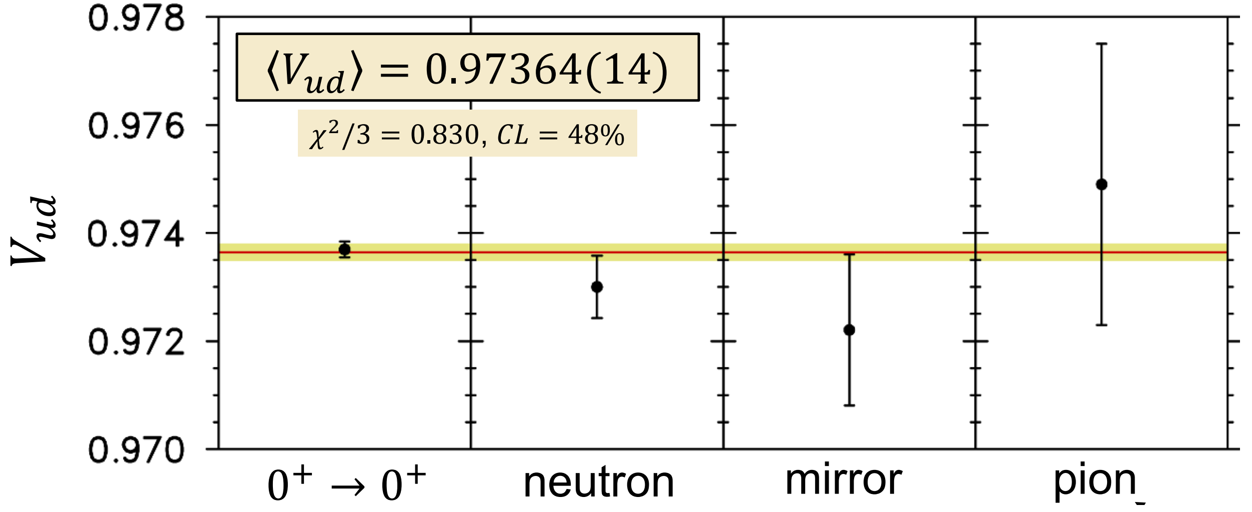
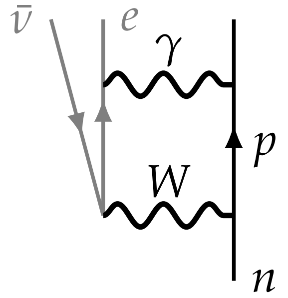


$$|M_F|^2 = |M_F^0|^2(1 + \delta_C)$$

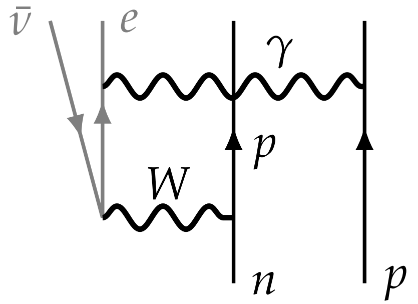
Isospin-symmetry breaking

$\delta'_R \sim$



Structure-independent radiative correction

$\delta_{NS} \sim$



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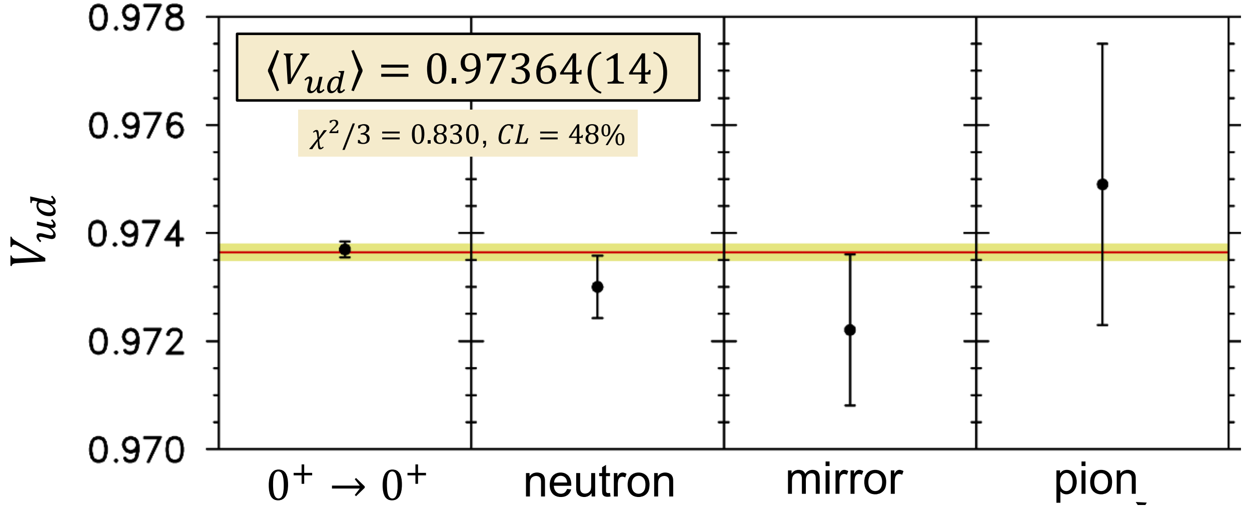
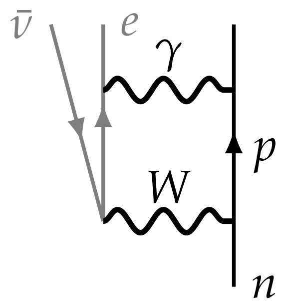


$$|M_F|^2 = |M_F^0|^2(1+\delta_C)$$ Isospin-symmetry breaking

$\delta'_R \sim$



Structure-independent radiative correction

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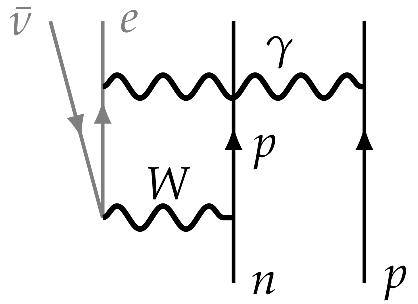


Structure-dependent radiative correction

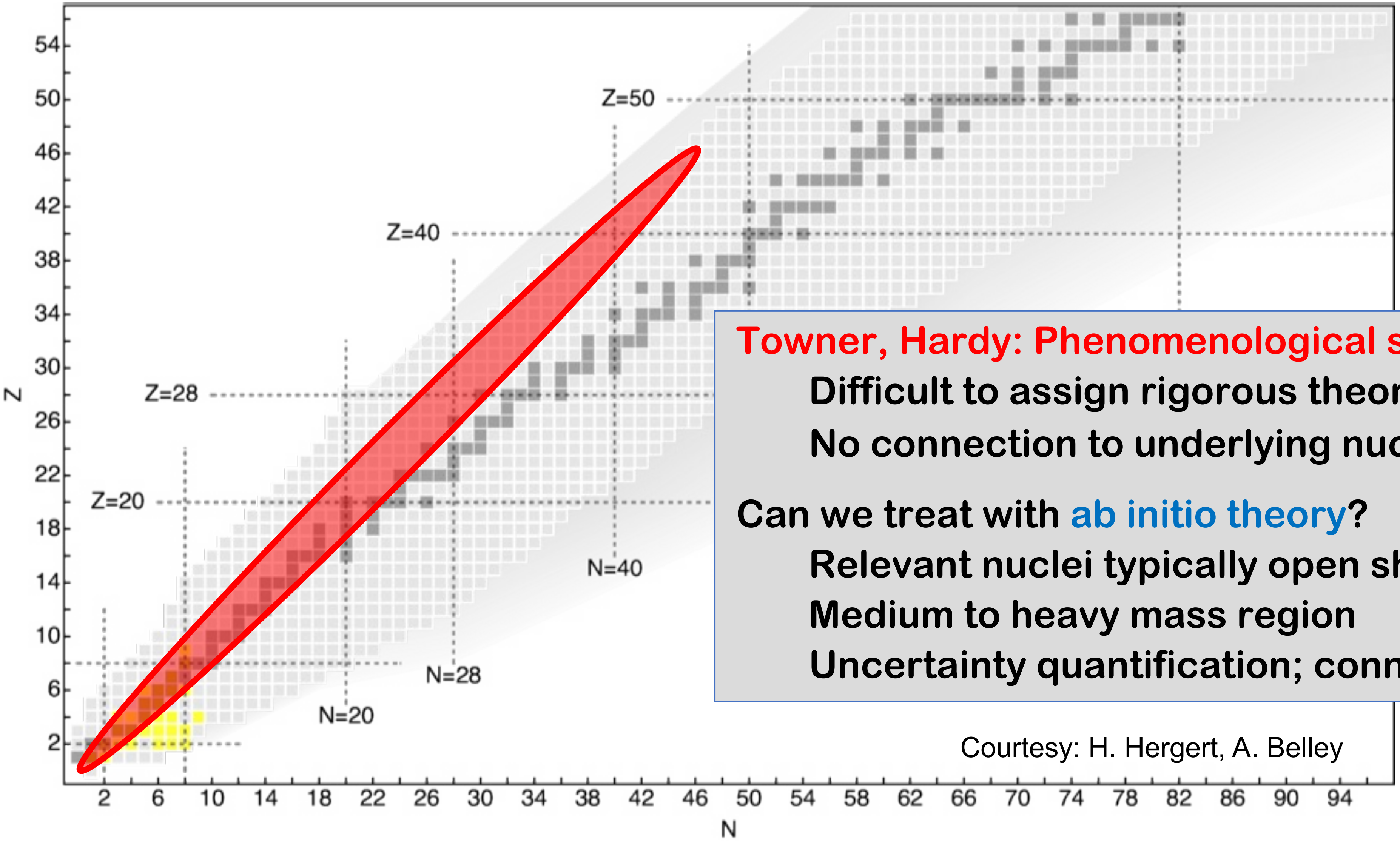
Nuclear structure theory

Isospin symmetry correction

dominates uncertainty in medium/heavy nuclei (and simple operator to calculate)

Progress of Ab Initio Theory Since 2010

2010: Limited capabilities for 3N forces; ^{16}O heaviest



Towner, Hardy: Phenomenological shell model

- **Difficult to assign rigorous theoretical uncertainties**
- **No connection to underlying nuclear/weak forces**

Can we treat with ab initio theory?

- **Relevant nuclei typically open shell**
- **Medium to heavy mass region**
- **Uncertainty quantification; connection to QCD**

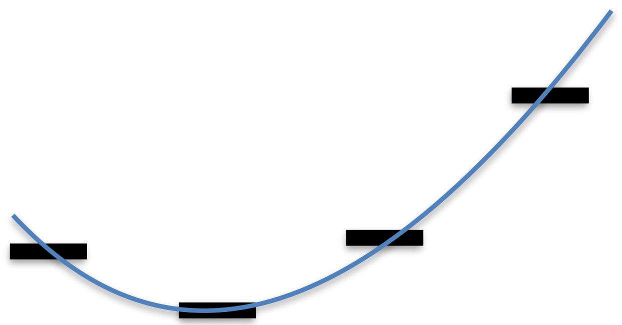
Courtesy: H. Hergert, A. Belley

TRIUMF

Explore ab initio isospin symmetry breaking

Isobaric mass multiplet equation (IMME) relates energies between members of multiplets

$$E(T_z) = a + bT_z + cT_z^2$$



Compare ab initio with experimental determination of IMME coefficients to gauge success

Calculate all nuclei relevant for superallowed transitions; 2 NN+3N forces

Ab initio IMME: bare vs IMSRG

Isobaric mass multiplet equation (IMME) relates energies between members of multiplets

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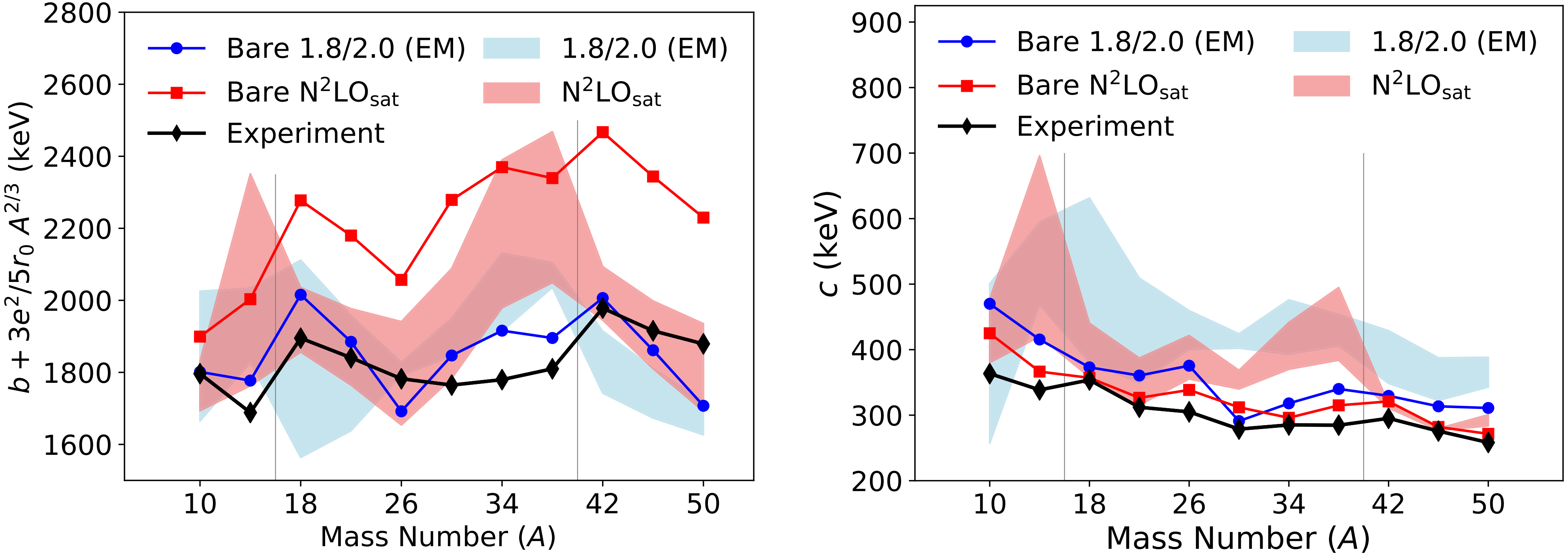


Bands: normal ordering reference dependence

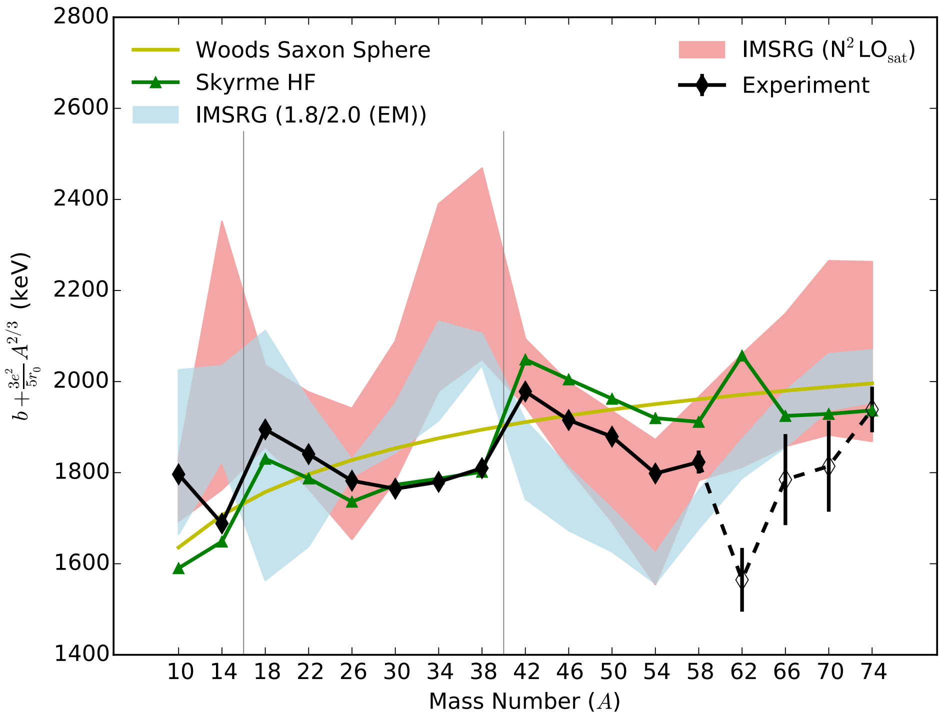
Overall little effect/improvement when applying IMSRG transformation for both b, c

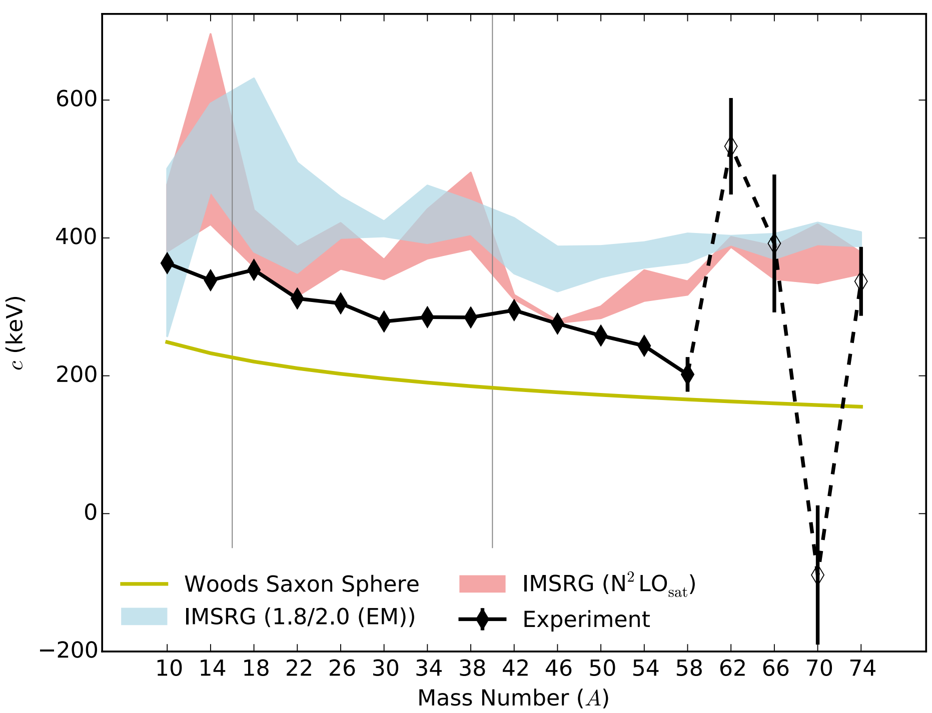
Ab initio IMME: bare vs IMSRG

Isobaric mass multiplet equation (IMME) relates energies between members of multiplets

$$E(T_z) = a + bT_z + cT_z^2$$

Compare VS-IMSRG b, c coefficients to HF and results from a uniform charged sphere





Systematics already largely captured (better) by mean field or charged sphere

Ambiguous results… turn to superallowed Fermi transitions

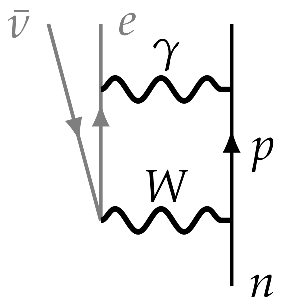
Superallowed Fermi Transitions

$0^+ \rightarrow 0^+$ transitions: most stringent constraint on V_{ud} from corrected (parameterized) lifetime

$$|M_F|^2 = |M_F^0|^2(1 + \delta_C)$$ Isospin-symmetry breaking

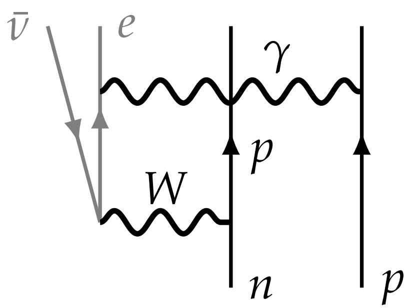
~ Effect of **correlations outside valence space**

$\delta'_R \sim$



Structure-independent radiative correction

$\delta_{NS} \sim$



Structure-dependent radiative correction

~ Effect of **two-body currents**

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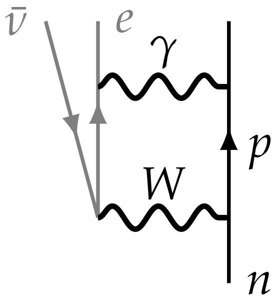

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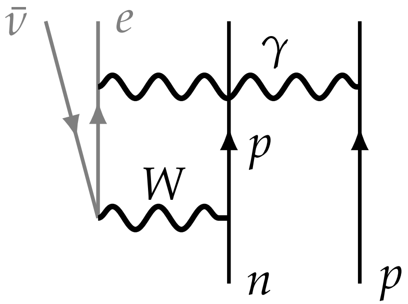
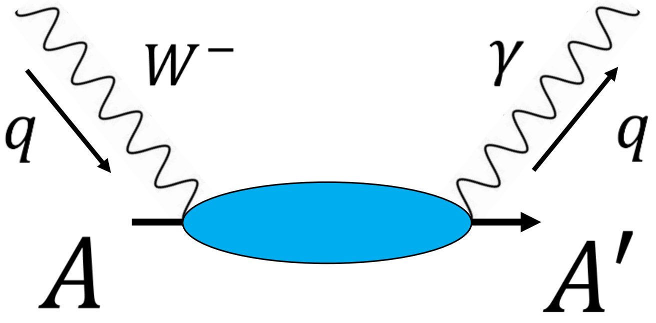


Structure-dependent radiative correction

~ Effect of **two-body currents**

Treatment of SD Radiative Corrections in NCSM

Compton amplitude in the NCSM



- Nuclear matrix elements for γW-box
  1) Express currents in momentum space
  2) Multipole expansion of current operators
  3) Connect currents to effective one–body operators

Lanczos continued fractions method to compute Green's functions!

$$T_3(q_0, Q^2) = -4\pi i \frac{q_0}{q}\sqrt{M_i M_f}\sum_{J=1}^{\infty}(2J+1)$$

$$\times \langle A\lambda_f J_f M_f \Big| \Big[T_{J0}^{mag}(q)\, G(M_f + q_0 + i\epsilon)\, T_{J0}^{5,el}(q) + T_{J0}^{el}(q)\, G(M_f + q_0 + i\epsilon)\, T_{J0}^{5,mag}(q)$$

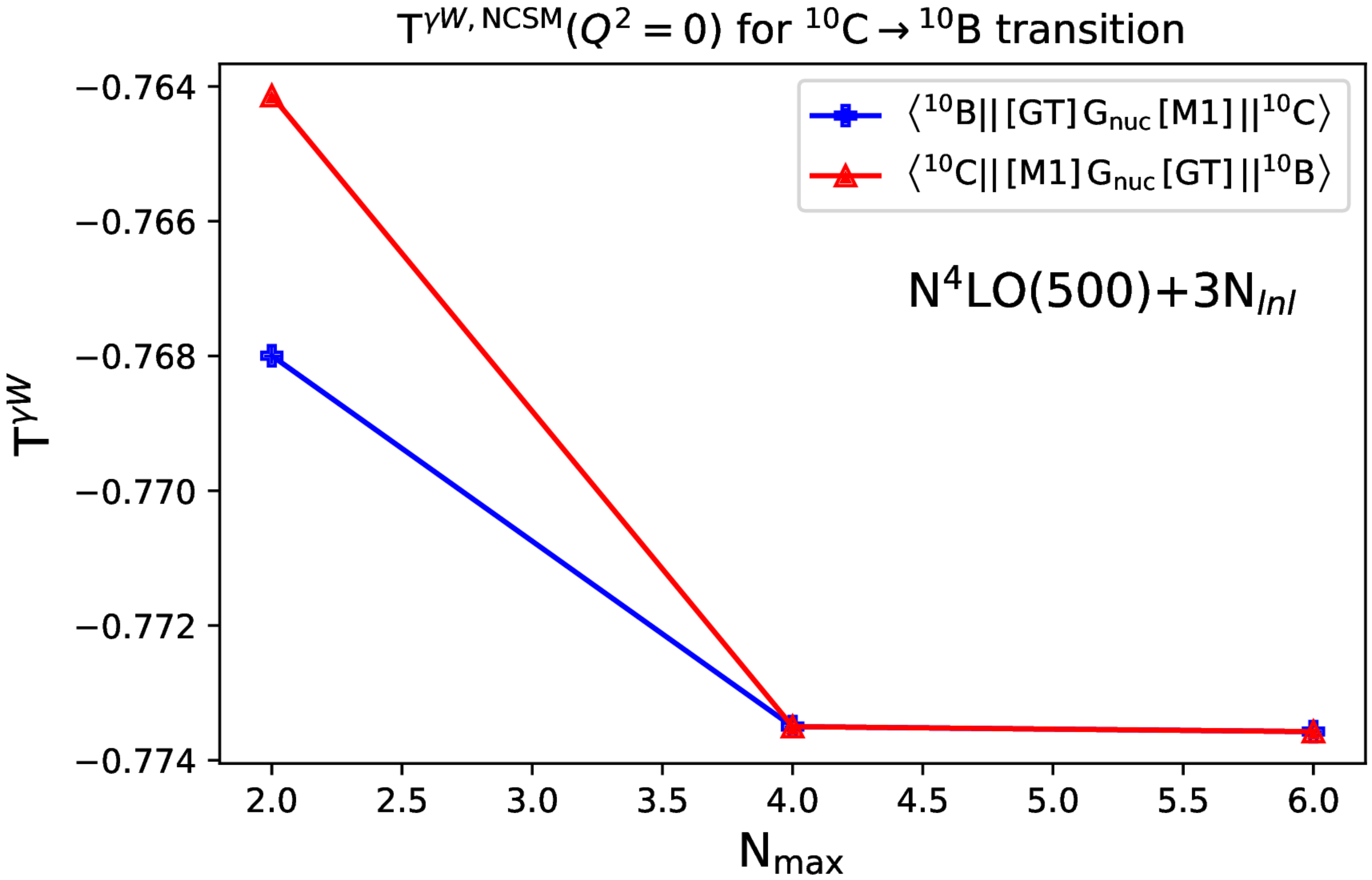
$$+ T_{J0}^{5,mag}(q)\, G(M_i - q_0 + i\epsilon)\, T_{J0}^{el}(q) + T_{J0}^{5,el}(q)\, G(M_i - q_0 + i\epsilon)\, T_{J0}^{mag}(q) \Big] \Big| A\lambda_i J_i M_i \rangle$$

Courtesy, M. Gennari

Treatment of SD Radiative Corrections in NCSM

Comment on many-body convergence

Preliminary



Next step: implement in VS-IMSRG for all superallowed nuclei

Courtesy, M. Gennari

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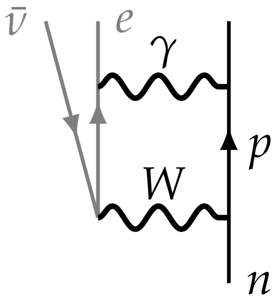

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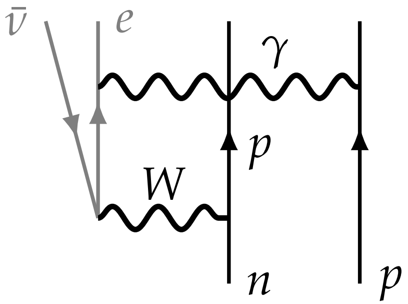

Structure-dependent radiative correction

~ Effect of **two-body currents**

Superallowed Fermi Transitions

Ab initio calculations of all cases with 1.8/2.0 (EM) interaction

Standard approach (T/H): Split contribution

$$\delta_C = \delta_{C1} + \delta_{C2}$$

Configuration mixing (→ δ_{C1})

wavefunction mismatch (→ δ_{C2})

Ab initio approach: calculate directly

$$|M_F|^2 = |M_F^0|^2(1 - \delta_C)$$

$$\delta_C = 1 - \frac{|M_F|^2}{2}$$

$$M_F = \langle \Psi_F || \tau || \Psi_i \rangle$$

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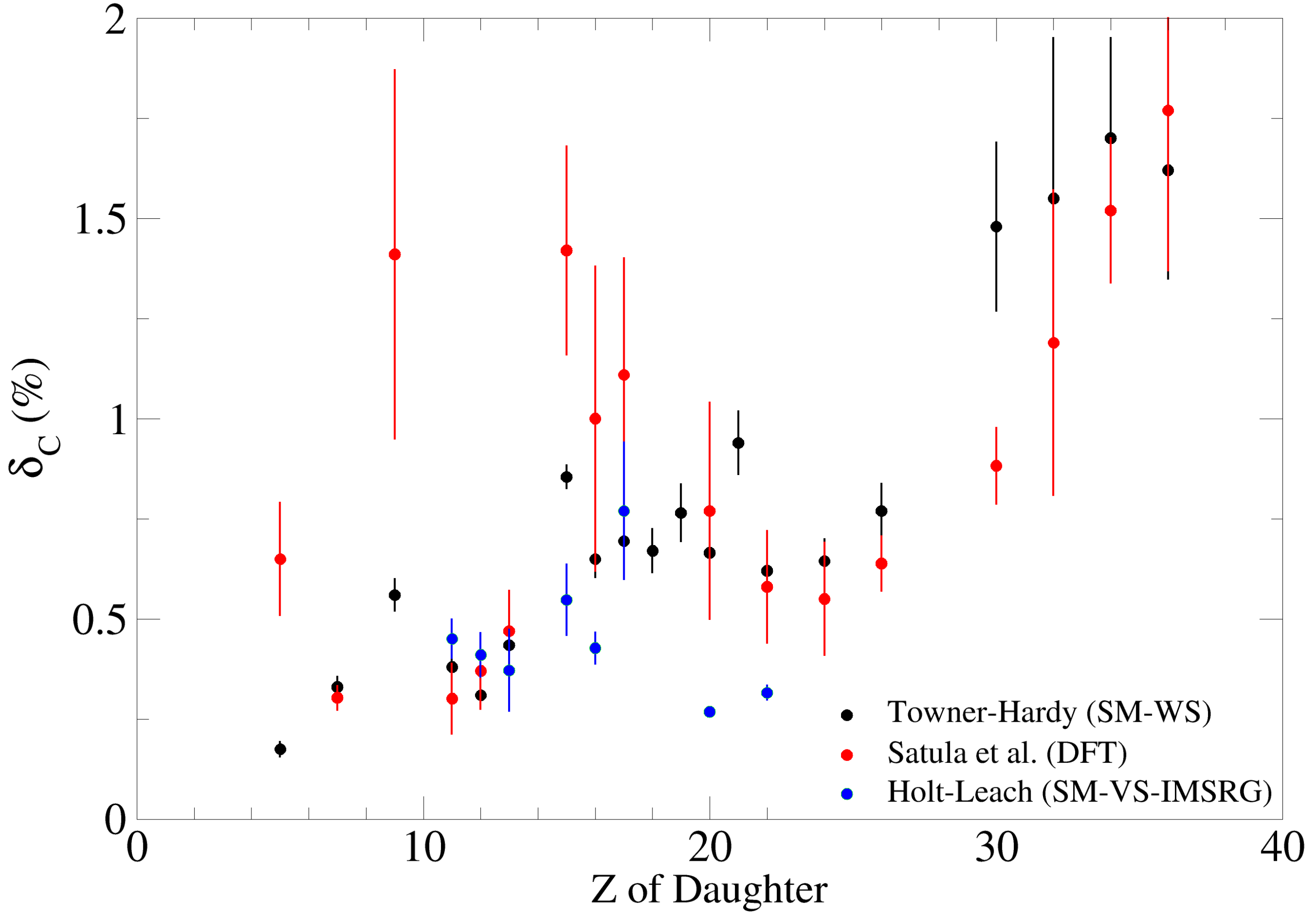
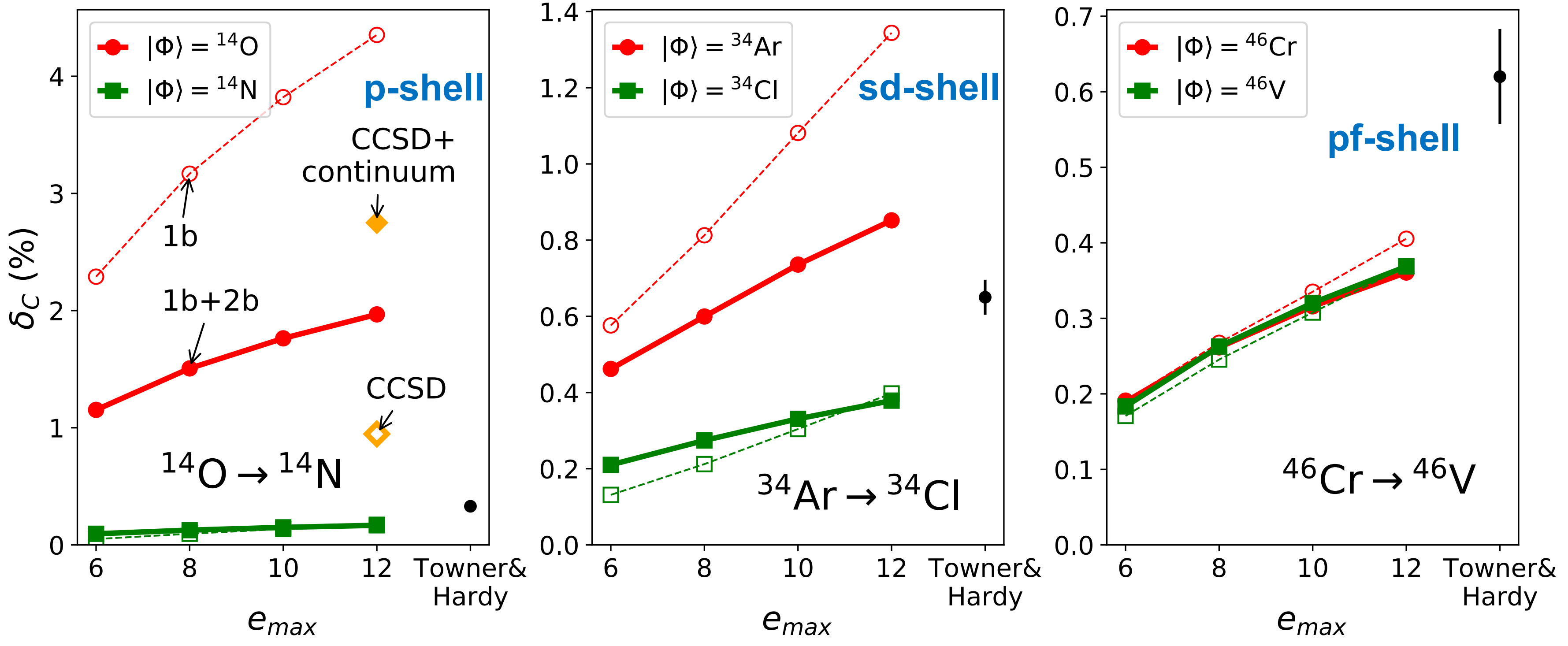


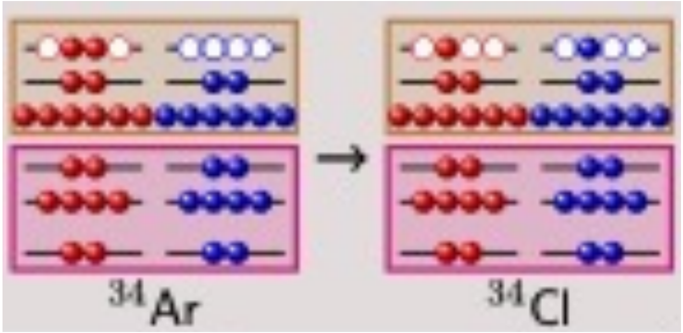
Leach, Holt, arXiv:1809.10793

Results comparable to T-H and DFT

Convergence Issues

Can we provide rigorous uncertainty estimates?





Significant effect from 1b to 1b+2b

Significant reference-state dependence in some cases; ι nvergence with e_{max}

Large effect from CC with continuum indicates generally difficult for ab inito

Potential Improvement: Natural Orbitals Basis

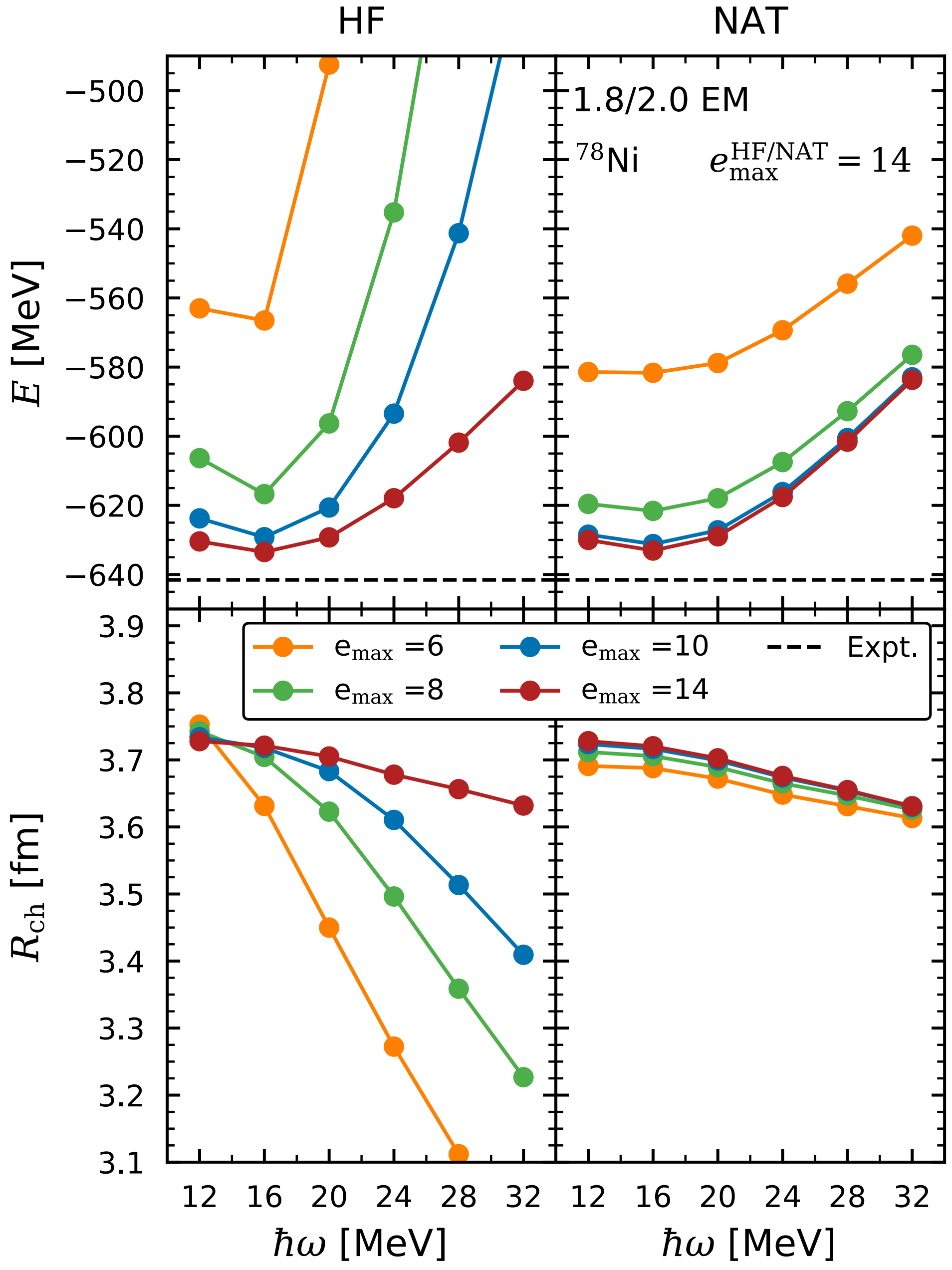
TRIUMF

Natural Orbitals (perturbatively improved) basis:

Add *perturbations* caused by interactions between particles to the HF-basis system

$$|\Psi\rangle = |\Phi\rangle + \sum_{n=1}^{\infty}\Big(\frac{H_I}{H_0 - E^{(0)}}\Big)^n|\Phi\rangle$$

$$E = E^{(0)} + \sum_{n=1}^{\infty}\Big\langle\Phi|H_I\Big(\frac{H_I}{H_0 - E^{(0)}}\Big)^n|\Phi\Big\rangle$$



Dramatic improvement in energies and radii

Can it help with superallowed convergence?

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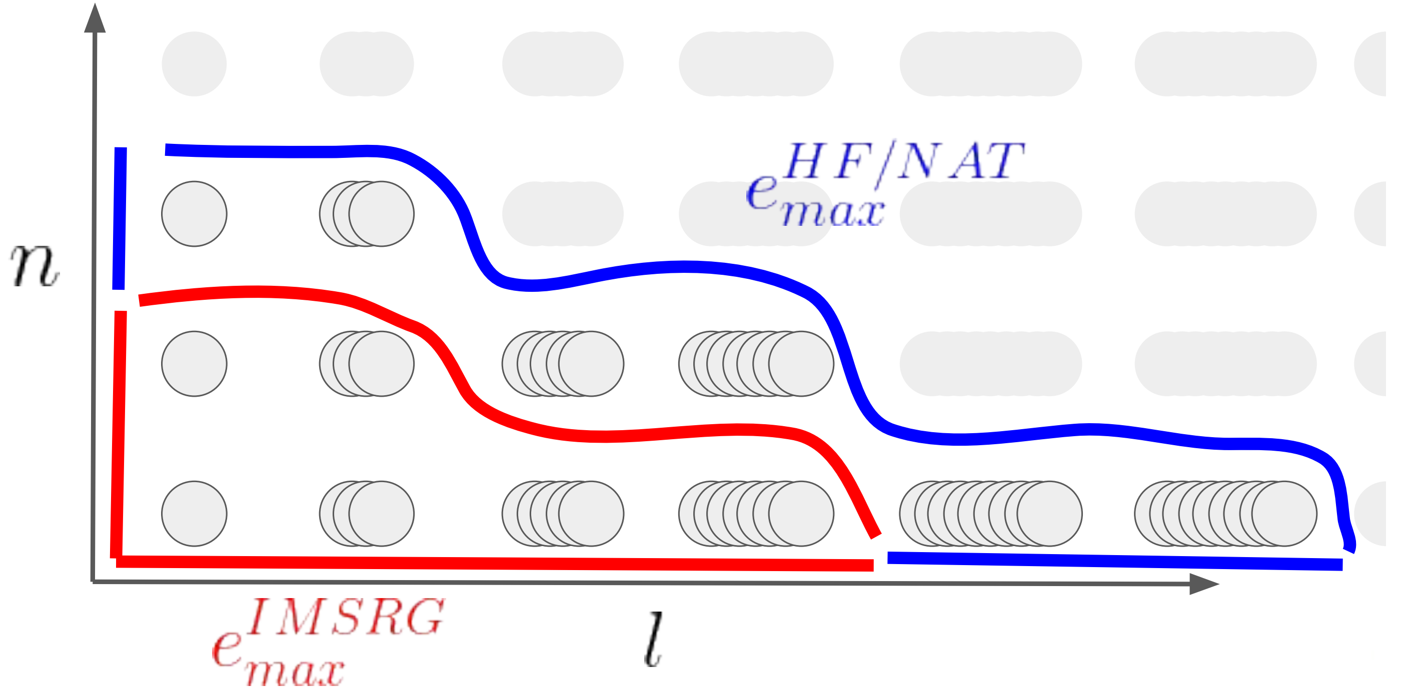

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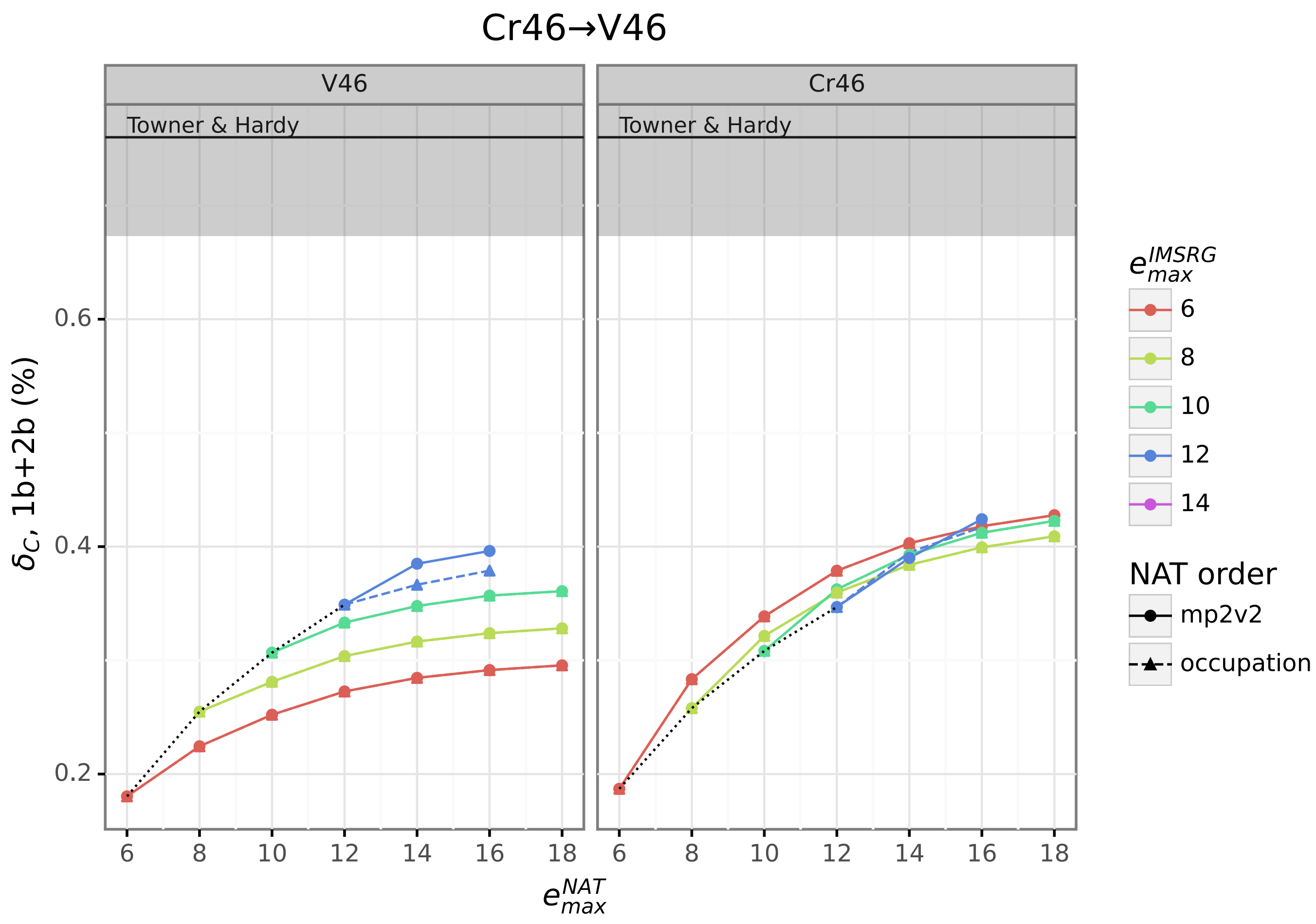
Medium mass:

- consistent results for NAT orbitals chosen
- potentially small reference-state dependence
- still unclear e_{max} convergence



Potential Improvement: Natural Orbitals Basis

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Medium mass:

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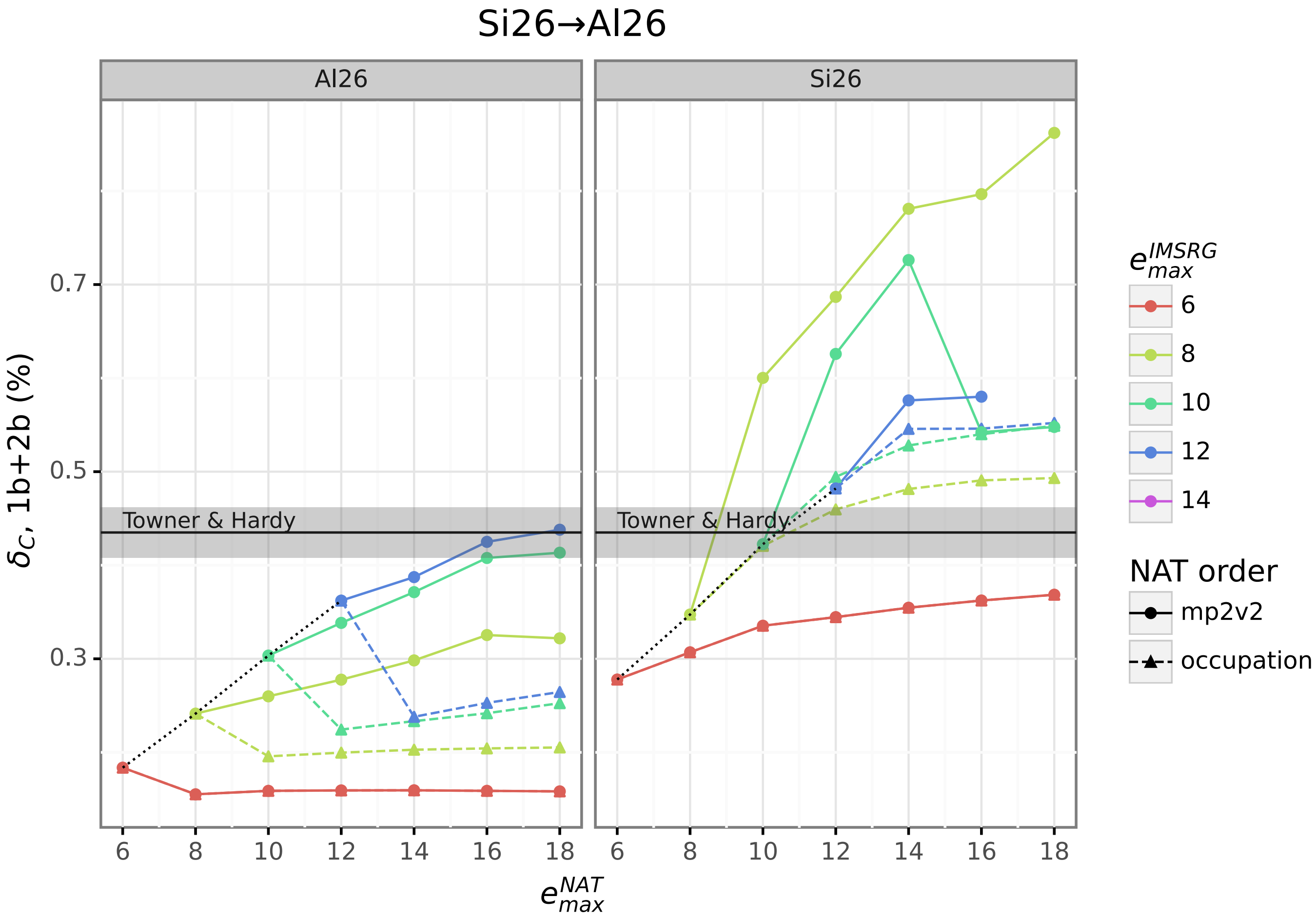
- potentially small reference-state dependence
- still unclear e_{max} convergence

Lighter systems

- "quirks" in convergence…



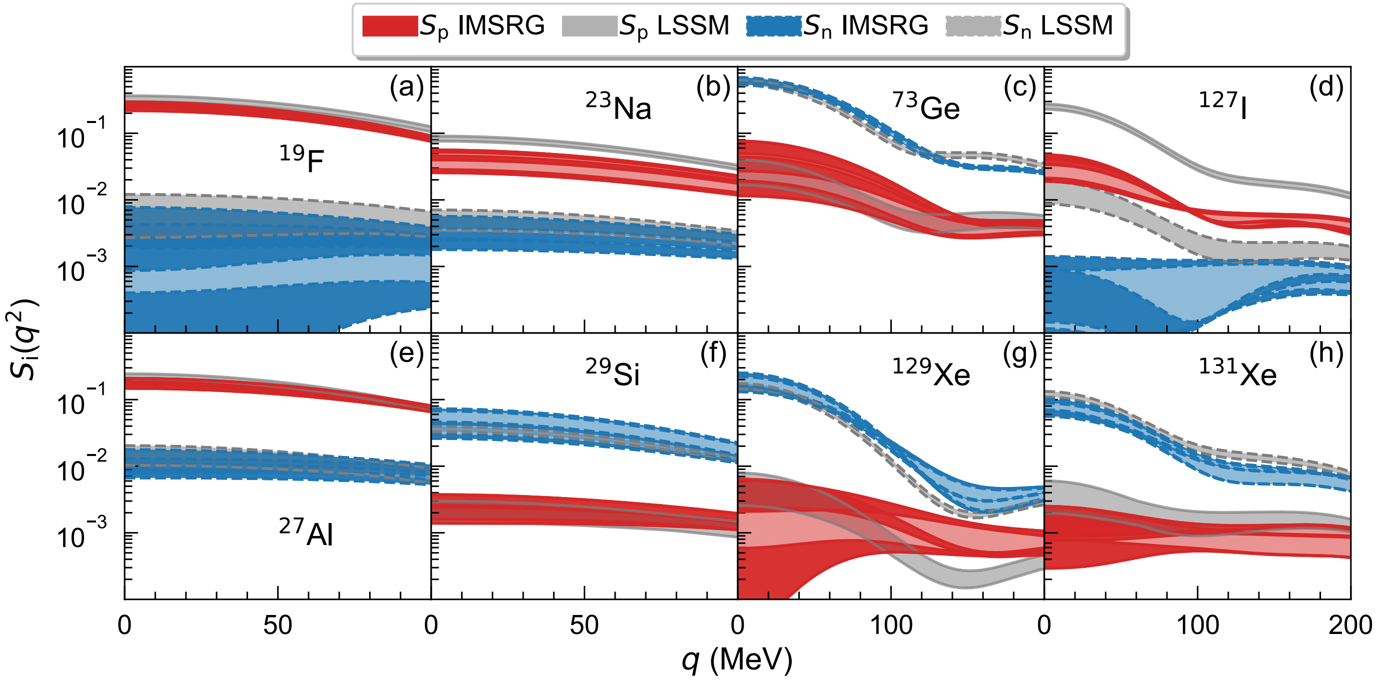
Work still in progress…

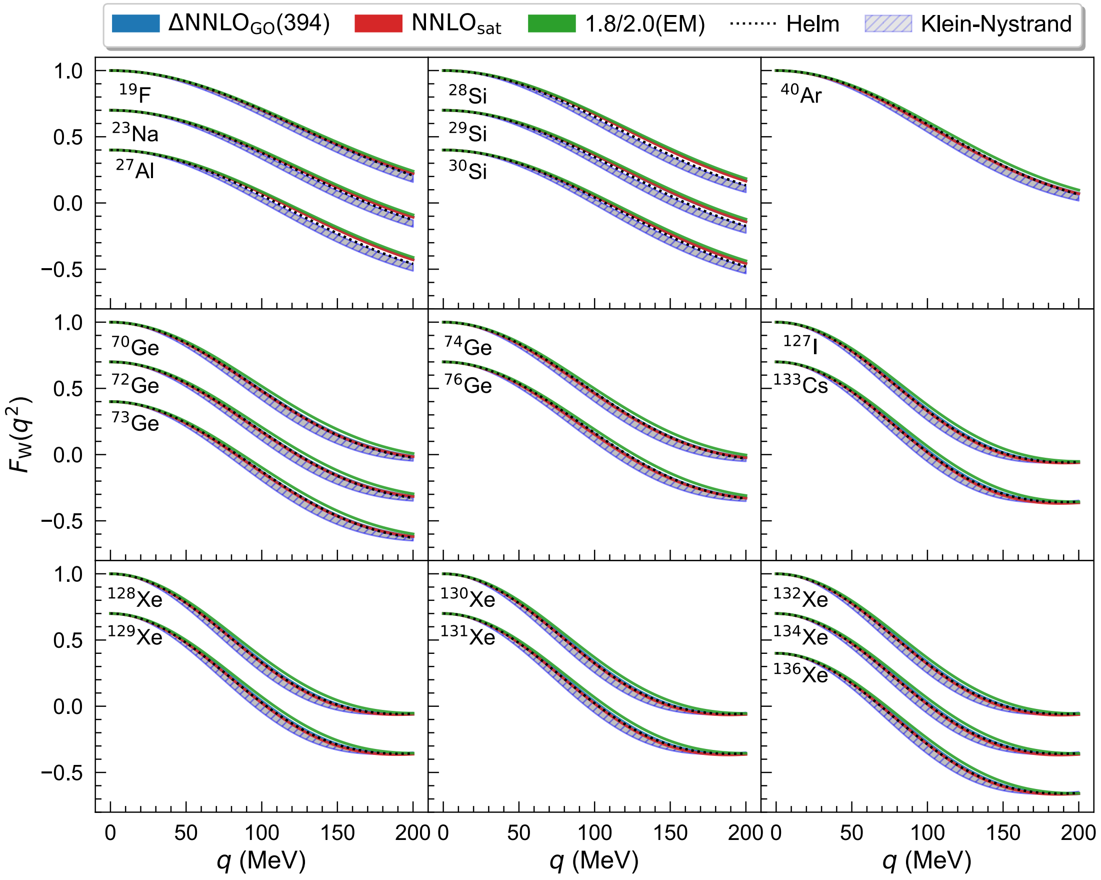
TRIUMF

Ab Initio SD WIMP/ν-Nucleus Response Overview

Use **three** NN+3N chiral interactions with consistent chiral currents

Overall similar to phenomenology at low q, largest discrepancies in ^{127}I





New structure functions for all SD direct-detection candidates