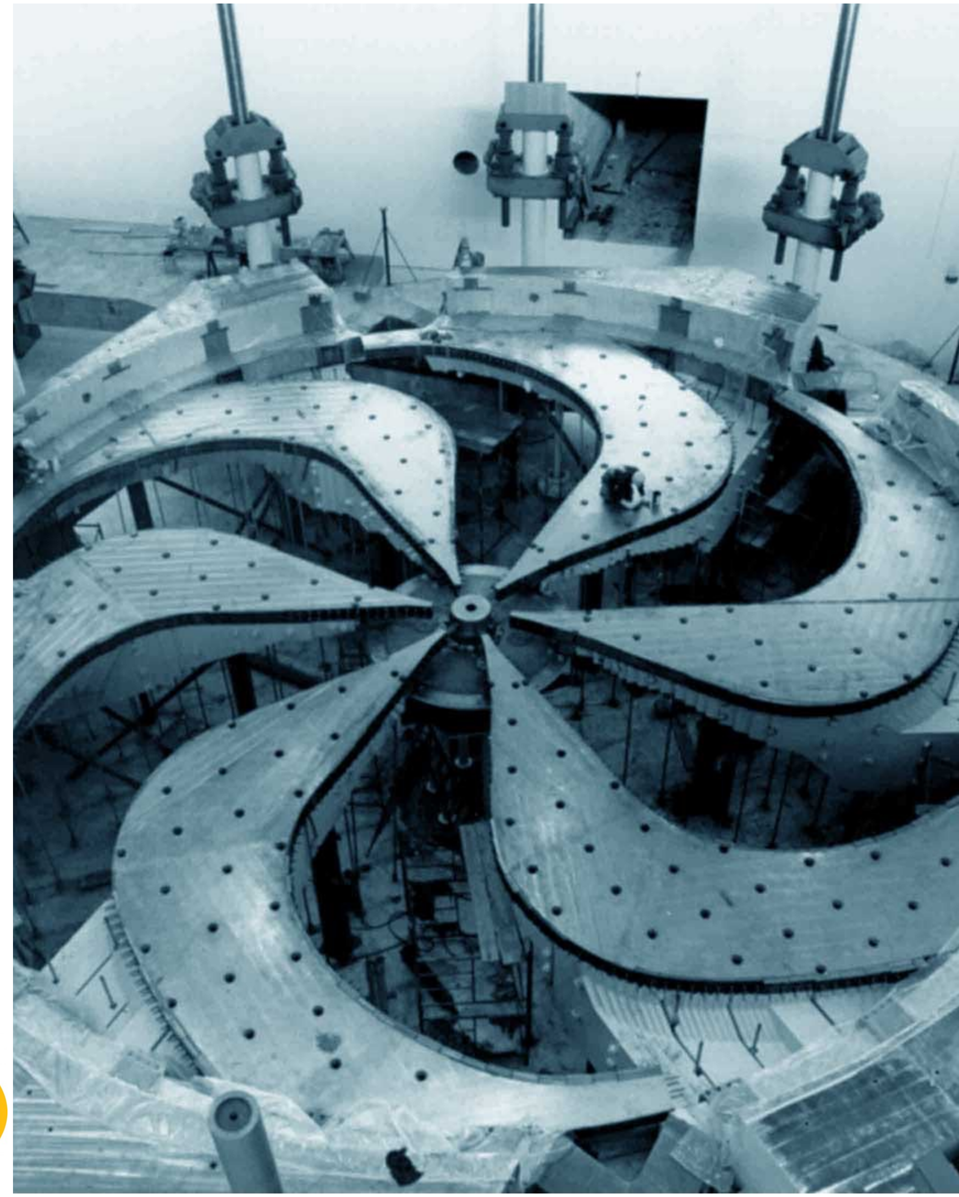
Global ab initio calculations for exotic and heavy nuclei

Jason D. Holt
TRIUMF, Theory Department
Theory Alliance Meeting, FRIB
May 18, 2023



Discovery, accelerated

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Major RIB Facilities Worldwide

Next-generation RIB facilities: unprecedented era of nuclear science

Thousands of new isotopes to be produced: **How does our field maximize this opportunity?**

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Major RIB Facilities Worldwide

Next-generation RIB facilities: unprecedented era of nuclear science

Thousands of new isotopes to be produced: **Meaningful interaction with theory!**

$4-5B worldwide investment

What is the fundamental, exciting physics?

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Major RIB Facilities Worldwide

Next-generation RIB facilities: unprecedented era of nuclear science

Thousands of new isotopes to be produced: **Meaningful interaction with theory!**

Role of theory

Motivation: robust predictions (**with uncertainties!**) where no data exists

Interpretation: model independent, connect to underlying forces of nature

$4-5B worldwide investment

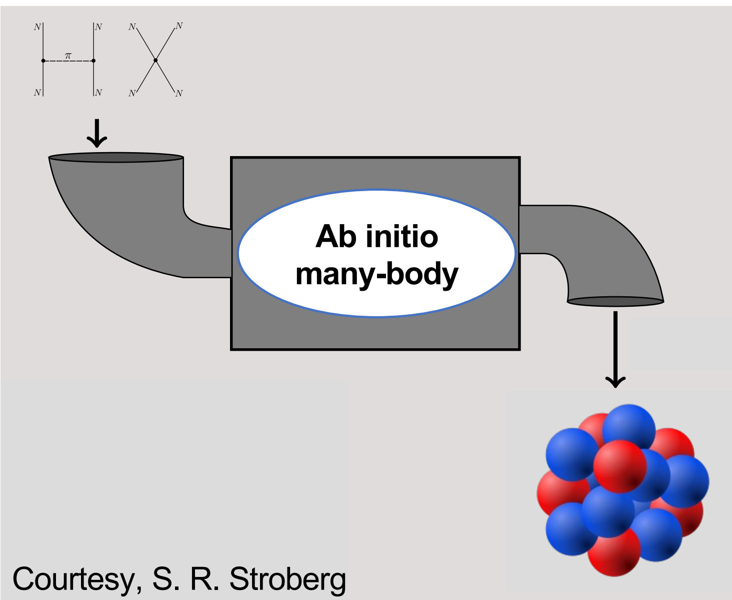
What is the fundamental, exciting physics?

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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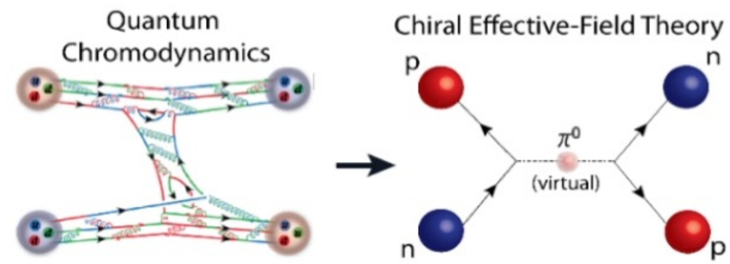
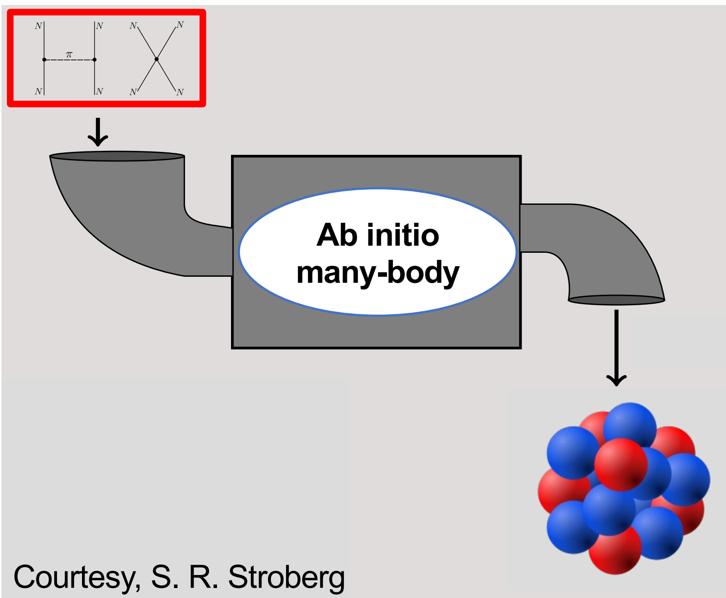




Courtesy, S. R. Stroberg

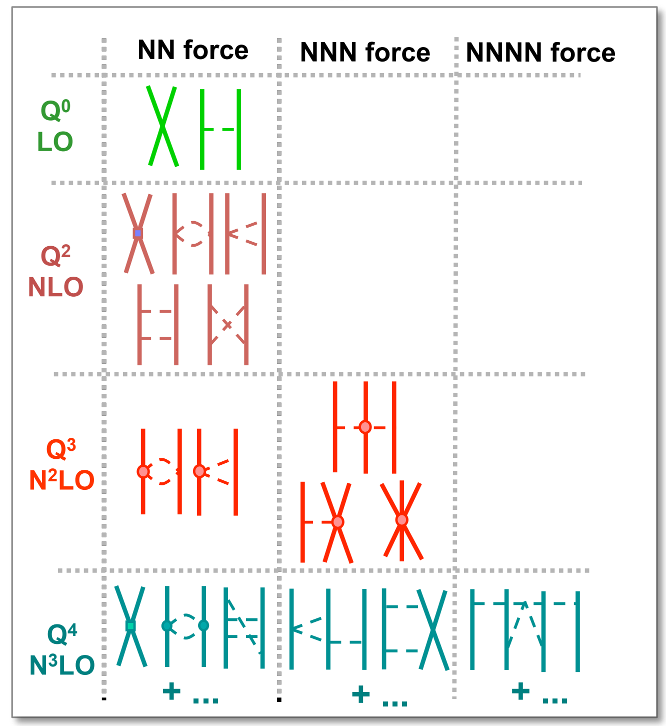
[Chiral Effective Field Theory]

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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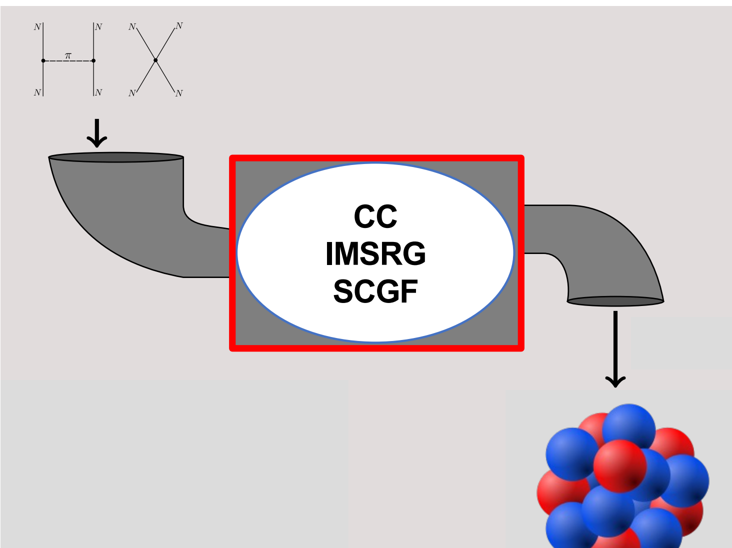

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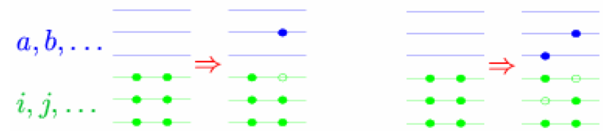
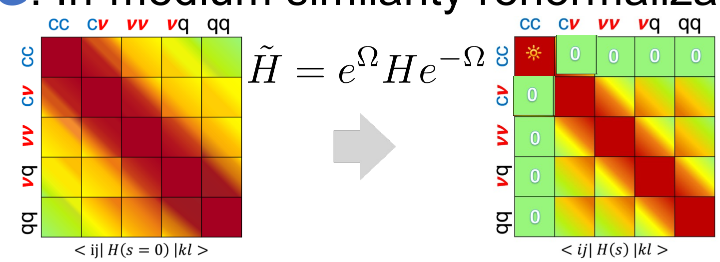
Ab Initio Cheat Sheet (polynomial scaling methods)

CC: Coupled cluster theory



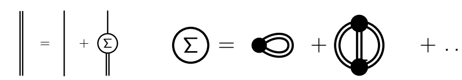
$$E = \langle\Phi|\overline{H}|\Phi\rangle$$
$$0 = \langle\Phi_i^a|\overline{H}|\Phi\rangle$$
$$0 = \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle$$
$$\overline{H} \equiv e^{-T}He^{T} = \left(He^{T}\right)_c$$

IMSRG: In-medium similarity renormalization group



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

SCGF: Self-consistent Green's function



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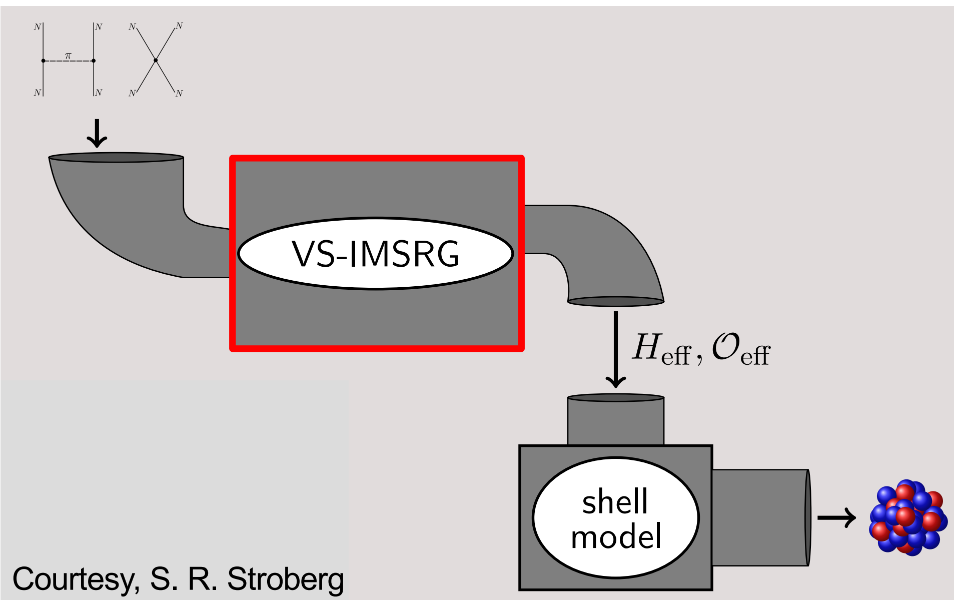

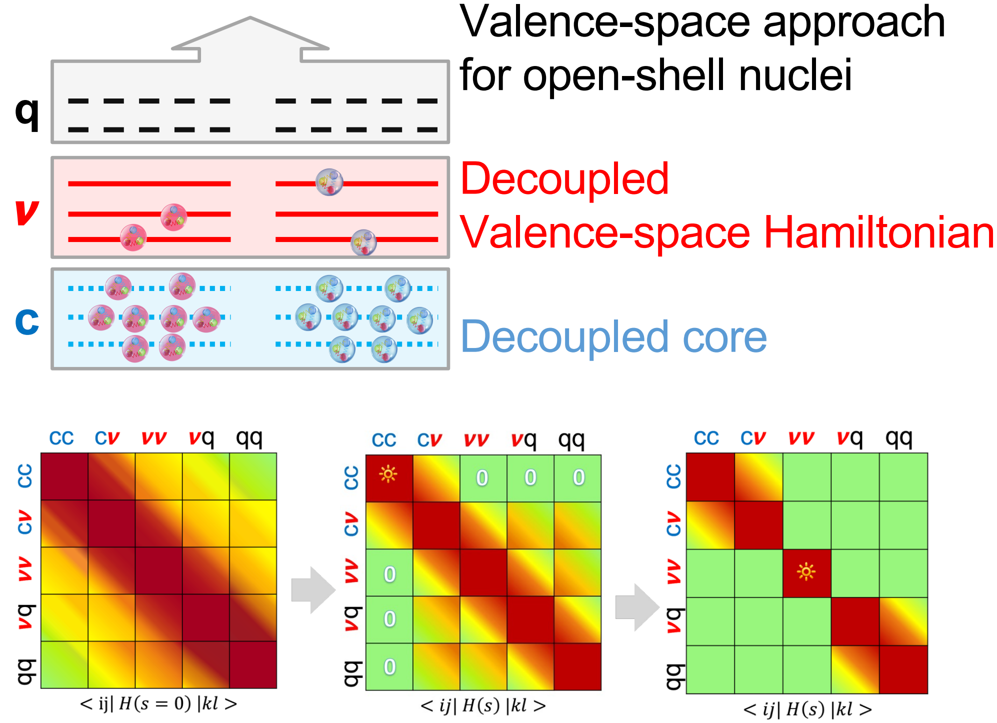

Extends ab initio to scope of traditional nuclear shell model

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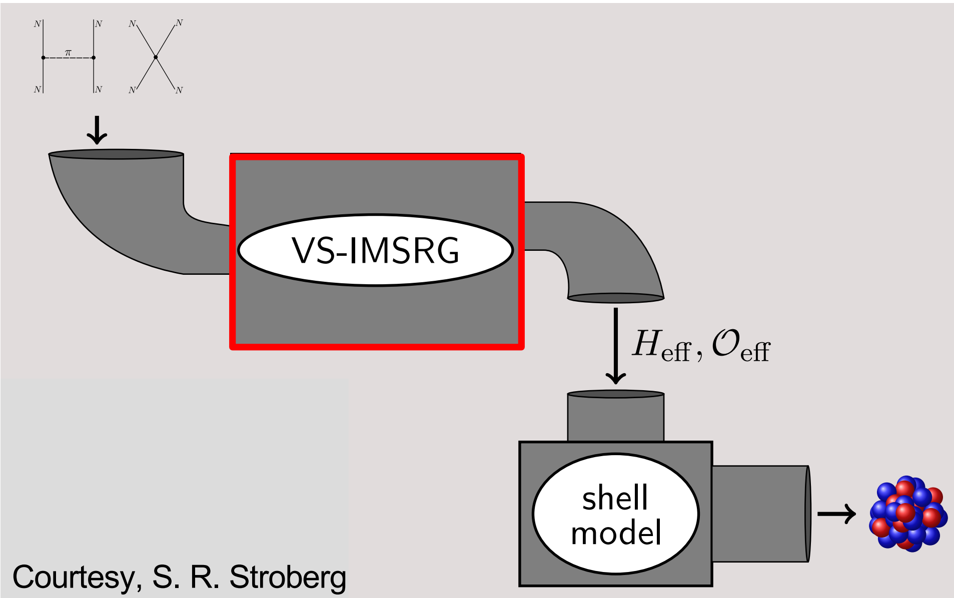

Methods Exact up to Truncations

- ✅ **Single-particle basis** $e_{\rm max} = 2n + l$
- ✅ **Storage limits of 3N forces** $e_1 + e_2 + e_3 \leq E_{3\rm max}$
- 🤷‍♂️ **Many-body operators: e.g., CCSD(T), IMSRG(2)**

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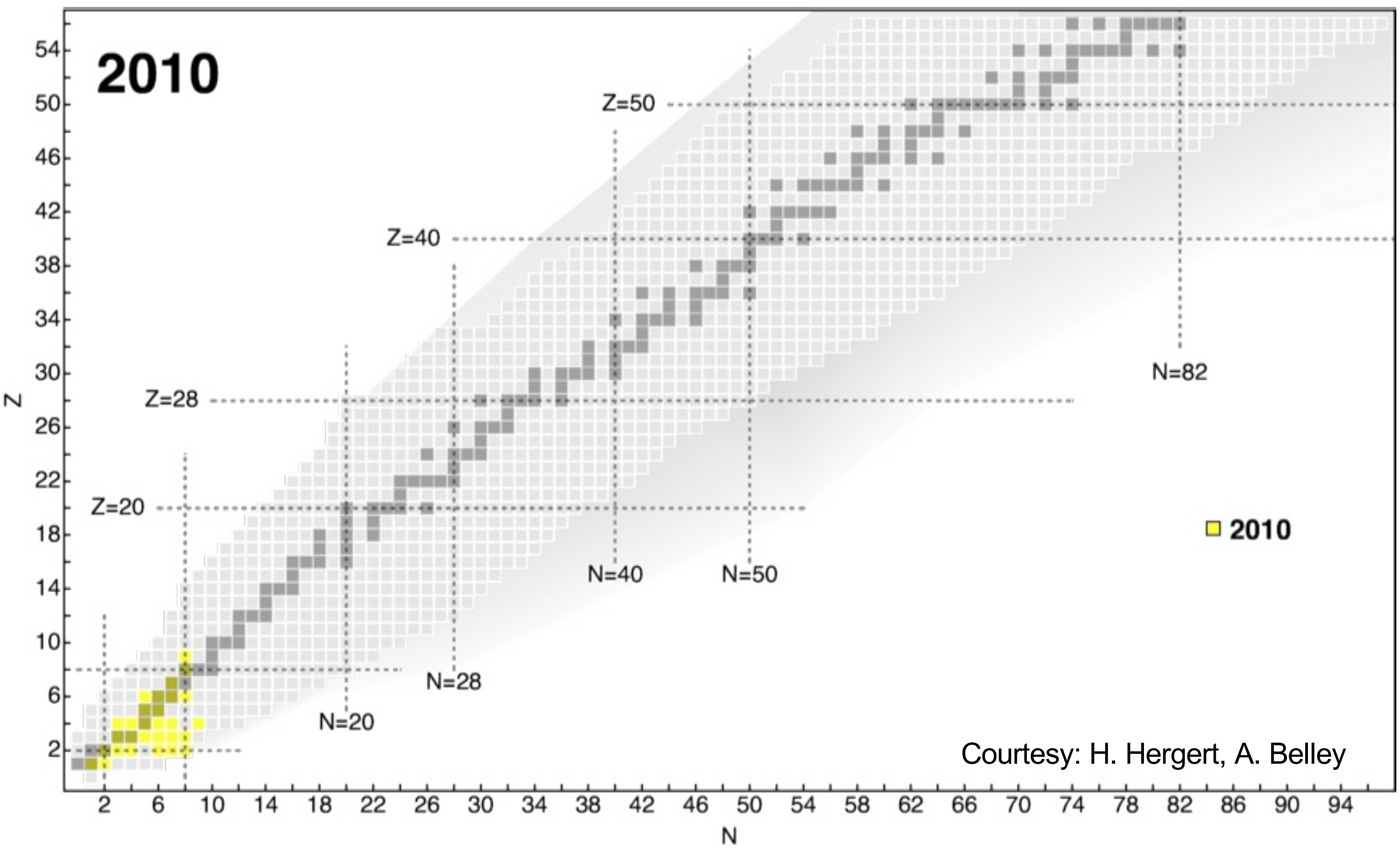
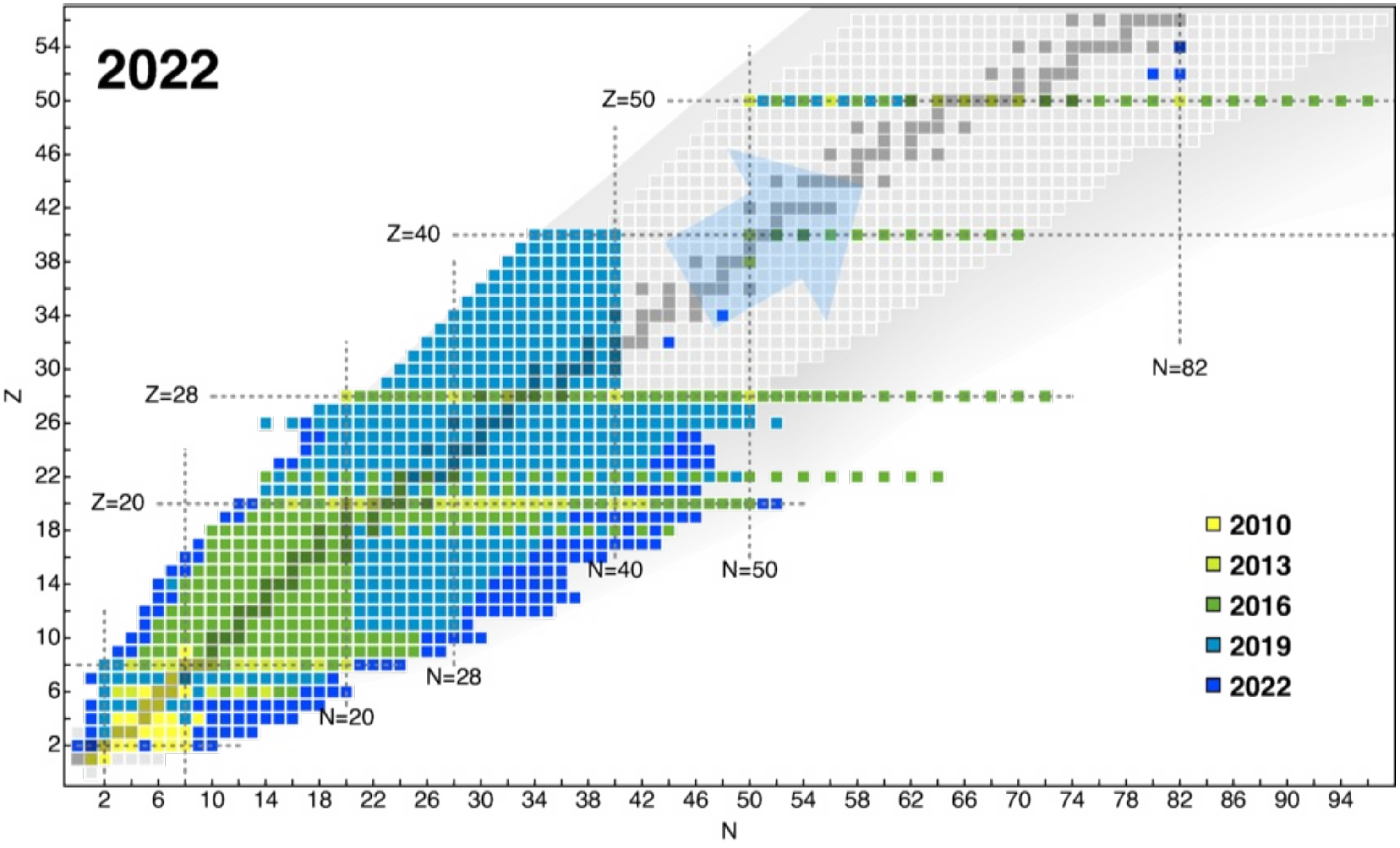
Progress of Ab Initio Theory Since 2010

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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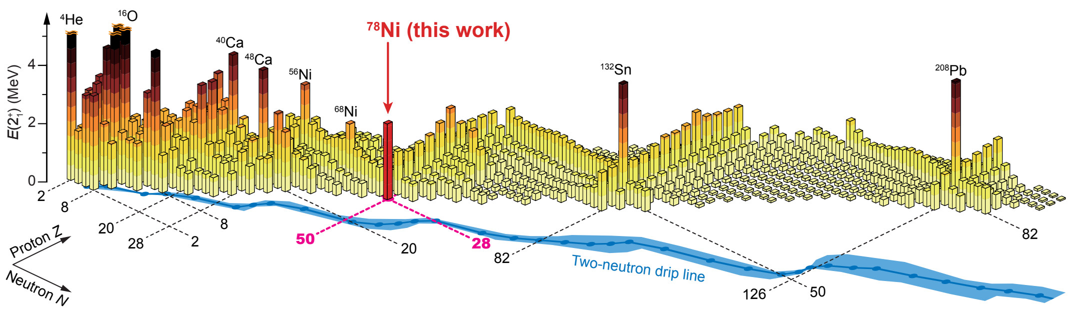
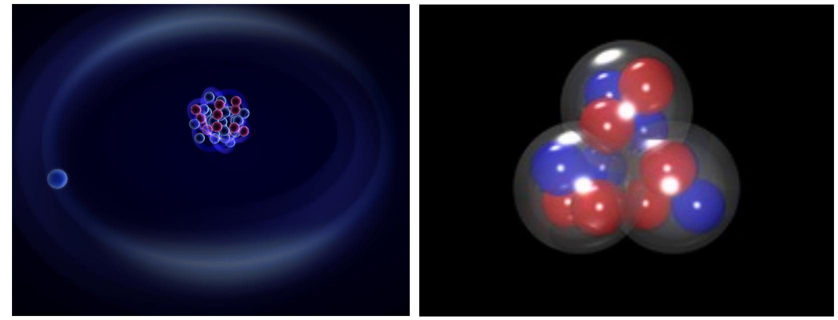
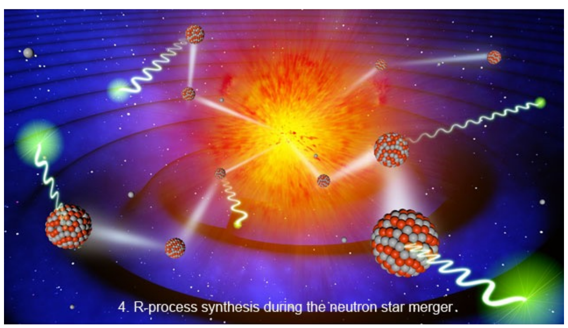
Major Questions in Nuclear Structure



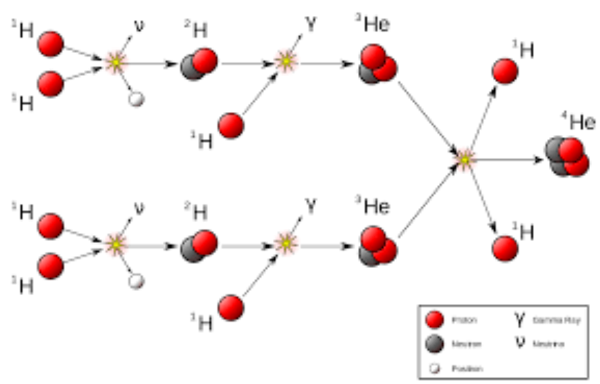
Limits of existence + formation/evolution of magic numbers



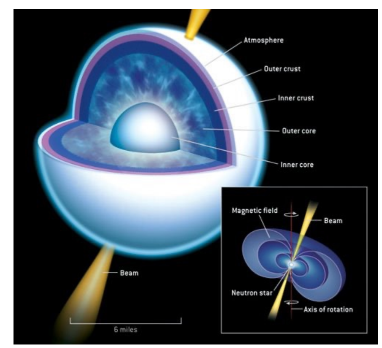
Nuclear skins/halos/clusters



Heavy Nuclei + r-process



Continuum and nuclear reactions



Infinite matter/Neutron stars

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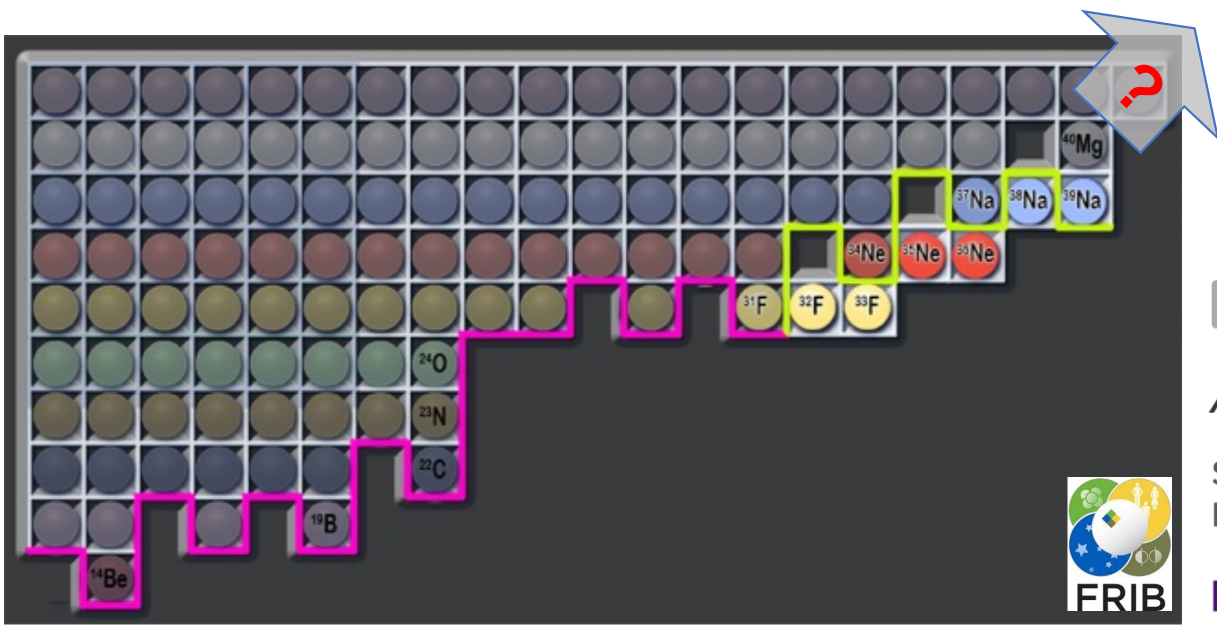
Global Ab Initio Calculations: Proton/Neutron Driplines



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

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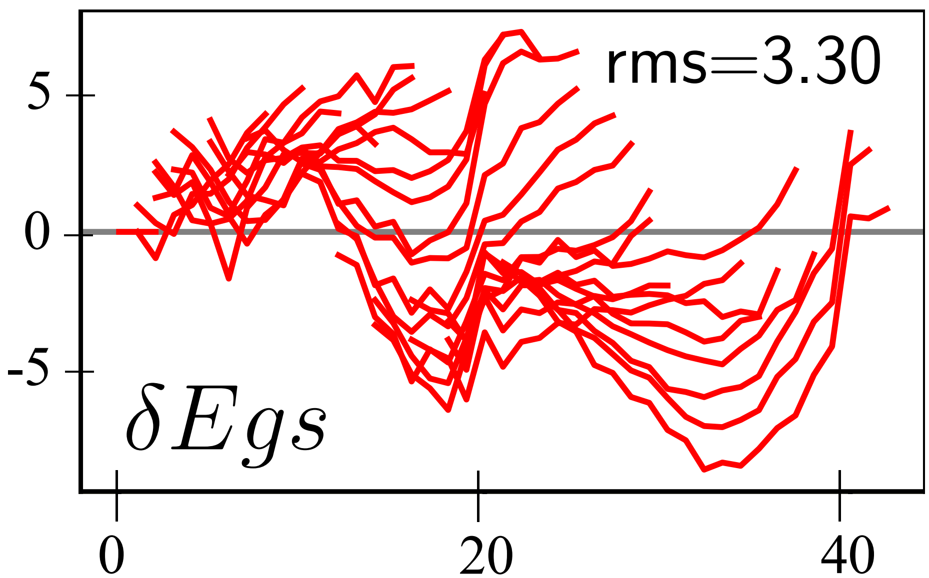
Ab Initio Goes Global!

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)

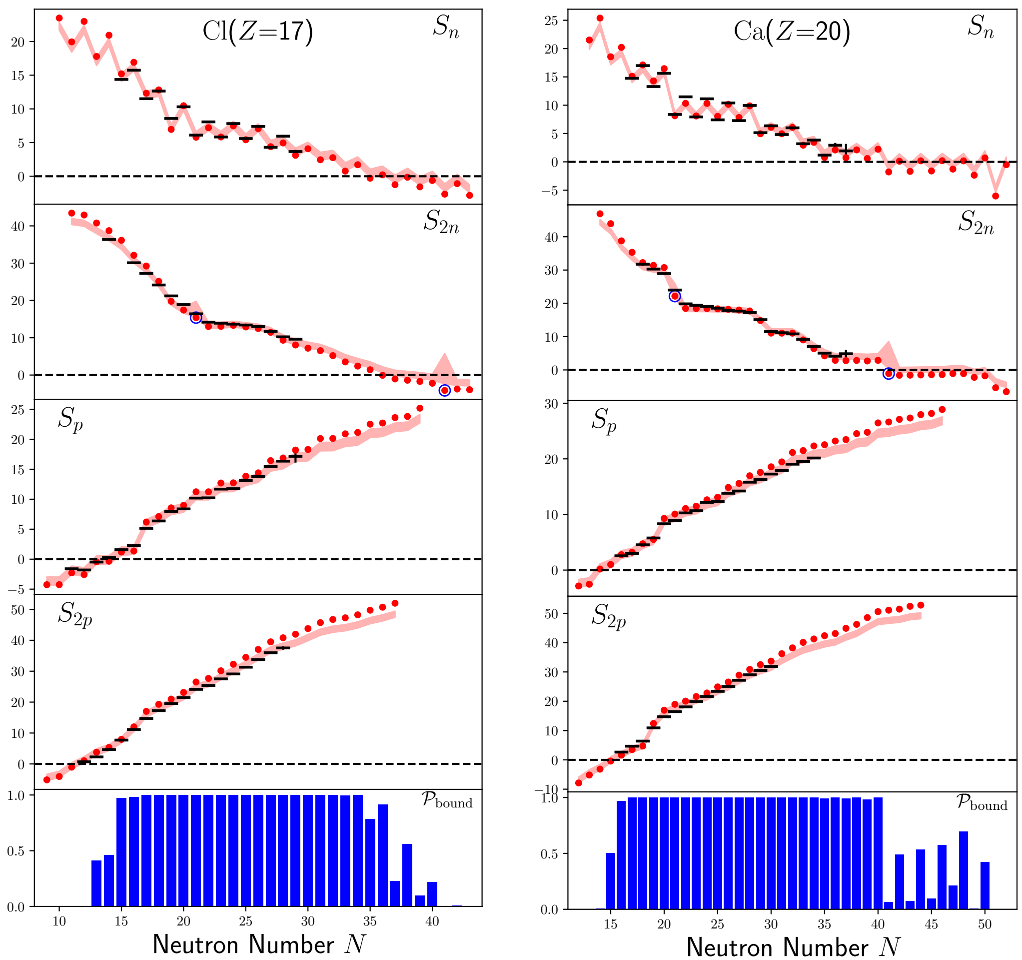
DFT: 0.6-2.0 MeV

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

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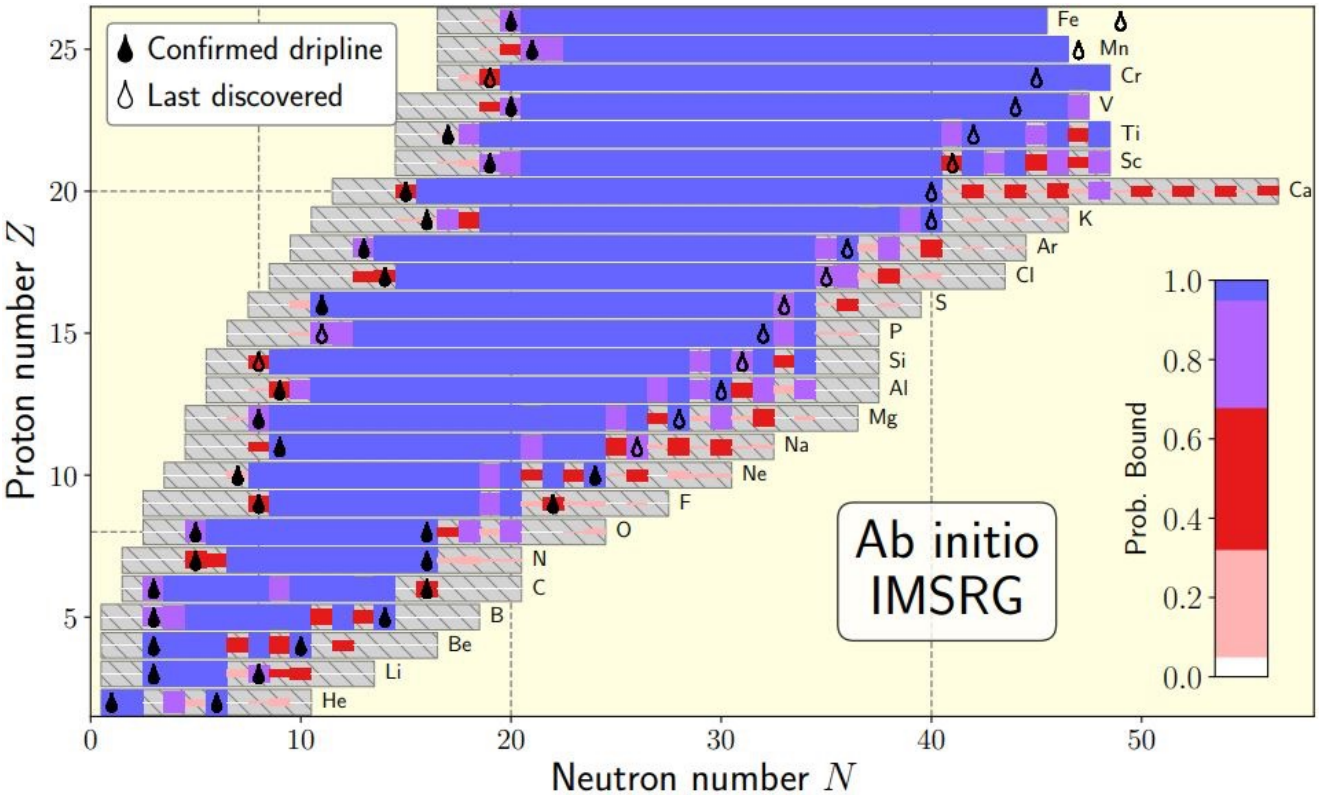
Dripline Predictions to Medium Mass Region

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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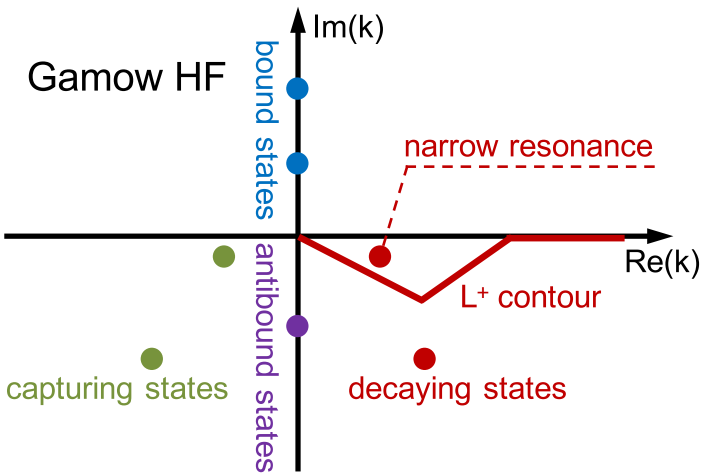
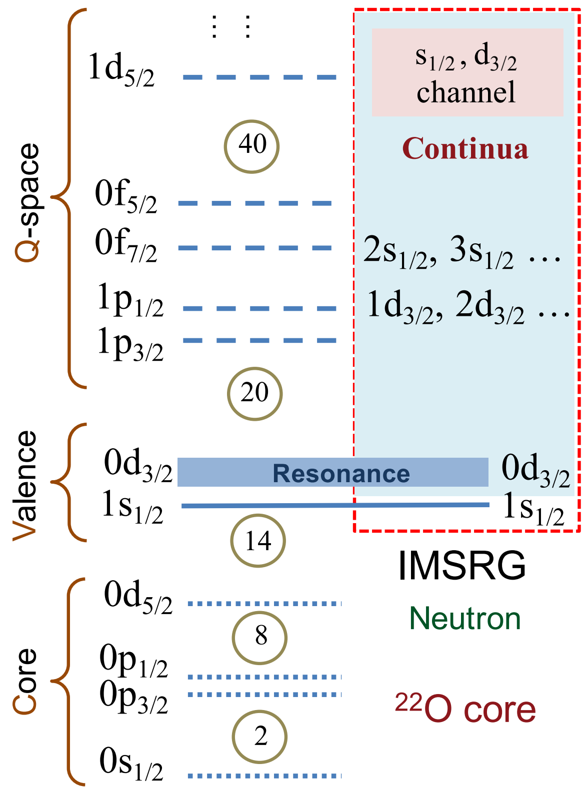
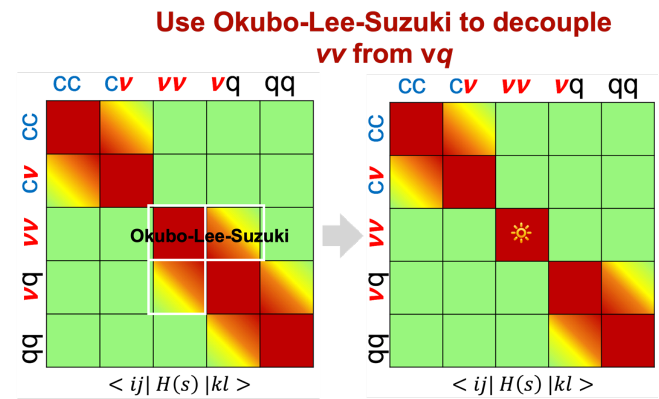
VS-IMSRG with Continuum

Use Gamow-Bergren basis for VS-IMSRG calculation







Continuum states complicate IMSRG - Solution similar to multi-shell

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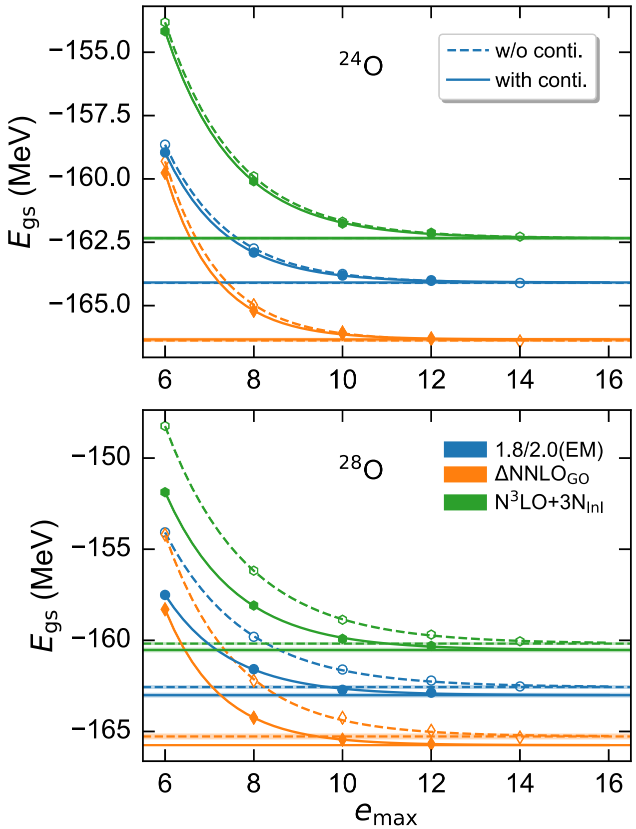
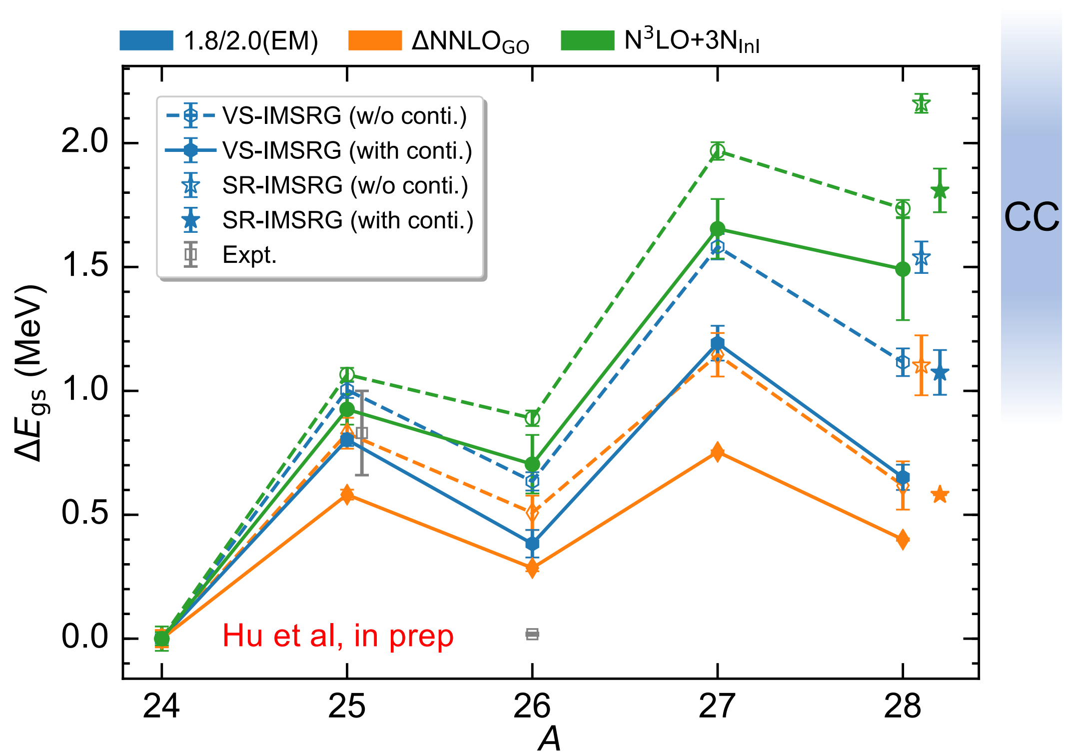
Existence of ^{28}O

New measurement at RIKEN of existence of energy in ^{28}O – apply VS-IMSRG w/ continuum





Chalmers + ORNL collab.

Continuum lowers calculated g.s. energy by ~300keV

In all cases ^{28}O predicted to be unbound… consistent with CC emulator predictions

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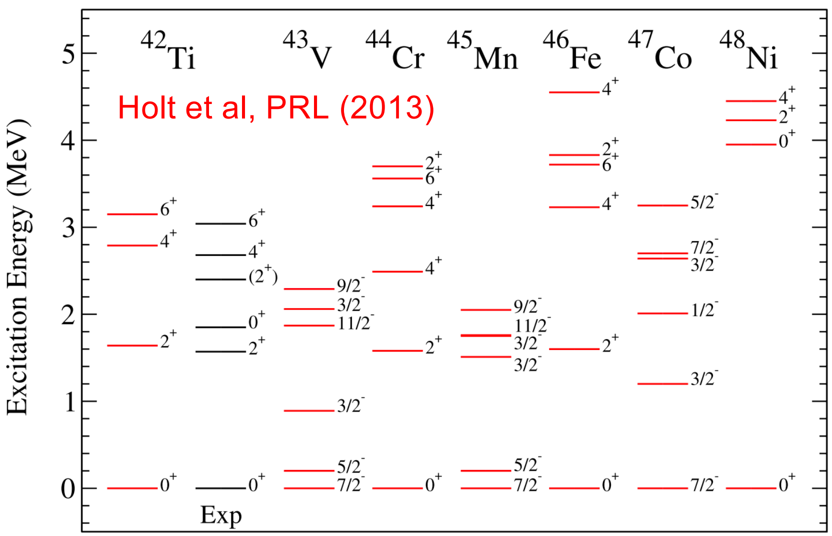
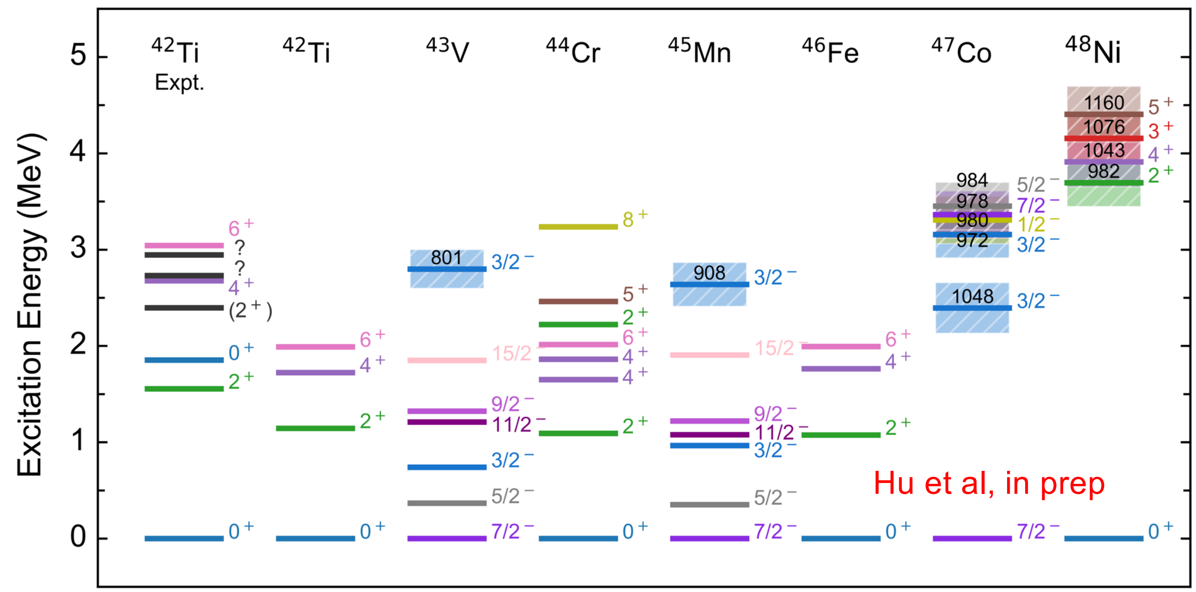
Existence of ^{48}Ni

Probe limits of existence at proton dripline ^{48}Ni – VS-IMSRG w/ continuum also necessary





Minor effect from continuum

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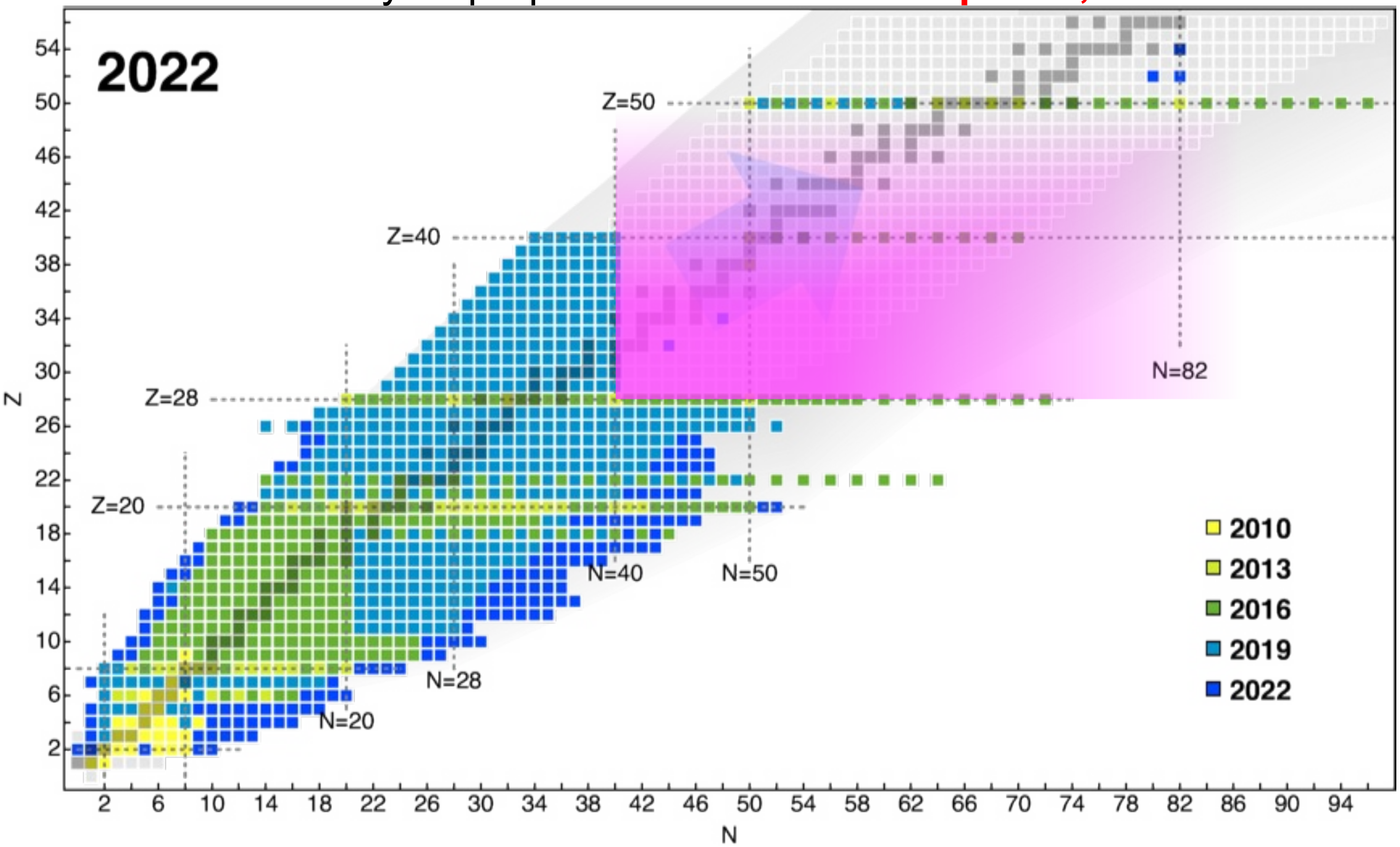
Ab Initio Progress: How Heavy Can We Go?

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

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



<u>Key Limitation</u>

3NF matrix element storage

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

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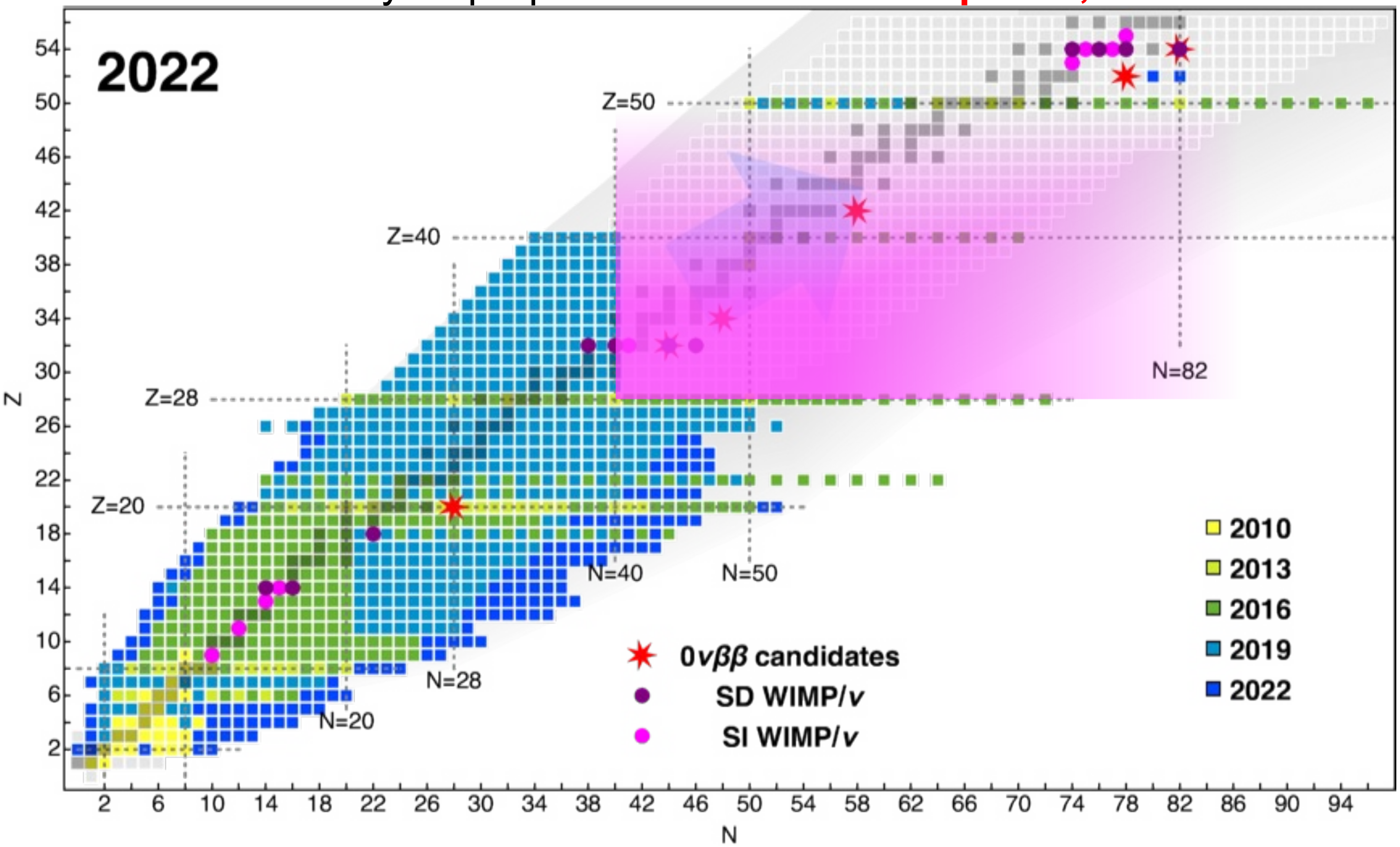

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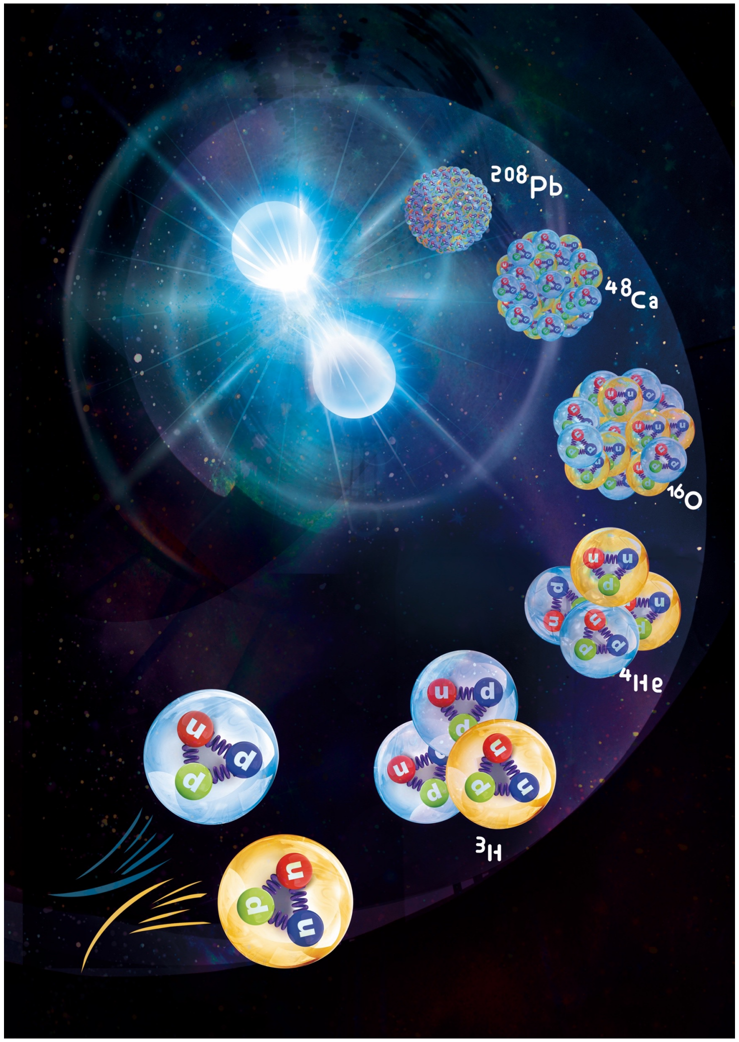
Converged Calculations in Heavy Nuclei



Converged *ab initio* calculations of heavy nuclei

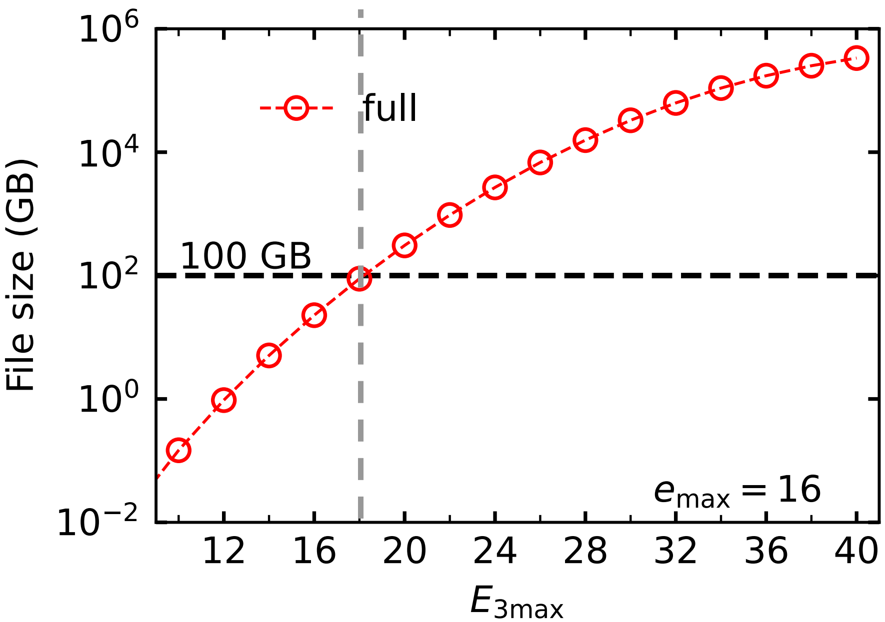
T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt

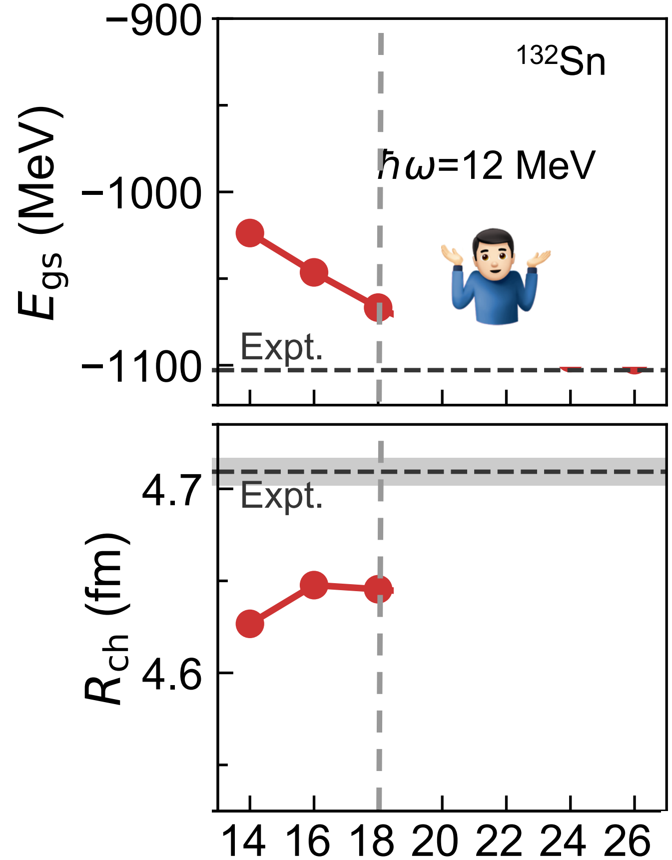
Phys. Rev. C **105**, 014302 – Published 3 January 2022

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}





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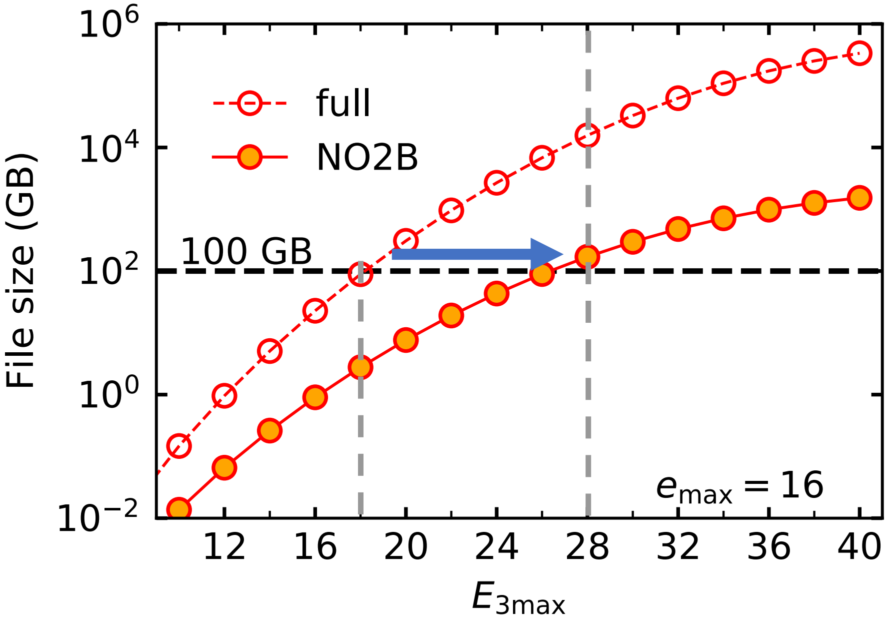
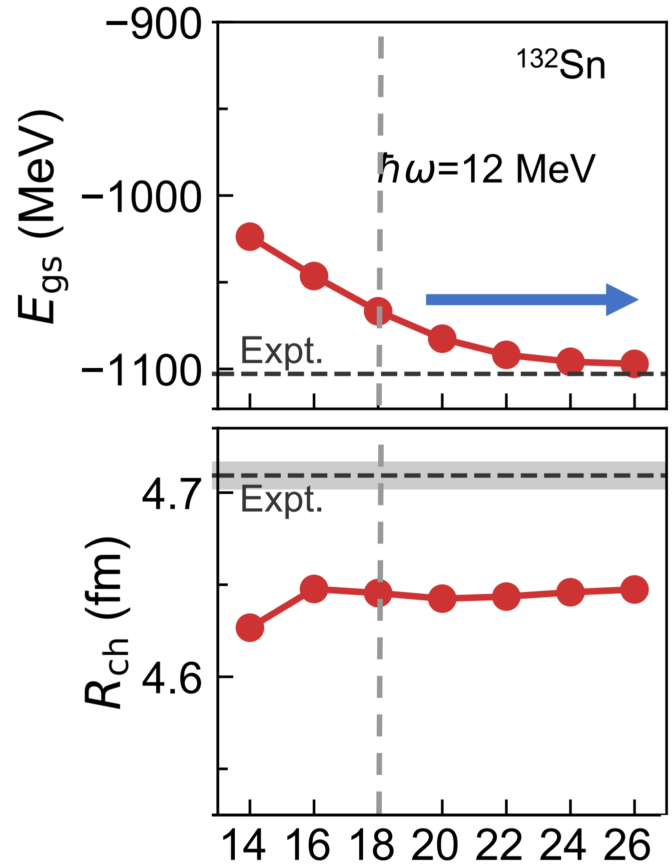
Ab Initio Calculations of Heavy Nuclei

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

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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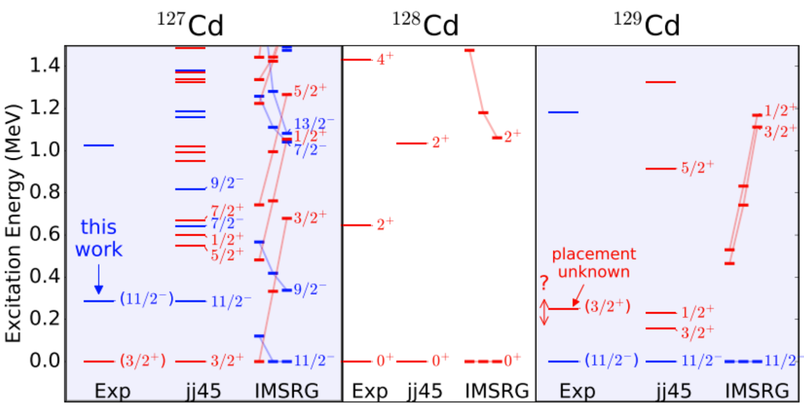
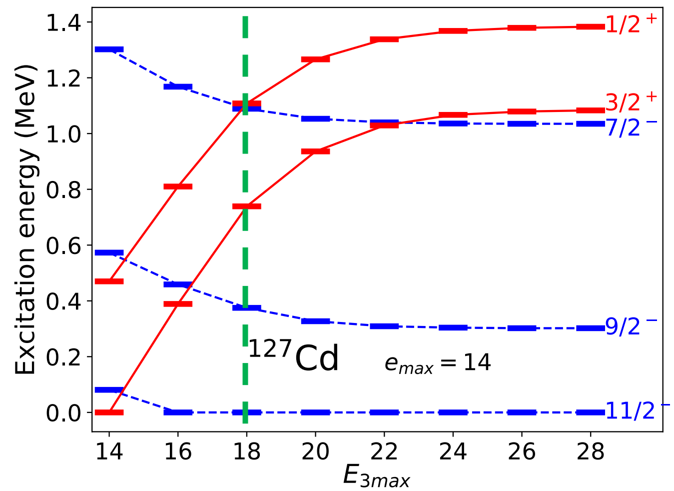
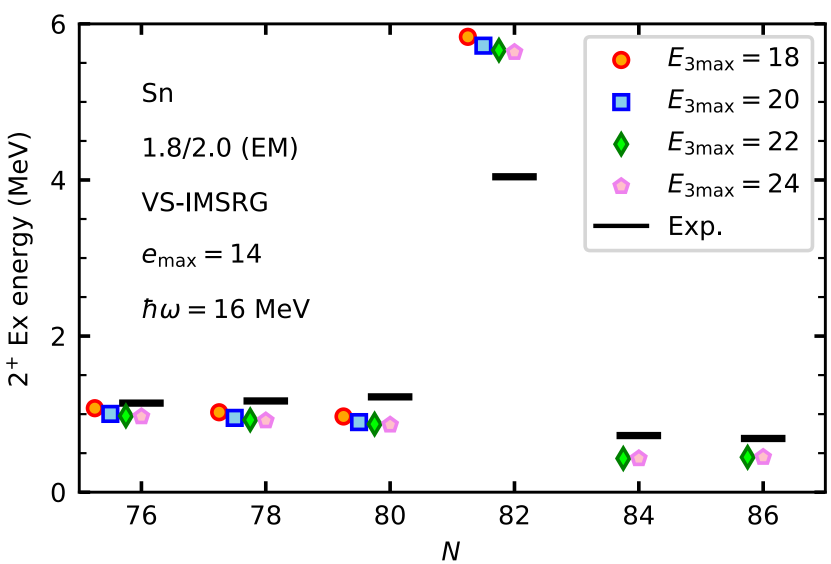
Convergence of N=82 Gap

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







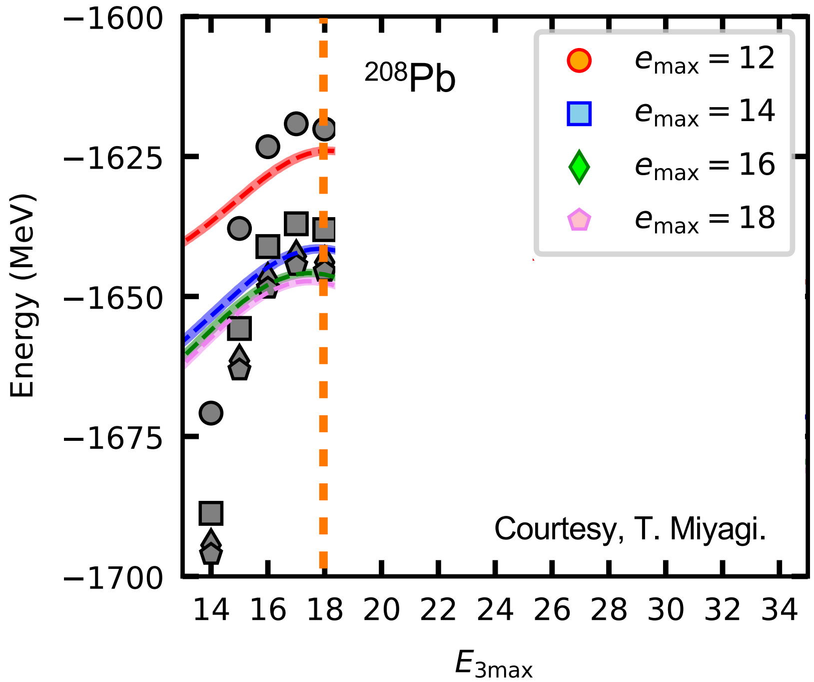
New capabilities: converged spectra in N=82 region

Converged (overpredicted) doubly magic ^{132}Sn

Can we go heavier?

Convergence in Heavy Nuclei: ^{208}Pb

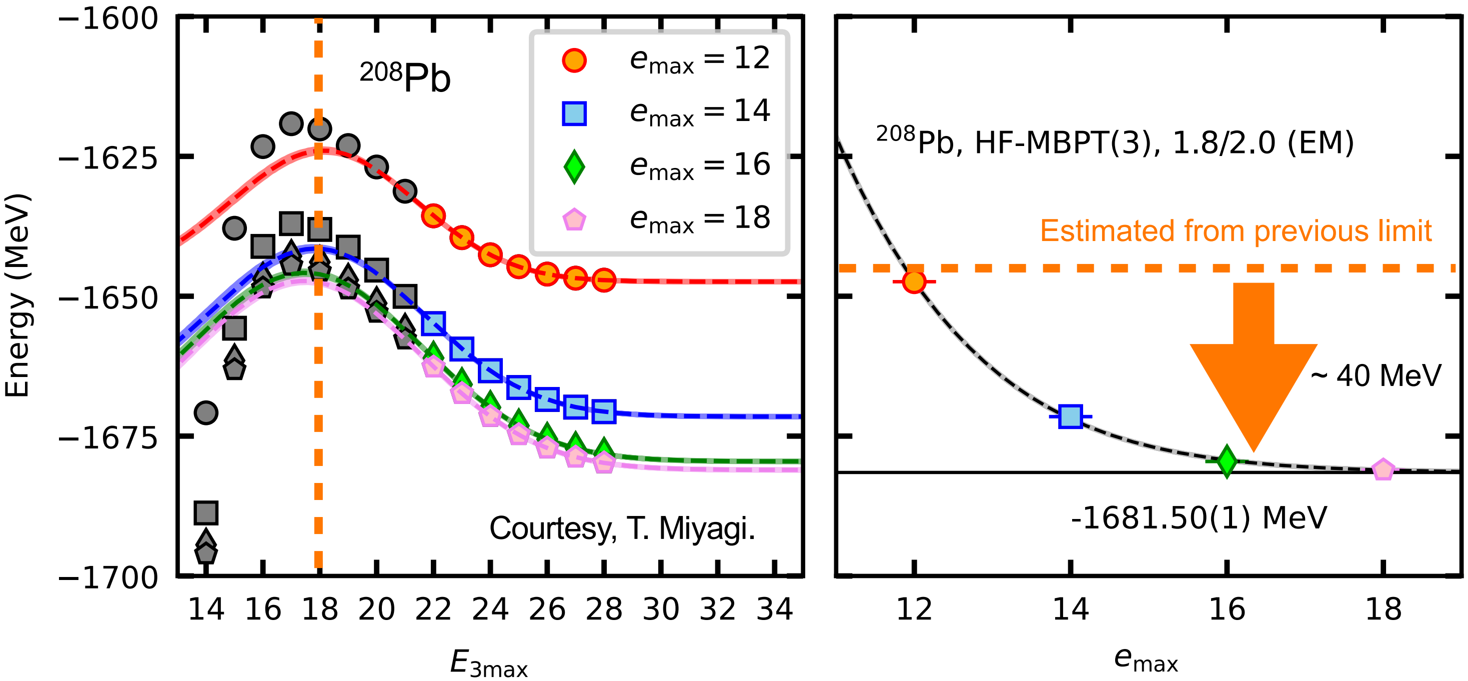
Previous limit, no hope of convergence in ^{208}Pb g.s. energy…



Convergence in Heavy Nuclei: ^{208}Pb

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

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



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

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

nature physics

ARTICLES

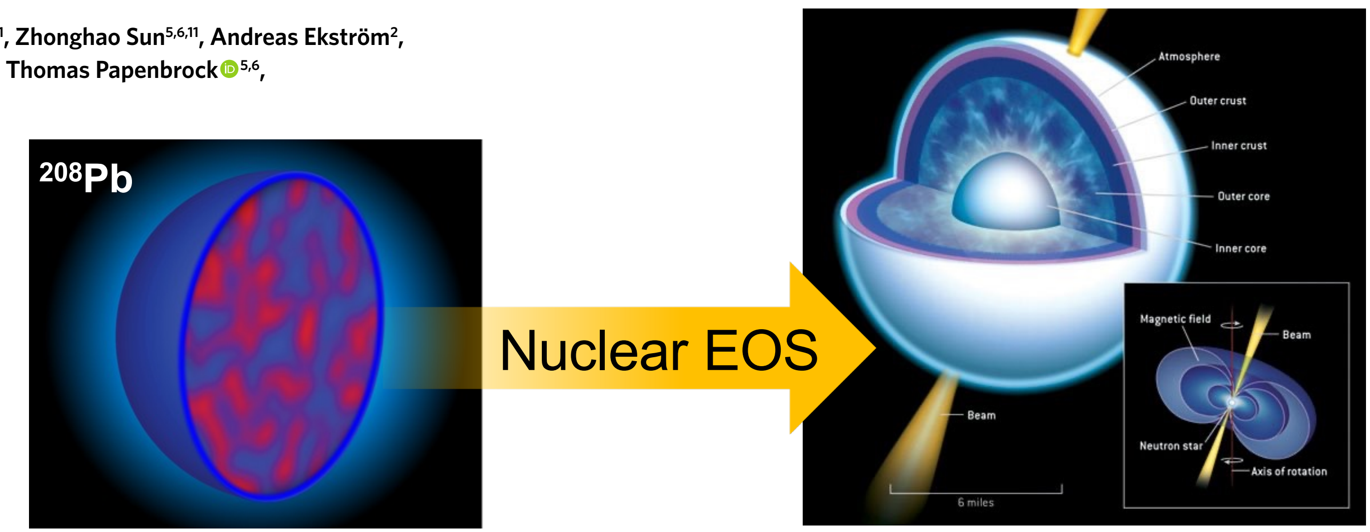
https://doi.org/10.1038/s41567-022-01715-8

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]



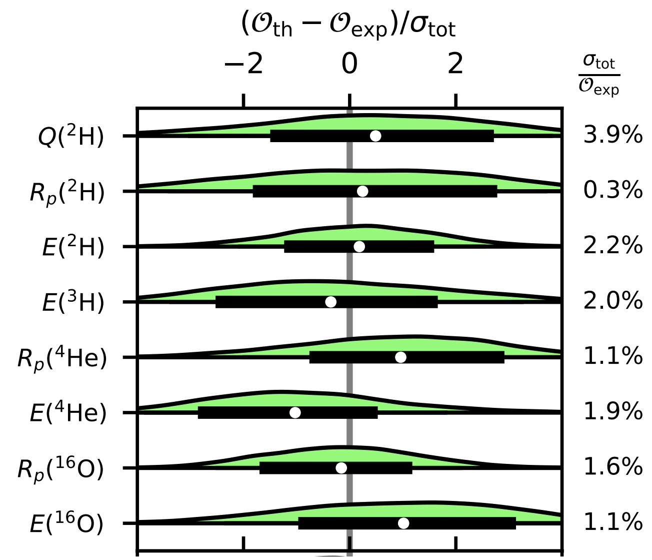
Neutron Skin of ^{208}Pb

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^2LO

34 non-implausible interactions



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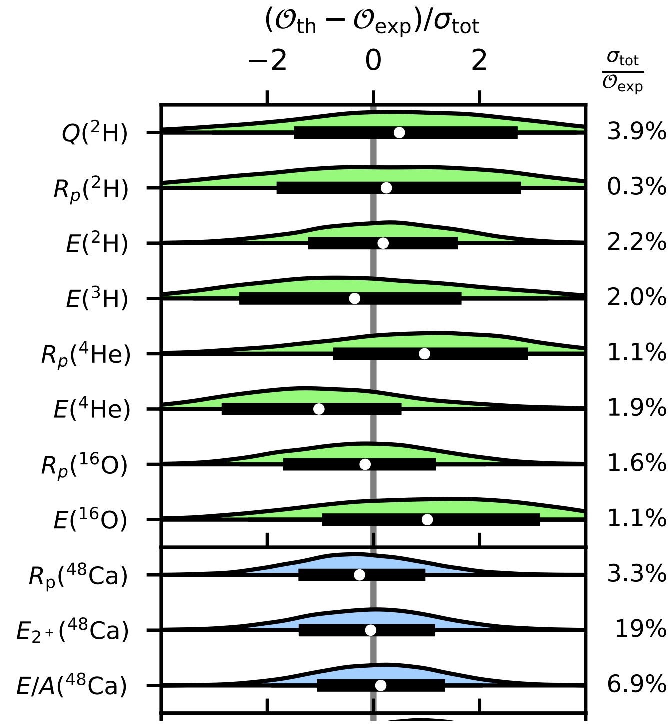
II: Calibration use ^{48}Ca E/A, E(2^+), R_p, dipole polarizability

Importance resampling – statistically weight interactions



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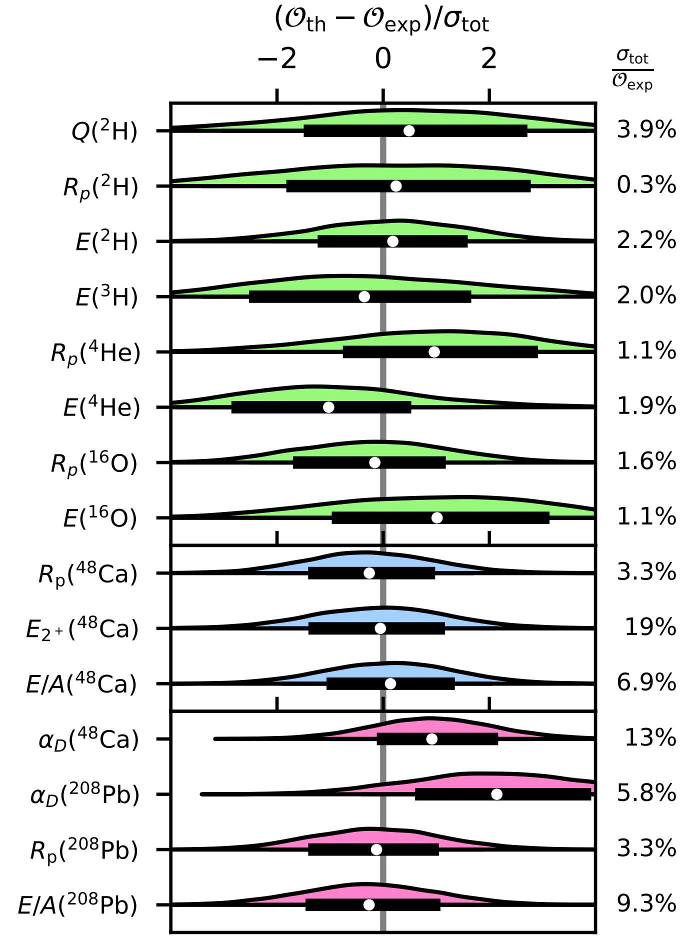
III: Validation ^{208}Pb E/A, R_p + ^{48}Ca/^{208}Pb DP from ab initio

Clear quality description of data



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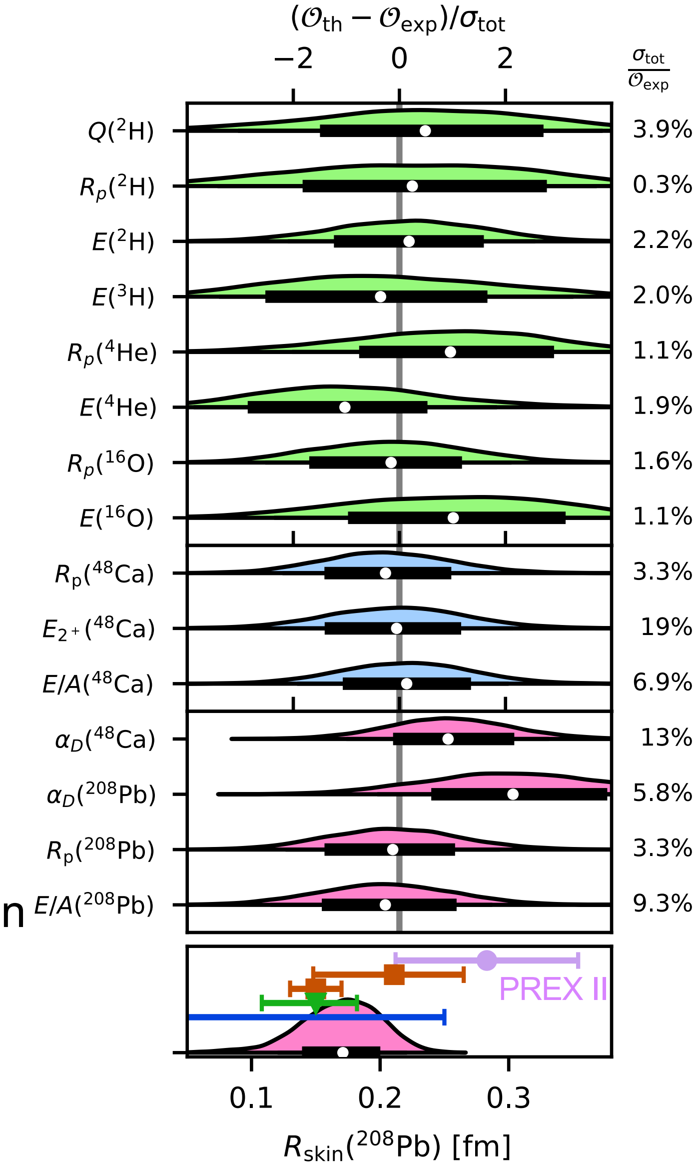
Clear quality description of data

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**



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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

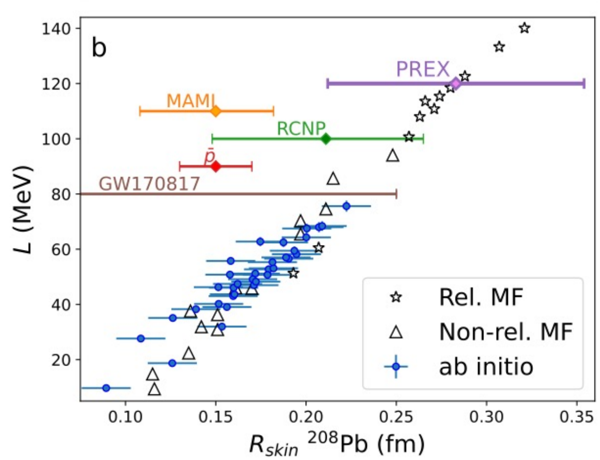
L = 37-63 MeV

Constrain forces potentially from:

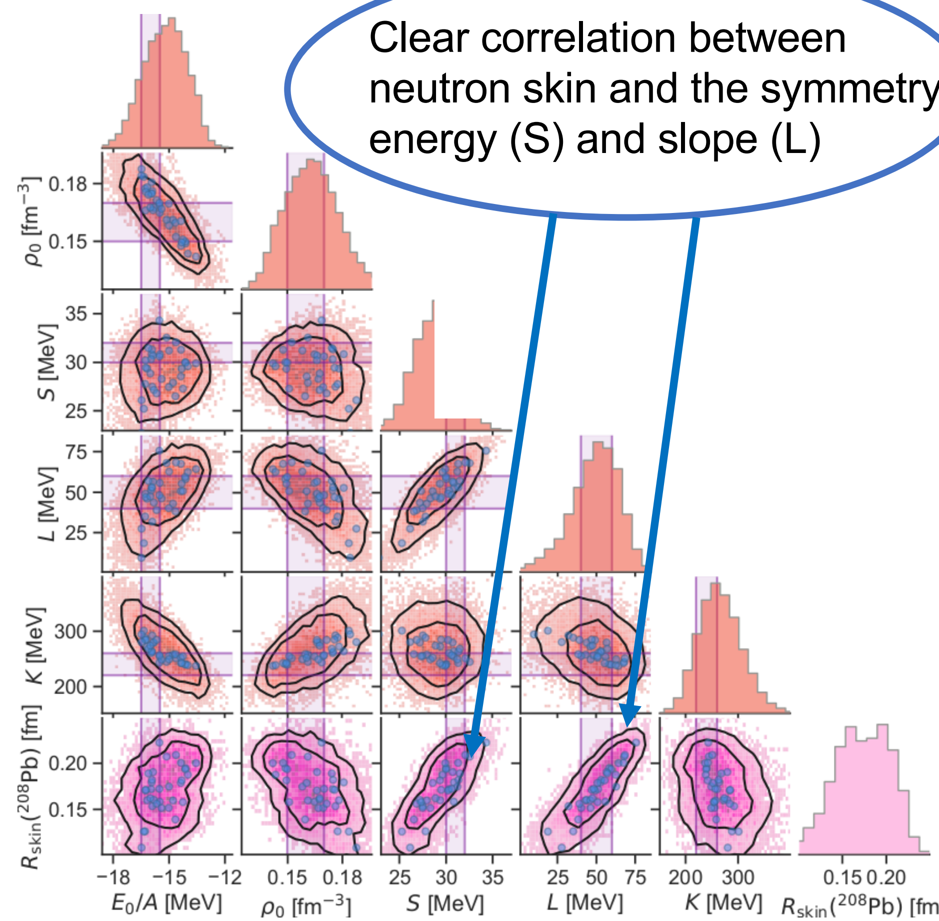
Neutron star radii/mergers

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)



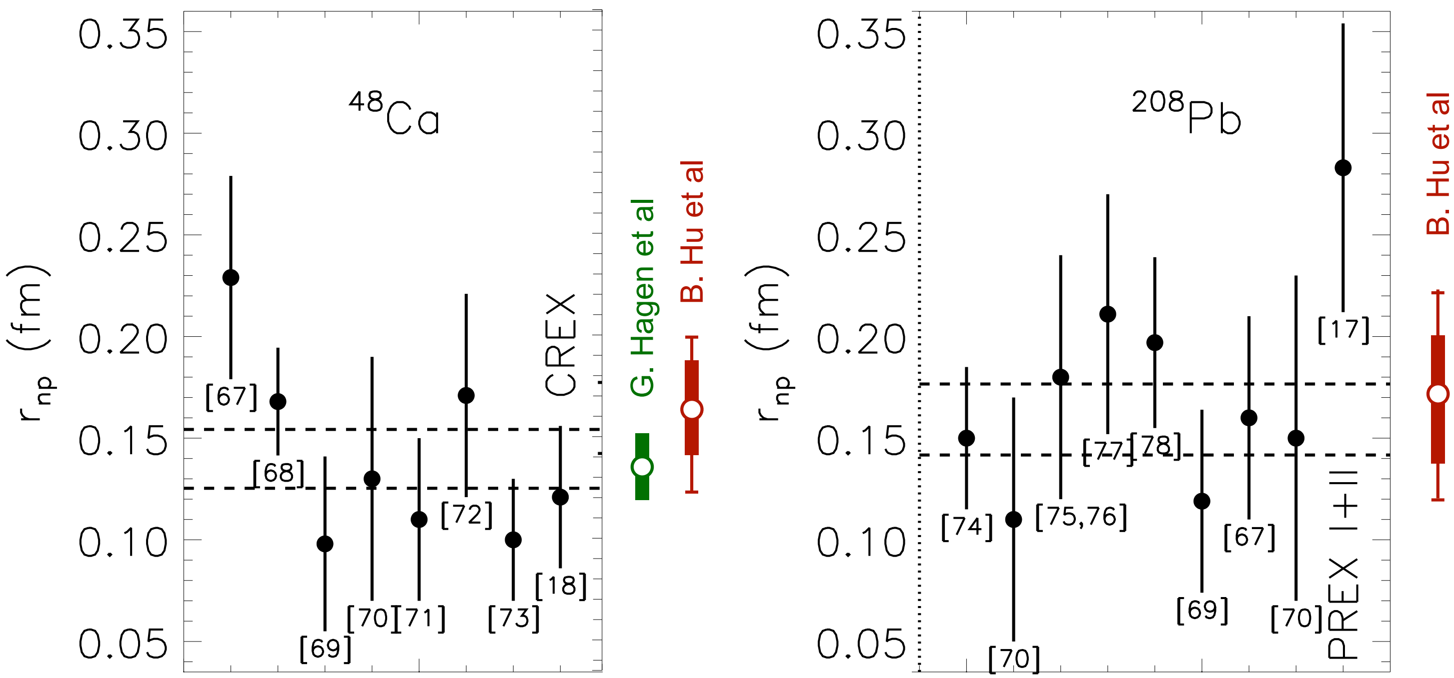
TRIUMF

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

Newly extracted neutron skin in ^{48}Ca

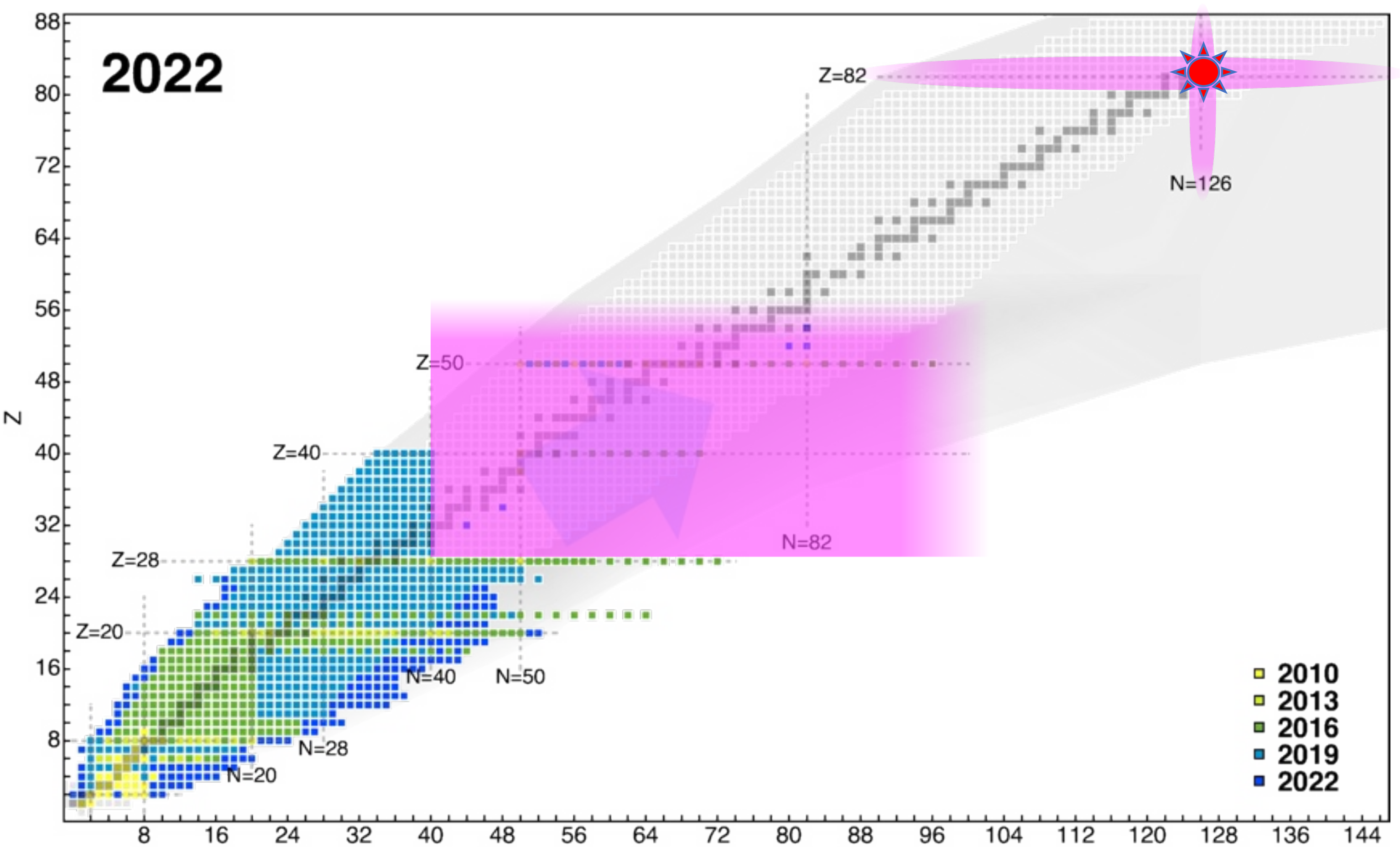
Use same 34 interactions – predictions in good agreement with CREX result

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

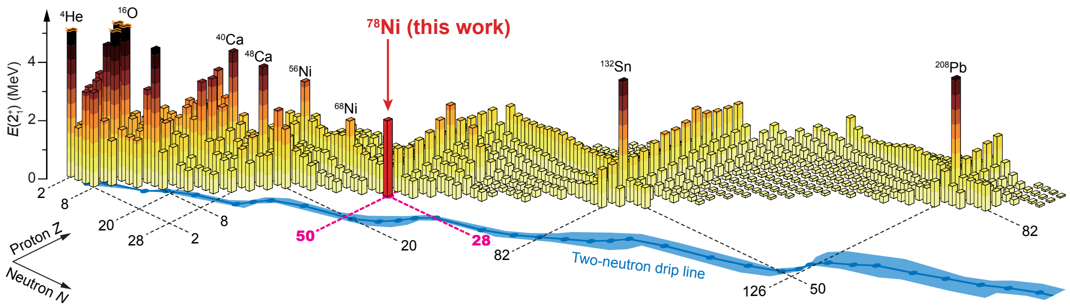


Recalibrating Ab Initio Progress

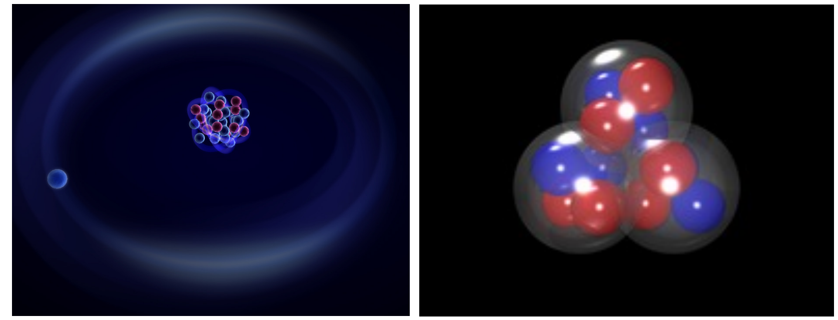
Rapid progress in ab initio reach, due to valence-space approach… up to...



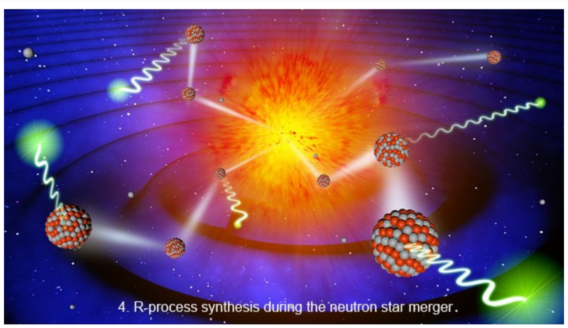
Major Questions in Nuclear Structure



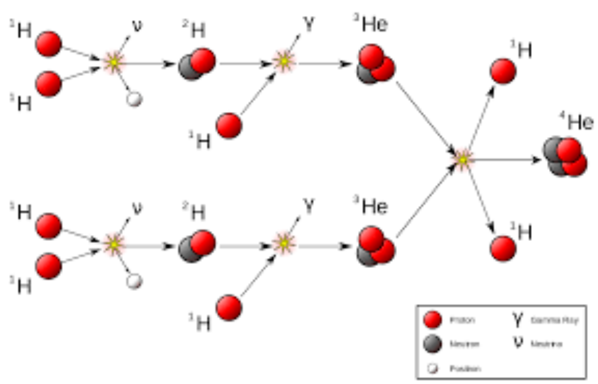
Limits of existence + formation/evolution of magic numbers



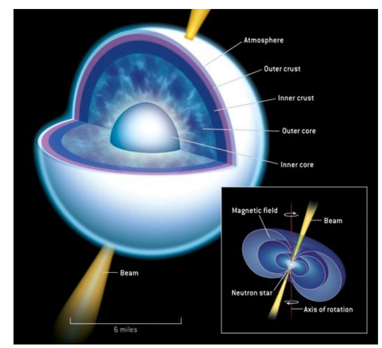
Nuclear radii/skins/halos/clusters



Heavy Nuclei + r-process



Continuum and nuclear reactions

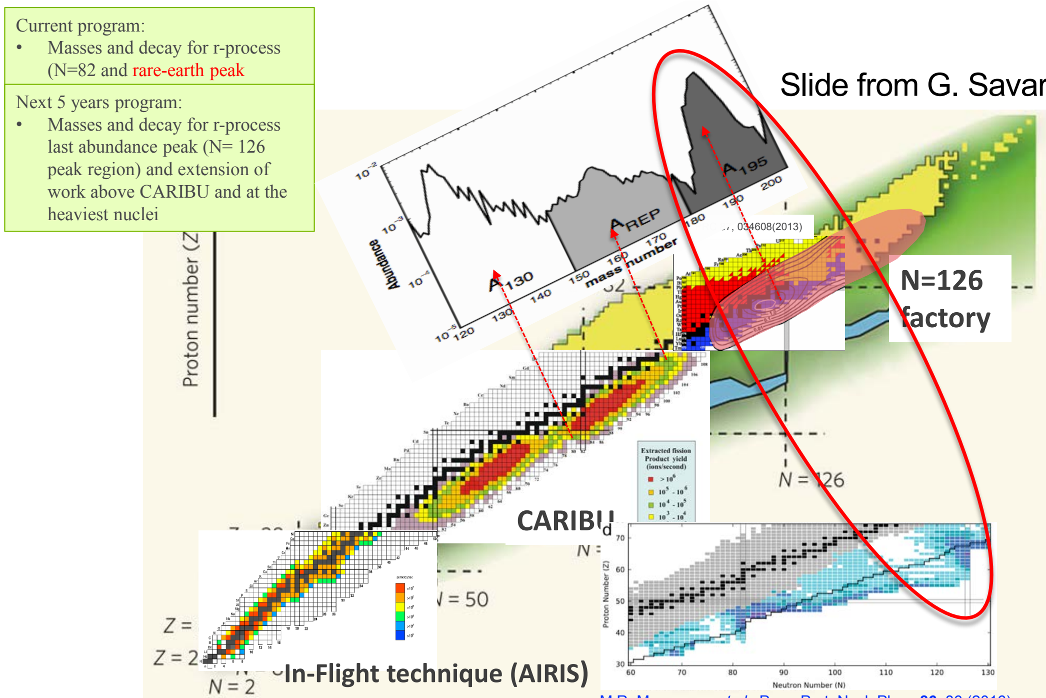


Infinite matter/Neutron stars

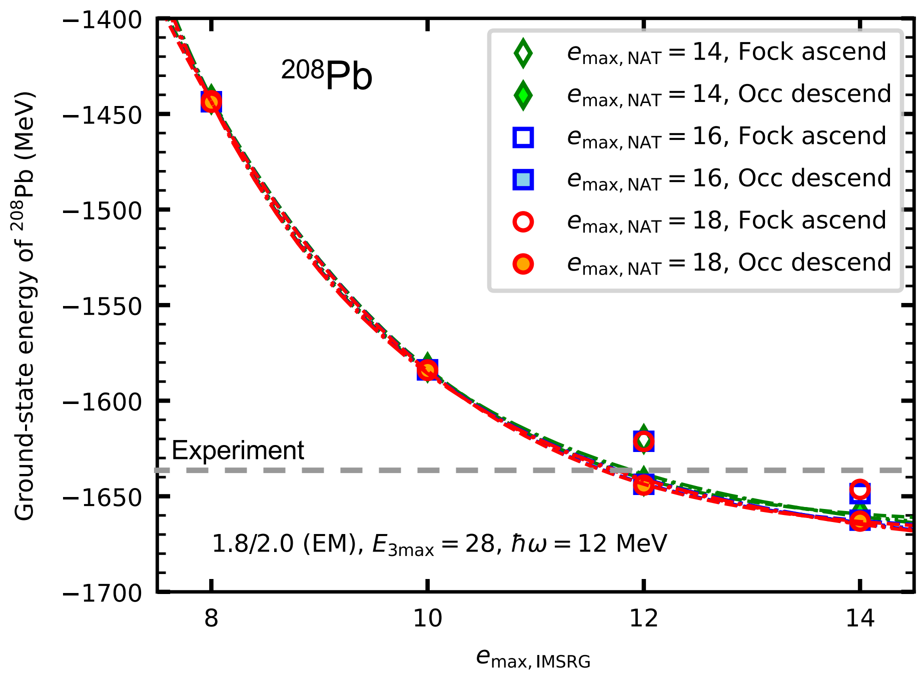
Ab Initio Theory for r-process

Information for nuclei along N=126 necessary for third r-process abundance peak

Slide from G. Savard



M.R. Mumpower *et al.*, Prog. Part. Nucl. Phys. **86**, 86 (2016)

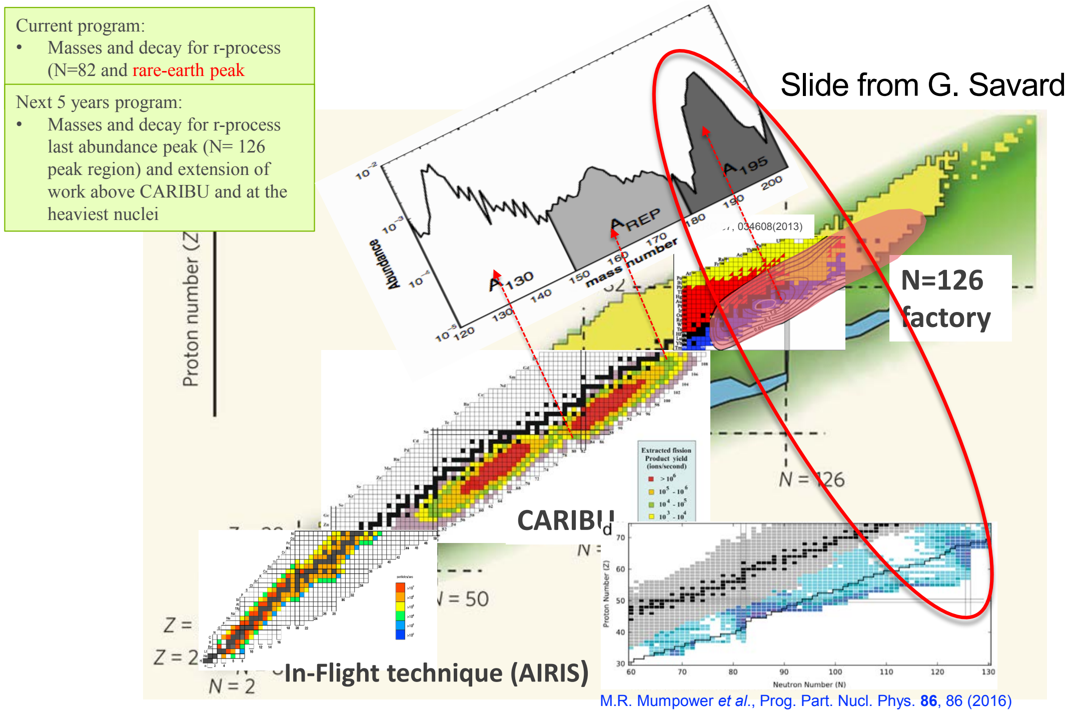


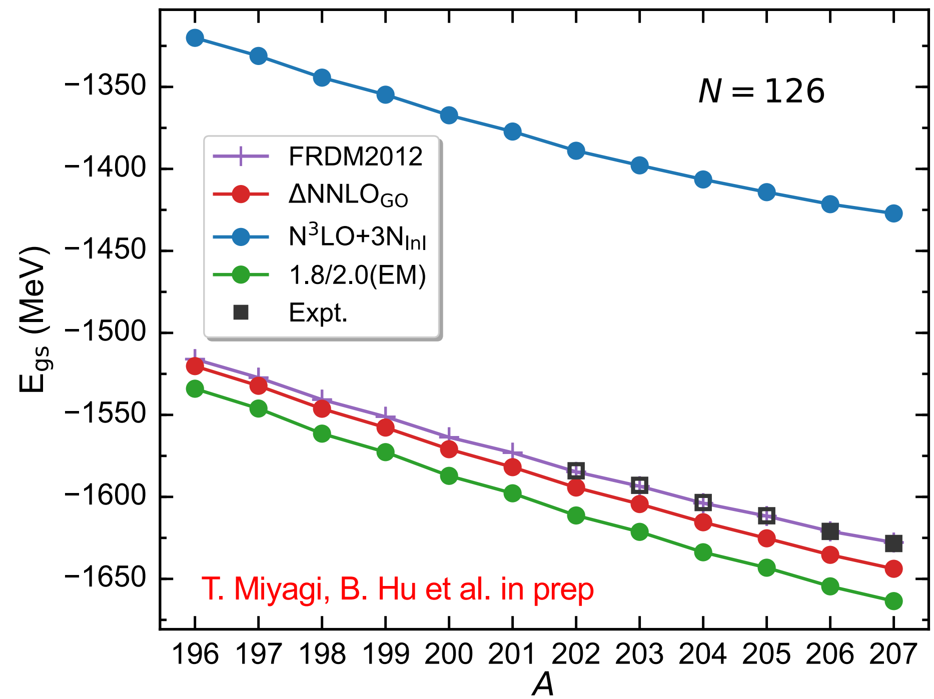
Natural Orbital Basis (NAT) allows for rapid convergence

TRIUMF

Ab Initio Theory for r-process

Information for nuclei along N=126 necessary for third r-process abundance peak



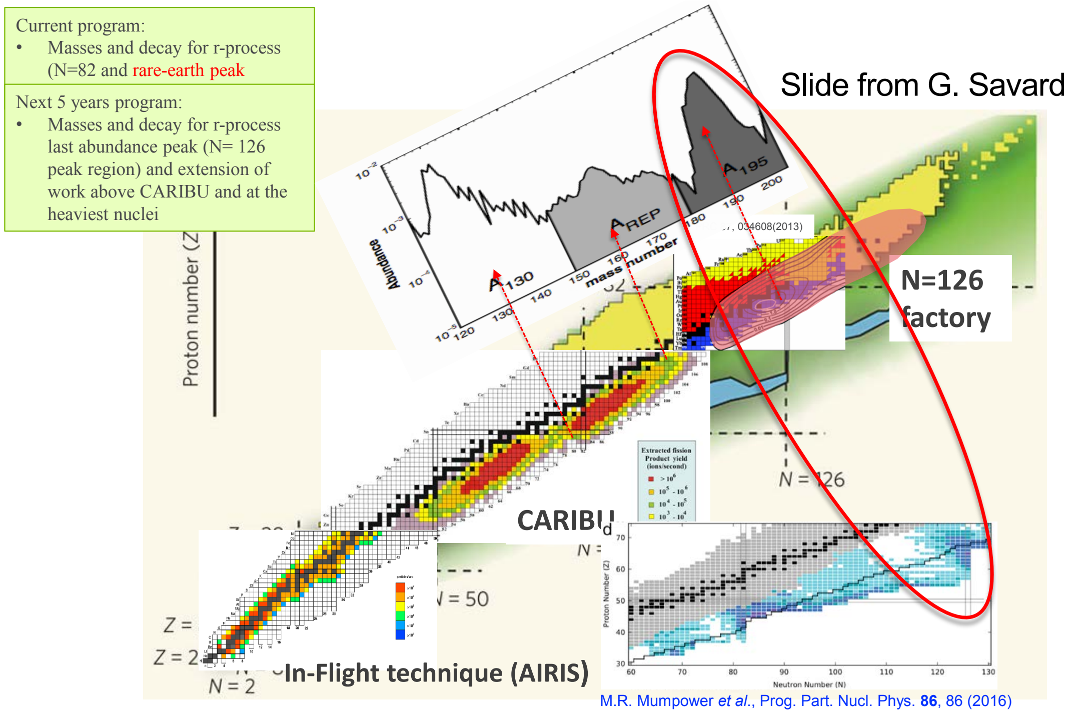


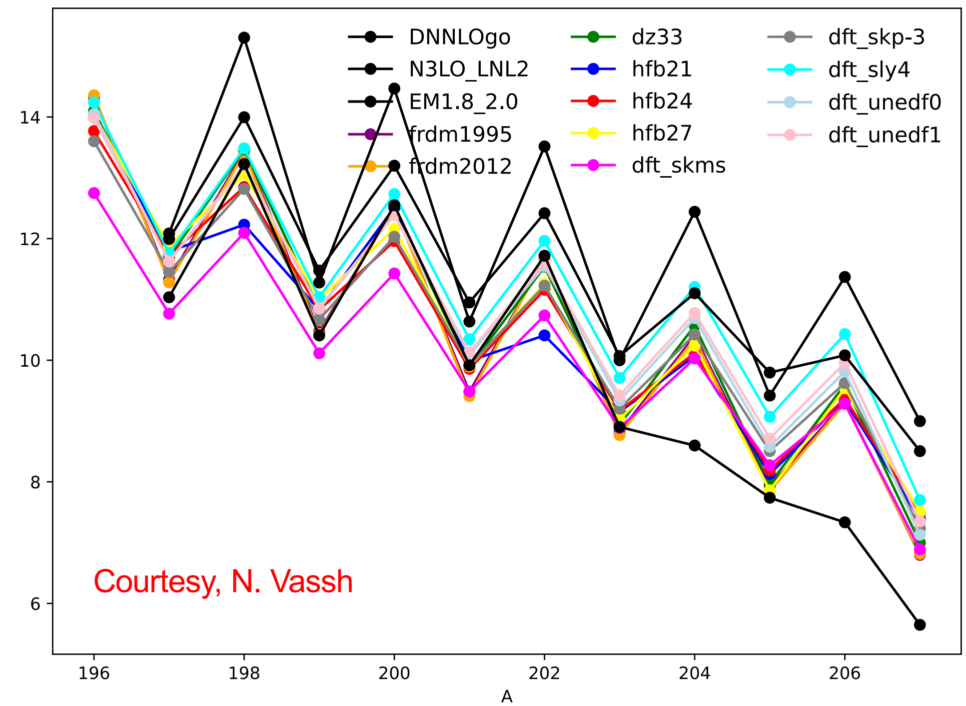
Natural Orbital Basis (NAT) allows for rapid convergence

Converged ground-state energies for Z=69-82

Ab Initio Theory for r-process

Information for nuclei along N=126 necessary for third r-process abundance peak



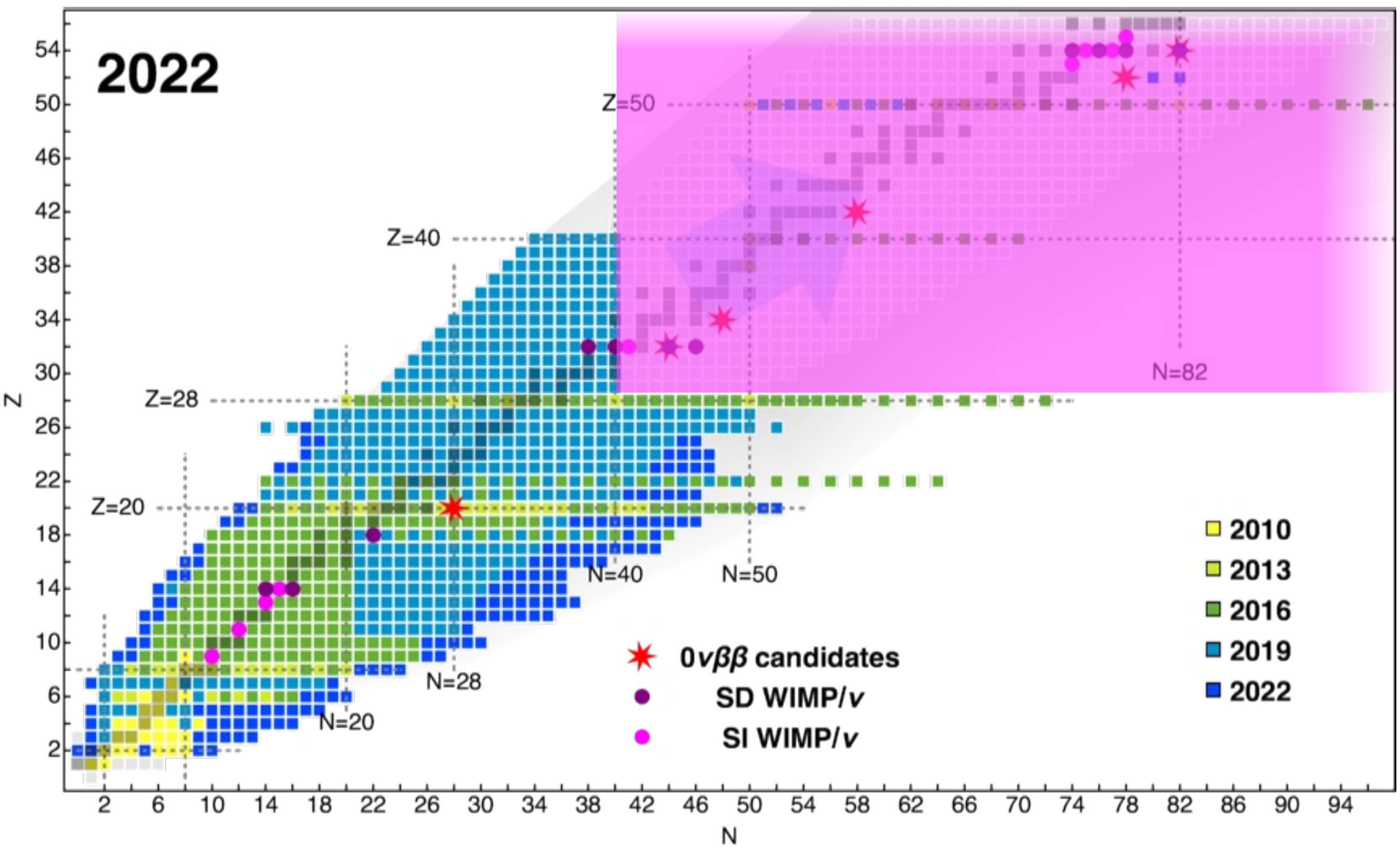


Natural Orbital Basis (NAT) allows for rapid convergence

Significant systematic differences from mass models for S_p

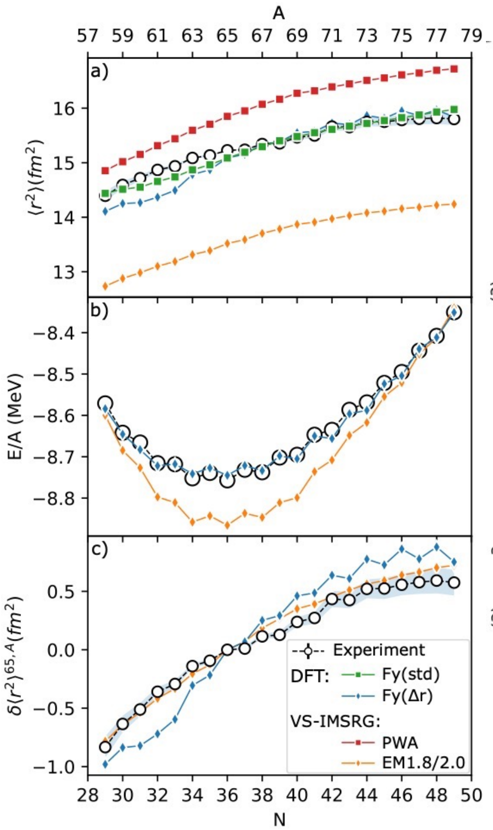
Recalibrating Ab Initio Progress

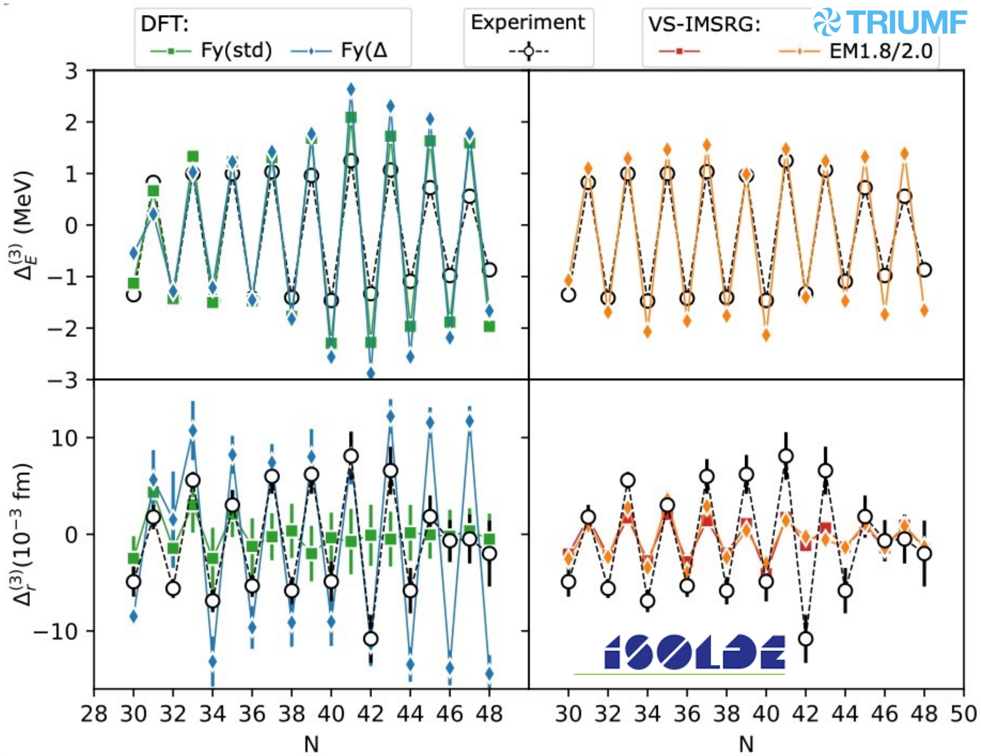
Rapid progress in ab initio reach, due to valence-space approach… up to...



Laser Spectroscopy: Charge Radii of Cu Isotopes

Odd-even staggering of charge radii across Cu chain





LETTERS

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

nature physics

OPEN

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

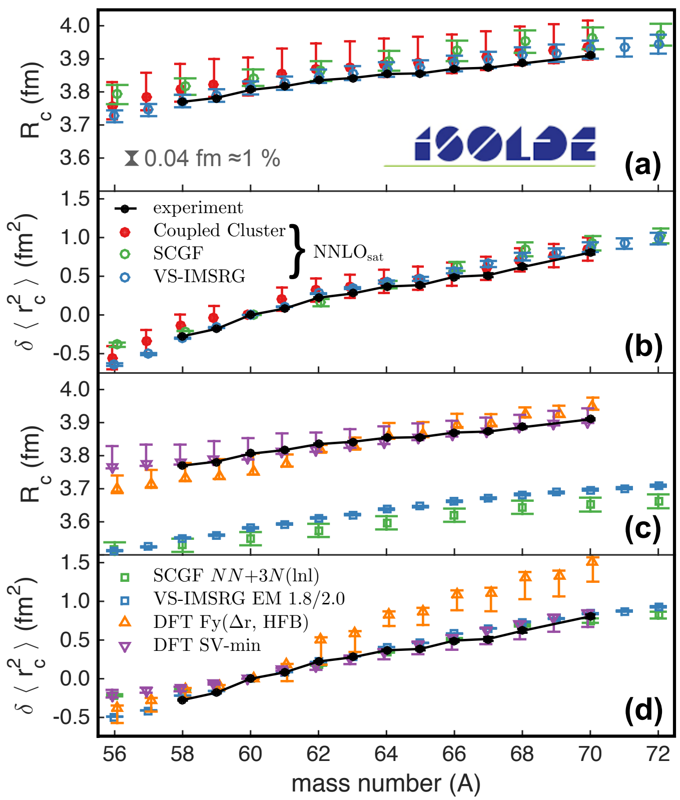
R. P. de Groote[1,2], J. Billowes[3], C. L. Binnersley[3], M. L. Bissell[3], T. E. Cocolios[1], T. Day Goodacre[4,5], G. J. Farooq-Smith[1], D. V. Fedorov[6], K. T. Flanagan[3], S. Franchoo[7], R. F. Garcia Ruiz[3,8,9], W. Gins[1,2], J. D. Holt[5,10], Á. Koszorús[1], K. M. Lynch[9], T. Miyagi[5], W. 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)

TRIUMF 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

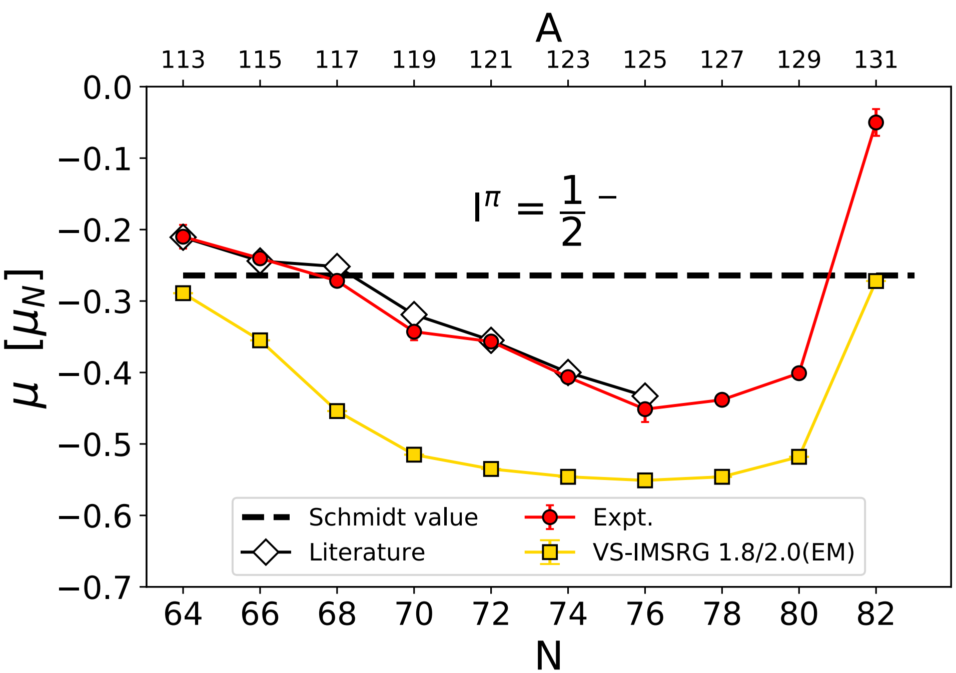
Multiple ab-initio methods largely agree within uncertainties

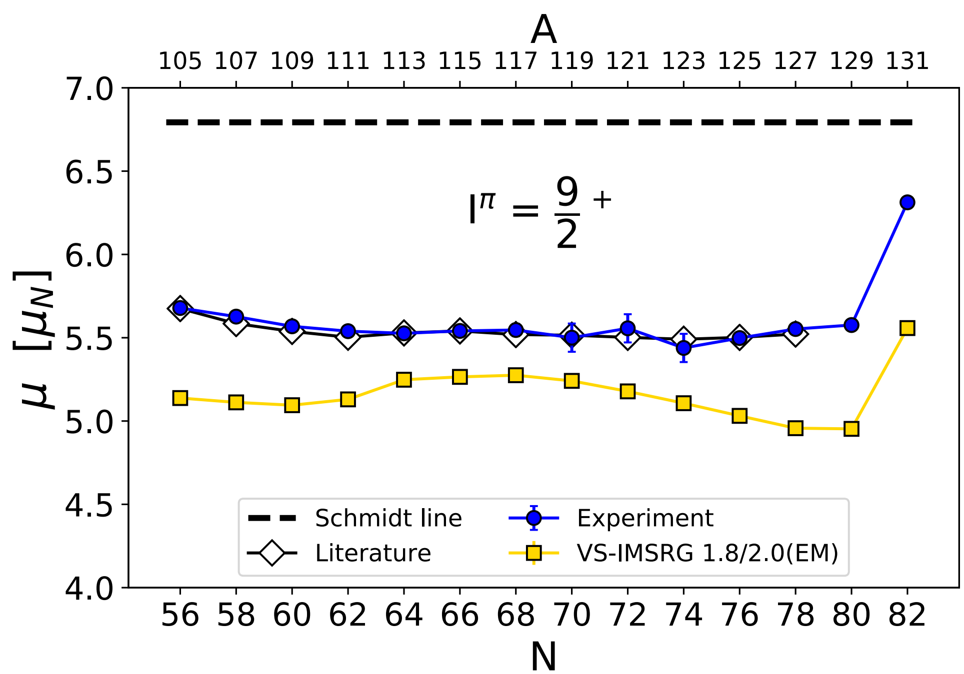
Ab initio (again) competitive/complementary with DFT

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

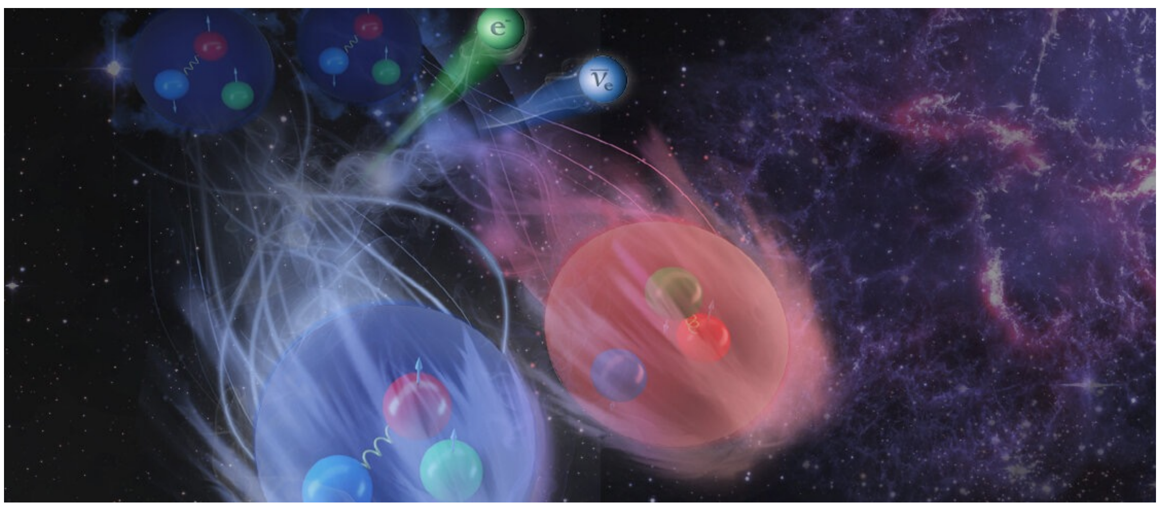
Nuclear moments of indium isotopes reveal abrupt change at magic number 82

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

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

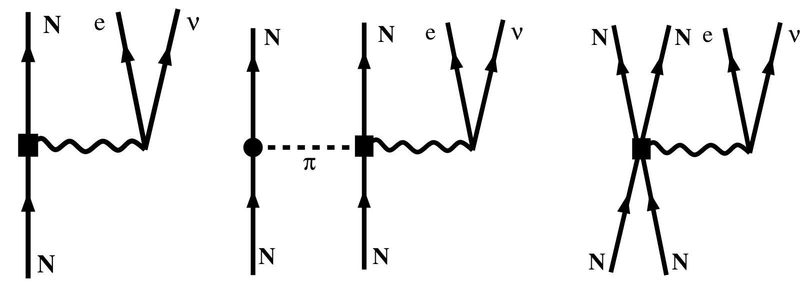
P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

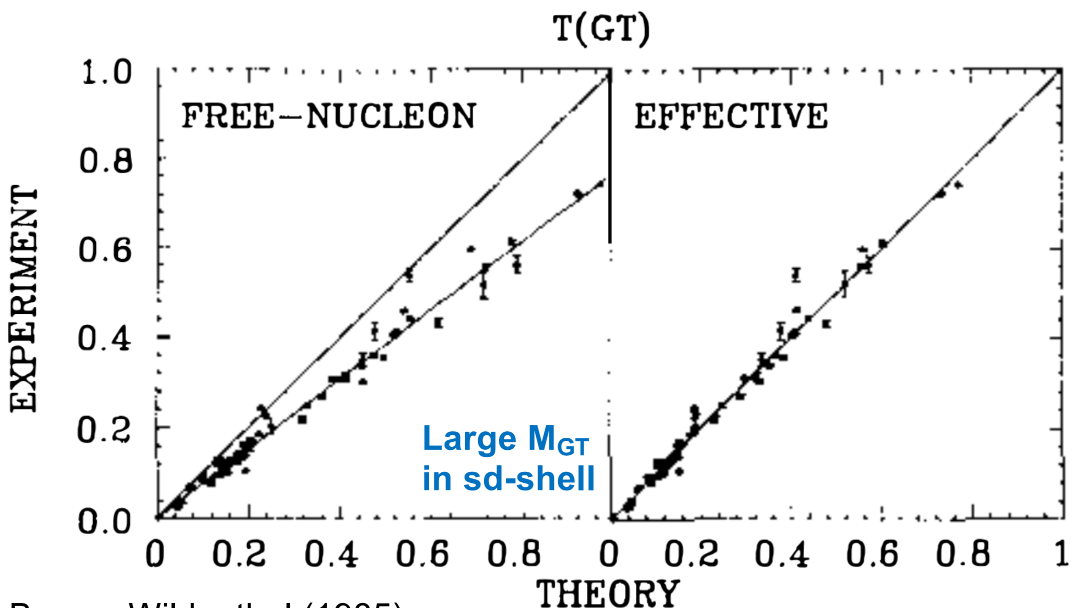
Beta-Decay "Puzzle": Quenching of g_A

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

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

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





Brown, Wildenthal (1985)

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

Explore in ab initio framework

TRIUMF Large-Scale Efforts for Ab Initio GT Transitions

Calculate **large GT matrix elements**

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

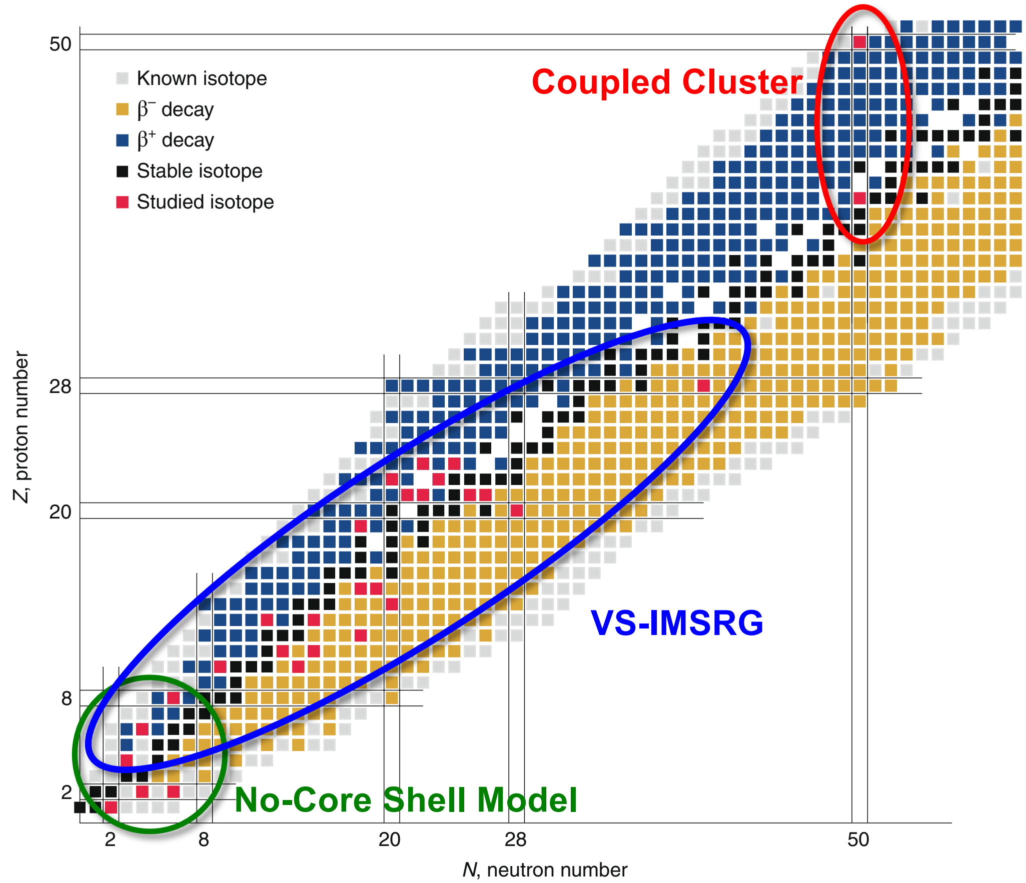
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}_{\sigma\tau}^{1\mathrm{b}} + \mathcal{O}_{2BC}^{2\mathrm{b}}$$

- 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

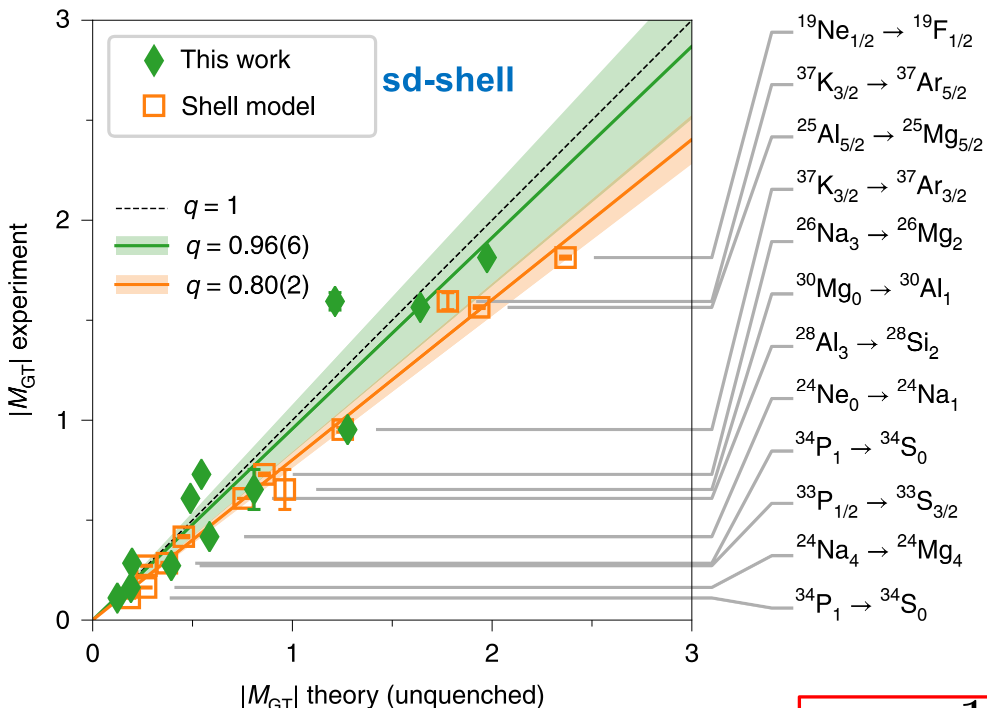
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.

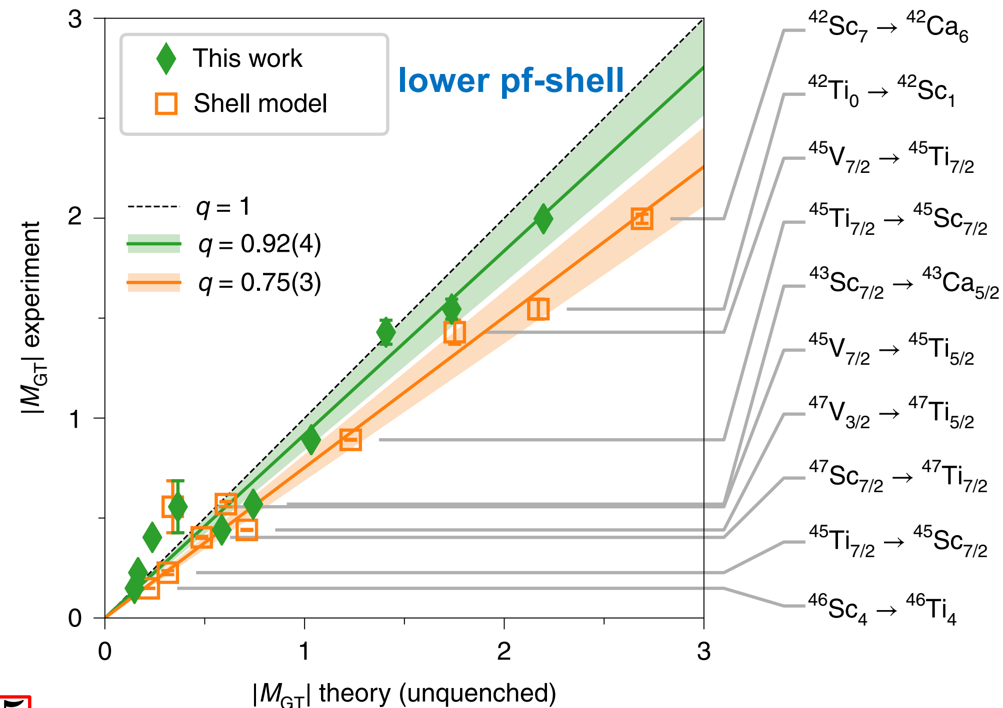


Solution to g_A-Quenching Problem

TRIUMF

VS-IMSRG calculations throughout sd and pf shells





$$g_A = 1.25$$

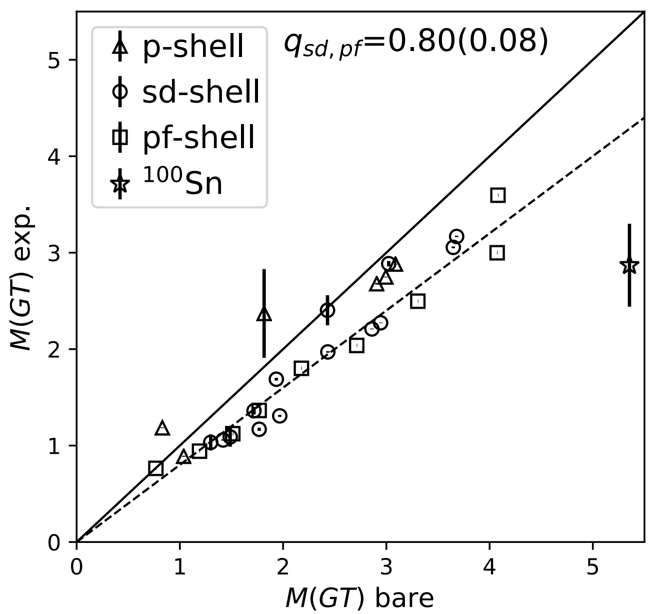
Ab initio calculations across the chart explain data with unquenched g_A

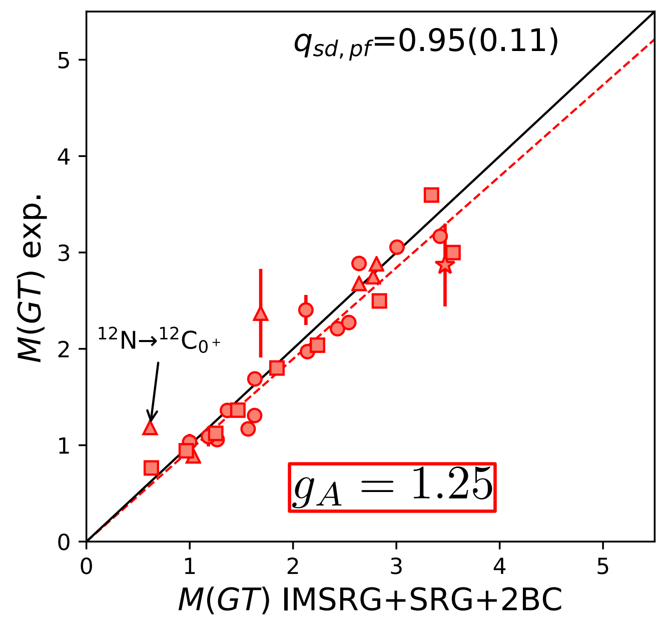
Refine results: improvements in forces and many-body methods

TRIUMF

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

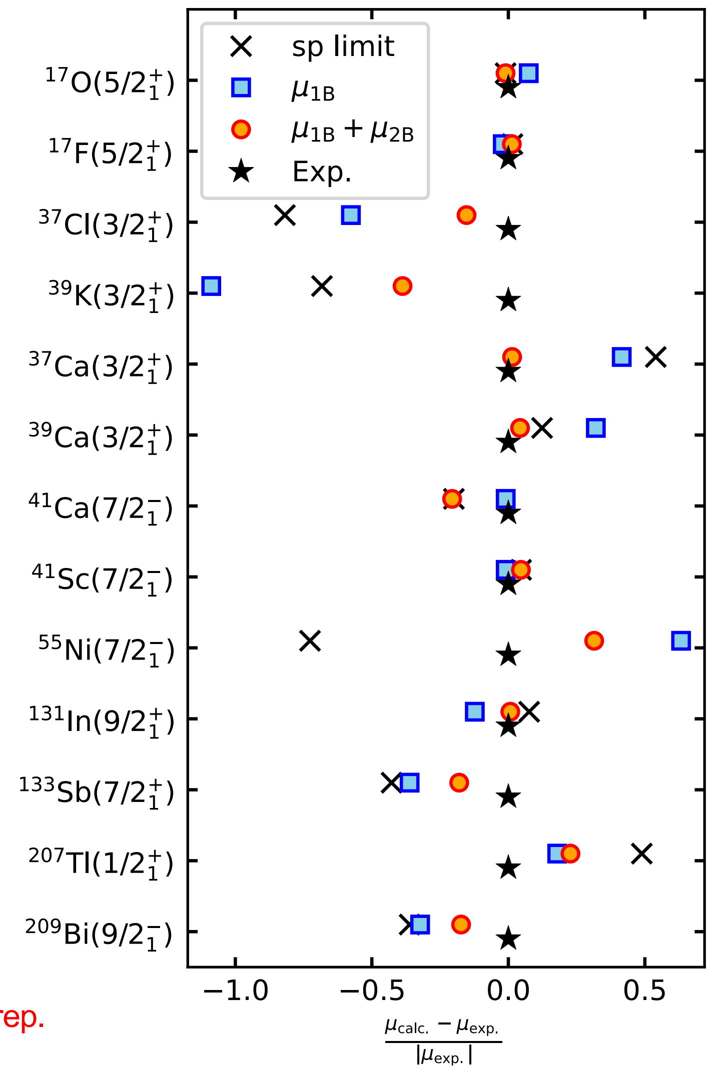
Including p-shell: q=0.99(21)

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.

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

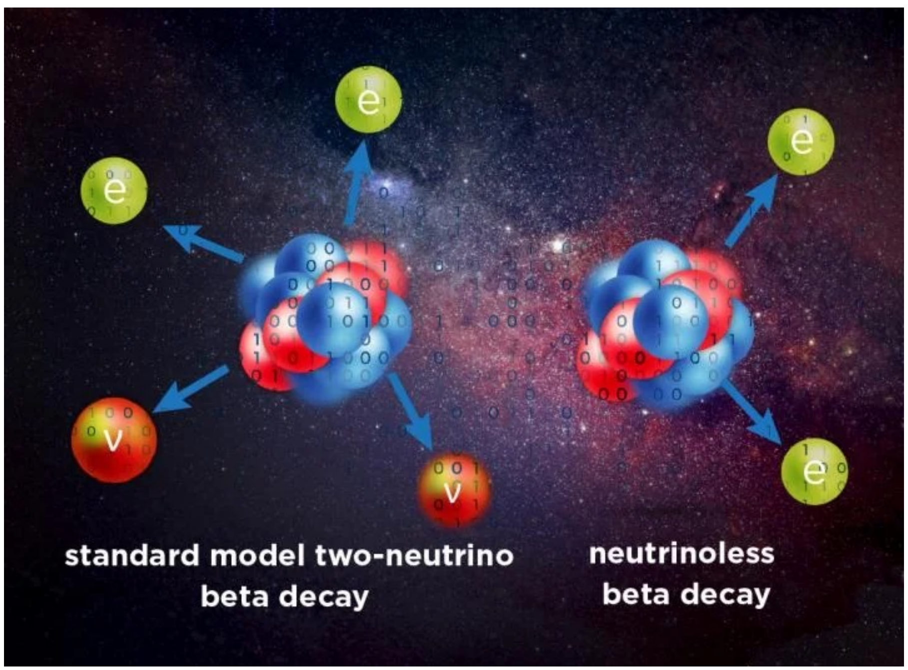
Higher-order many-body physics: IMSRG(3)
Monte Carlo shell model diagonalization
Extension to superheavy nuclei

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 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

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

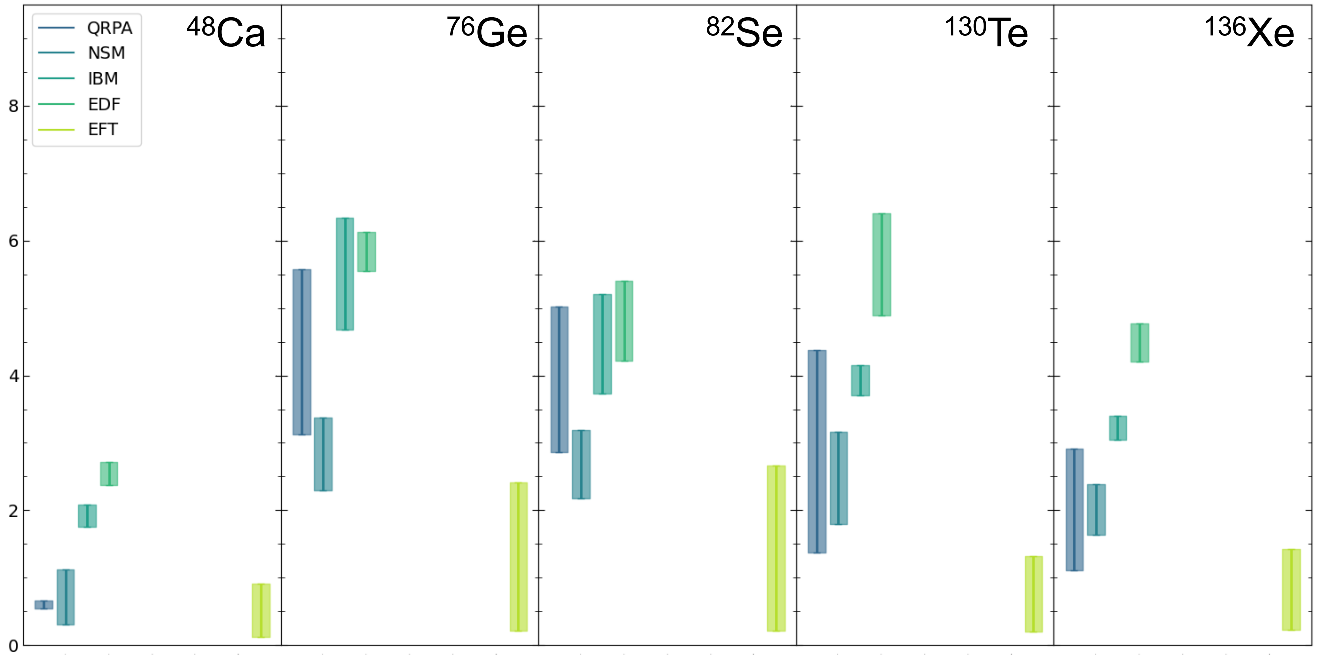
Coupled-Cluster Calculations of Neutrinoless Double-β Decay in ^{48}Ca

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

TRIUMF

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)

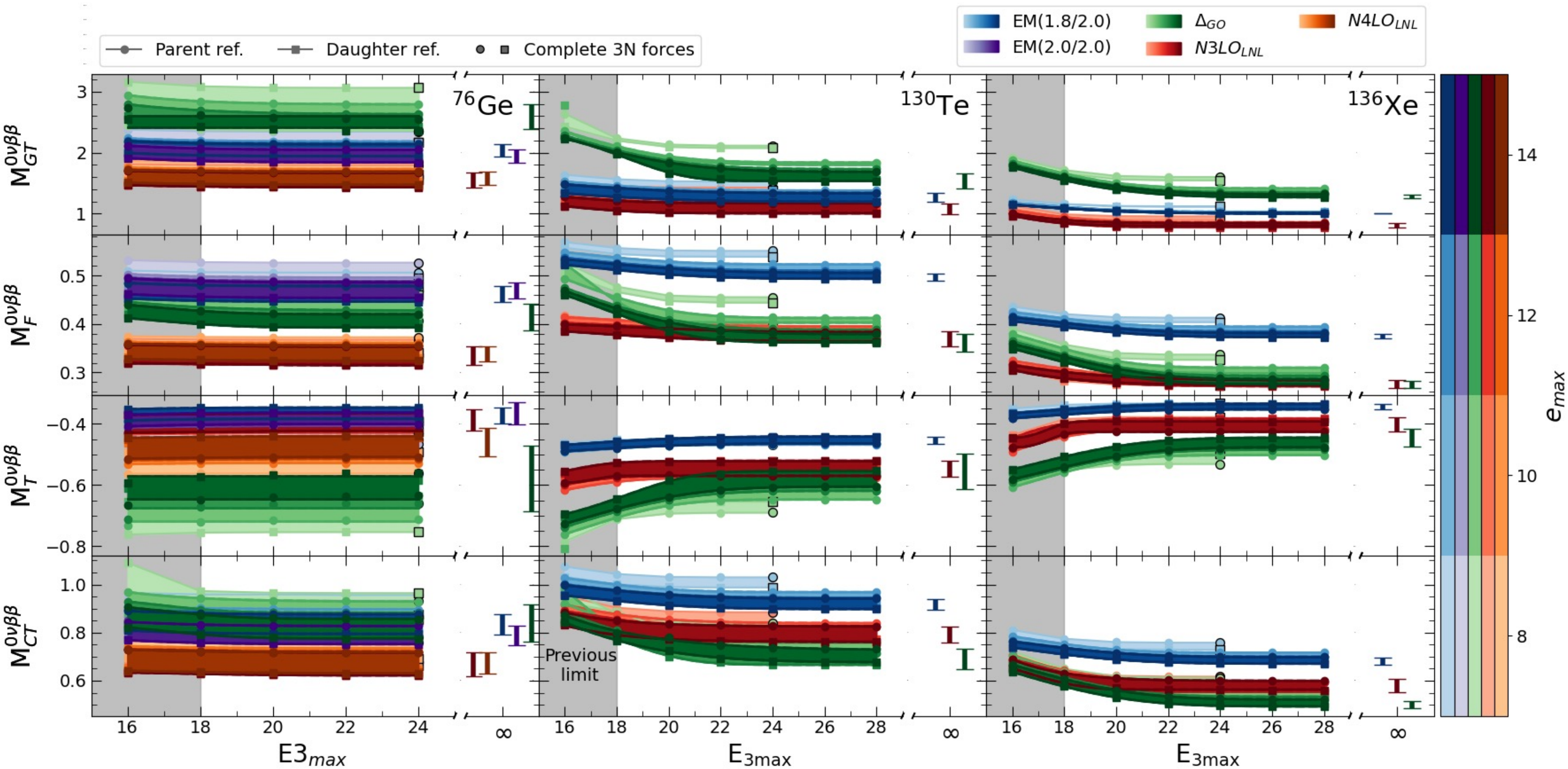
All models missing essential physics: correlations, single-particle levels, two-body currents

Address with ab initio theory

TRIUMF

Ab Initio Predictions in Heavy Nuclei

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



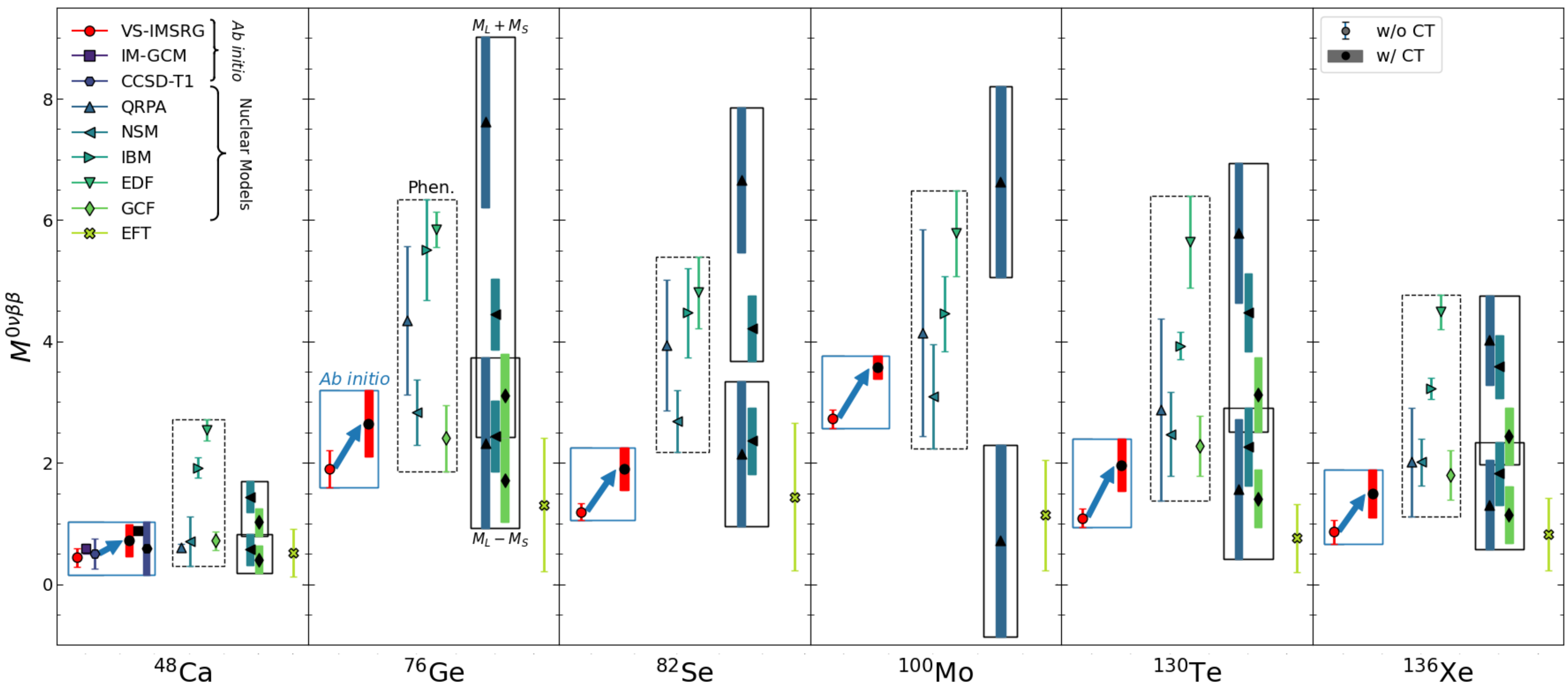
Belley et al, in prep

TRIUMF

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**

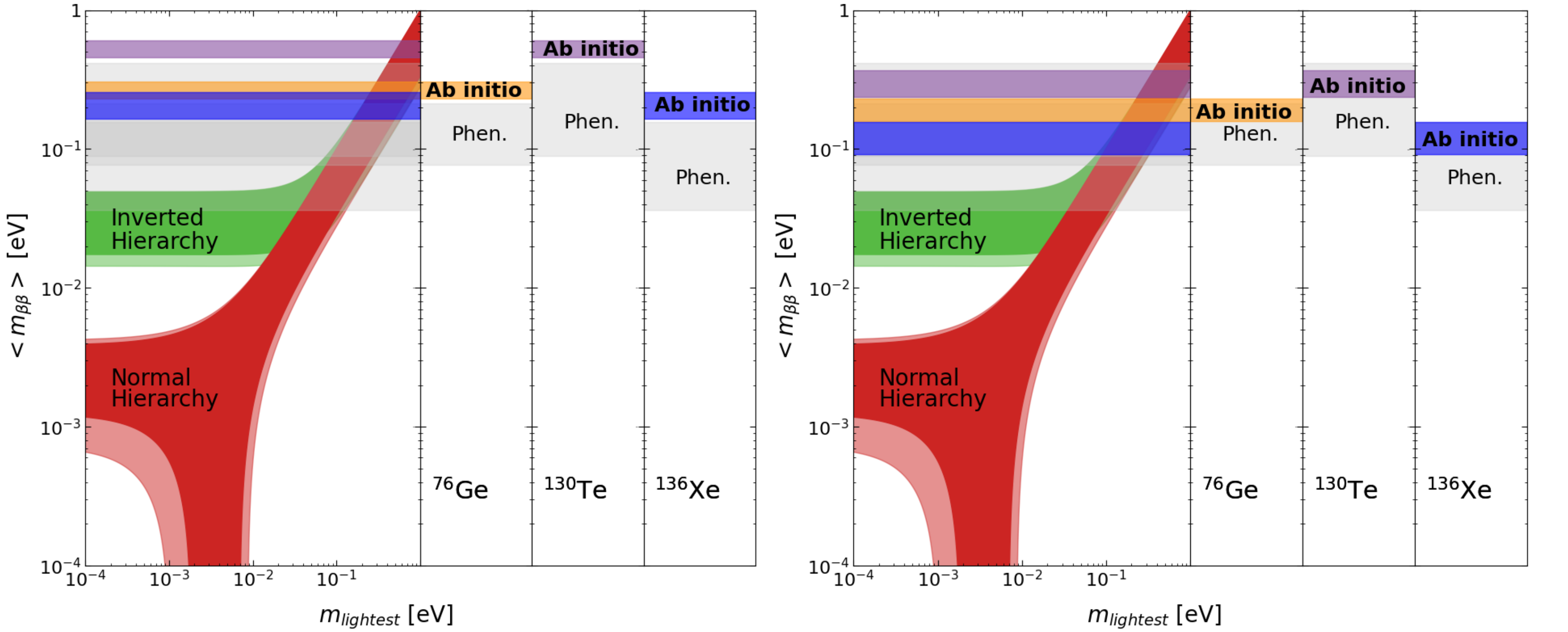


Belley et al, in prep

Impact of Ab Initio NMEs on Worldwide Searches

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

Current experimental reach – improved with effects of contact term,



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

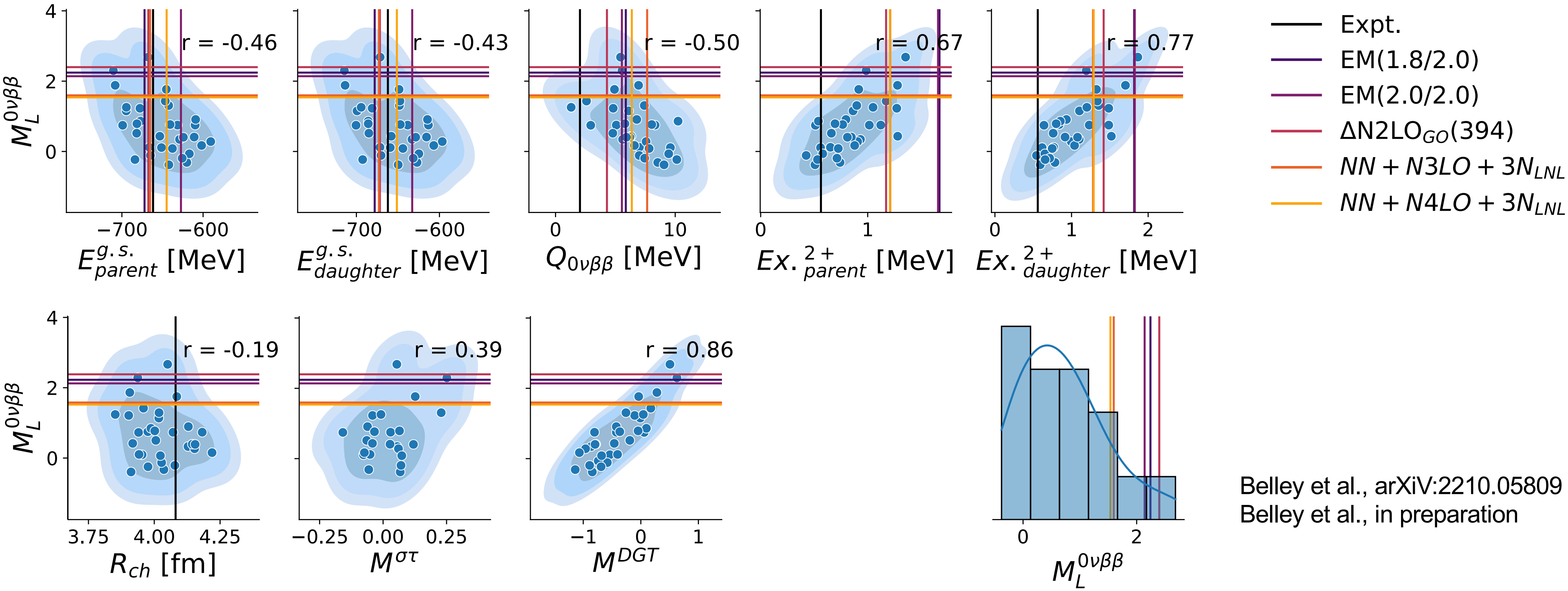
Belley et al, in prep

TRIUMF

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

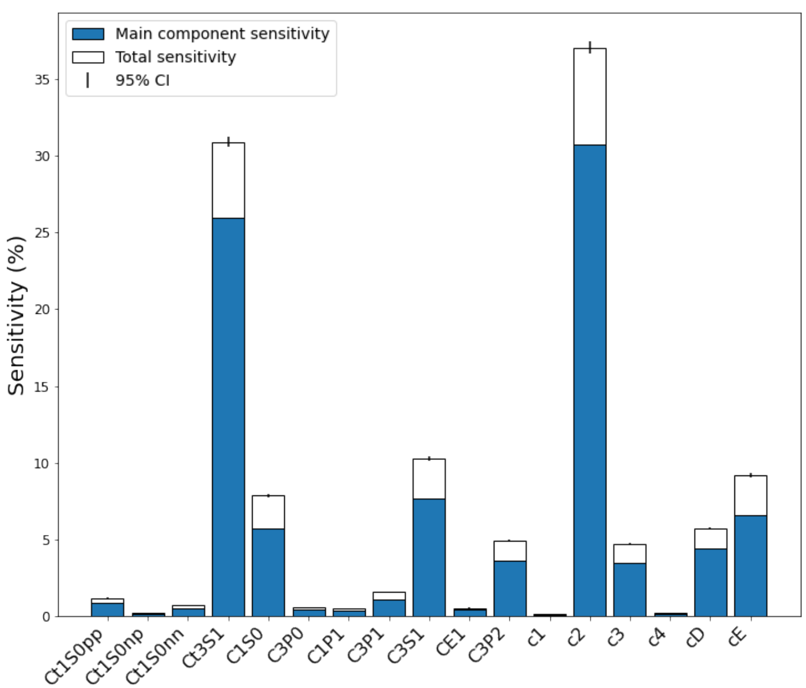
Maybe with first excited 2⁺ states?

MM-DGP Emulator: Sensitivity Analysis

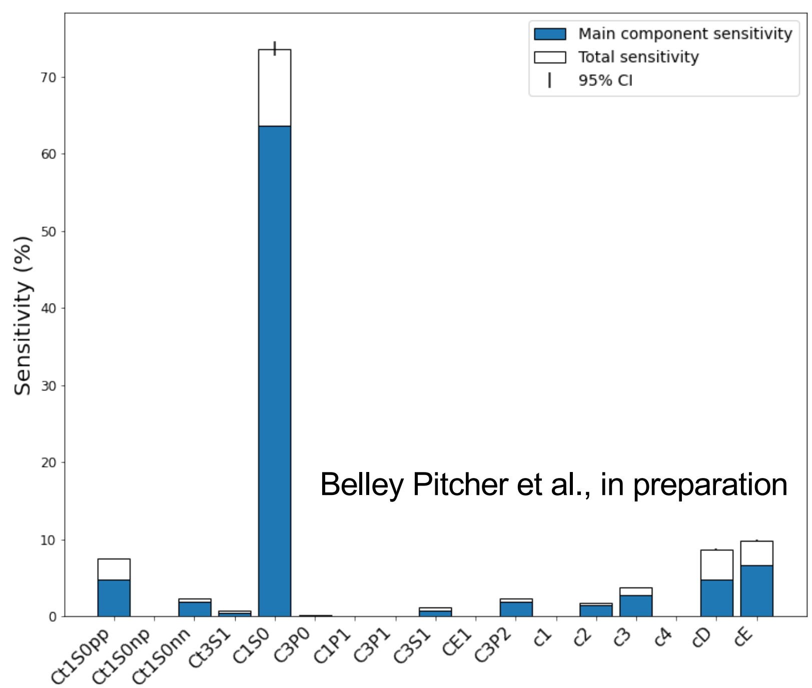
Explore correlations with other observables from systematic analysis (34 interactions)

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

Ground state energies



$M_L^{0\nu}$



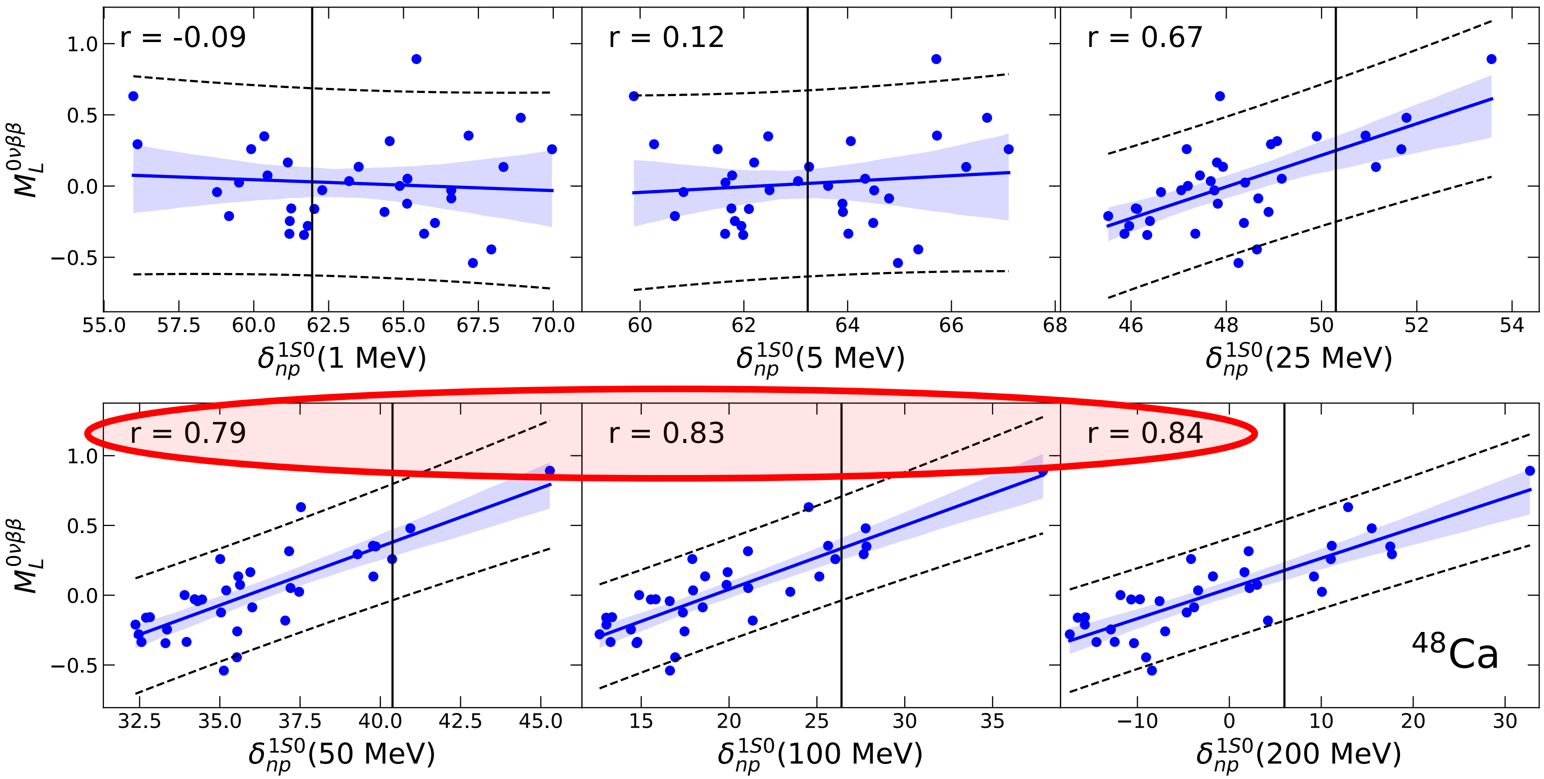
Highly sensitive to C1S0 – possible correlation with $^1S_0$ phase shift (observable!)

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

TRIUMF

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

Long-range component in ^{48}Ca



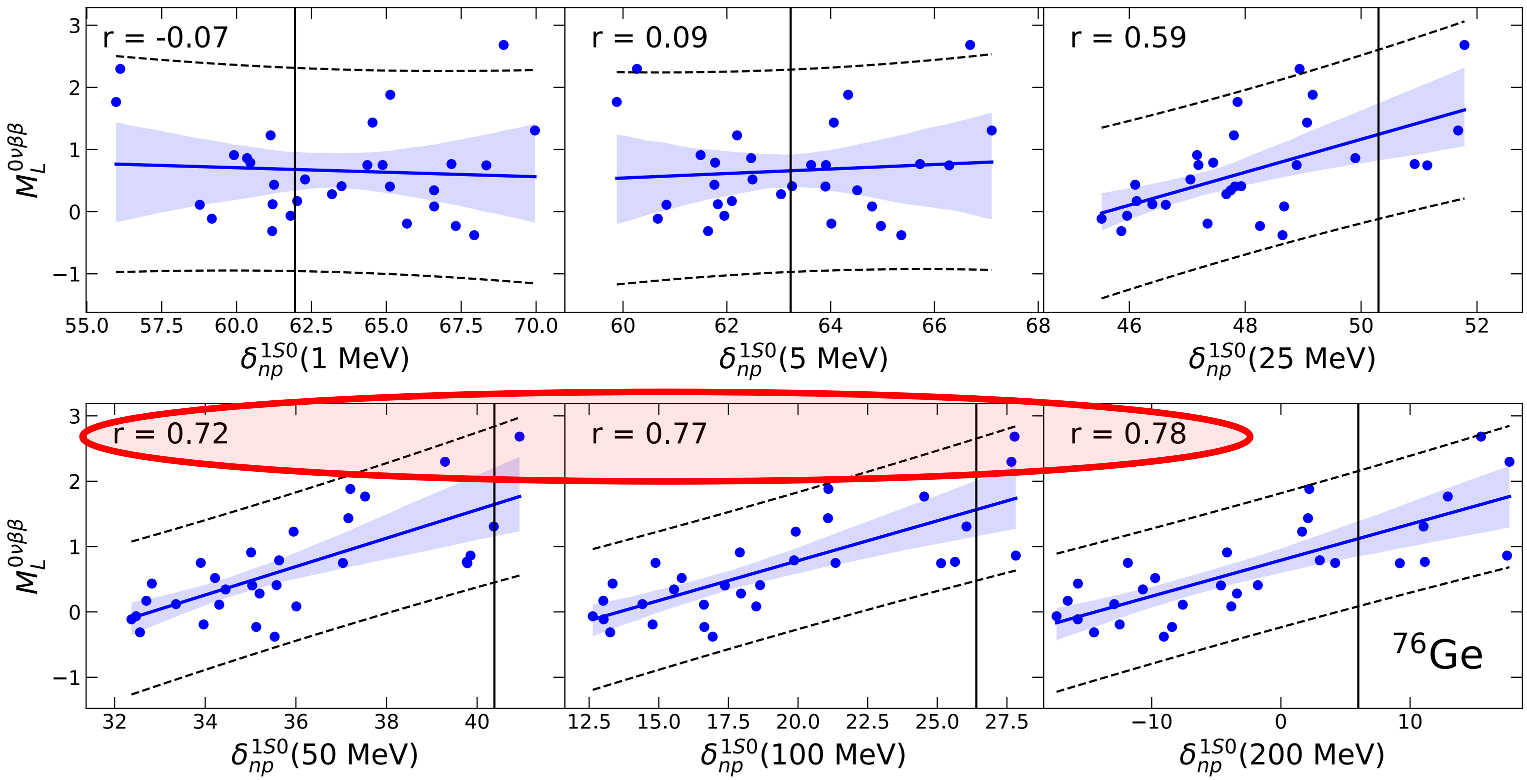
Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

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

TRIUMF

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

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



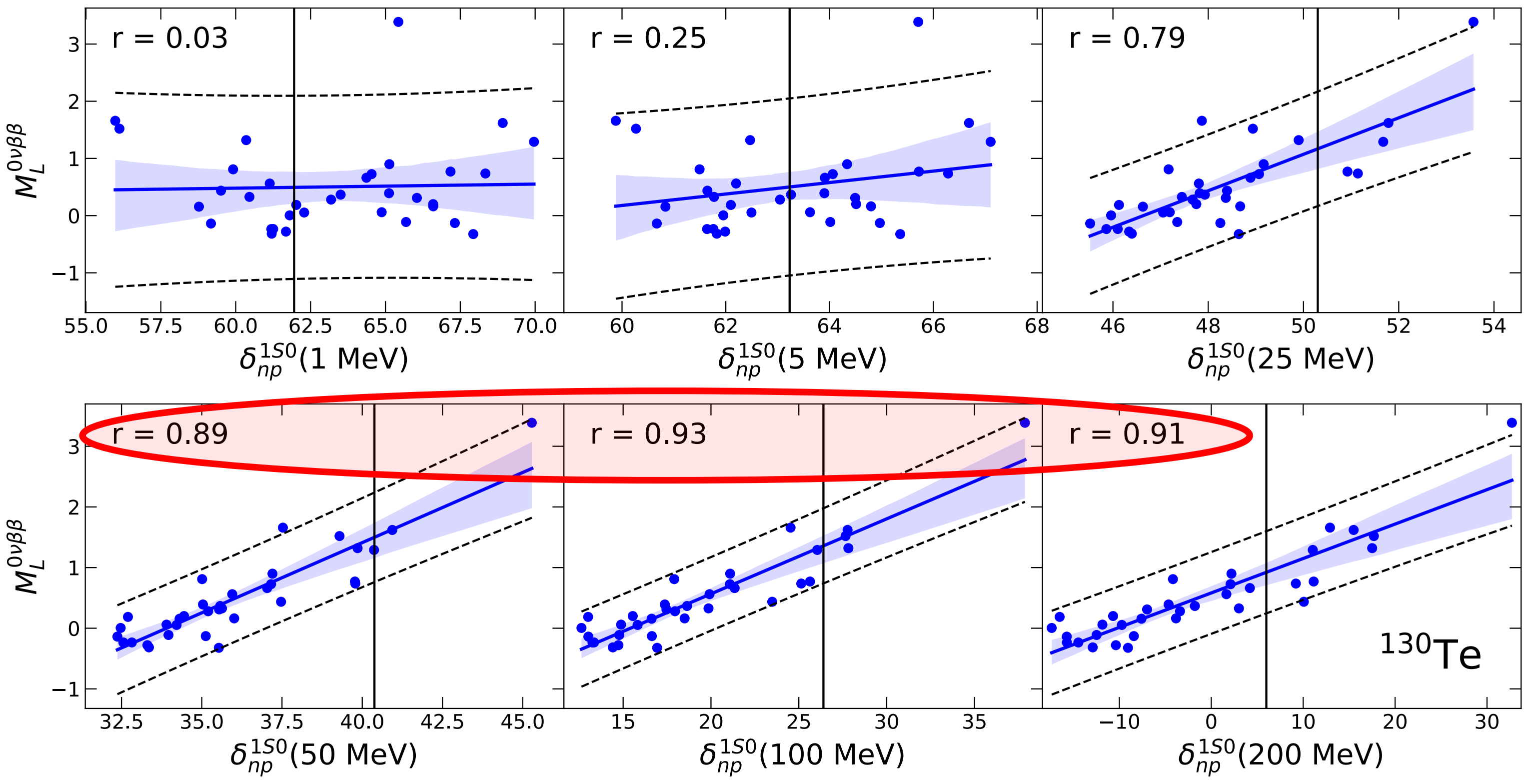
Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

TRIUMF

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, ^{130}Te



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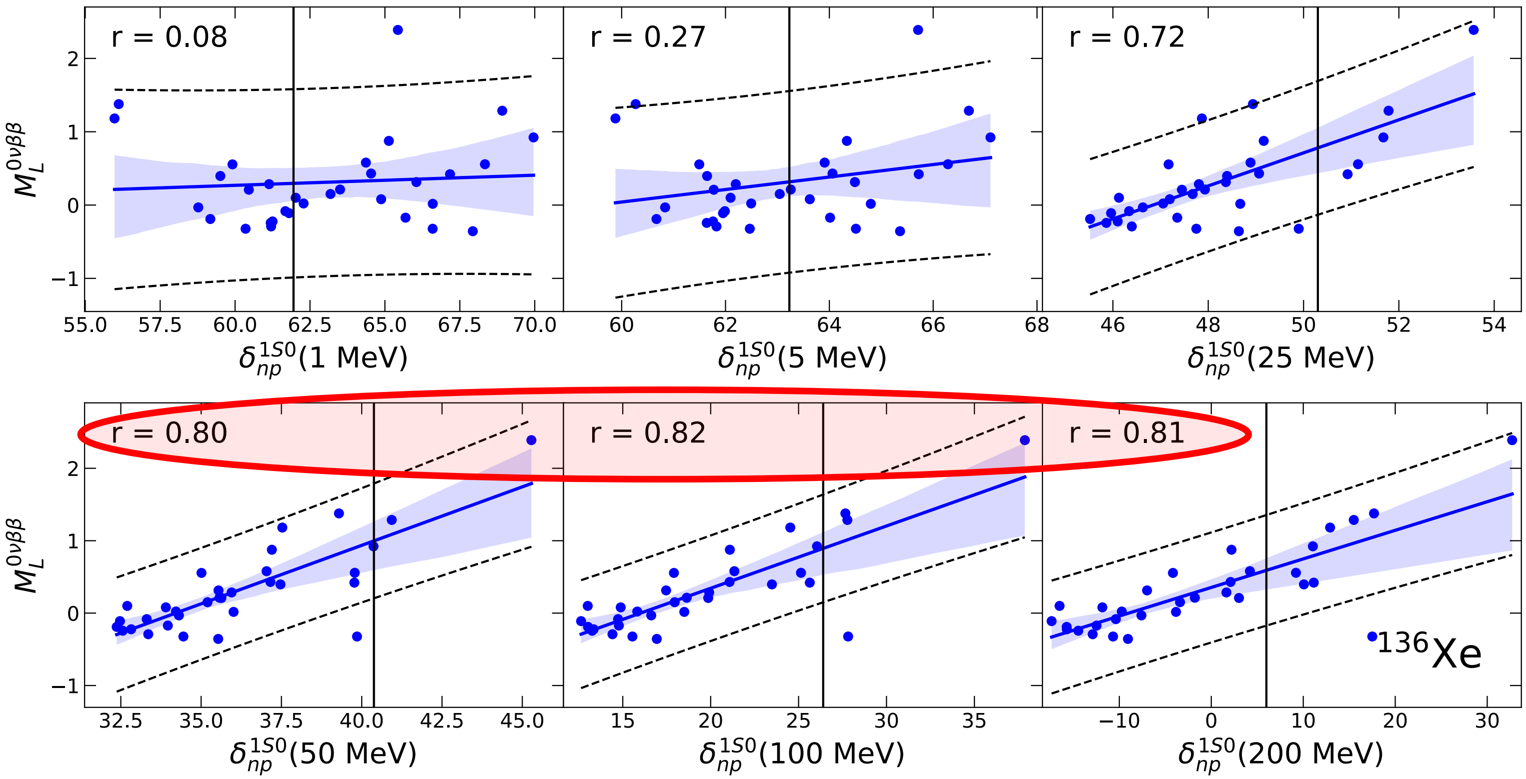
Long-range component in ^{48}Ca, ^{76}Ge, ^{130}Te, ^{136}Xe

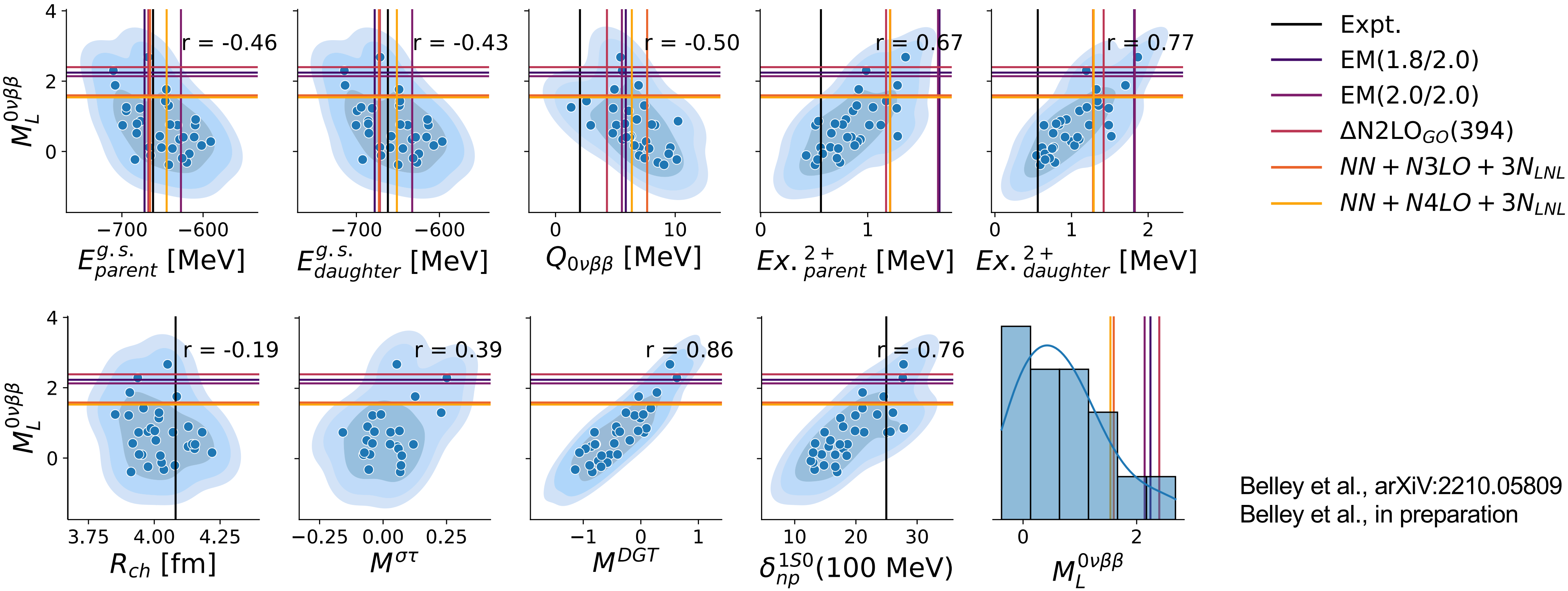


Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

TRIUMF Strategy III: Correlation with Structure Observables

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

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



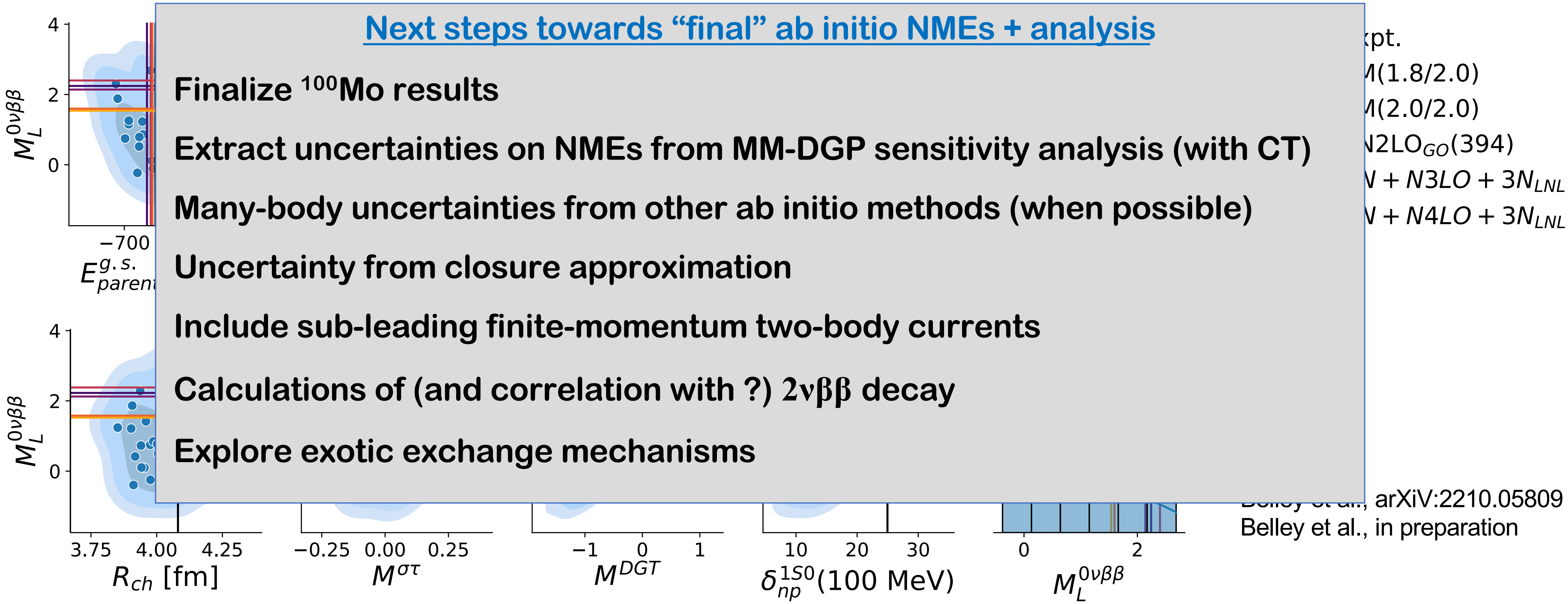
Belley et al., arXiV:2210.05809
Belley et al., in preparation

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

Strategy III: Correlation with Structure Observables

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

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

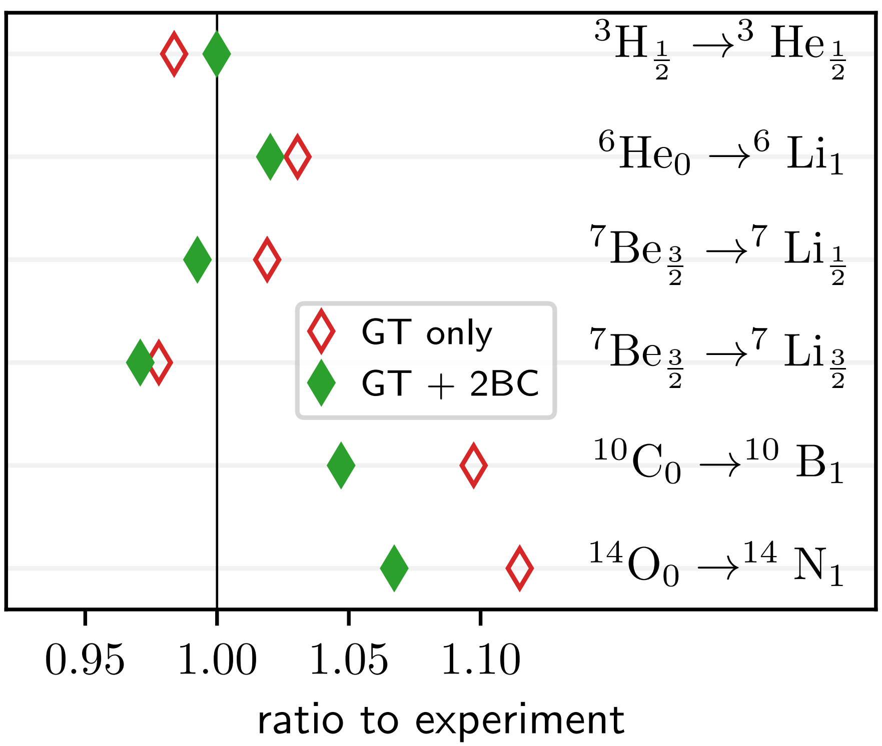
Explore exotic exchange mechanisms

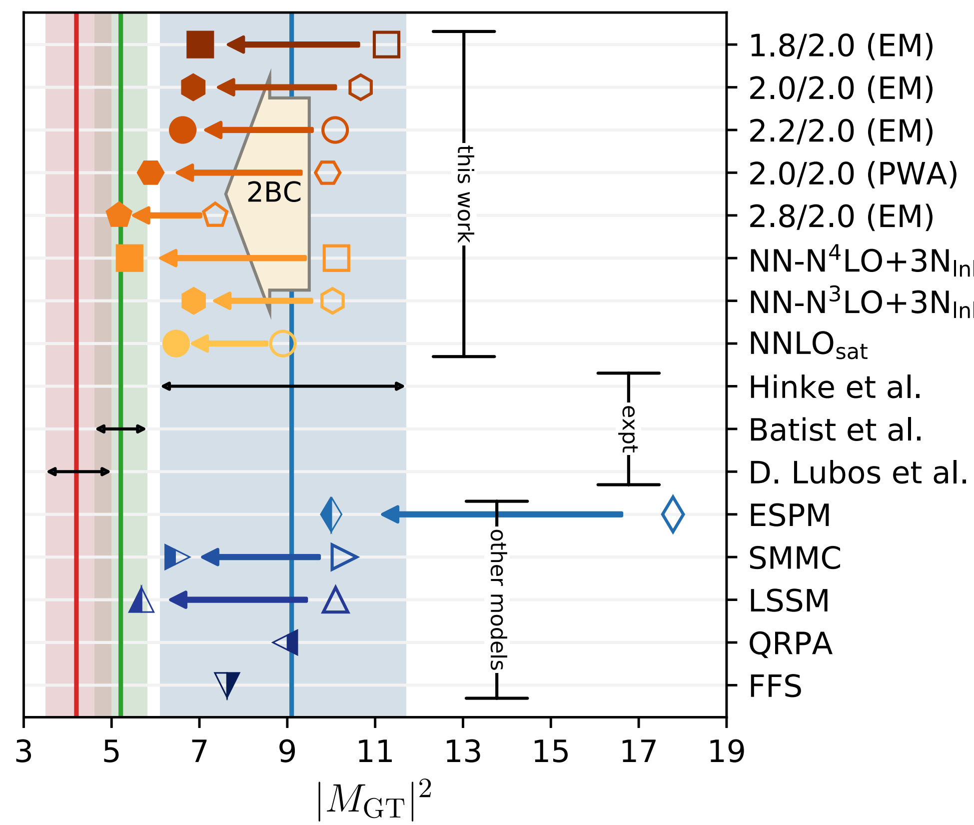
Now clear correlation with **measured** $^1S_0$ phase shift!

GT Transitions in Light Nuclei + ^{100}Sn

TRIUMF

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

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

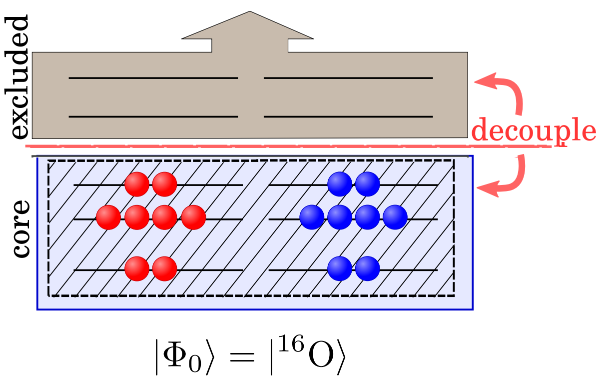
$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \qquad \eta = \frac{1}{2}\arctan\left(\frac{2H_{\text{od}}}{\Delta}\right) - \text{h.c.}$$

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

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?

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

Valence-Space IMSRG

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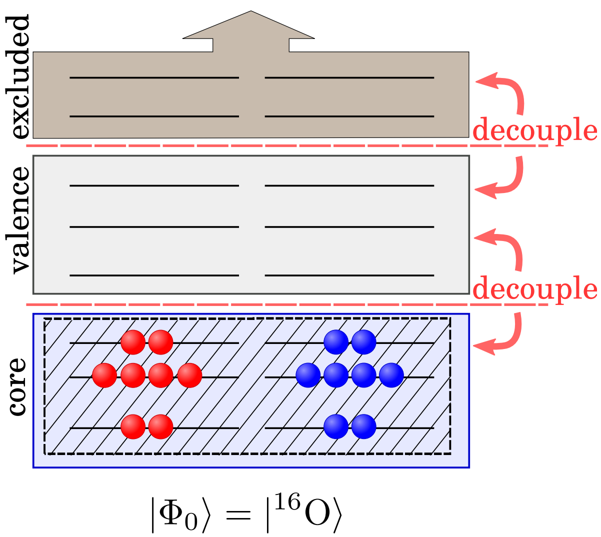
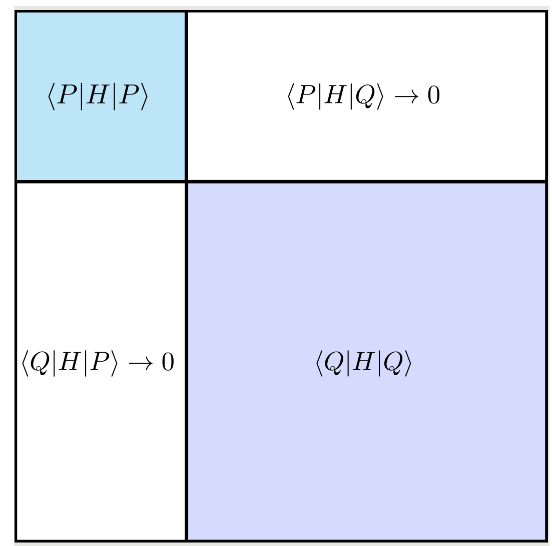


Step 1: Decouple core

Step 2: Decouple valence space

Can we achieve accuracy of large-space methods?

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



Valence-Space IMSRG

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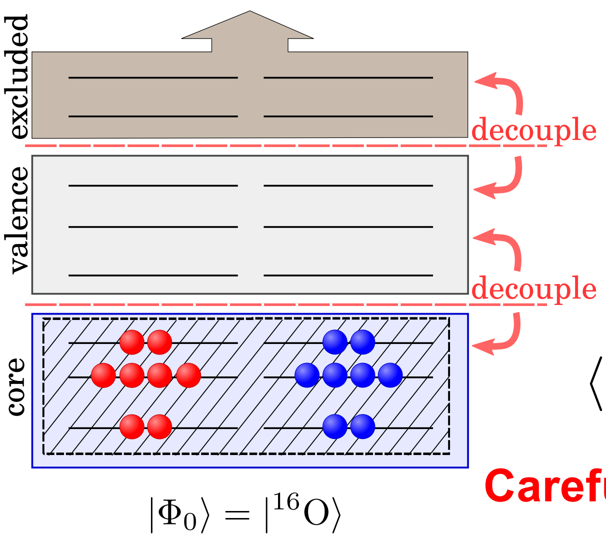
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

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

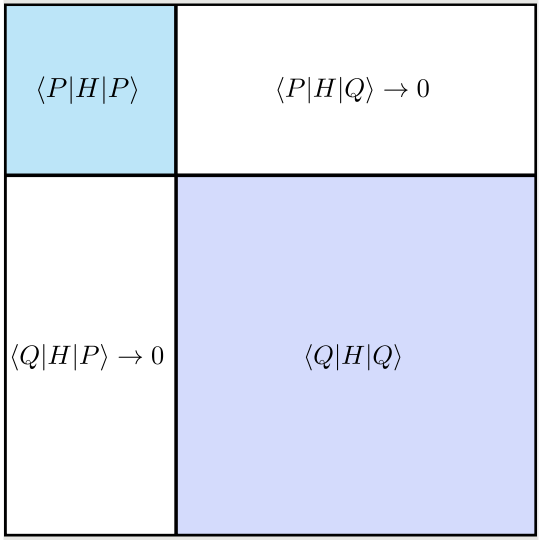


Step 1: Decouple core
Step 2: Decouple valence space
Step 3: Decouple additional operators

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

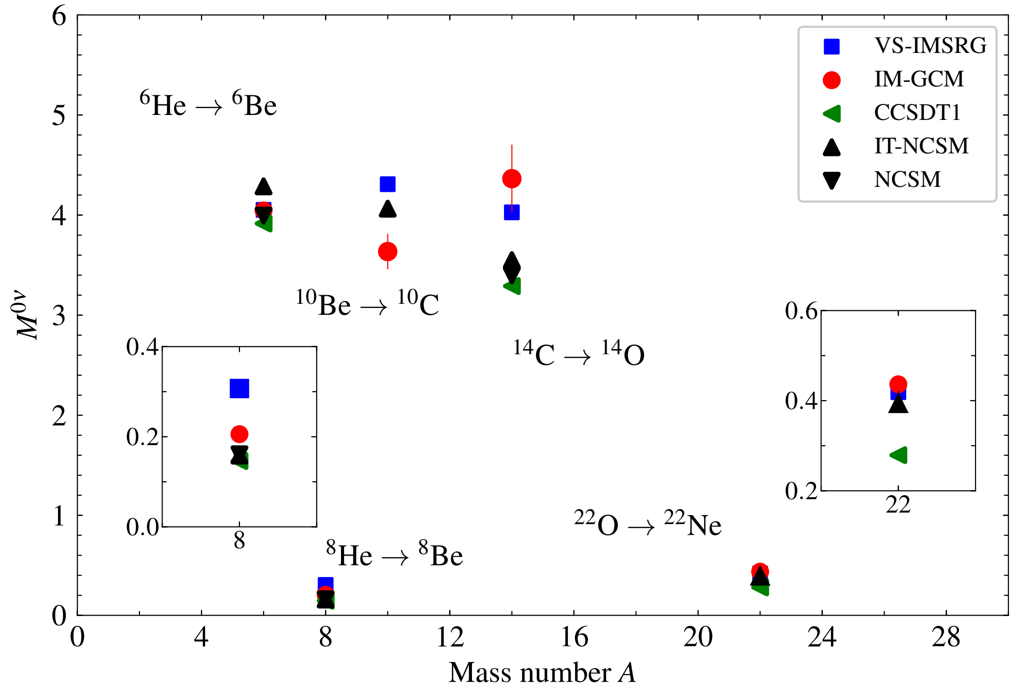
$$\langle \tilde{\Psi}_n | P \tilde{M}_{0\nu} P \mid \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$

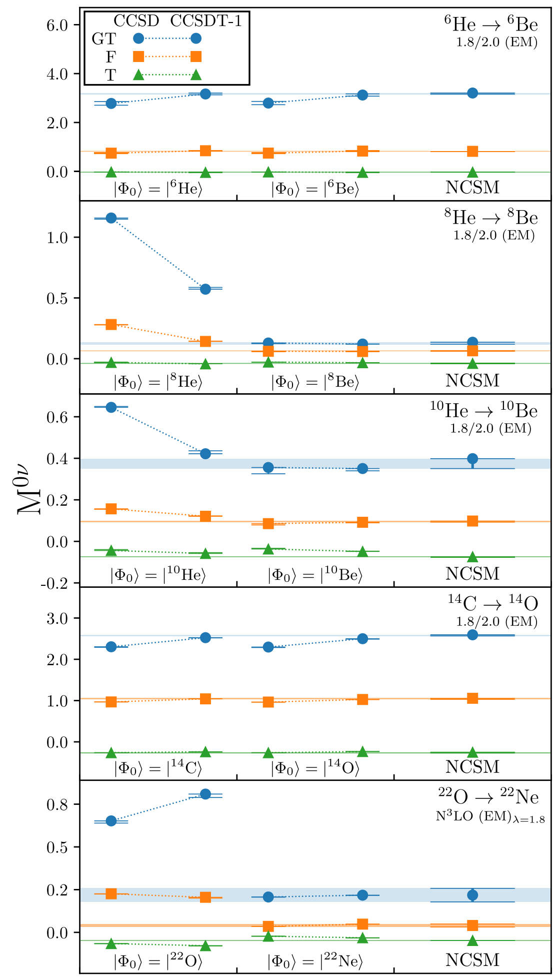
Careful benchmarking essential



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

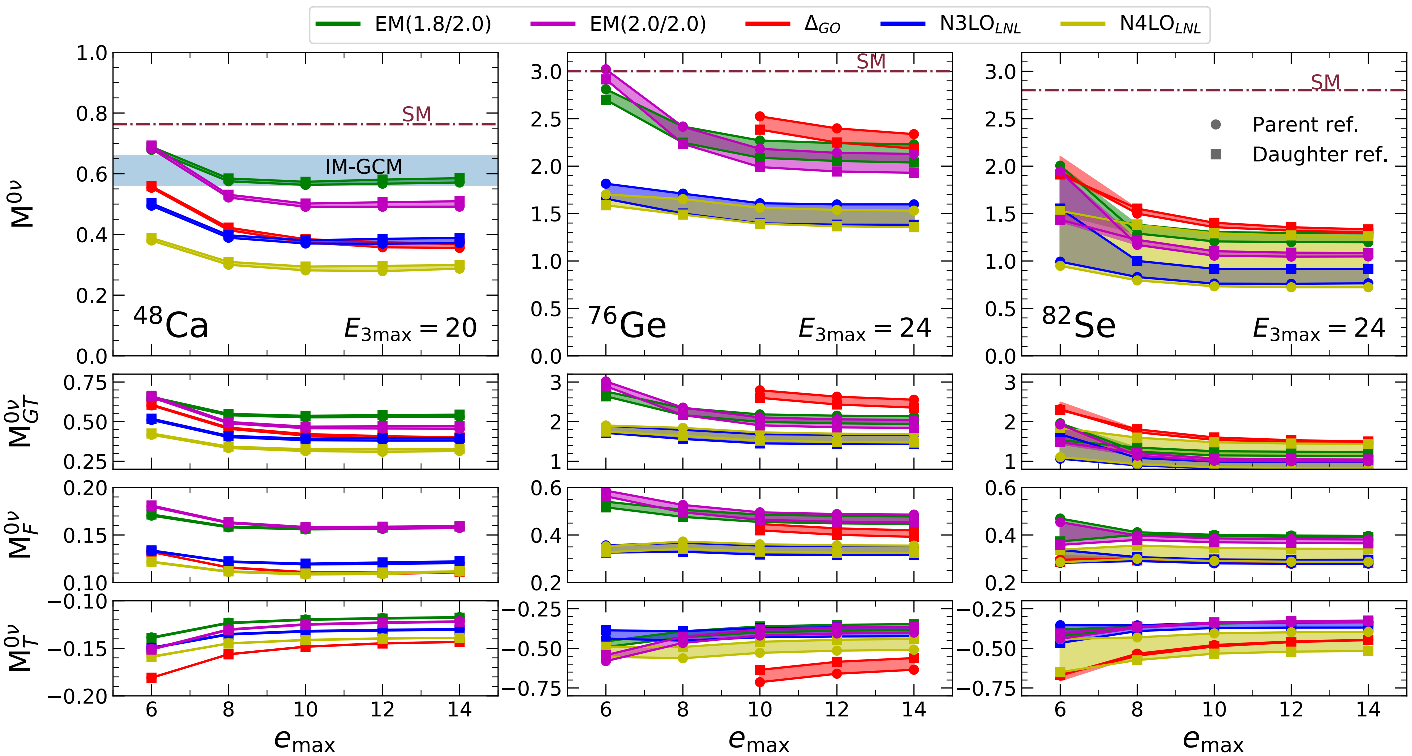
Pursue true double-beta decay candidates!

TRIUMF

Strategy II: "Uncertainties" from Input Forces

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

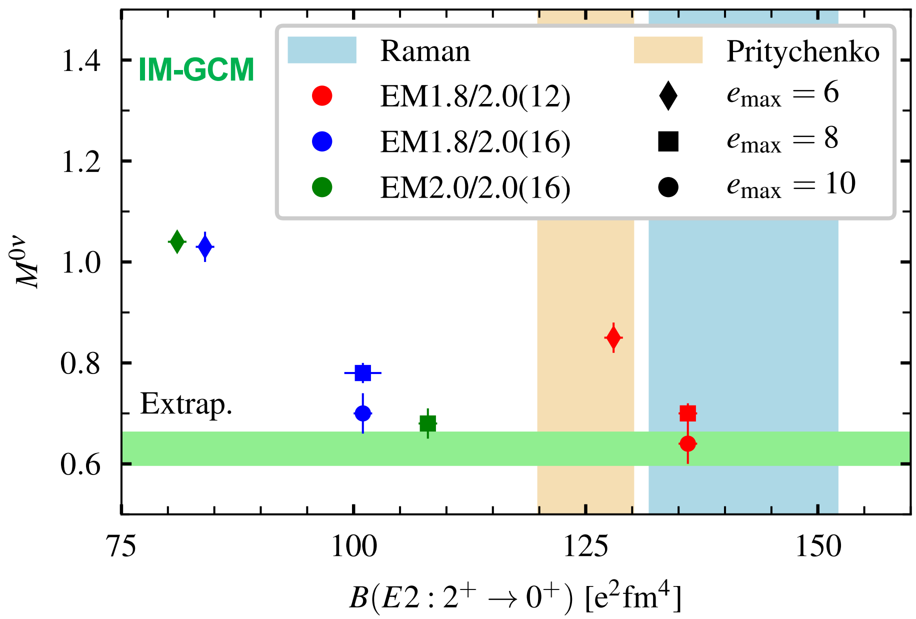
VS-IMSRG: clear convergence for ^{48}Ca, ^{76}Ge, ^{82}Se

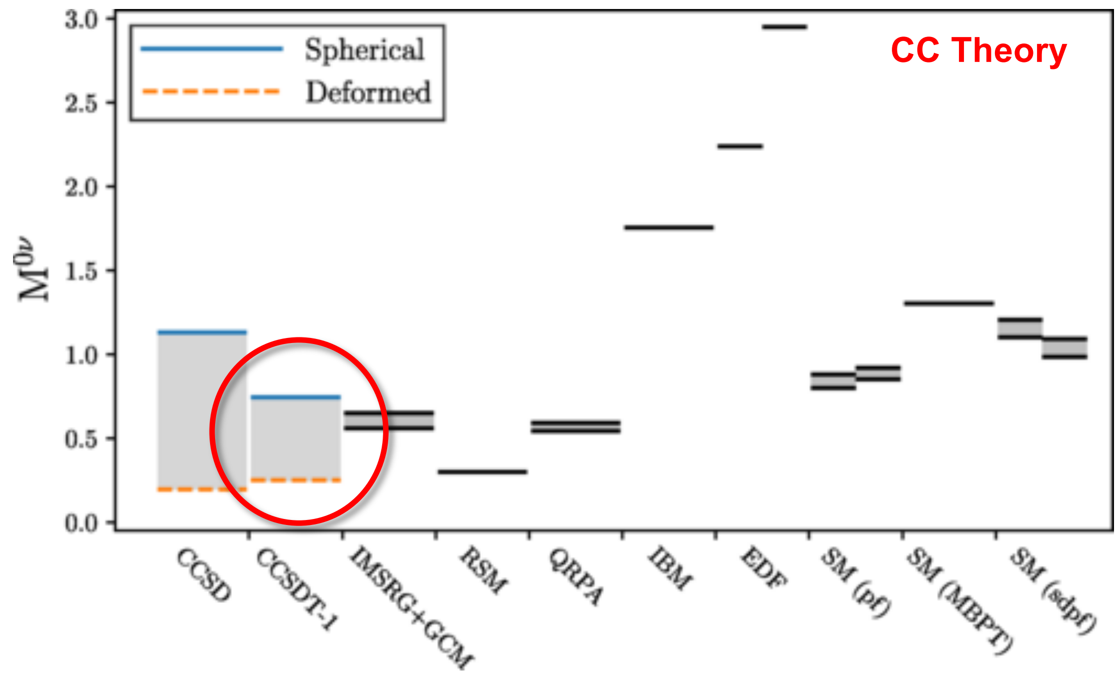


TRIUMF Strategy II: “Uncertainties” from Many-Body Methods

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

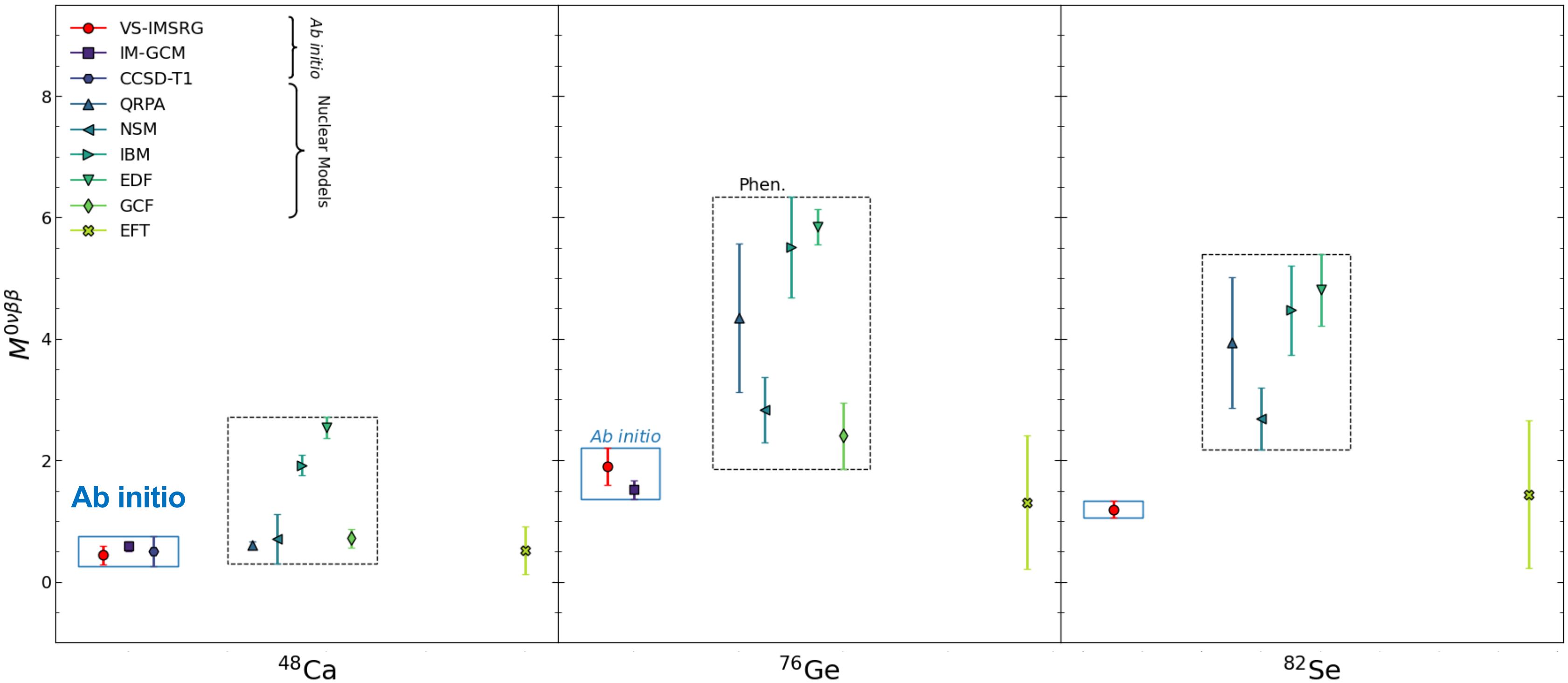
Key development: **treatment of deformation** in CC and IMSRG





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

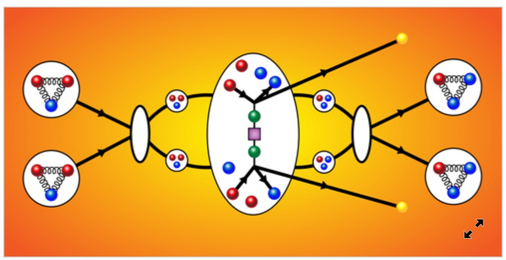
Proper renormalization requires short-range contact term at leading order

Physics — SYNOPSIS

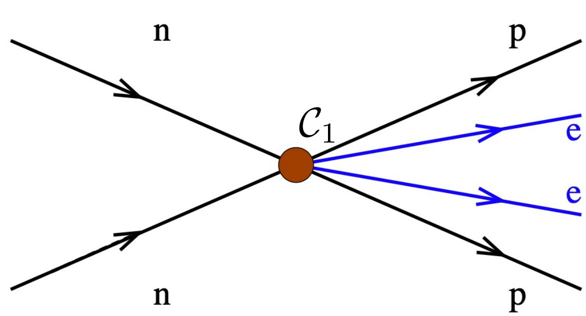
A Missing Piece in the Neutrinoless Beta-Decay Puzzle

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



New physics inside blob:
High-energy ν exchange

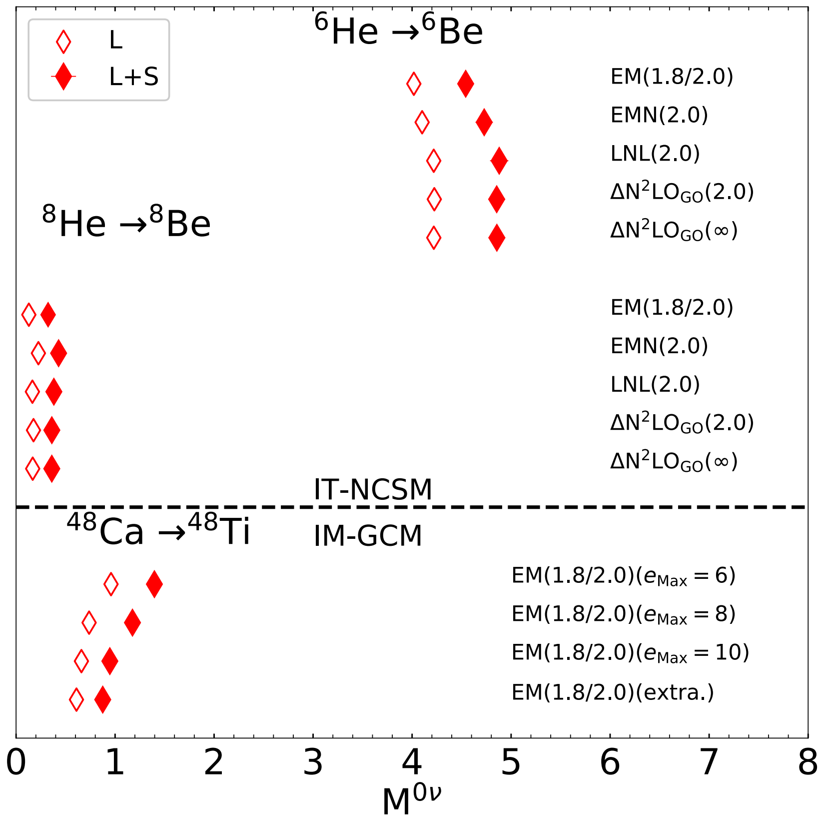
Cirigliano et al. PRL (2018)

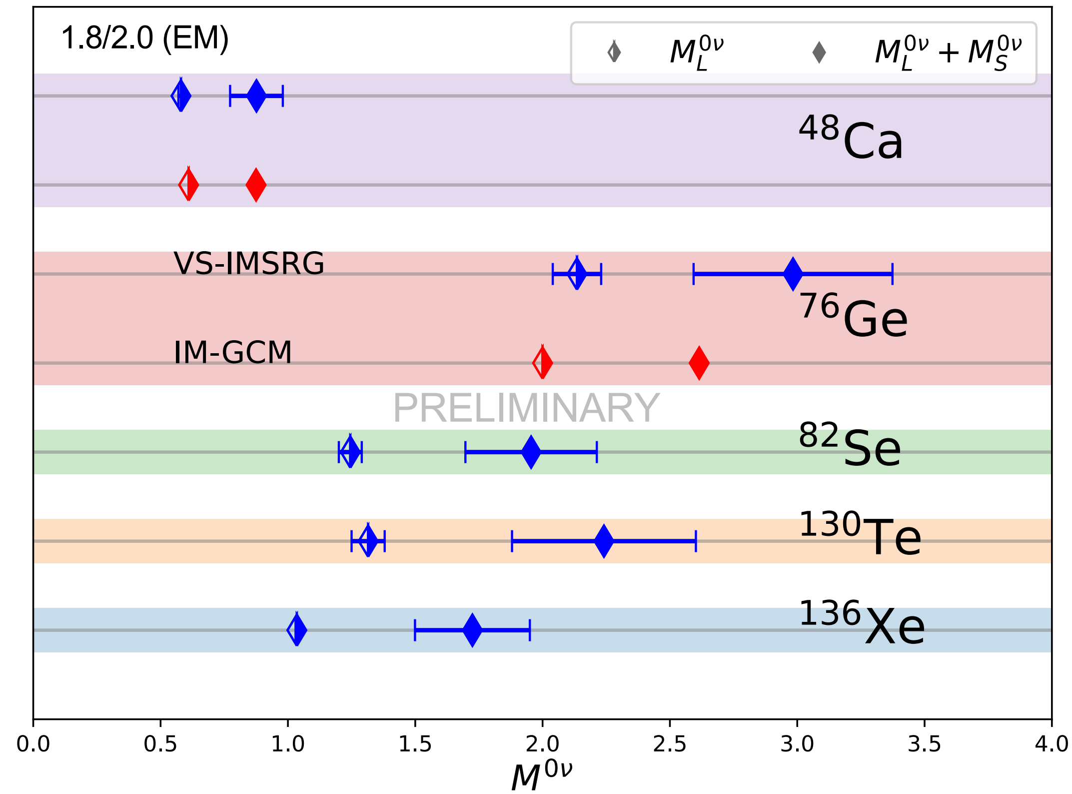
New paradigm for 0νββ decay: include long- and short-range terms

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

TRIUMF The Year We Regained Hope: Coupling Constant Fit

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





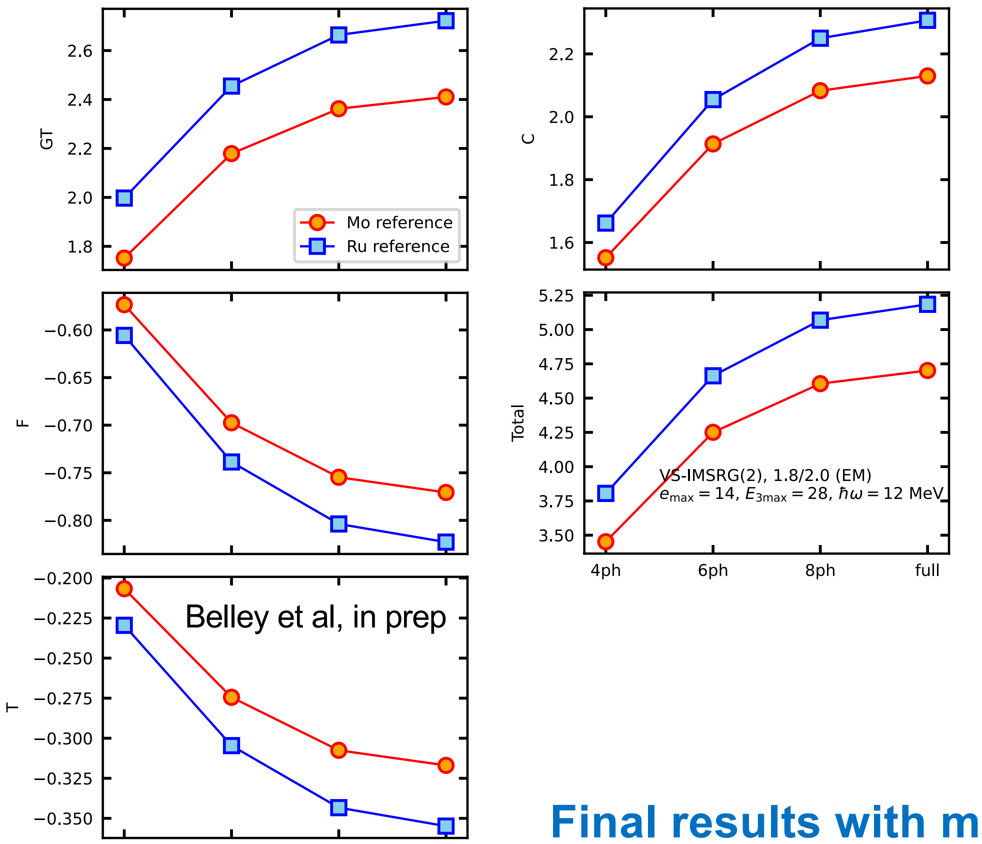
Increase of 40% (^{76}Ge) to 60% (^{130}Te/^{136}Xe)

TRIUMF

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!

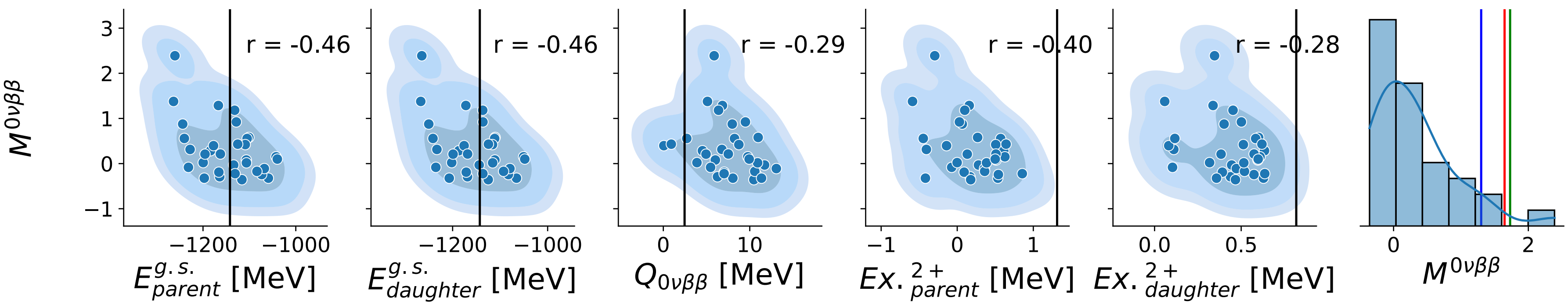
TRIUMF

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^+



Strategy IIIb: Sensitivity Analysis

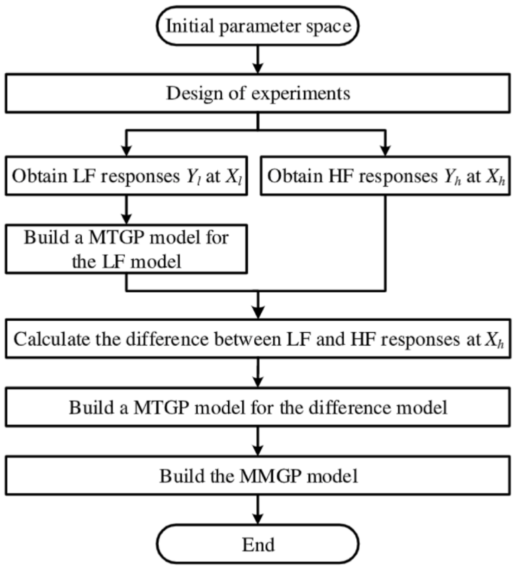
Explore dependence on chiral EFT LECs: requires many samples (as in ^{208}Pb)

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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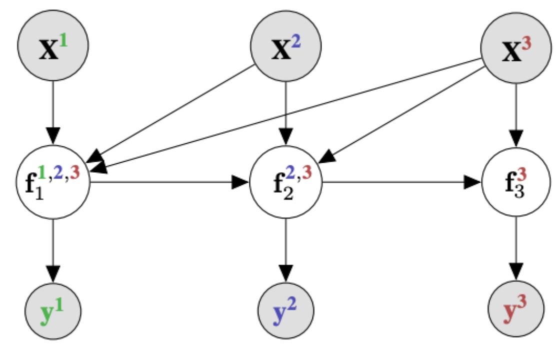
Difference function fit with Gaussian process: predict HF from LF

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)



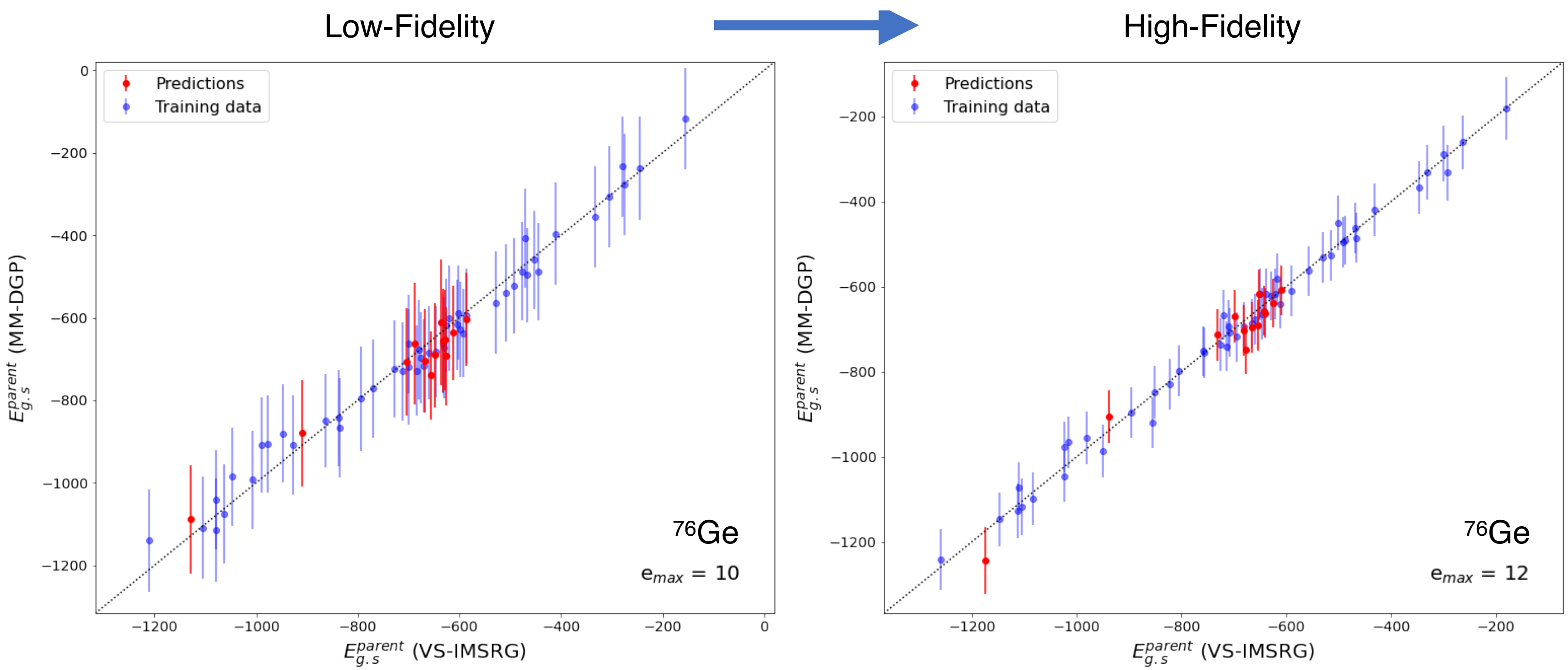
Belley Pitcher et al., in preparation

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.

TRIUMF

MM-DGP Emulator: 0νββ-Decay

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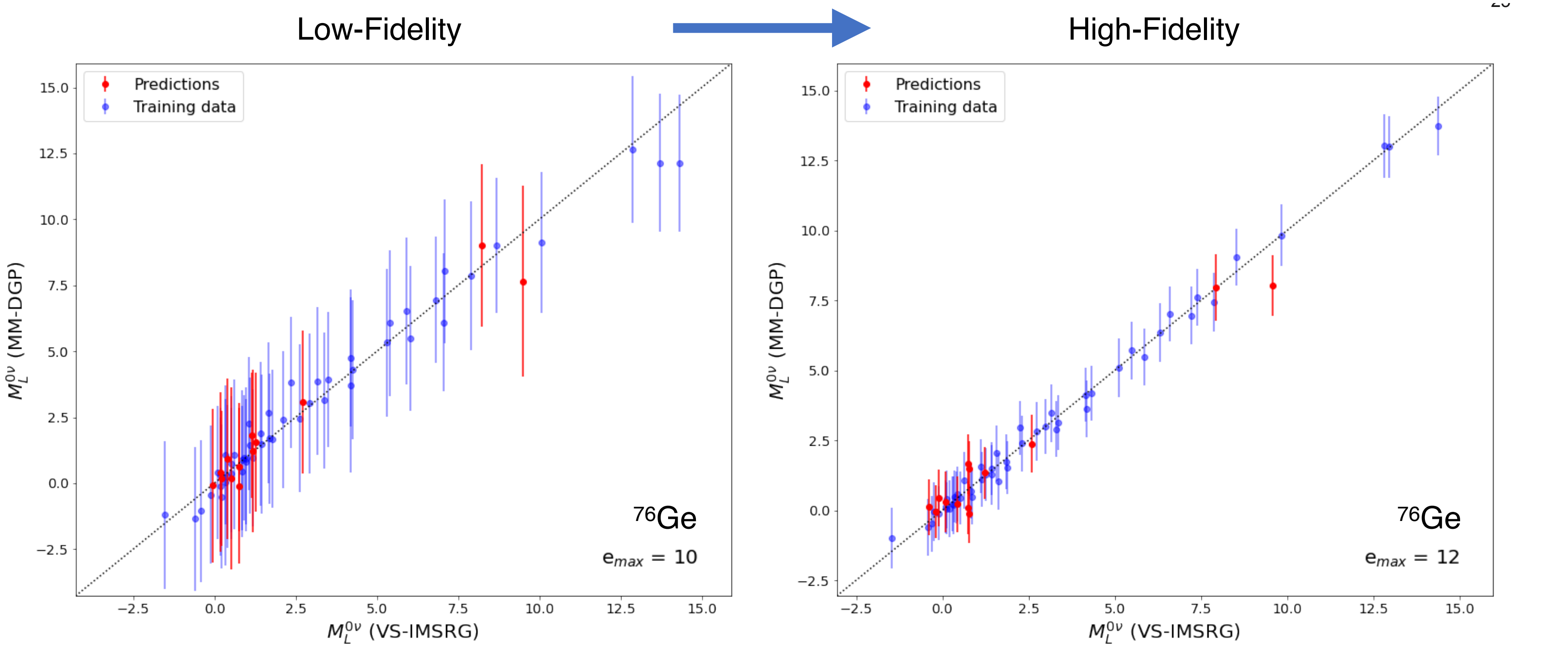

Belley, Pitcher et al. in prep.