Ab Initio Theory for Heavy Nuclei and Beyond Standard Model Physics

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TRIUMF, Theory Department
LANSPA
June 17, 2024

Discovery, accelerated

TRIUMF — Major RIB Facilities Worldwide

Next-generation **R**are **I**sotope **B**eam facilities → unprecedented era of nuclear science

Thousands of new isotopes produced… **Q: How does our field capitalize on this opportunity?**

~$1B FRIB

>$5B worldwide investment

Major RIB Facilities Worldwide

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Next-generation rare isotope beam facilities → unprecedented era of nuclear science

Thousands of new isotopes produced… **A: Meaningful interaction with theory (of course!)**

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What is the exciting physics? Connect to fundamental properties of nature?

Major RIB Facilities Worldwide

Next-generation rare isotope beam facilities → unprecedented era of nuclear science

Thousands of new isotopes produced… **A: Meaningful interaction with theory (of course!)**

Role of theory

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

Interpretation: model independent, connect to underlying forces of nature

Next-generation facilities require next-generation theory!

~$1B FRIB

>$5B worldwide investment

What is the exciting physics? Connect to fundamental properties of nature?

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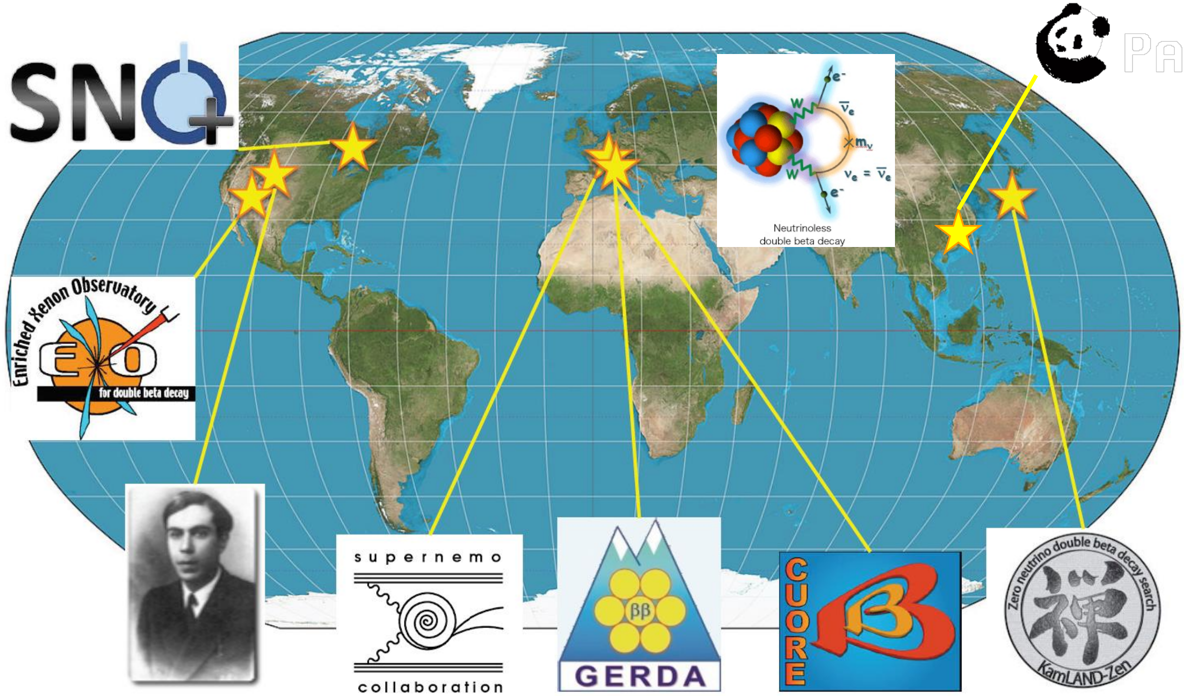
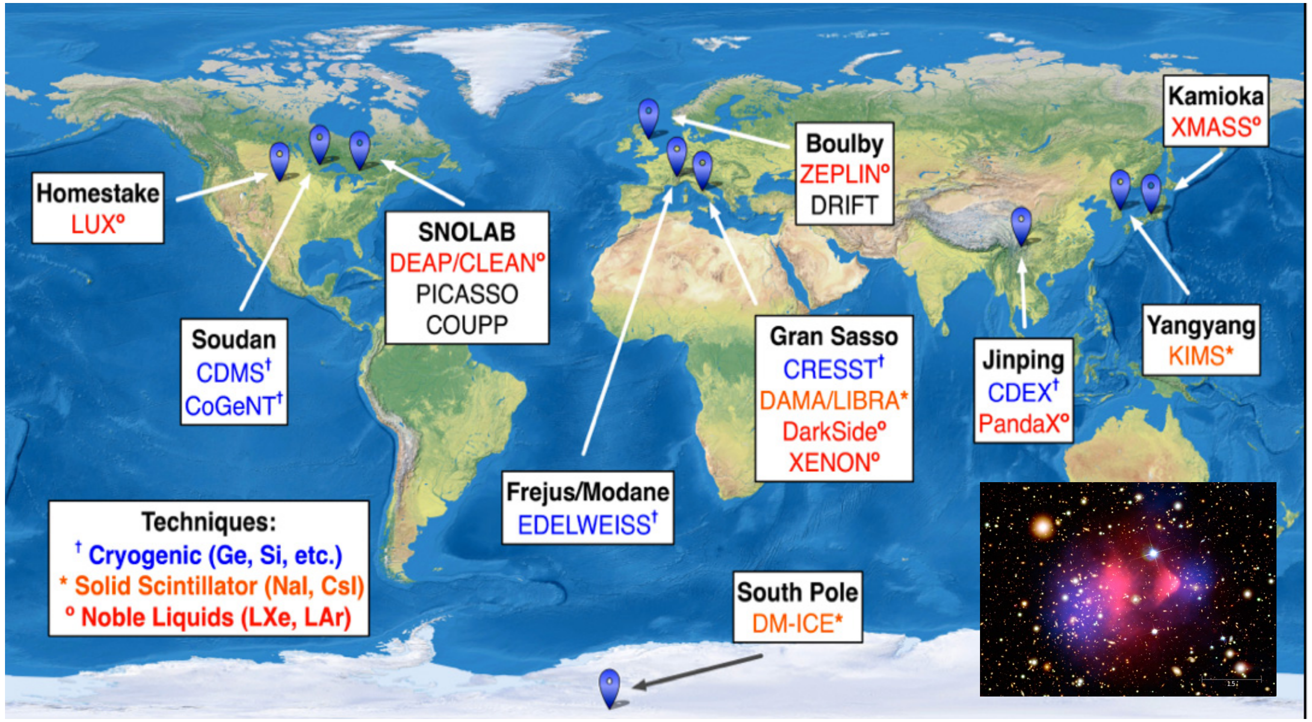
Major Underground Facilities Worldwide

Worldwide searches for BSM physics involving neutrinos and dark matter

$0\nu\beta\beta$ Decay



Dark Matter Direct Detection

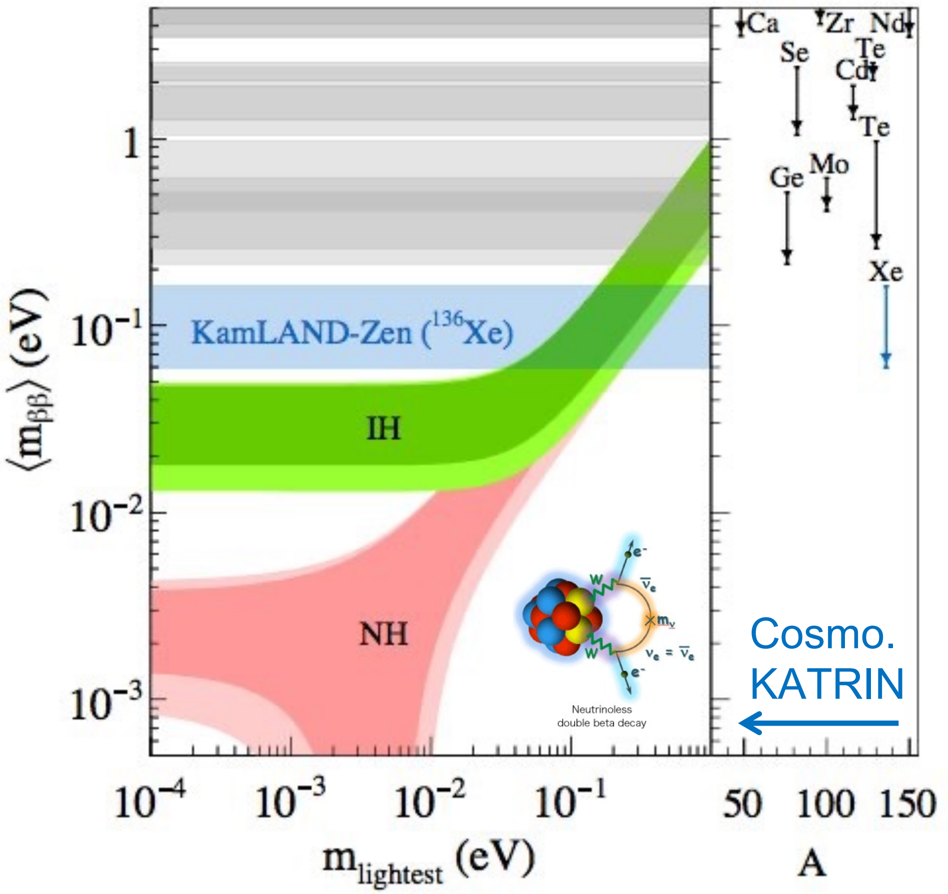


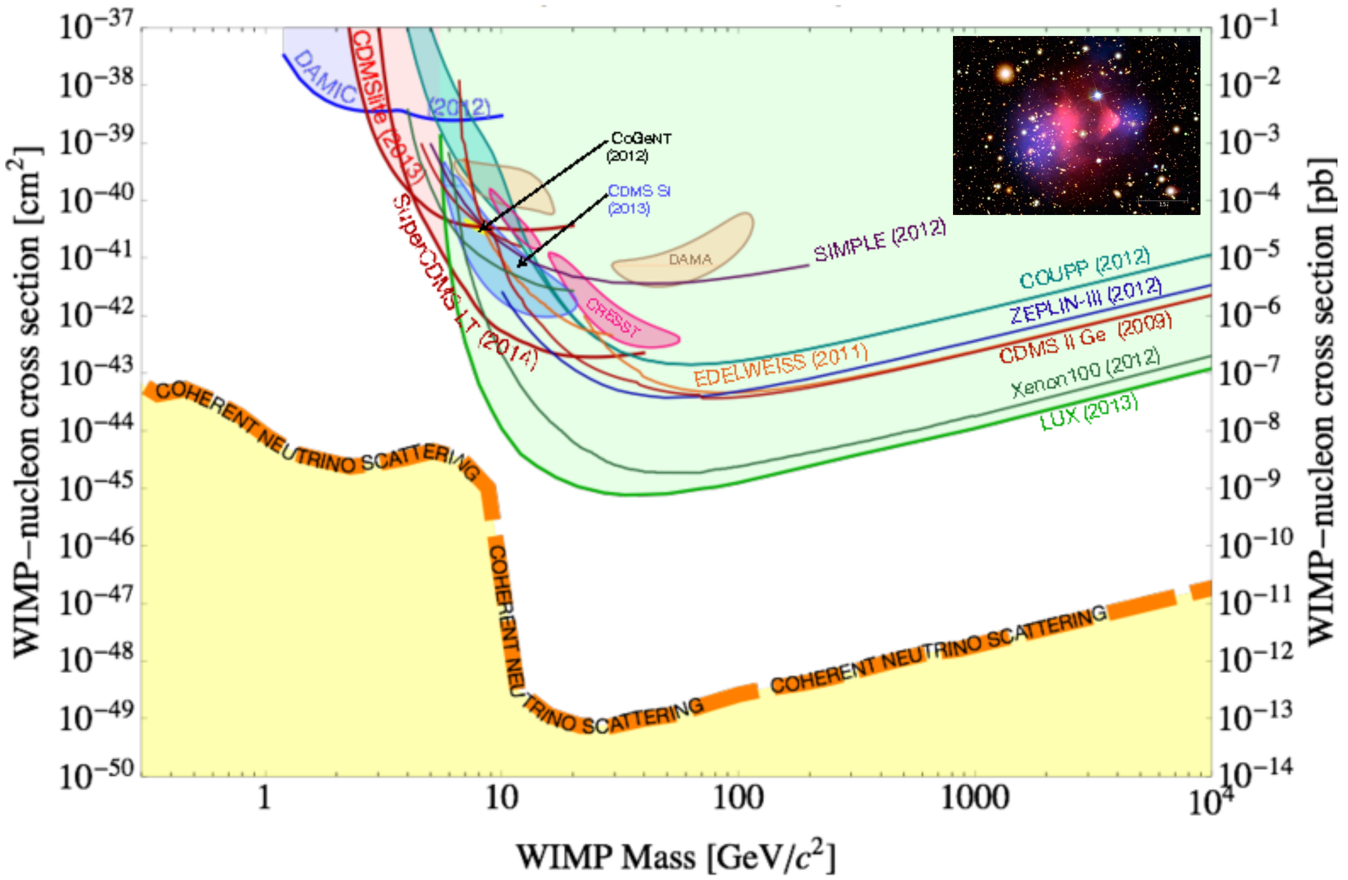
Billions invested worldwide

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

Nuclear Theory for BSM Searches

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





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

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

Nuclear Theory for BSM Searches

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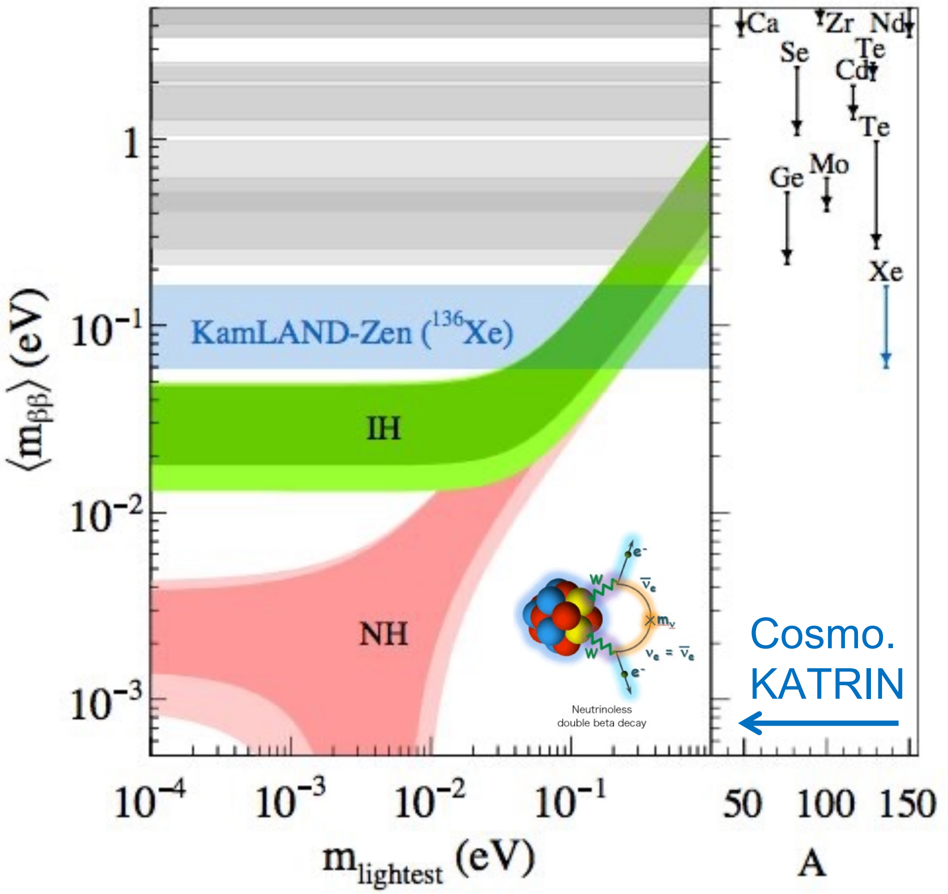

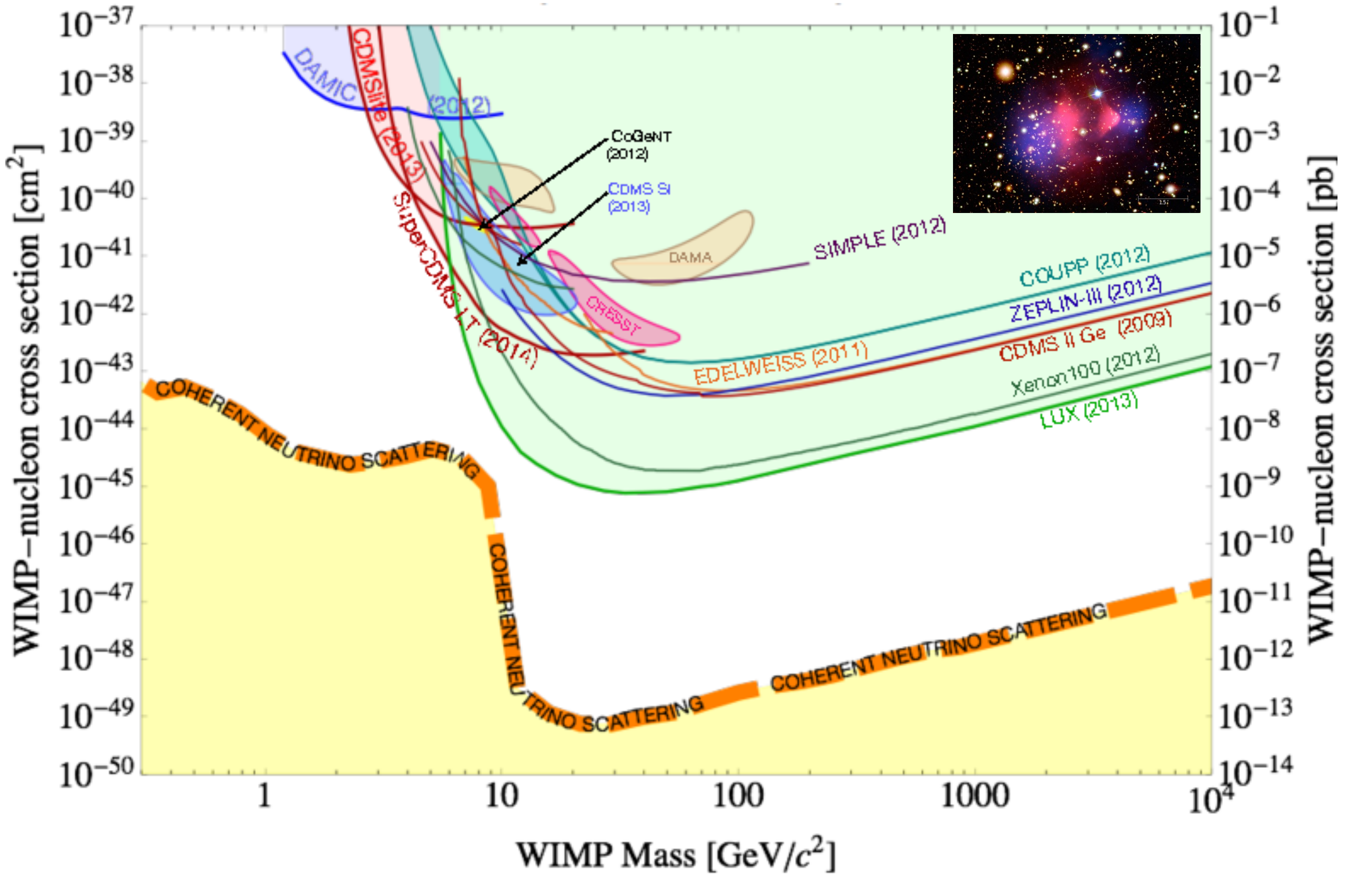

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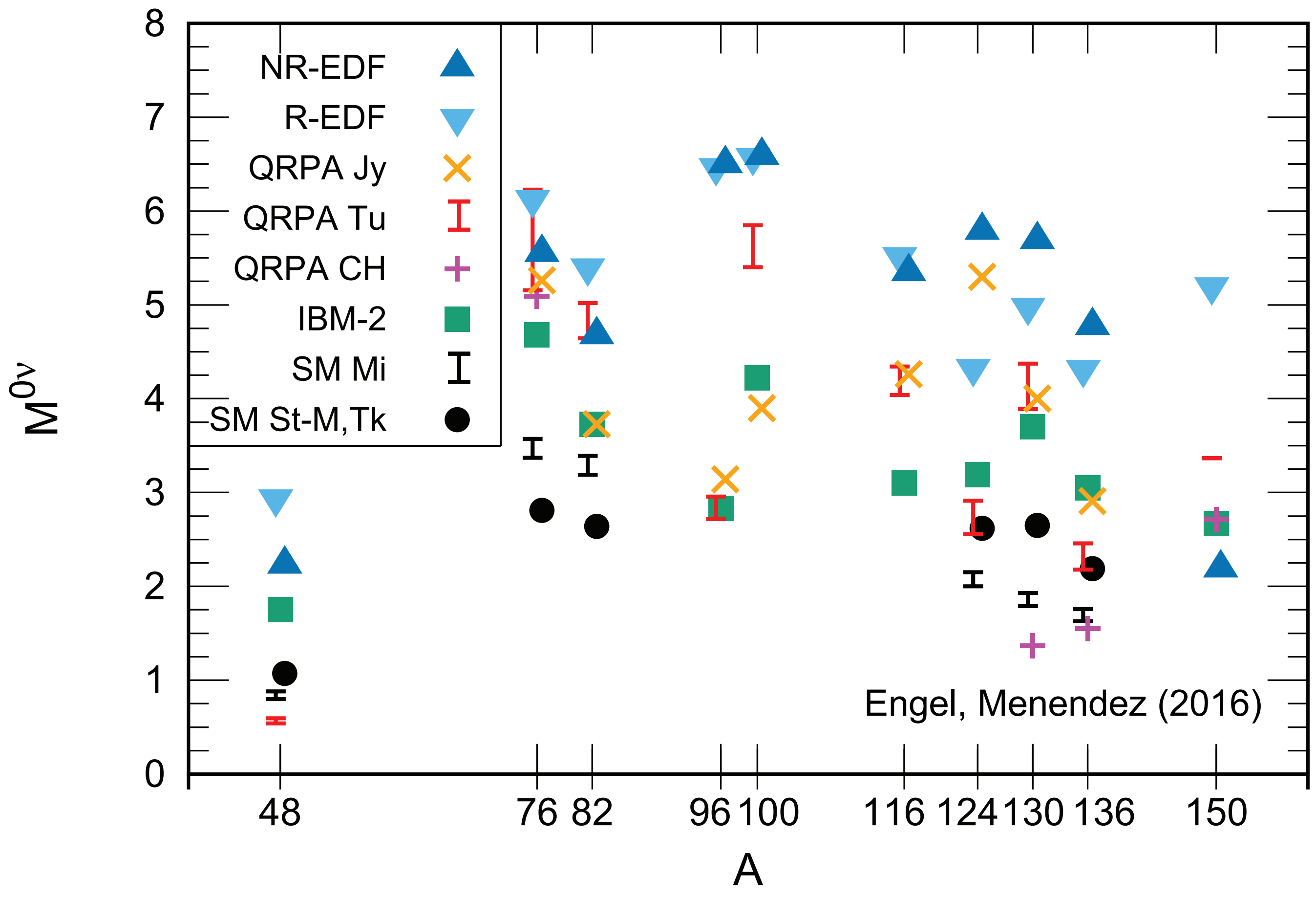
Nuclear matrix element: rate of decay

Structure functions for WIMP/ν scattering

Status of 0νββ-Decay Matrix Elements

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

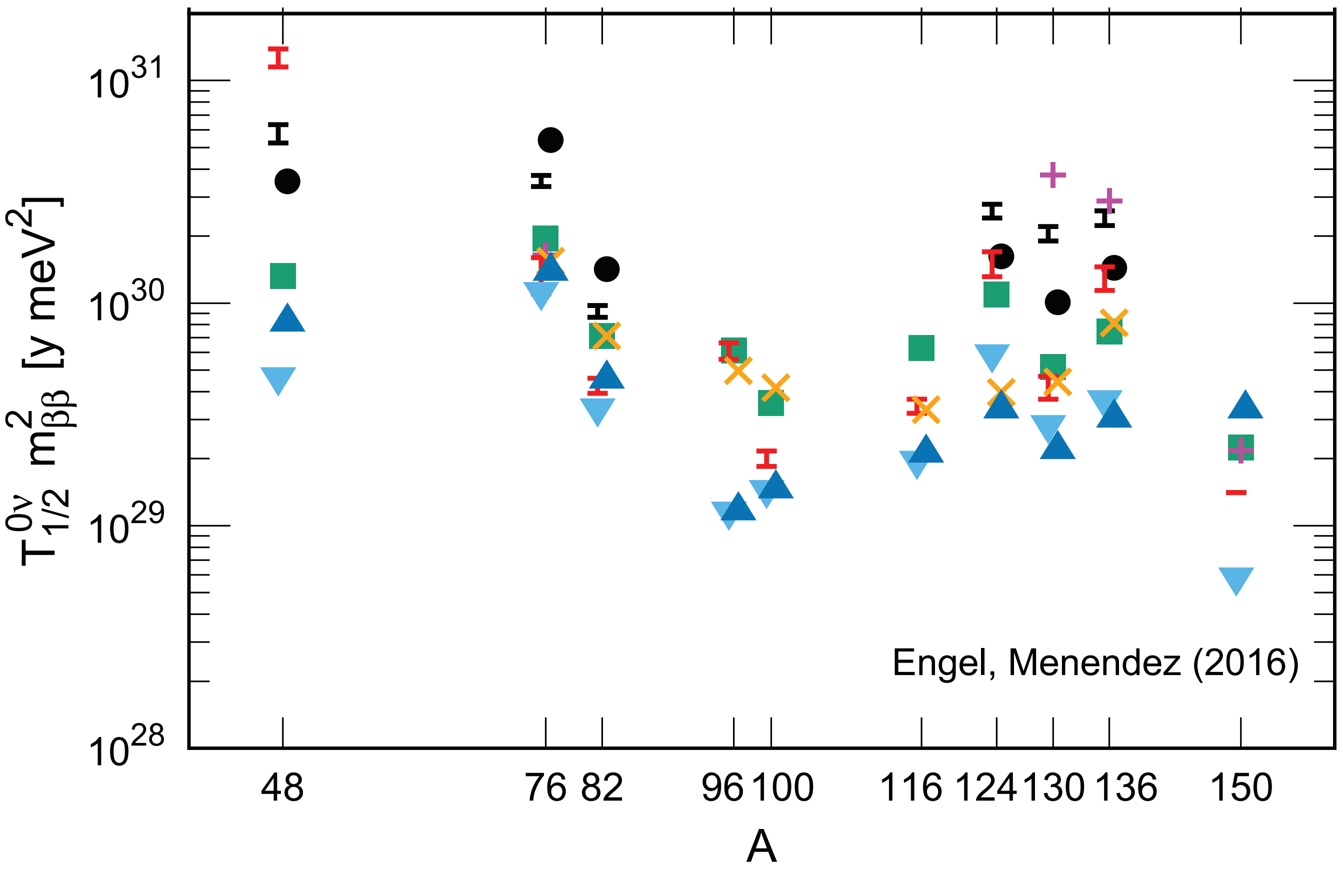


All models missing essential physics: correlations, single-particle levels, two-body currents

Impossible to assign rigorous uncertainties… but, hey, could be worse

Status of 0νββ-Decay Matrix Elements

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



Order of magnitude spread →

Order of magnitude more time/material

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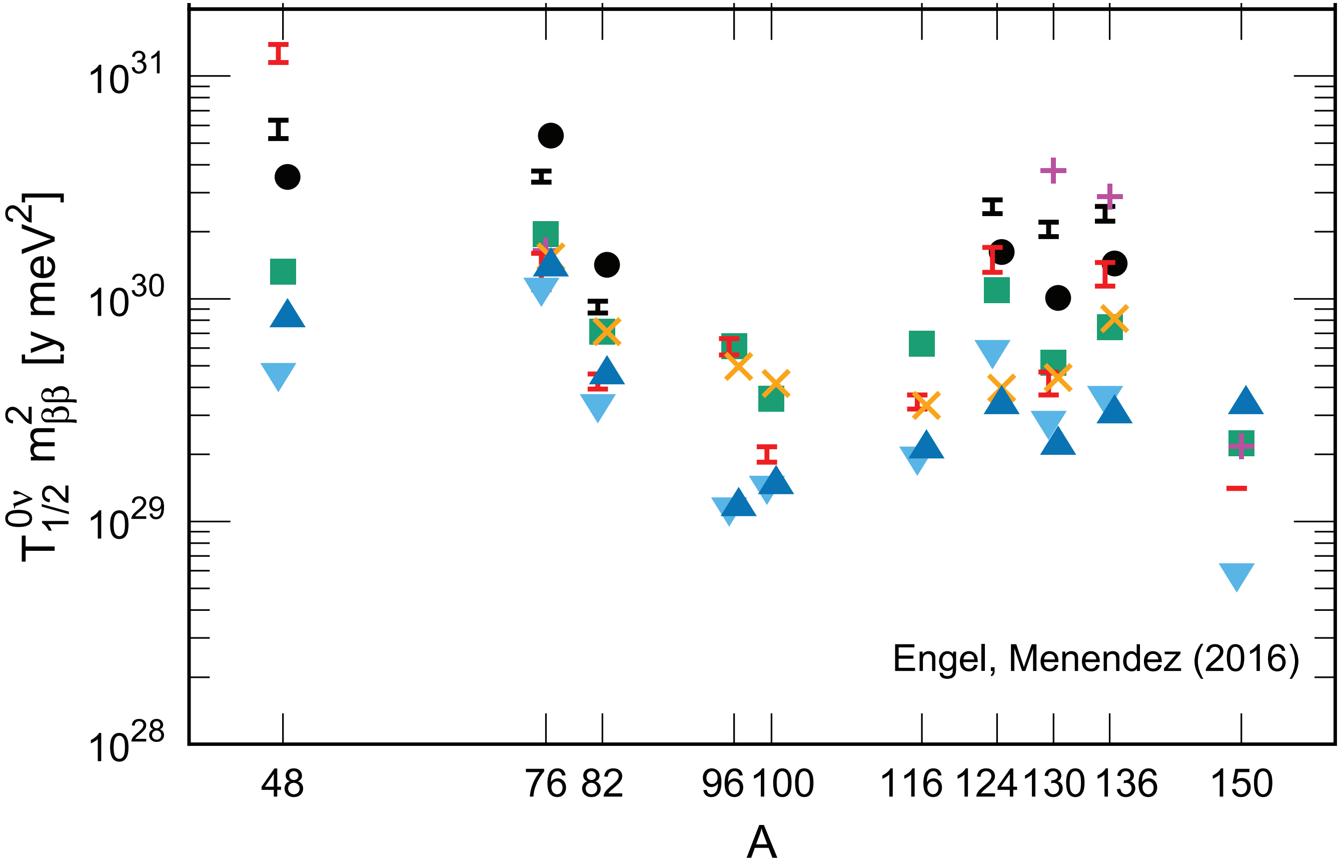

Order of magnitude spread →

Order of magnitude more time/material (i.e., more **$$$$**)

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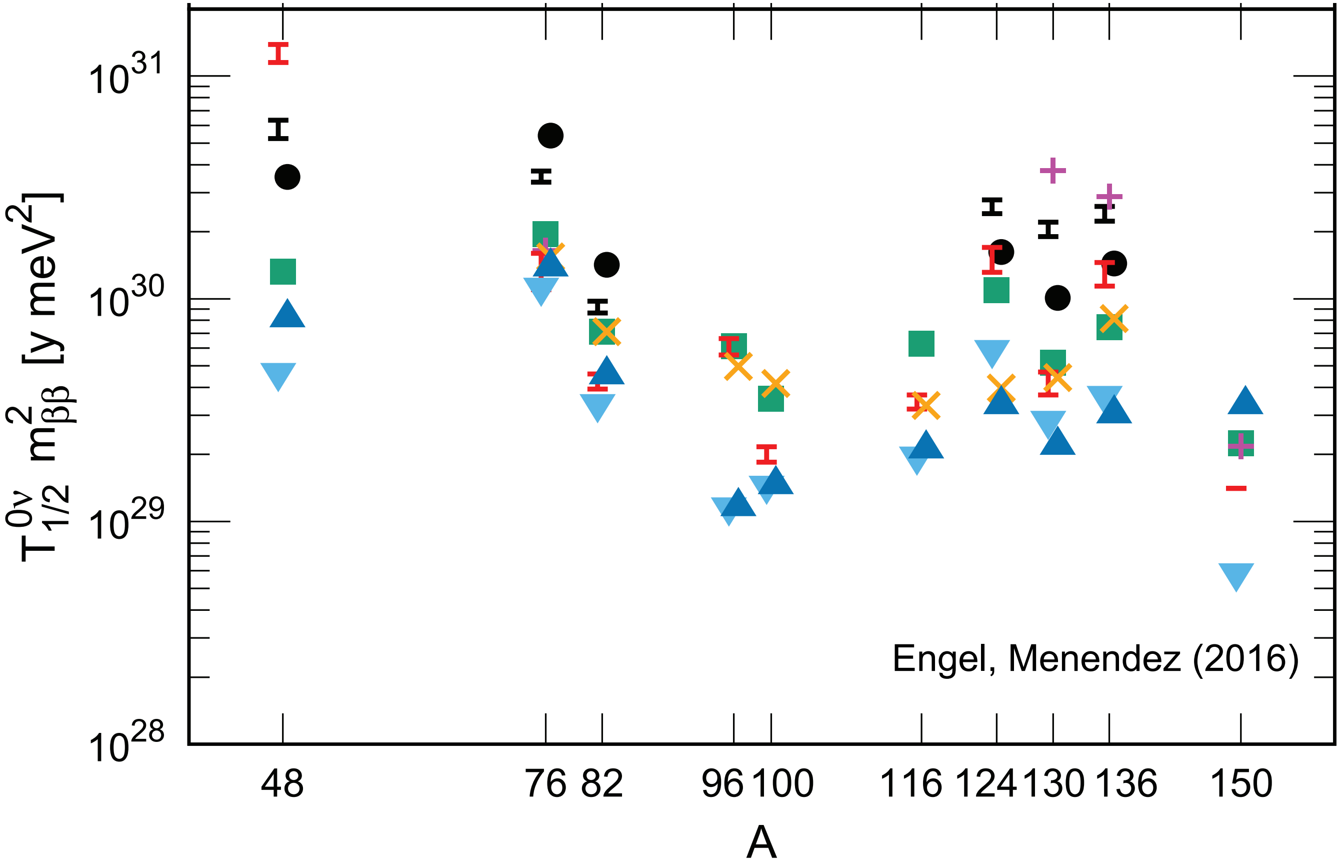

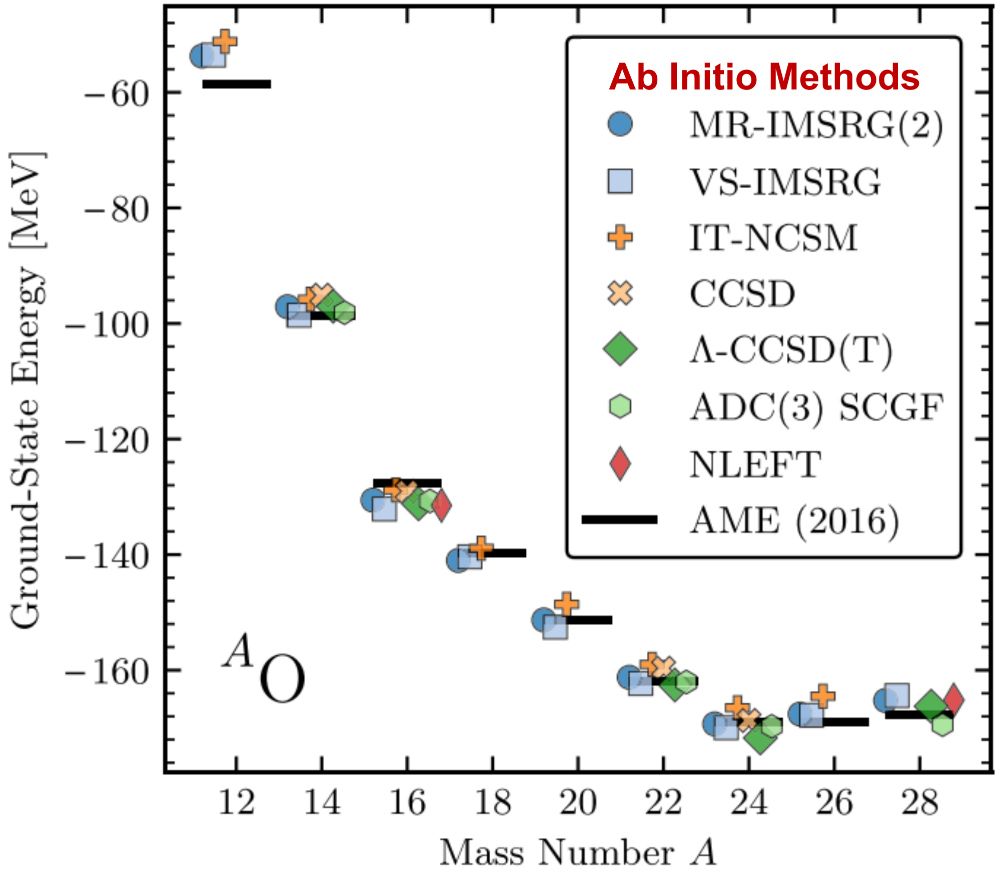

New approach to NME calculations: **ab initio theory** consistent results when extrapolated

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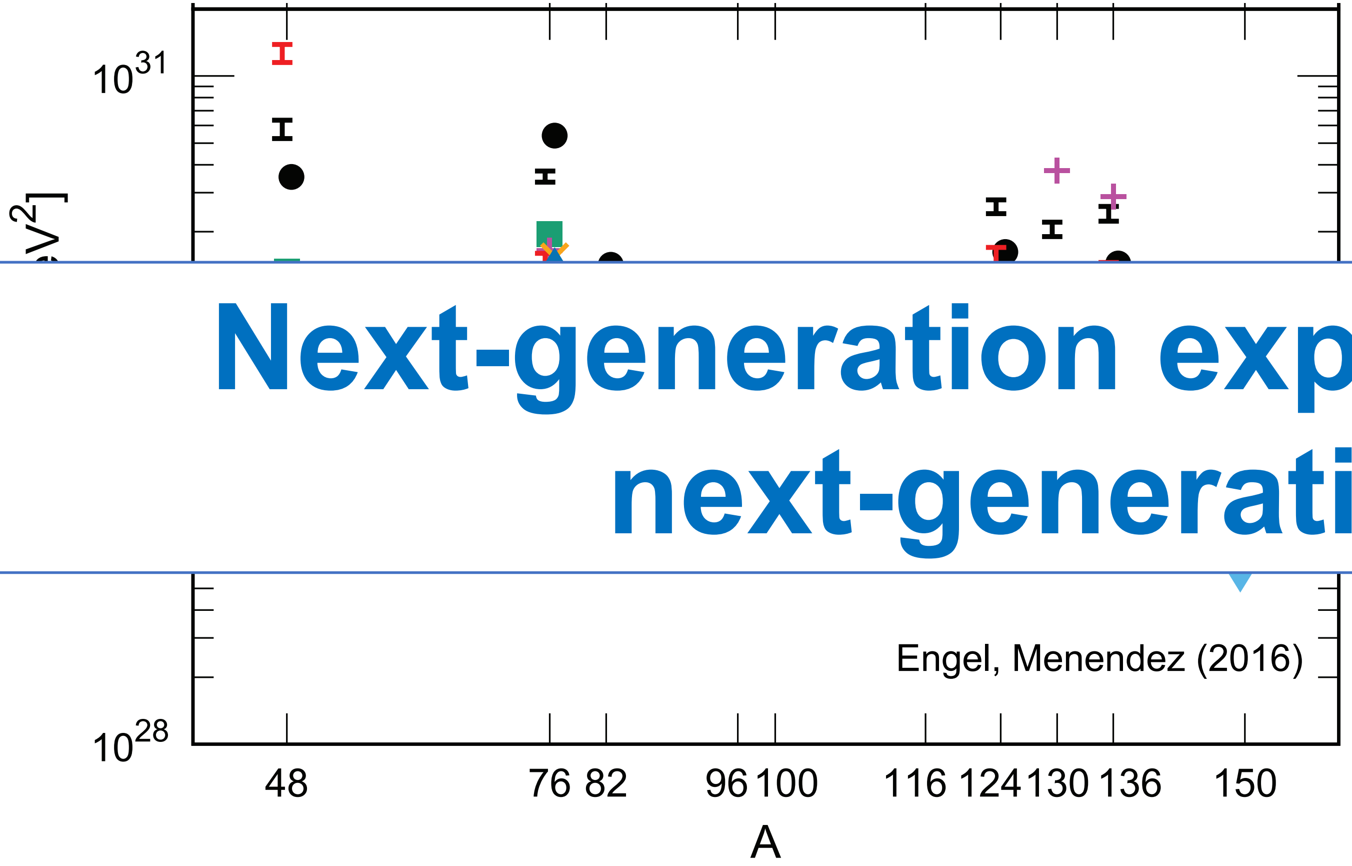
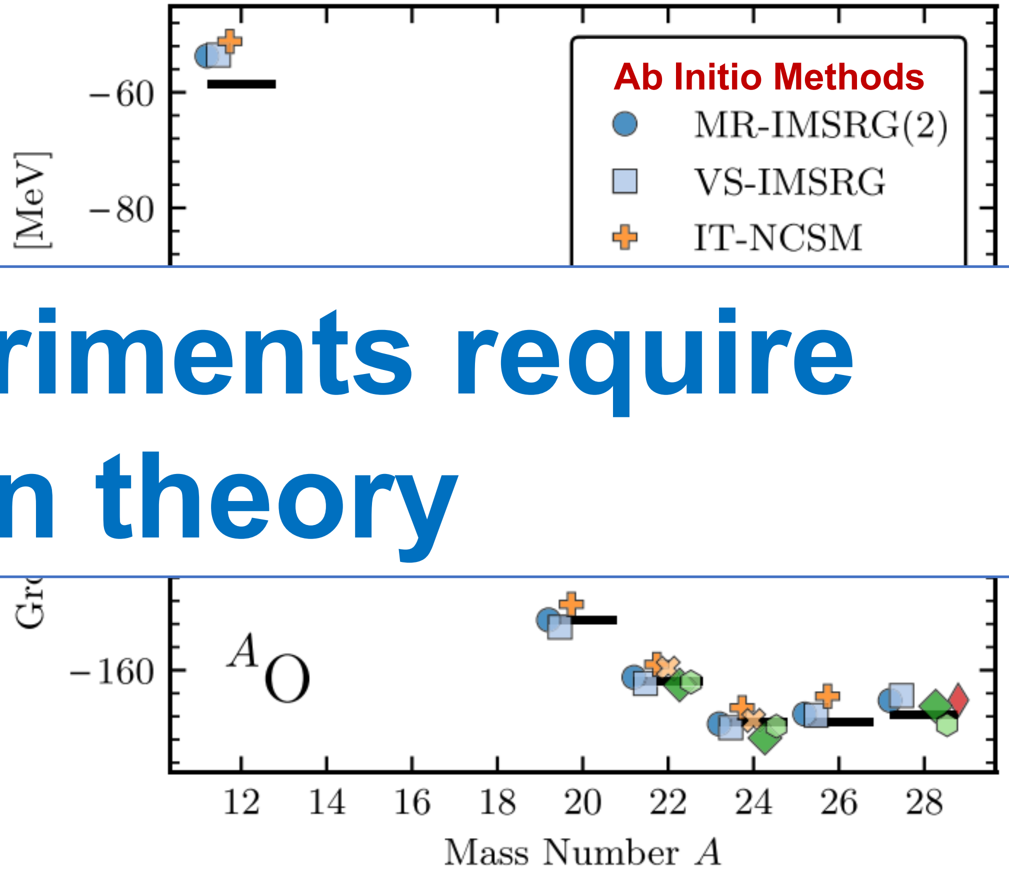
Status of $0\nu\beta\beta$-Decay Matrix Elements

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





Next-generation experiments require next-generation theory

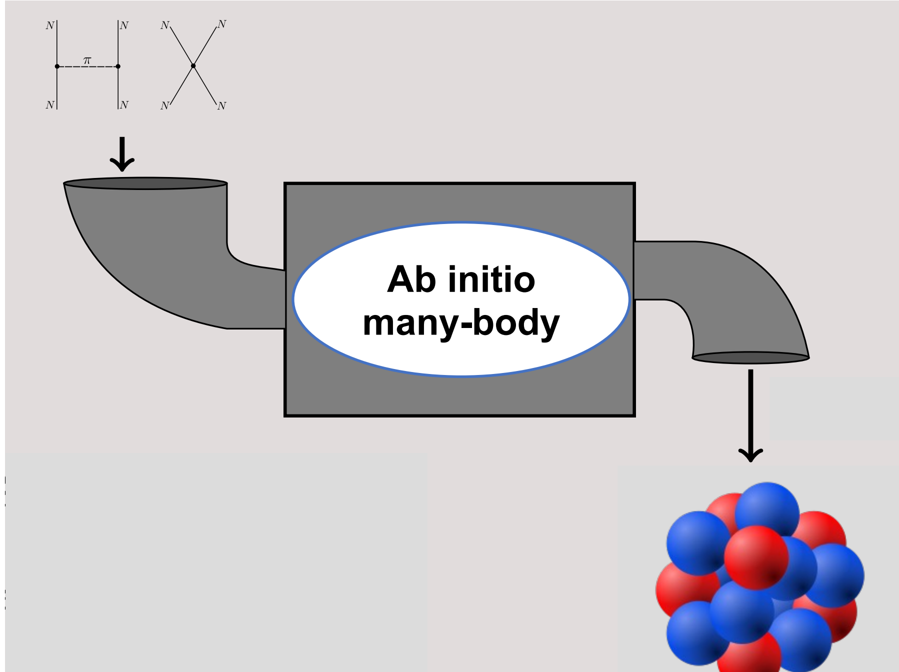
New approach to NME calculations: **ab initio theory** consistent results when extrapolated

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

$$H\psi_n = E_n\psi_n$$



Courtesy, S. R. Stroberg

Ab Initio Approach to Nuclear Forces

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

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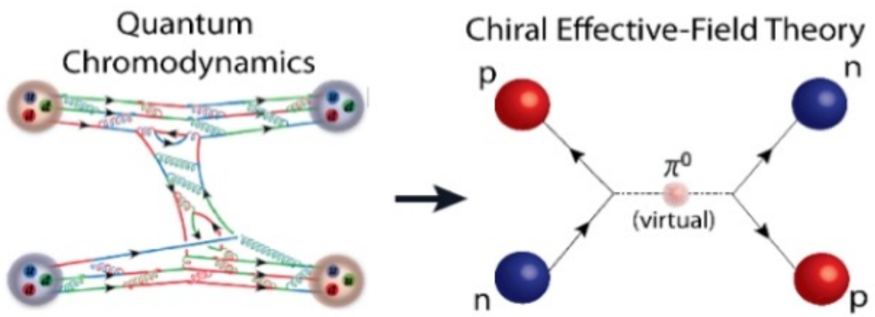
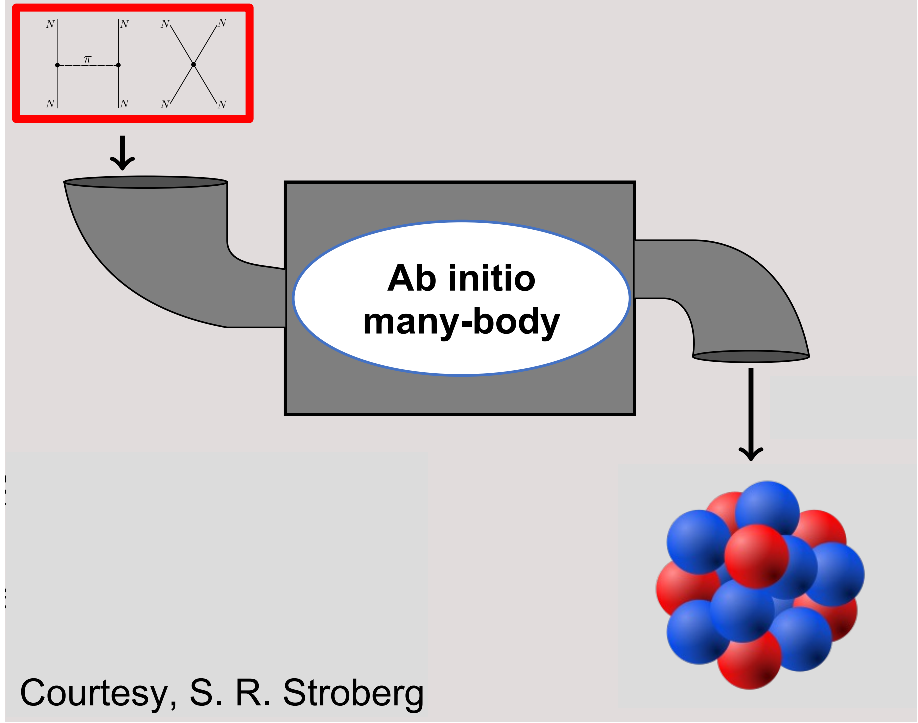
$$\boxed{H}\psi_n = E_n\psi_n$$





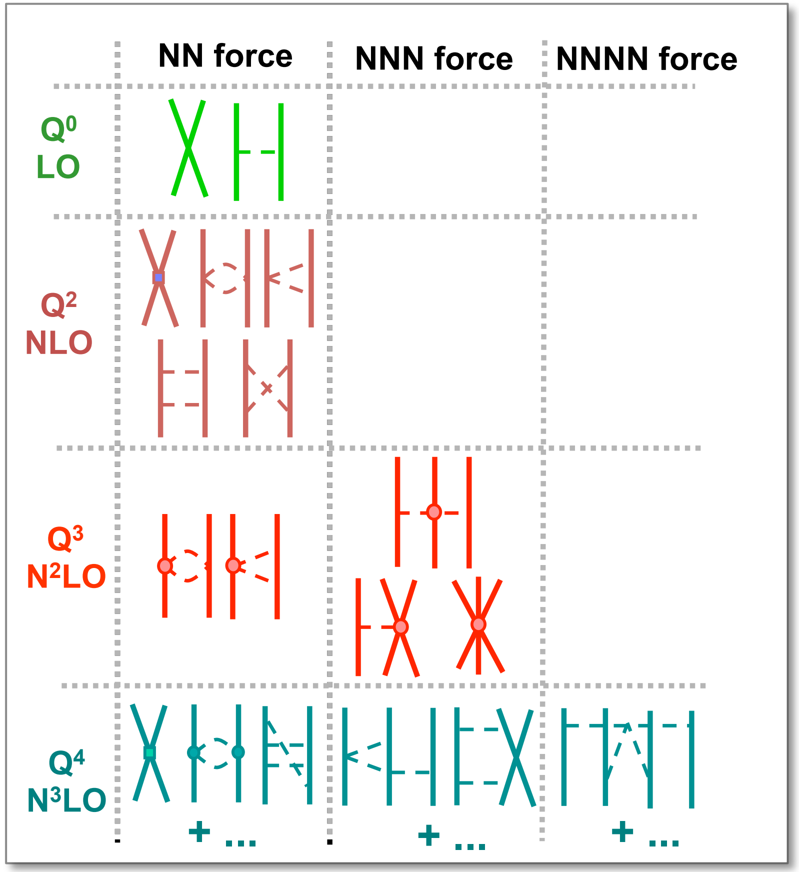
Chiral Effective Field Theory

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

Quantifiable uncertainties

Interactions

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

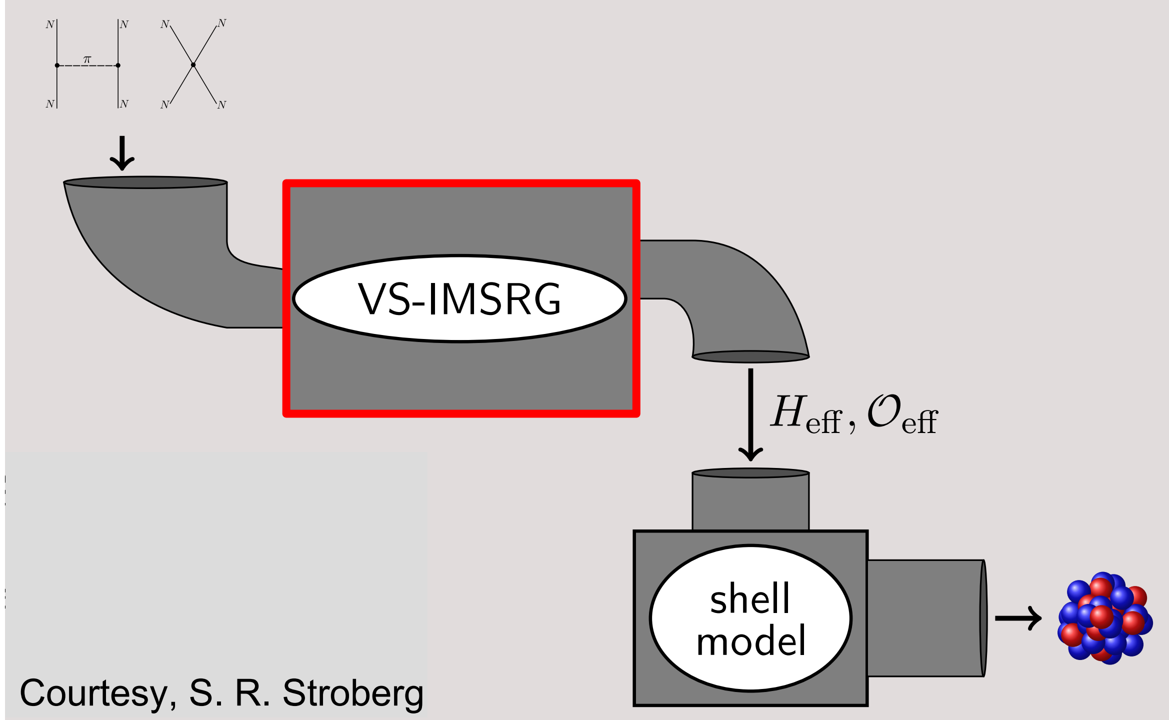


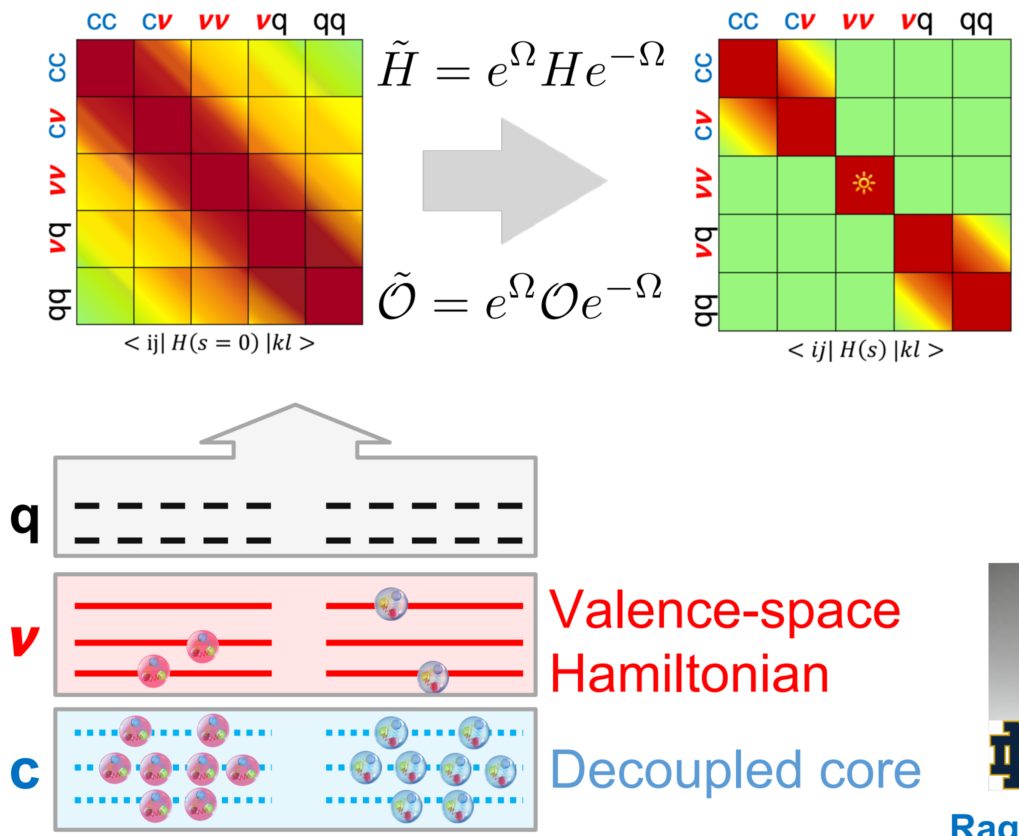
Key Advance Novel Valence-Space Approach

Polynomially scaling methods tailored for doubly magic, semi-magic chains

Valence-space IMSRG: Novel approach for all open-shell nuclei

$$\boxed{H\psi_n = E_n\psi_n}$$





Ragnar Stroberg

Ab initio → scope of nuclear shell model

Nucleus-Dependent Valence-Space Approach to Nuclear Structure

S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk

Phys. Rev. Lett. **118**, 032502 – Published 20 January 2017

Ab Initio Approach to Nuclear Structure

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

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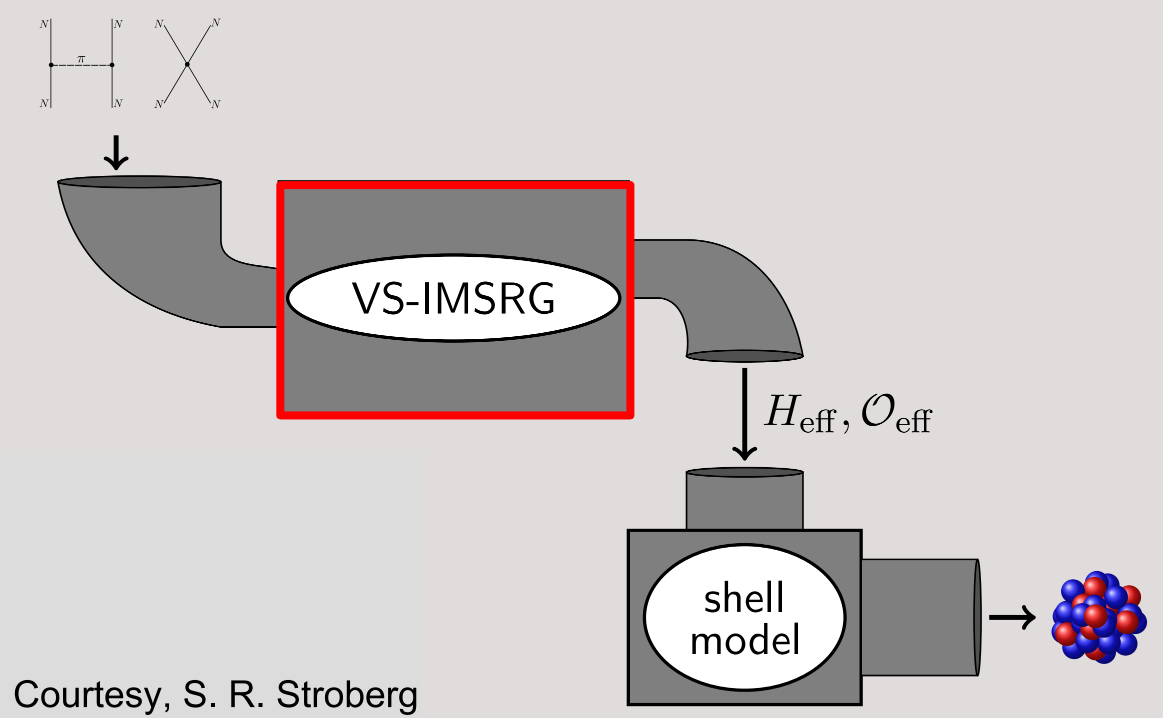


Courtesy, S. R. Stroberg

Methods Exact up to Truncations

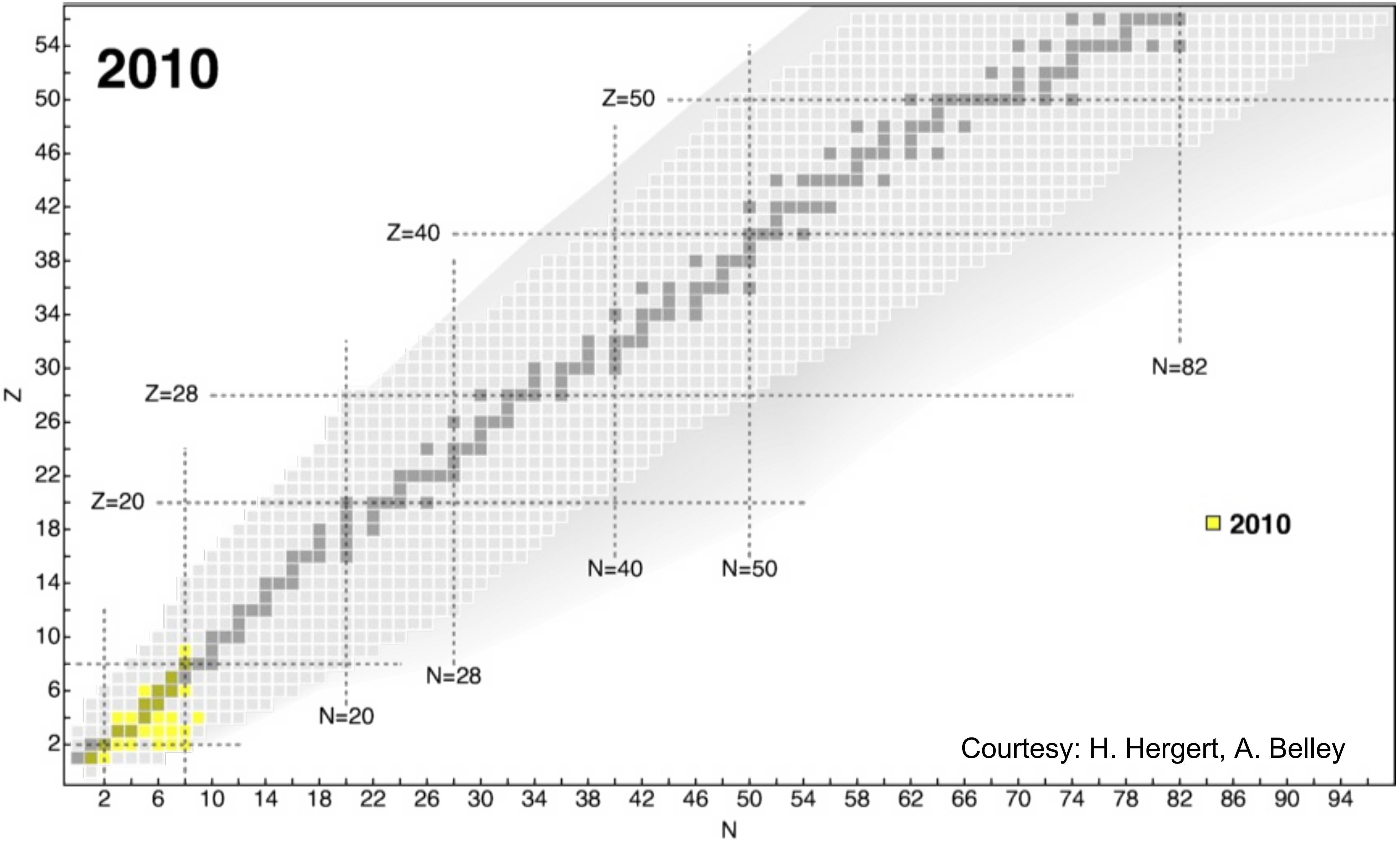
✅ **Single-particle basis** $e_{\max} = 2n + l$

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

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

Ab Initio 2010

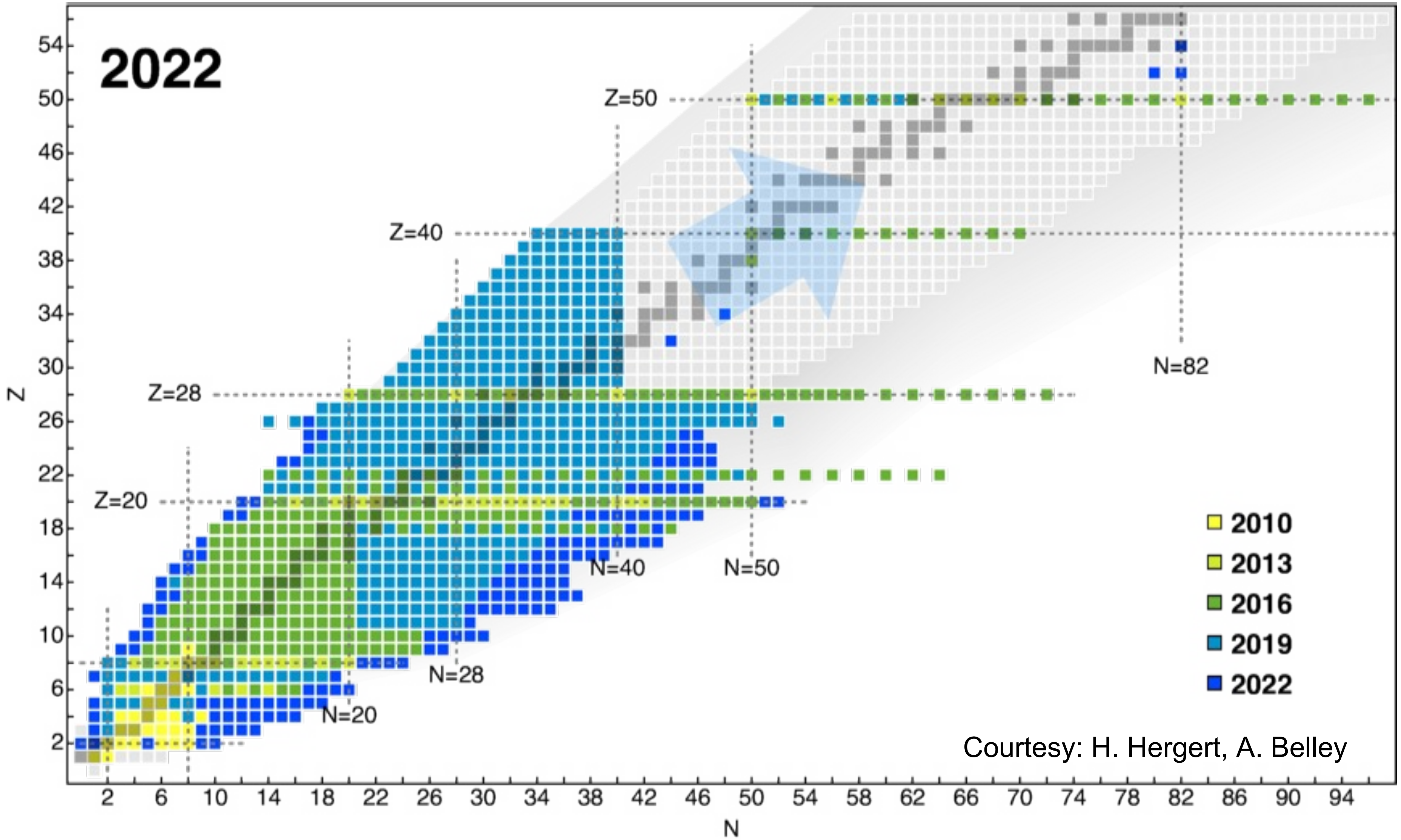
2010 Quasi-exact methods for light nuclei (^{16}O); limited capability for 3N forces



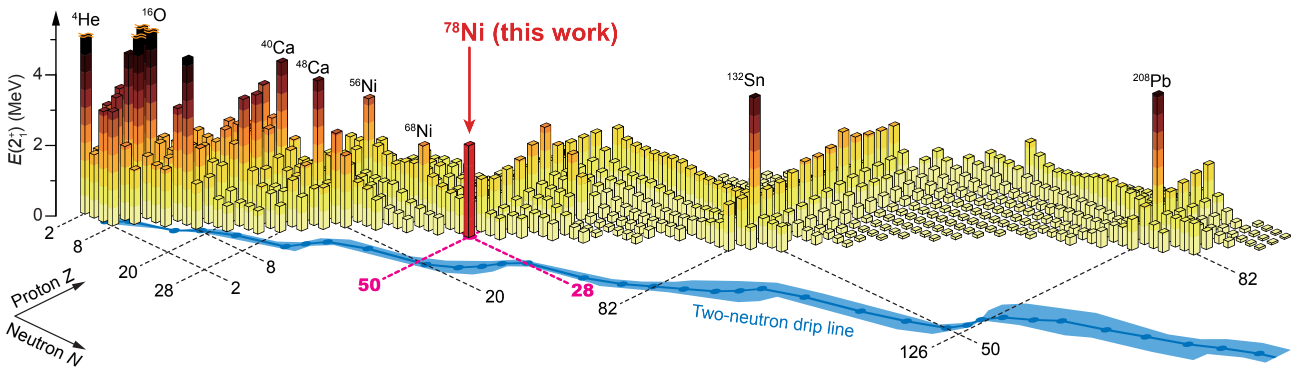
The 5-Year Revolution: 2022

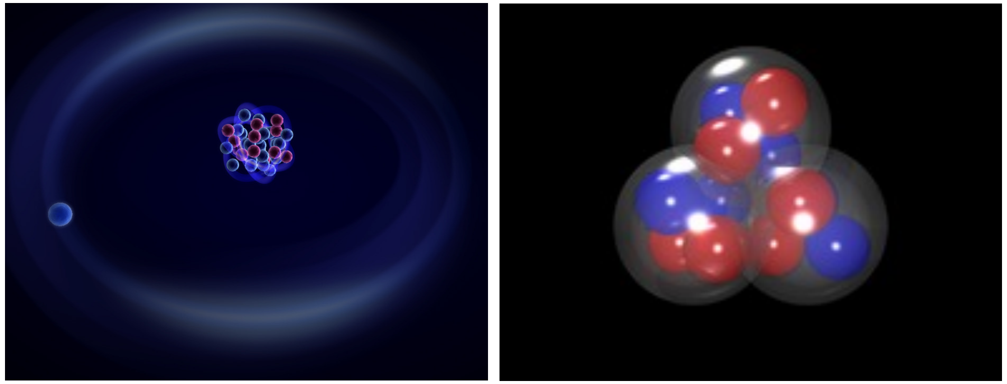
2022 Valence-space approach: essentially *all* properties of *all* nuclei

What can we do with this advance?



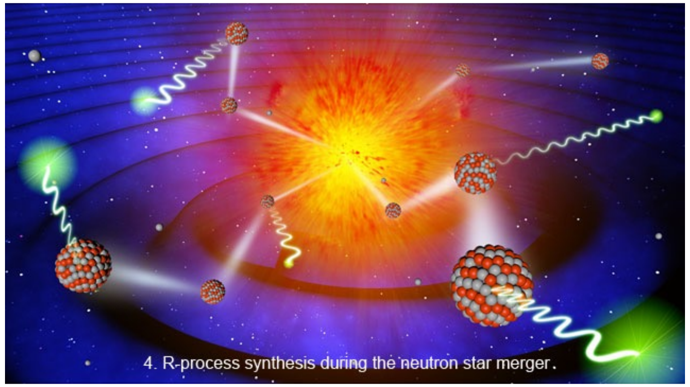
TRIUMF Major Questions in Nuclear Structure/Astrophysics

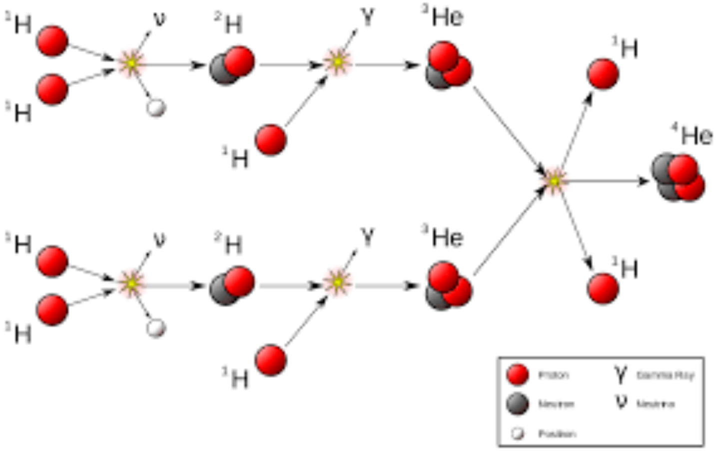


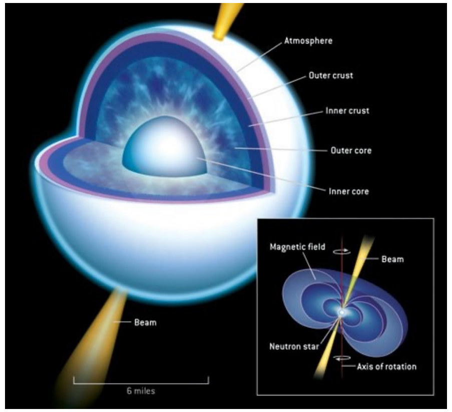


Limits of existence + formation/evolution of magic numbers

Nuclear skins/halos/clusters





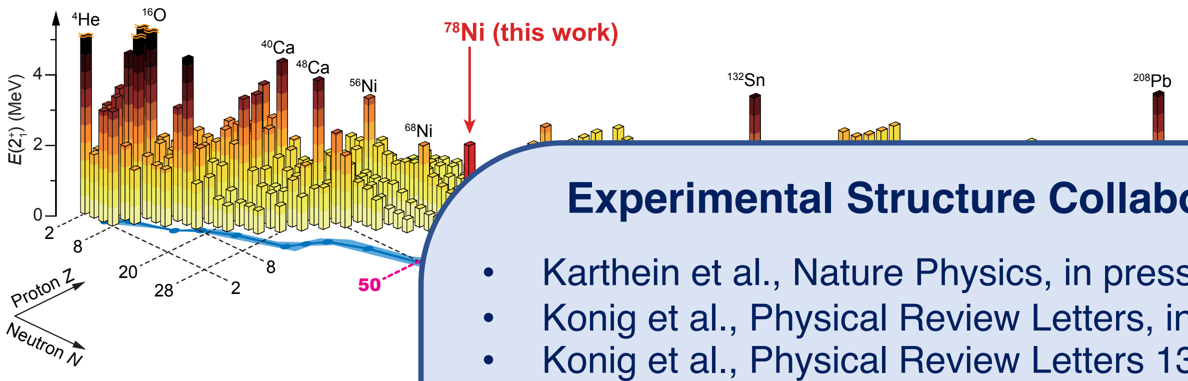


Heavy Element Nucleosynthesis

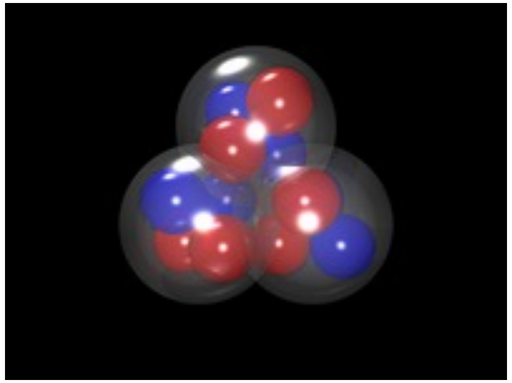
Continuum and nuclear reactions

Infinite matter/Neutron stars

Major Questions in Nuclear Structure/Astrophysics



Limits of existenc



kins/halos/clusters

Experimental Structure Collaborations: Recent Highlights

- Karthein et al., Nature Physics, in press (2024)
- Konig et al., Physical Review Letters, in press (2024)
- Konig et al., Physical Review Letters 131, 102501 (2023)
- Vernon et al., Nature 607, 260 (2022)
- Sommer et al., Physical Review Letters 129, 132501 (2022)
- Malbrunot et al., Physical Review Letters 128, 022502 (2022)
- De Groote et al., Nature Physics 16, 120 (2020)

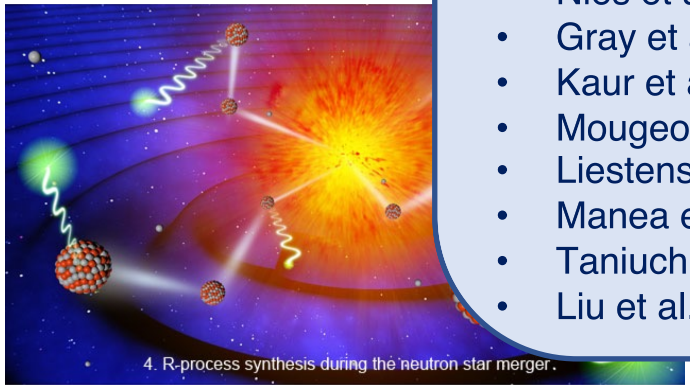
EM Moments

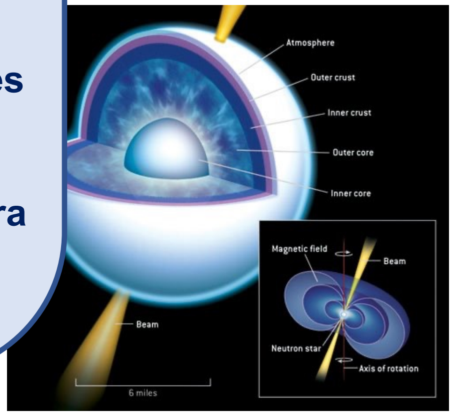
Radii

- Nies et al., Physical Review Letters 131, 022502 (2023)
- Gray et al., Physical Review Letters 130, 242501 (2023)
- Kaur et al., Physical Review Letters 129, 142502 (2022)
- Mougeot et al., Nature Physics 17, 1099 (2021)
- Liestenschneider et al., Physical Review Letters 126, 042501 (2021)
- Manea et al., Physical Review Letters 124, 092502 (2020)
- Taniuchi et al., Nature 569, 63 (2019)
- Liu et al., Physical Review Letters 122, 072502 (2019)

Masses

Spectra





Heavy Element Nucleosynthesis

Continuum and nuclear reactions

Infinite matter/Neutron stars

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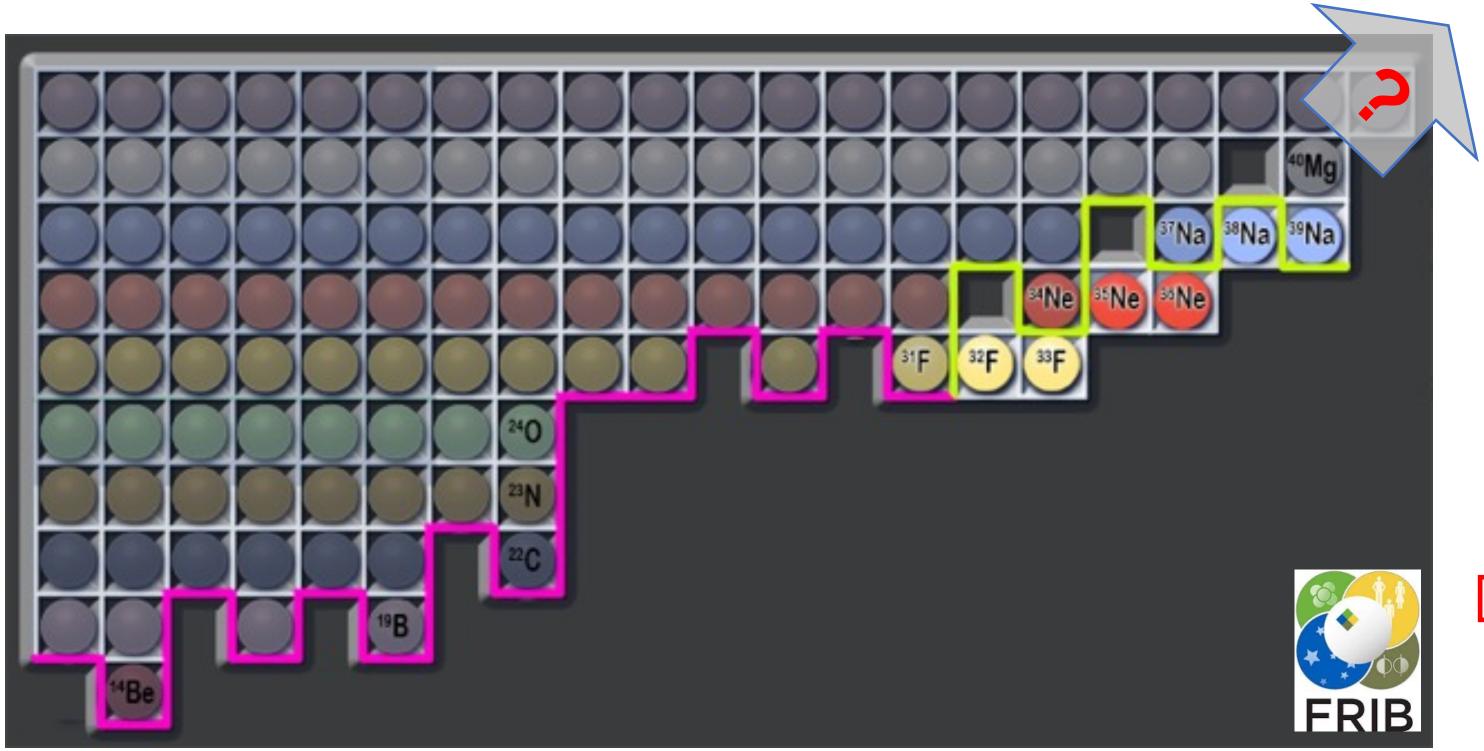
Milestone Result

Global Ab Initio Calculations: Limits of Nuclear Existence



Ragnar Stroberg

Featured in Physics | Editors' Suggestion

Ab Initio Limits of Atomic Nuclei

101

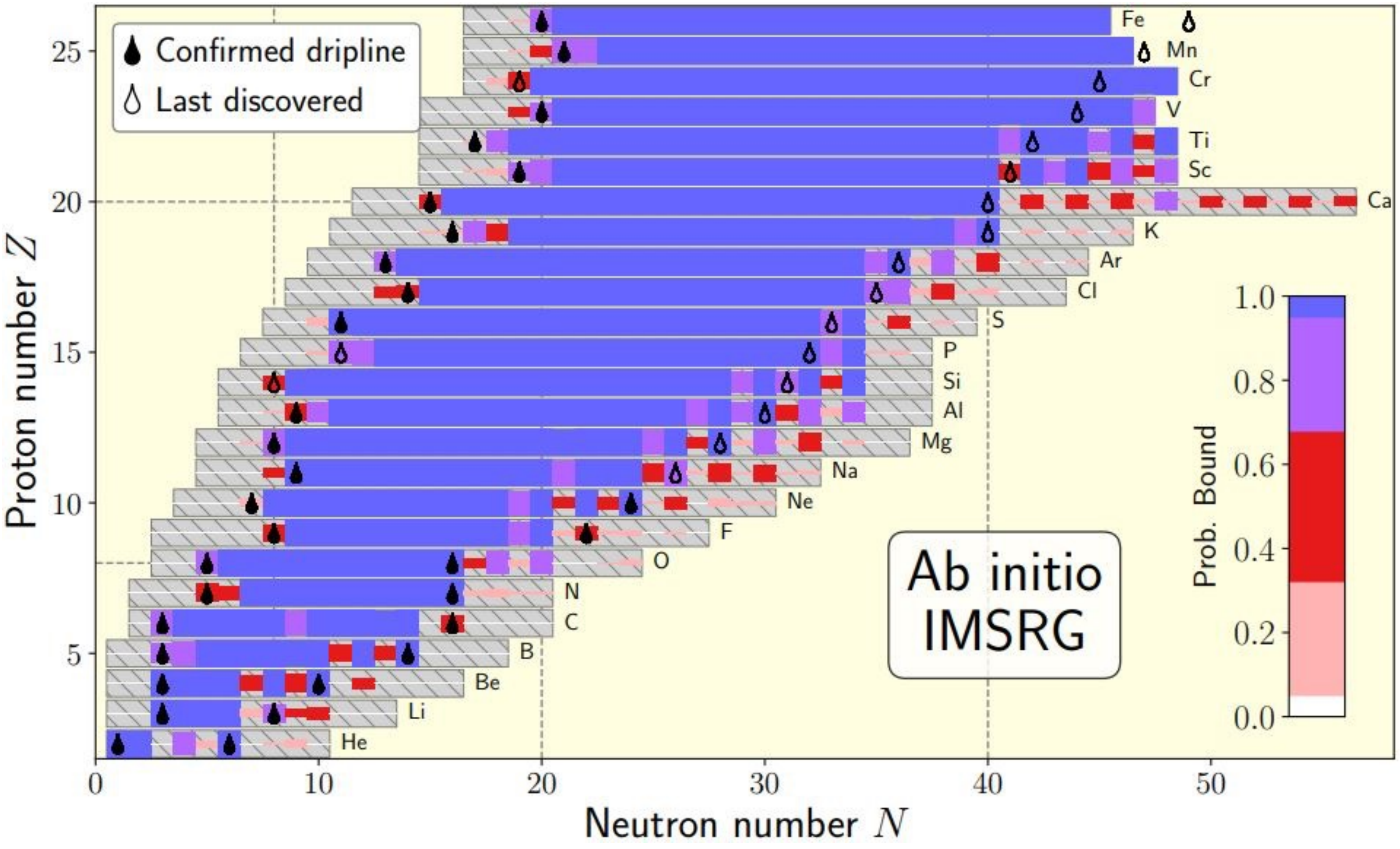
S. R. Stroberg, J. D. Holt, A. Schwenk, and J. Simonis

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

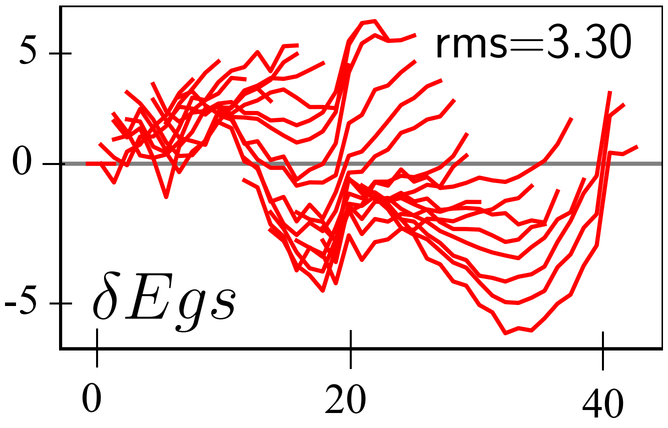
Physics See synopsis: Predicting the Limits of Atomic Nuclei

Limits of Existence in Medium-Mass Region

Ab initio calculations of ~700 nuclei from He to Fe



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



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

Physical Review Letters **126**, 022501 (2021)

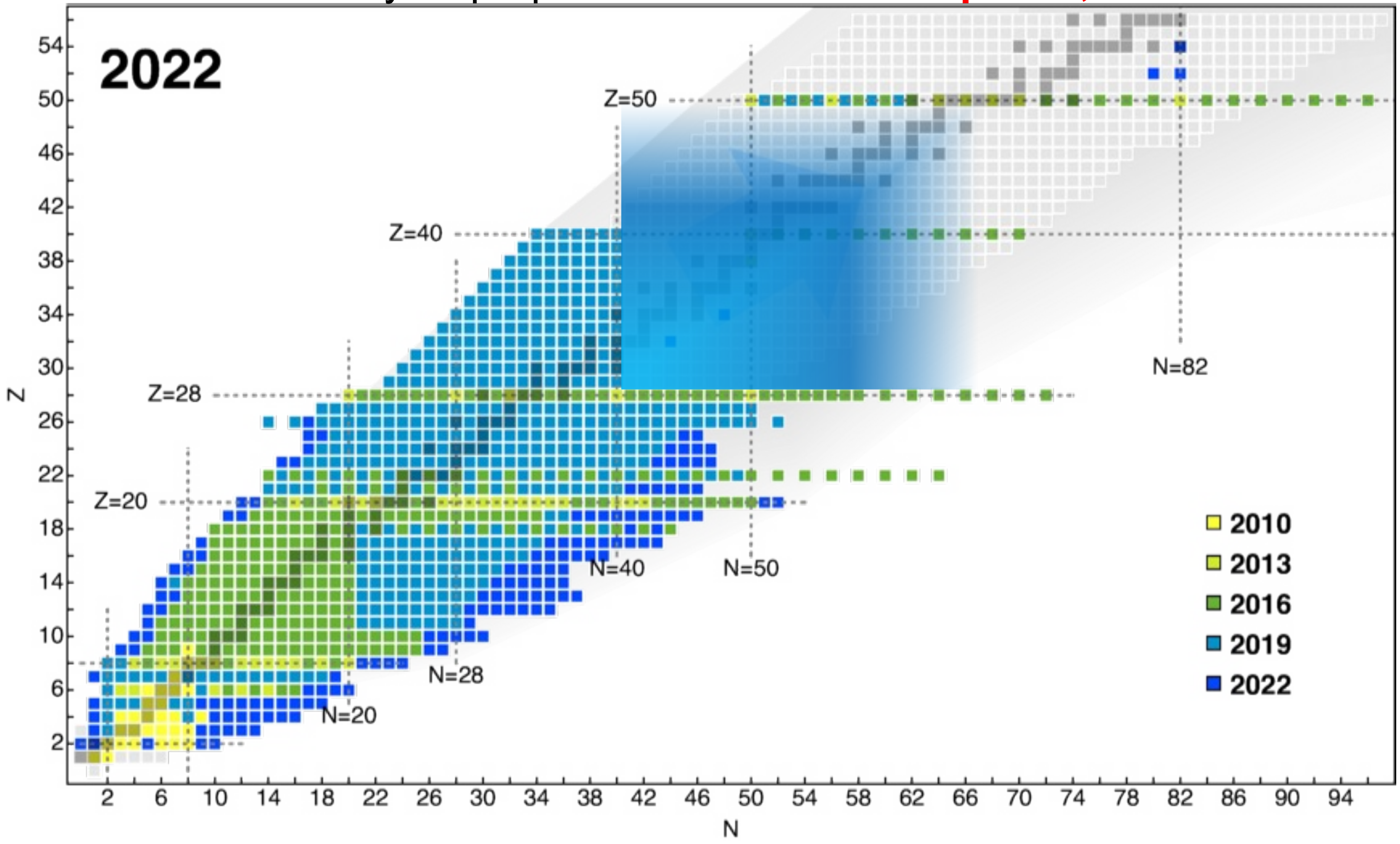
Known drip lines predicted within uncertainties

Ab initio guide for neutron-rich driplines

Ab Initio Progress: How Heavy Can We Go?

Tremendous progress in ab initio reach, largely due to valence-space IMSRG

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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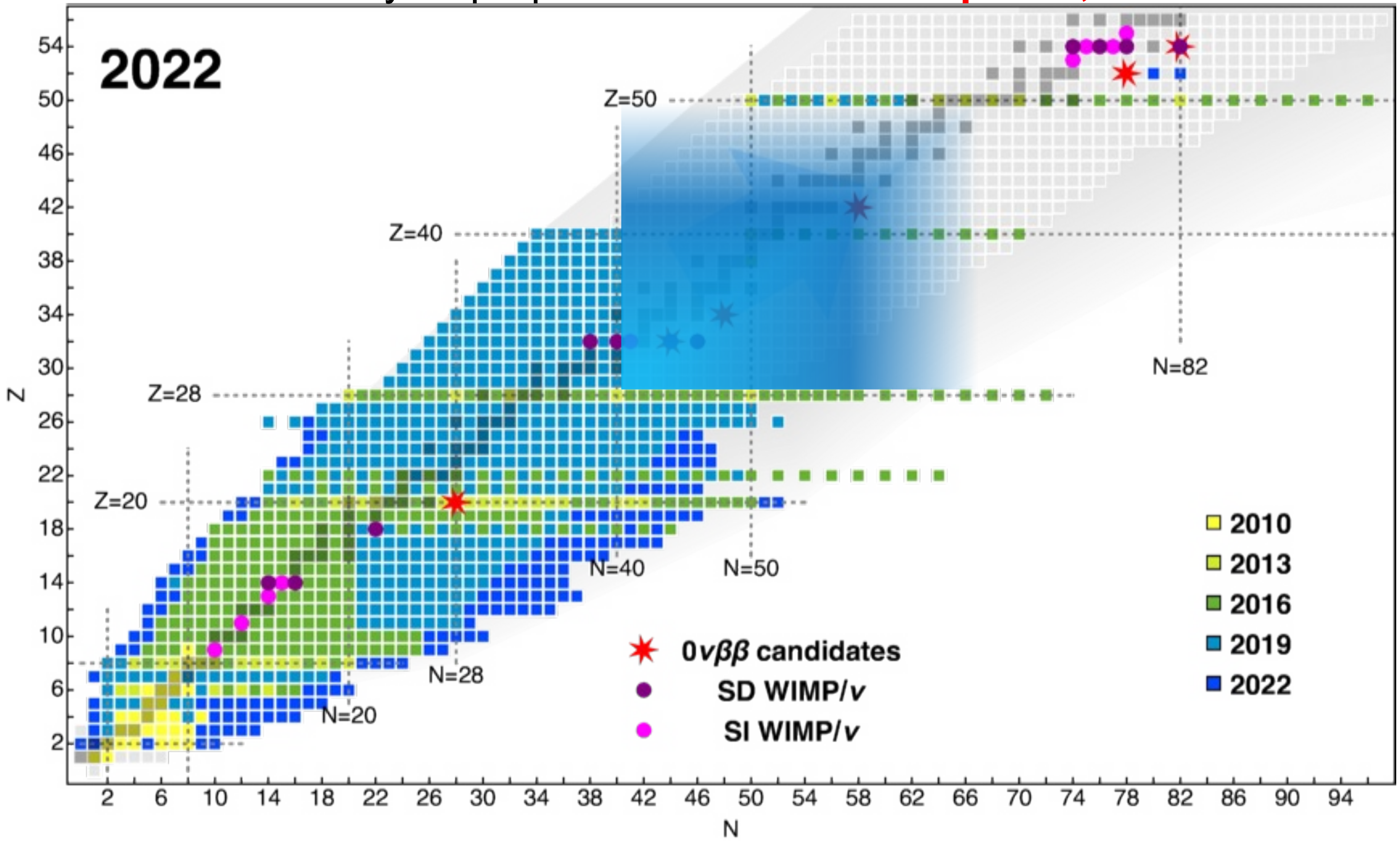

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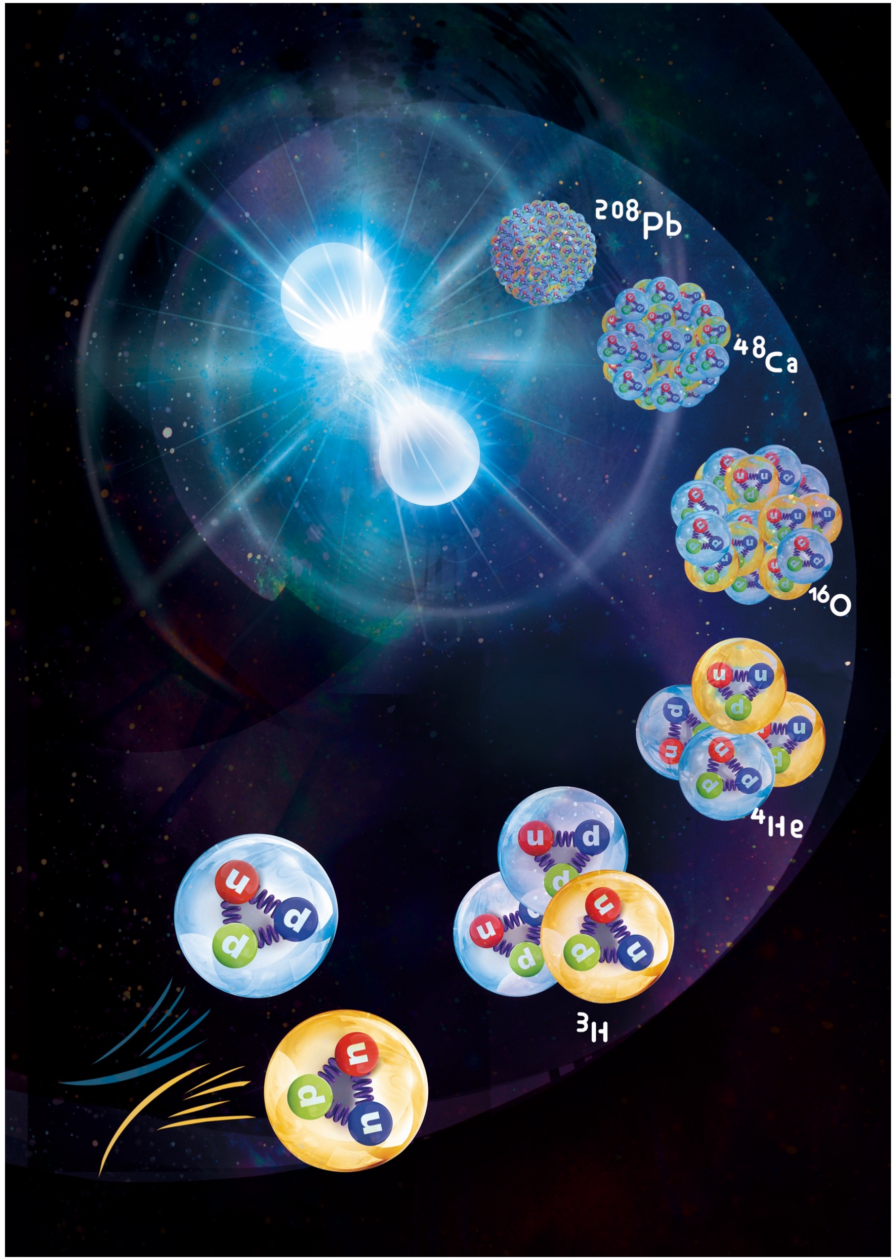
KEY ADVANCE

Converged Calculations of Heavy Nuclei

筑波大学
University of Tsukuba

Takayuki Miyagi



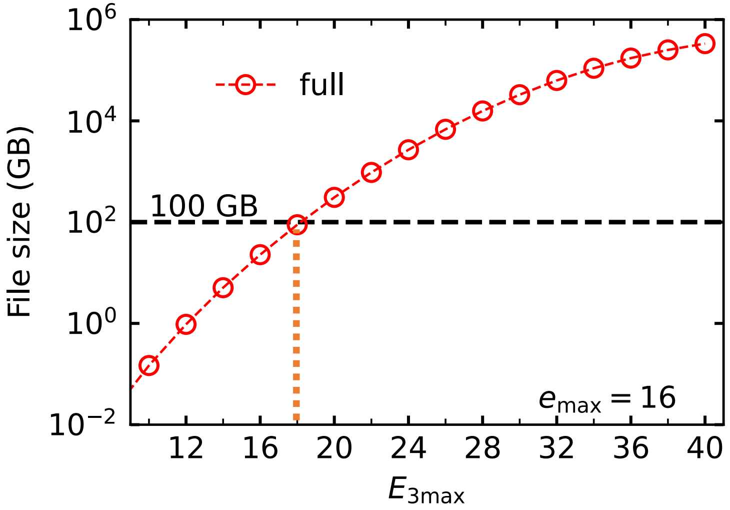
Converged *ab initio* calculations of heavy nuclei

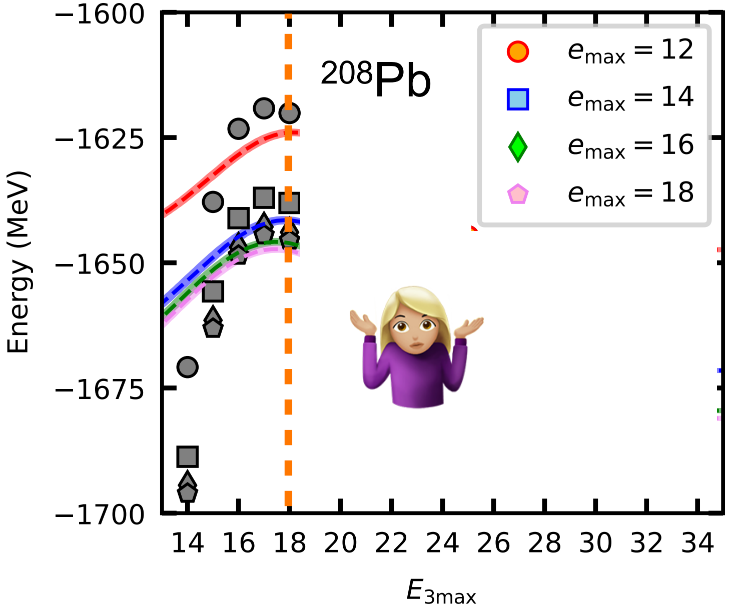
T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt
Phys. Rev. C **105**, 014302 – Published 3 January 2022

Ab Initio Calculations of Heavy Nuclei

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

No convergence in ^{208}Pb (heaviest doubly magic nucleus)





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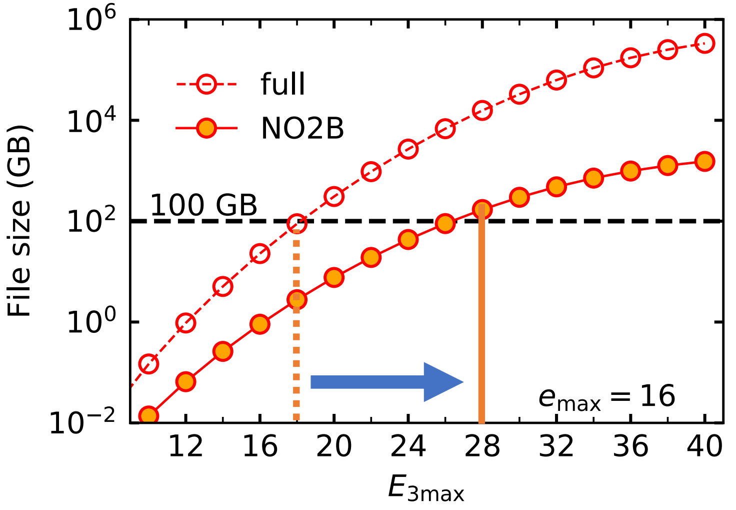
Ab Initio Calculations of Heavy Nuclei

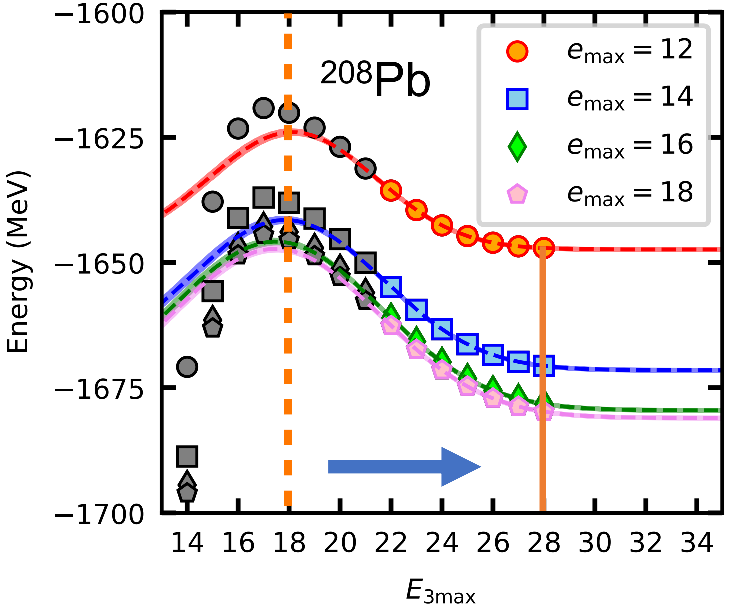
Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3\max} = 18$

Clever storage reduces needs: TB → GB



^{208}Pb now straightforward:

Solving the Schrodinger equation for 200+ nucleons!



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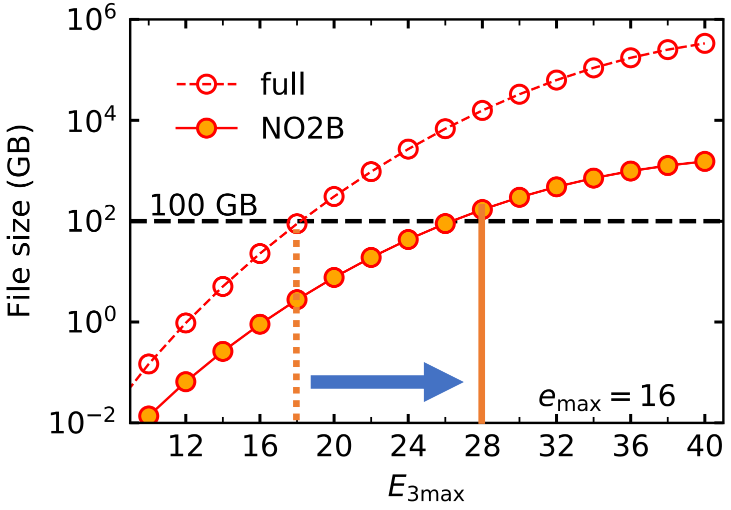

^{208}Pb now straightforward:

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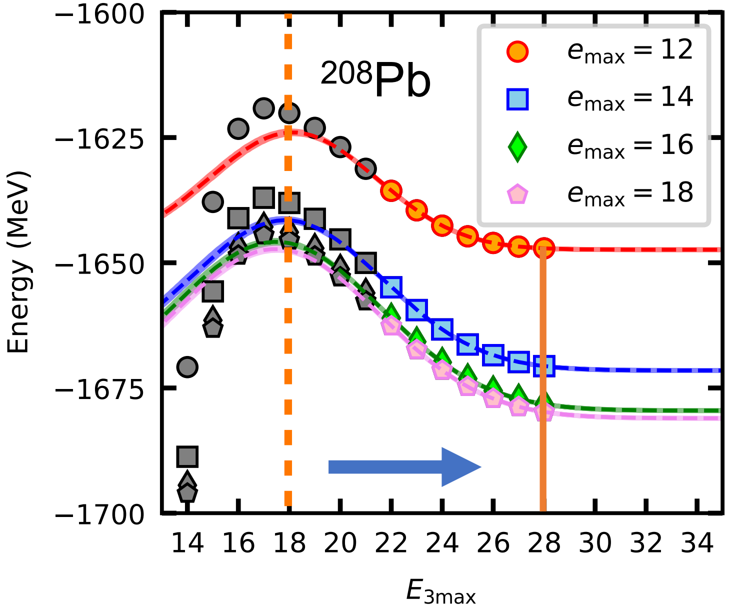
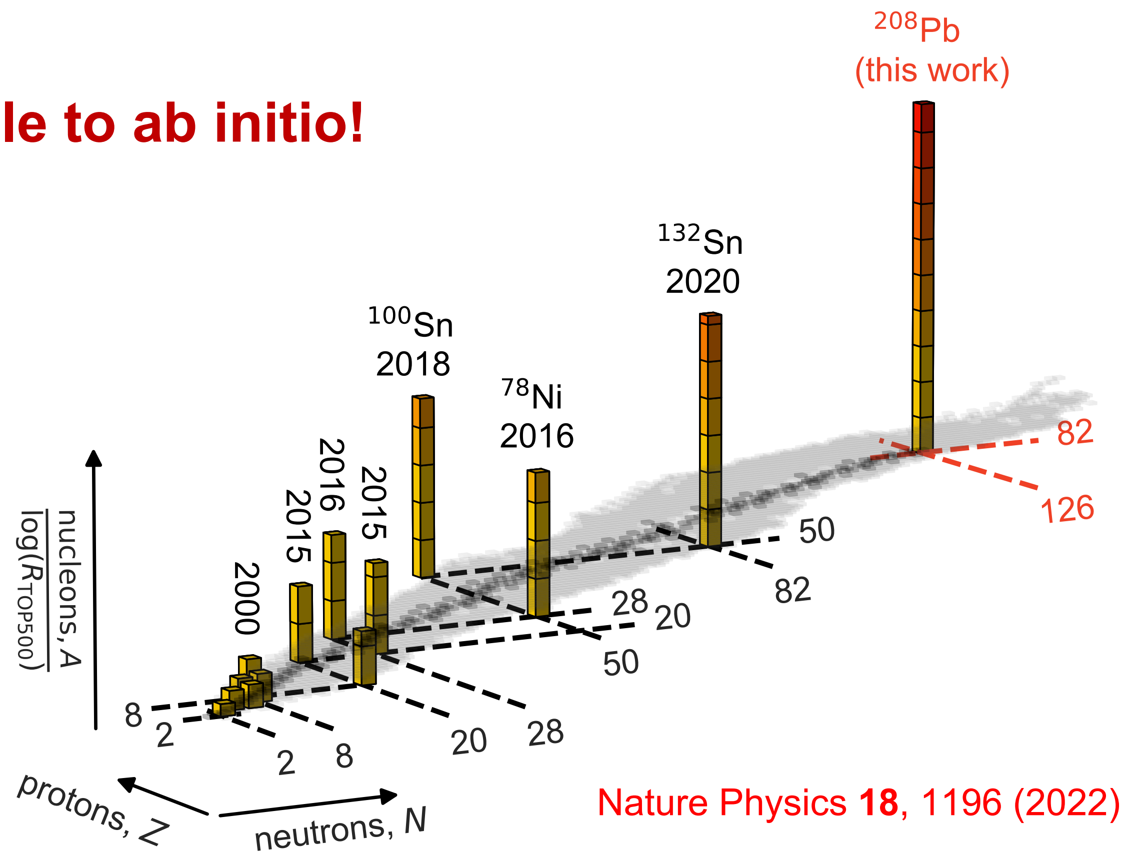
(Super)heavy accessible to ab initio!



16 years: ^{16}O → ^{56}Ni

6 years: ^{56}Ni → ^{208}Pb



Nature Physics **18**, 1196 (2022)

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Milestone Result

Ab Initio Neutron Skin of ^{208}Pb Linked to Neutron Star Properties

nature physics

ARTICLES

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

Check for updates

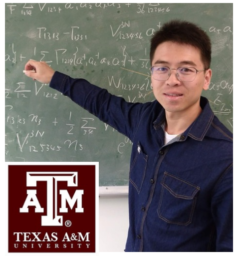
OPEN

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

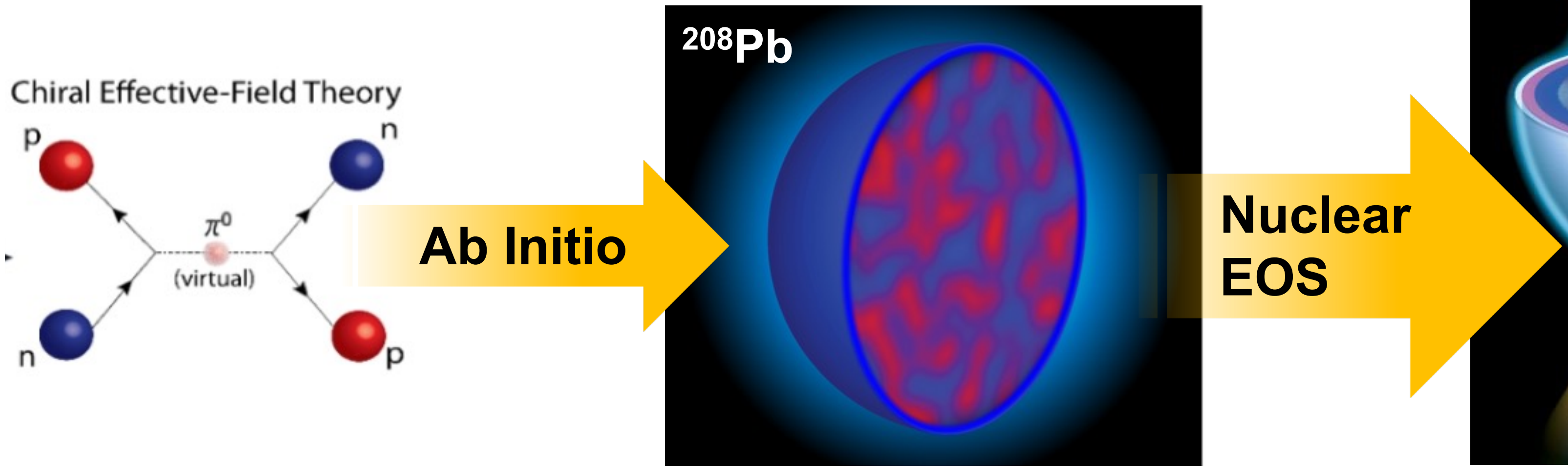
280

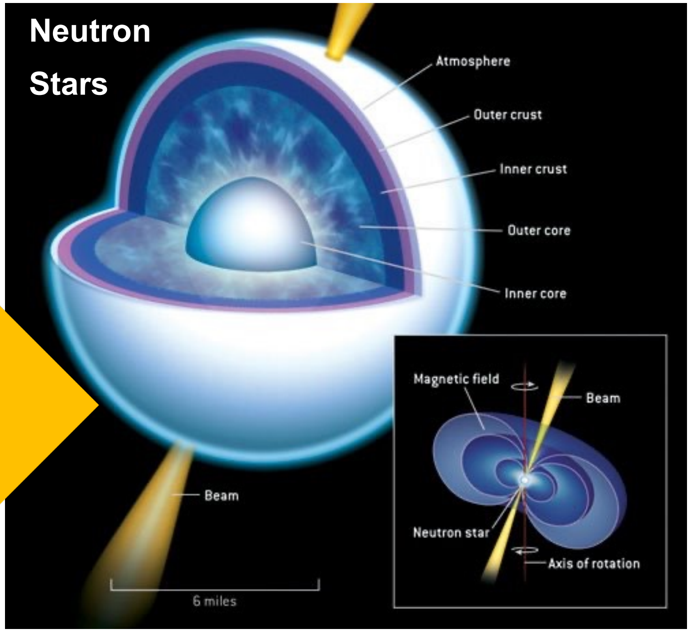
Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

Takayuki Miyagi



Baishan Hu





Ab Initio Neutron Skin of ^{208}Pb

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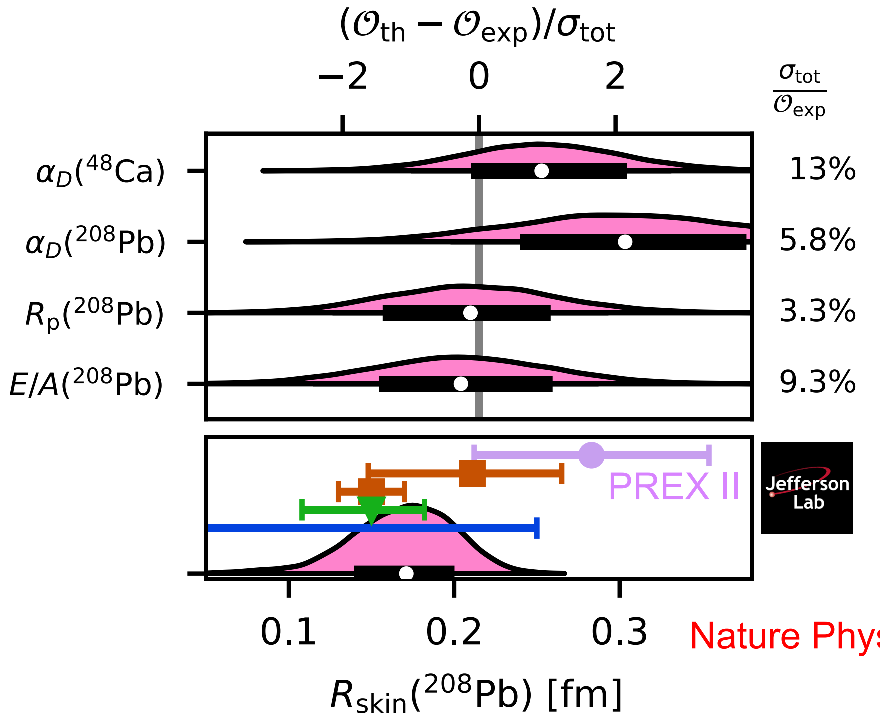
Combine ab initio + machine learning advances

I: History Matching: 34 "non-implausible" interactions

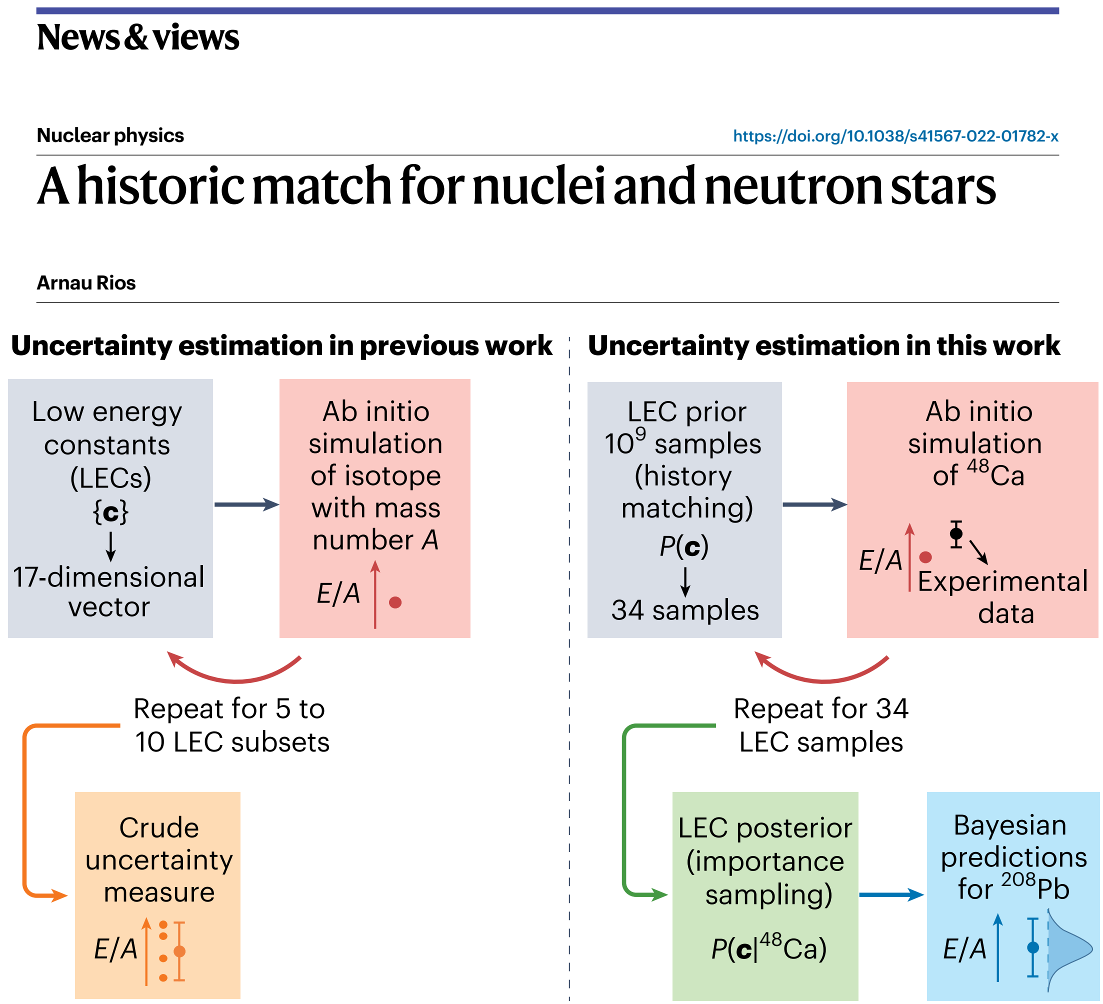
II: Calibration/importance sampling: ^{48}Ca properties

III: Validation: ^{208}Pb properties from ab initio

IV: Prediction: PPD for neutron skin



Nature Physics **18**, 1196 (2022)


News & views

Nuclear physics

https://doi.org/10.1038/s41567-022-01782-x

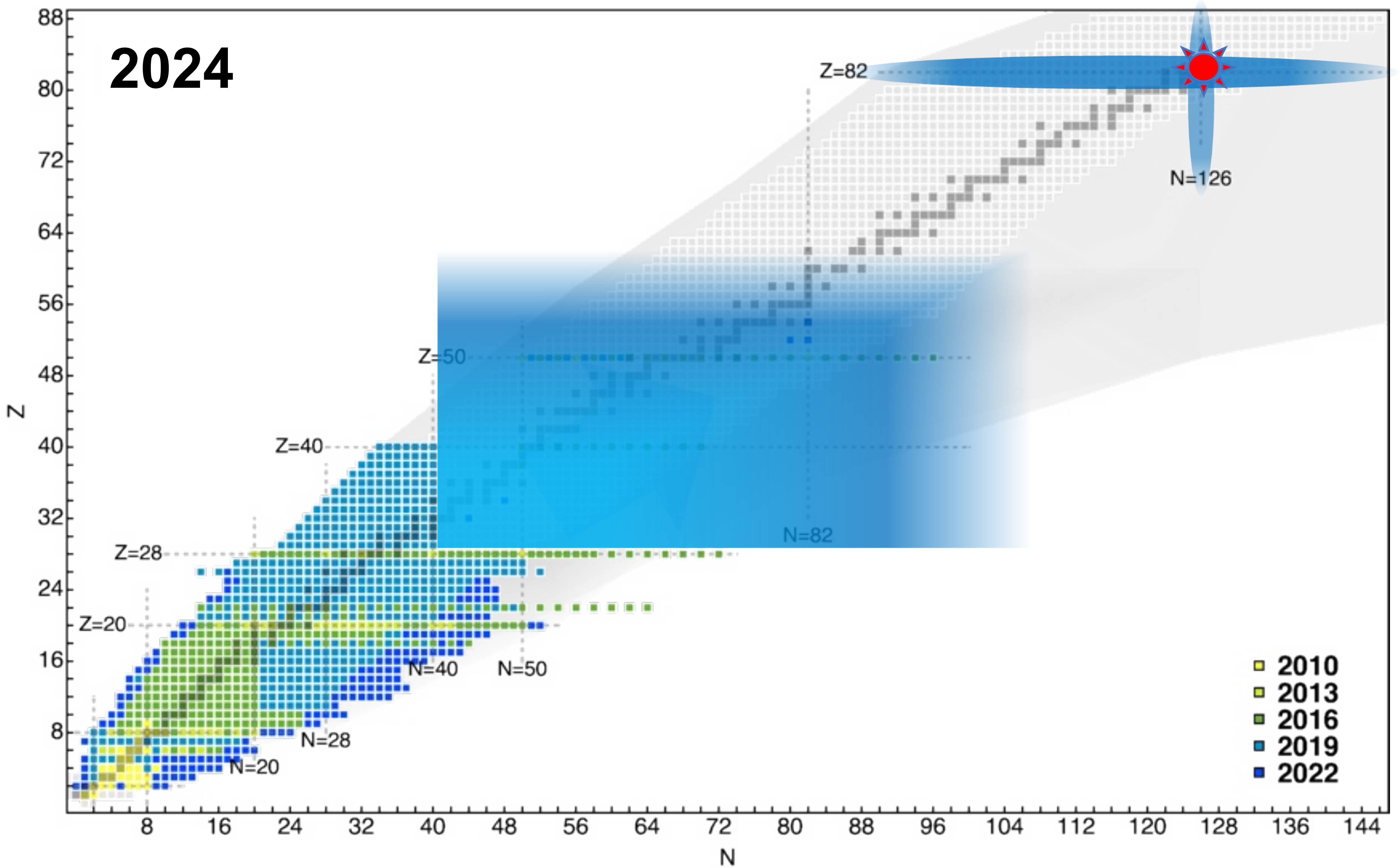
A historic match for nuclei and neutron stars

Arnau Rios

$R_{skin}(^{208}\mathrm{Pb})$=0.14-0.20fm – consistent with **PREXII**

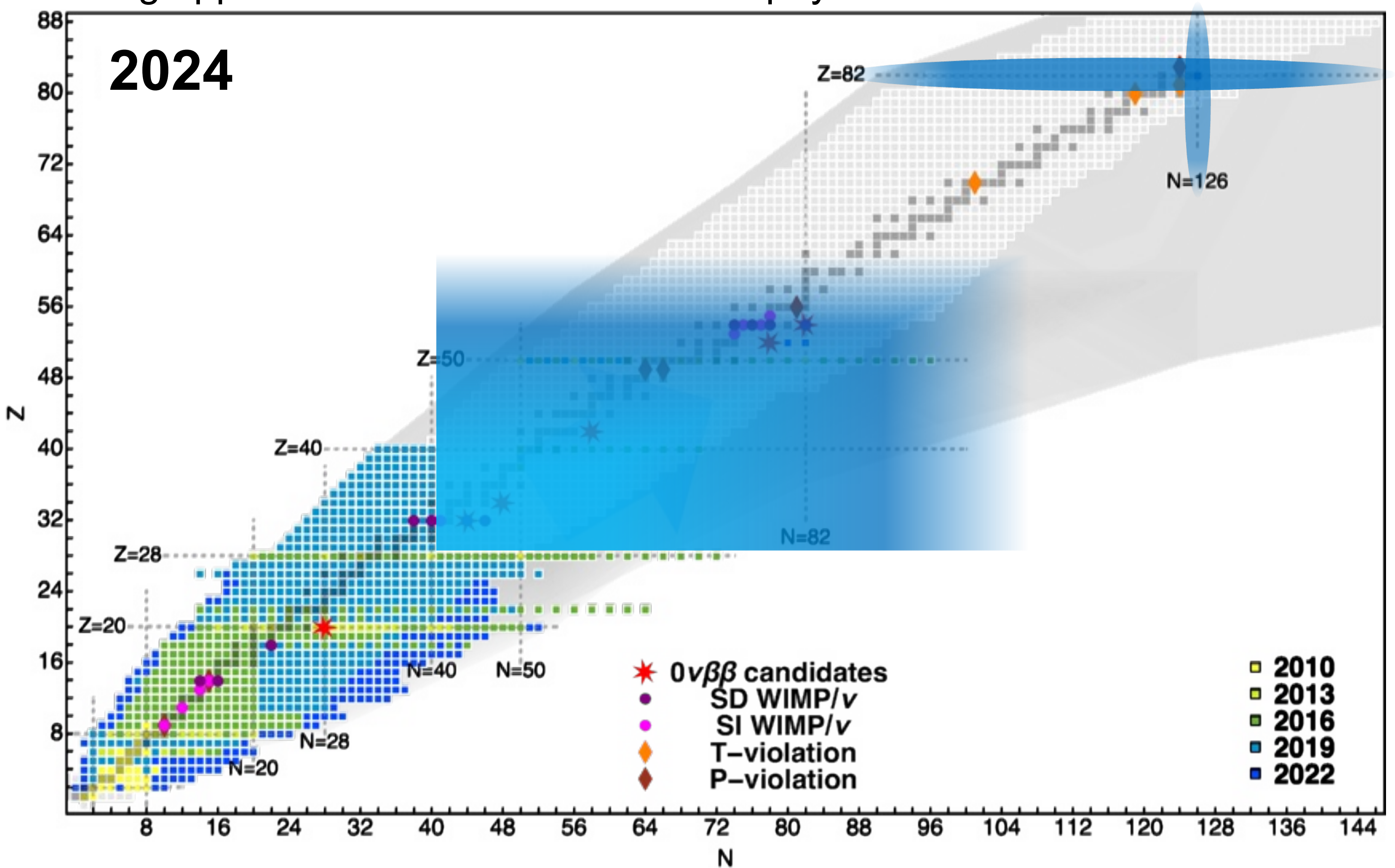
New Scope of Ab Initio Theory

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



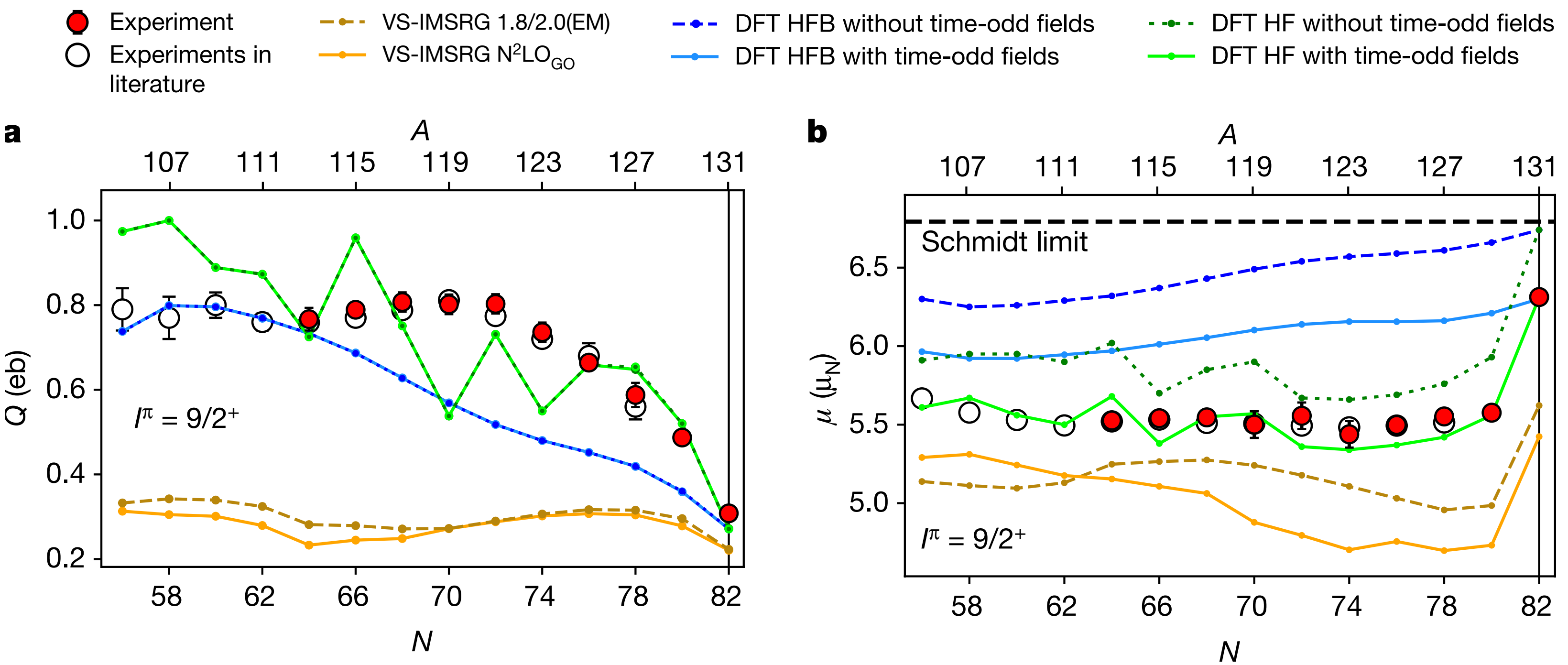
New Scope of Ab Initio Theory

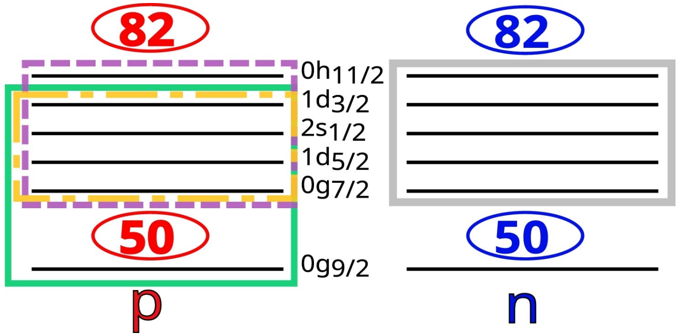
Rapid progress in ab initio reach, due to valence-space approach… up to...
Exciting applications to searches for BSM physics!

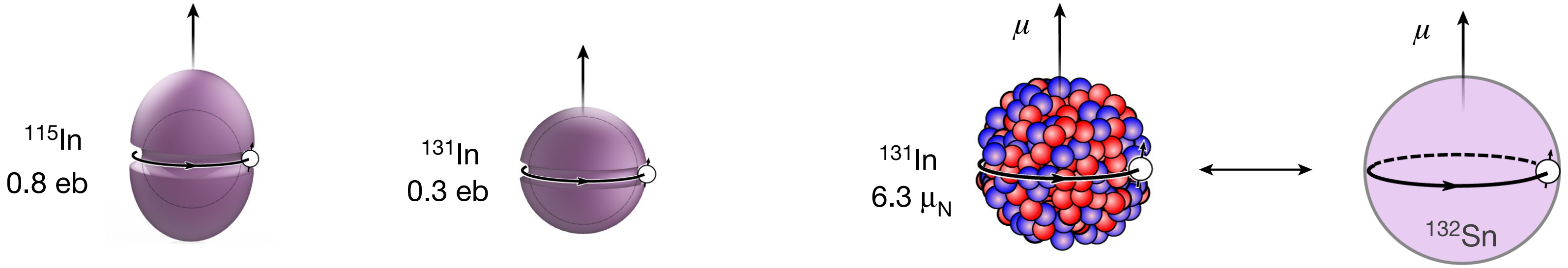


Systematic studies in Sn region: In Isotopes

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







Ab initio reproduces trends of new measurements

Q missing correlations, μ missing physics?

Article

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

https://doi.org/10.1038/s41586-022-04818-7
Received: 10 June 2021
Accepted: 28 April 2022
Published online: 13 July 2022

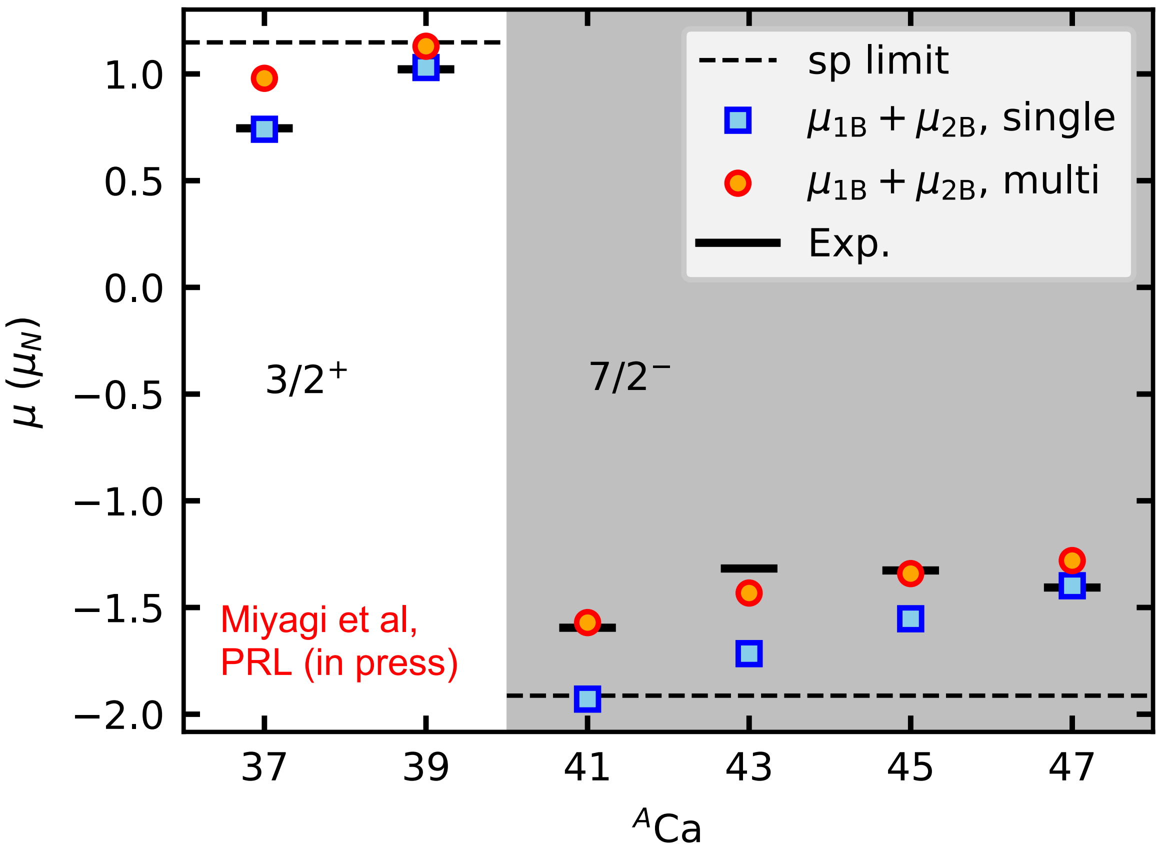
A. R. Vernon[1,2,3], R. F. Garcia Ruiz[2,4], T. Miyagi[5], C. L. Binnersley[1], J. Billowes[1], M. L. Bissell[1], J. Bonnard[6], T. E. Cocolios[3], J. Dobaczewski[6,7], G. J. Farooq-Smith[3], K. T. Flanagan[1,8], G. Georgiev[9], W. Gins[3,10], R. P. de Groote[3,10], R. Heinke[4,11], J. D. Holt[5,12], 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]

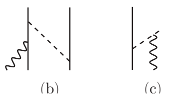
TRIUMF

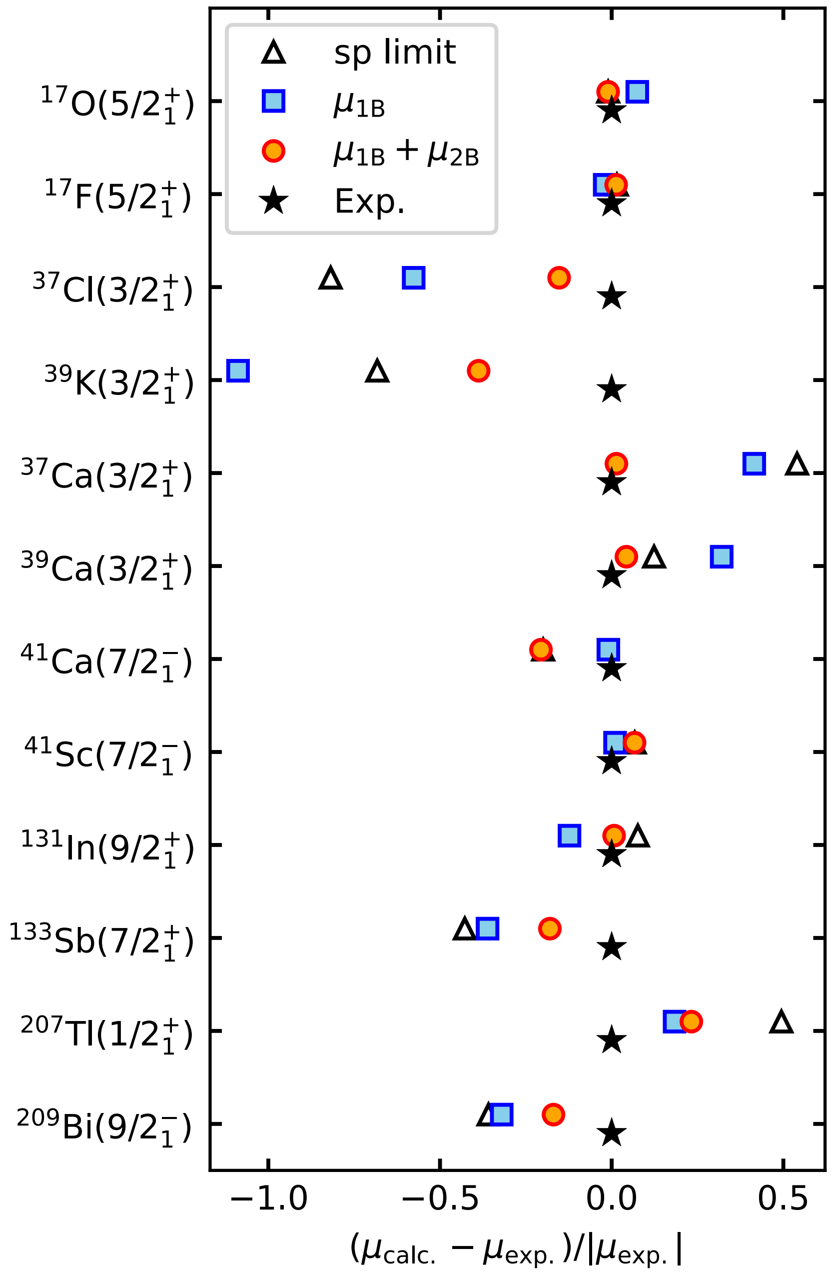
VS-IMSRG μ Moments: O → Pb

Ab initio calculations throughout the nuclear chart w/ 2BC

Ca discrepancies solved with multi-shell approach





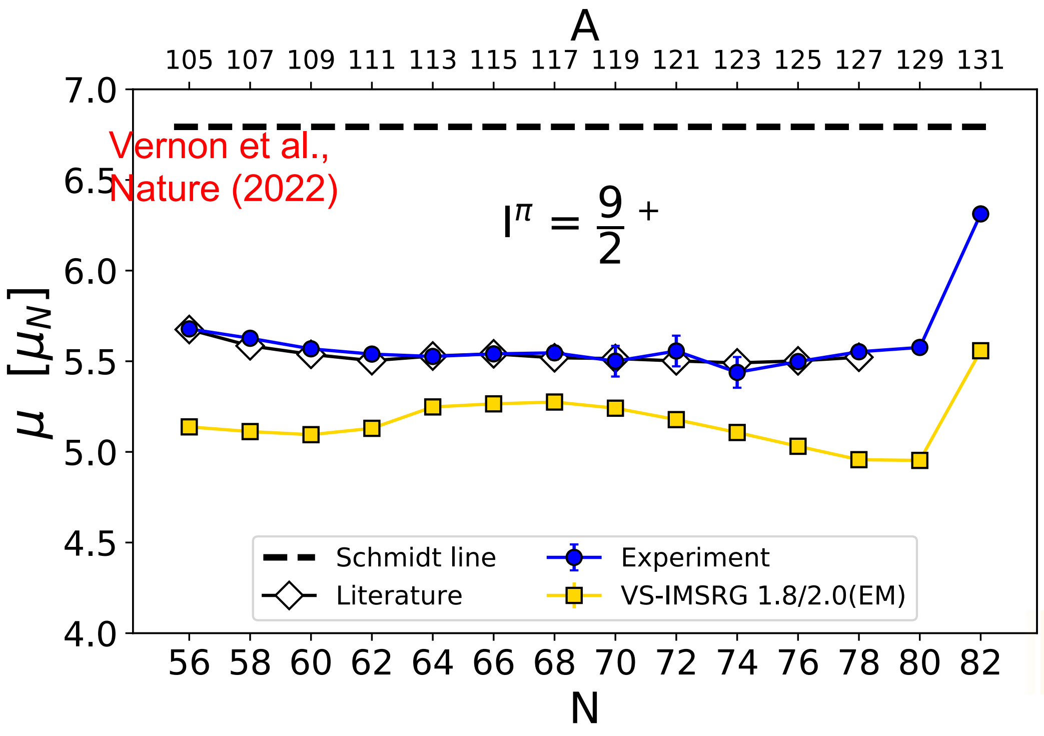


Magnetic moments significantly improved across chart!

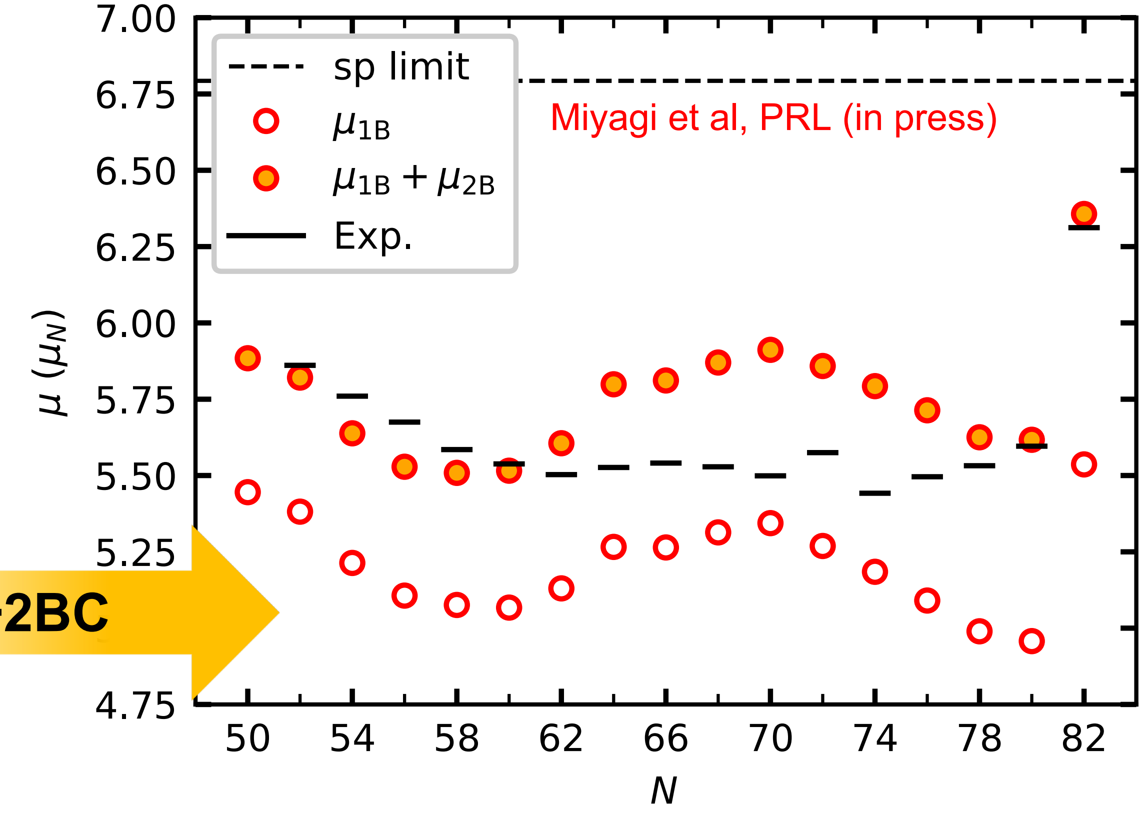
VS-IMSRG μ Moments: In Isotopes

Revisit discrepancies in In isotopes with addition of 2BC

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



+2BC

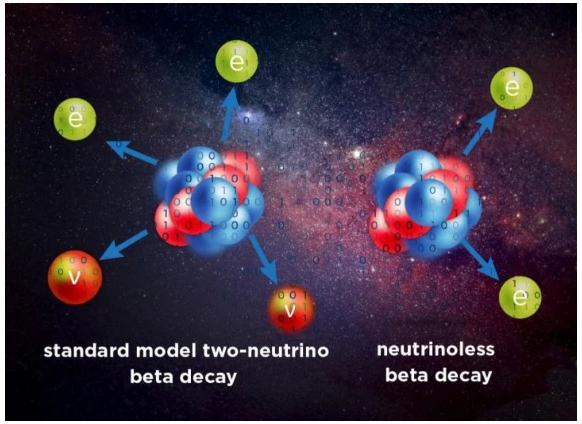


PHYSICAL REVIEW LETTERS **132**, 232503 (2024)

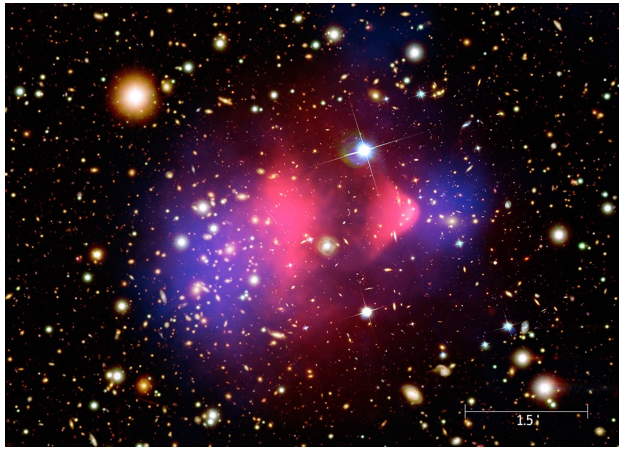
Impact of Two-Body Currents on Magnetic Dipole Moments of Nuclei

T. Miyagi,[1,2,3,*,‡‡] X. Cao,[4,†] R. Seutin,[3,1,2,‡] S. Bacca,[5,6,§] R. F. Garcia Ruiz,[7,∥] K. Hebeler,[1,2,3,¶] J. D. Holt,[8,9,**] and A. Schwenk[1,2,3,††]

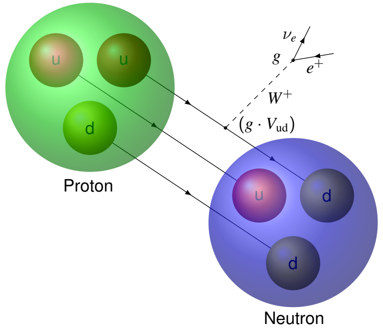
Searches for BSM Physics



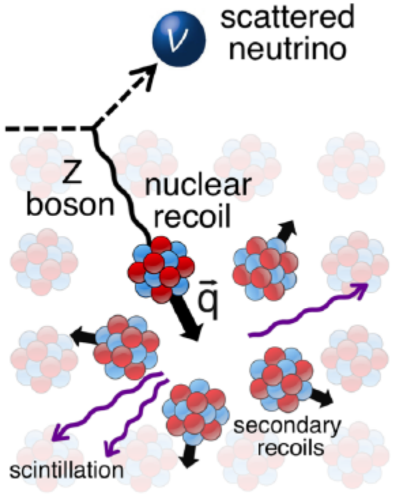
Neutrinoless double beta decay



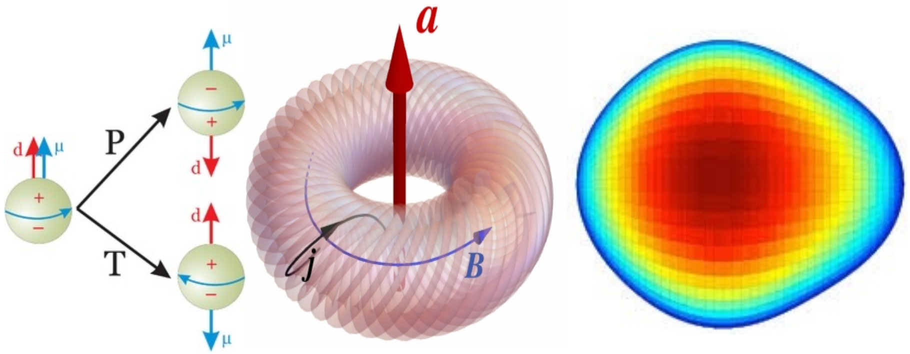
Dark matter direct detection



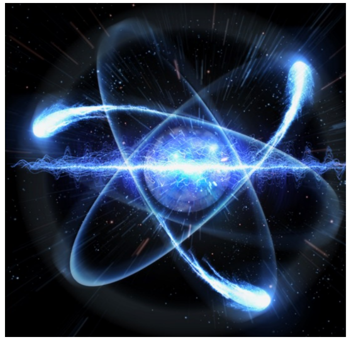
Superallowed Fermi transitions



Neutrino scattering



Symmetry-violating moments

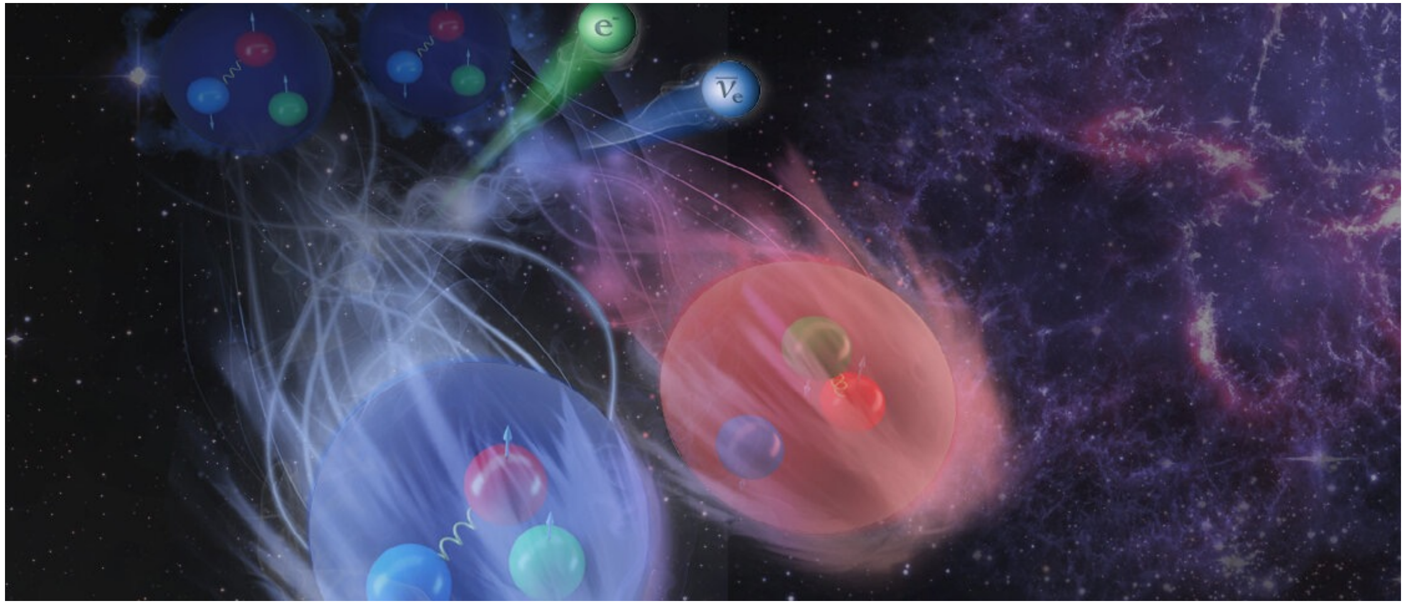


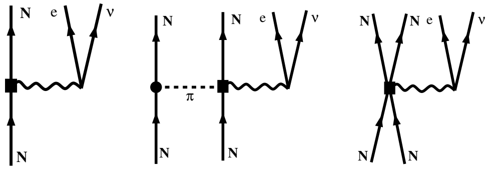
Atomic theory

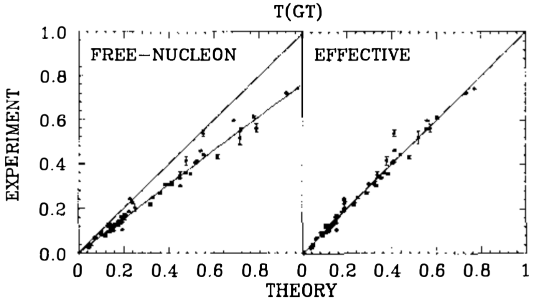
TRIUMF

Milestone Result

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

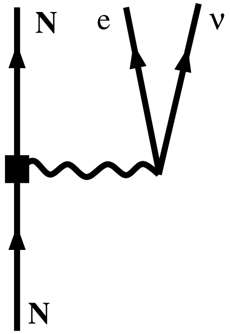
68

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

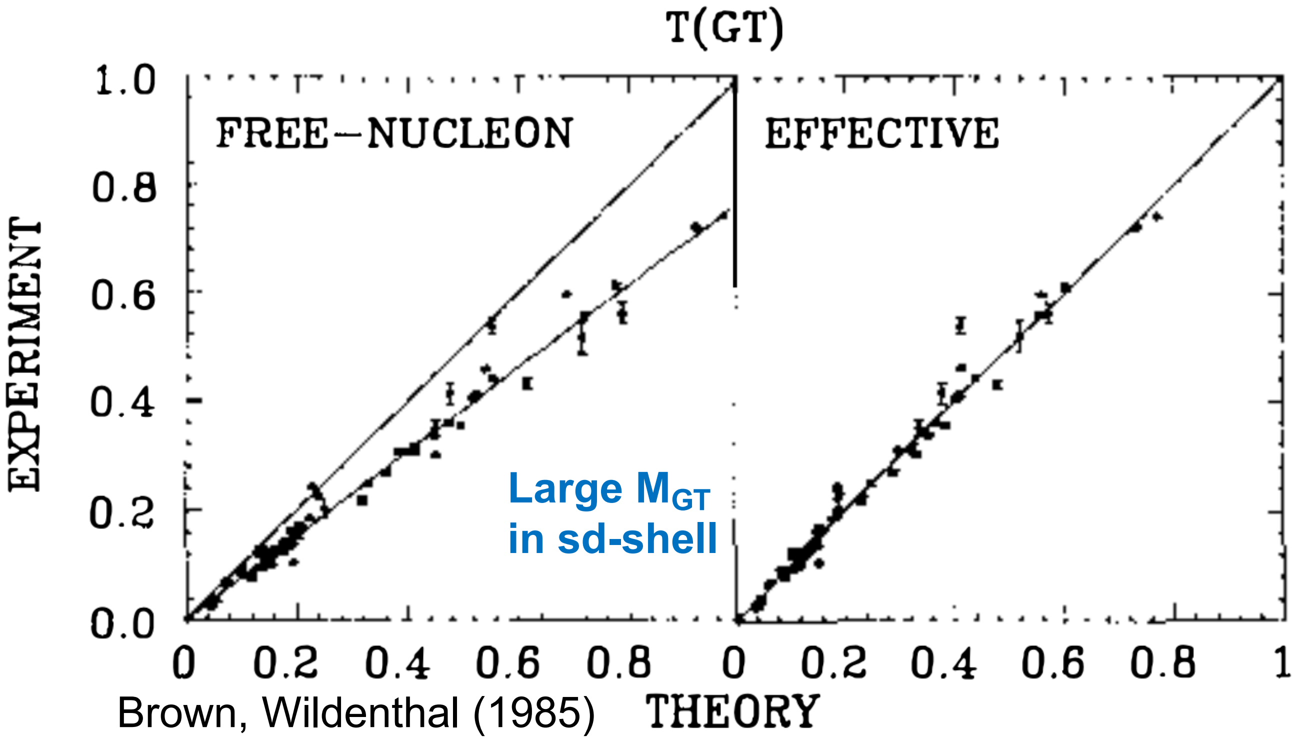
Long-standing problem[1] in weak decays **experimental values systematically smaller than theory**

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



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

Re-evaluate in modern framework?



Brown, Wildenthal (1985)

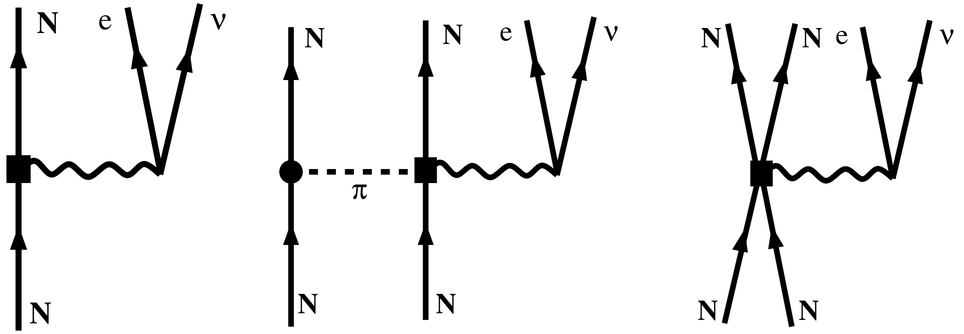
[1] papers from the 1970's

Large-Scale Ab Initio GT Transitions

Ab initio survey of **large GT matrix elements**

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

2BC: Coupling of weak force to two nucleons



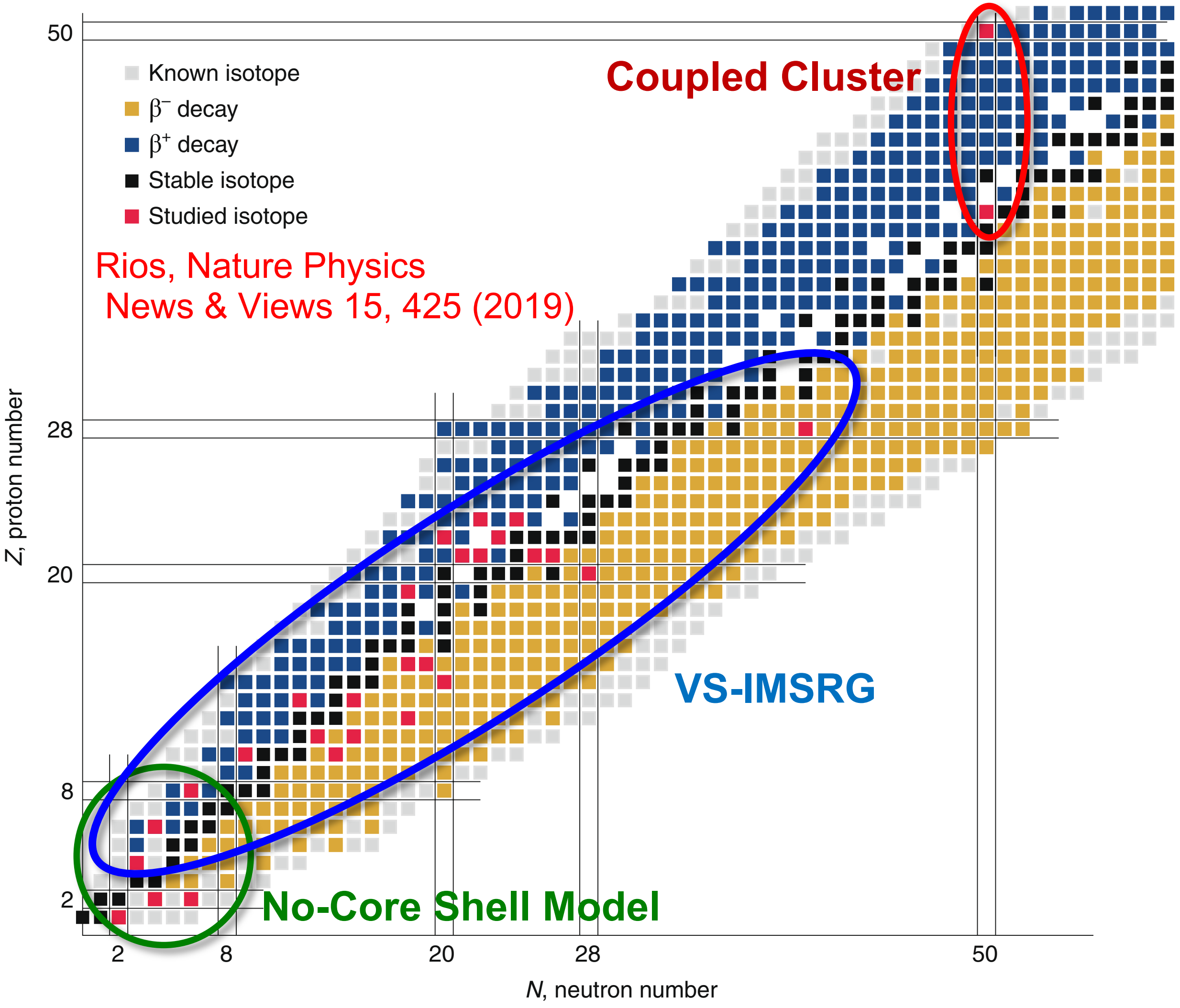
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

- Light → heavy mass regions
- Many-body correlations
- Consistent NN+3N forces + 2BC

NUCLEAR PHYSICS — news & views

Beta decay gets the ab initio treatment

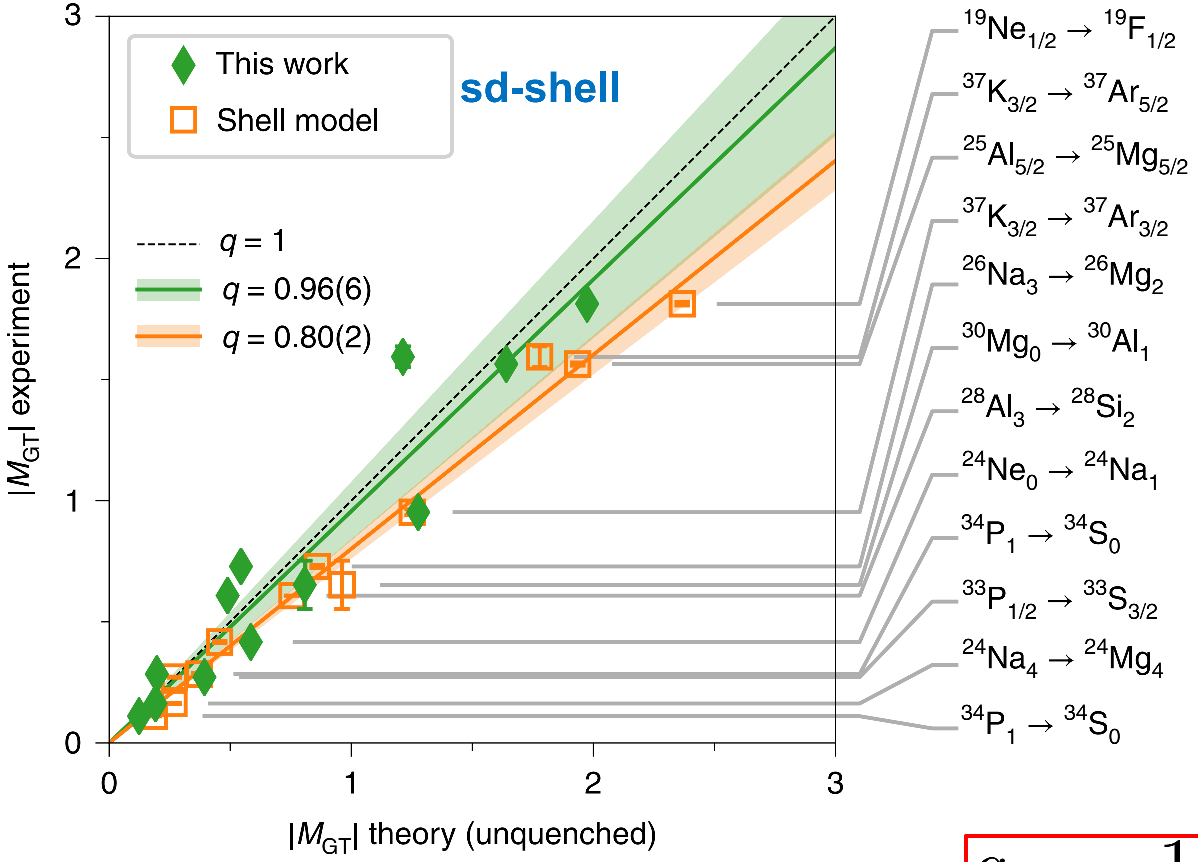
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.

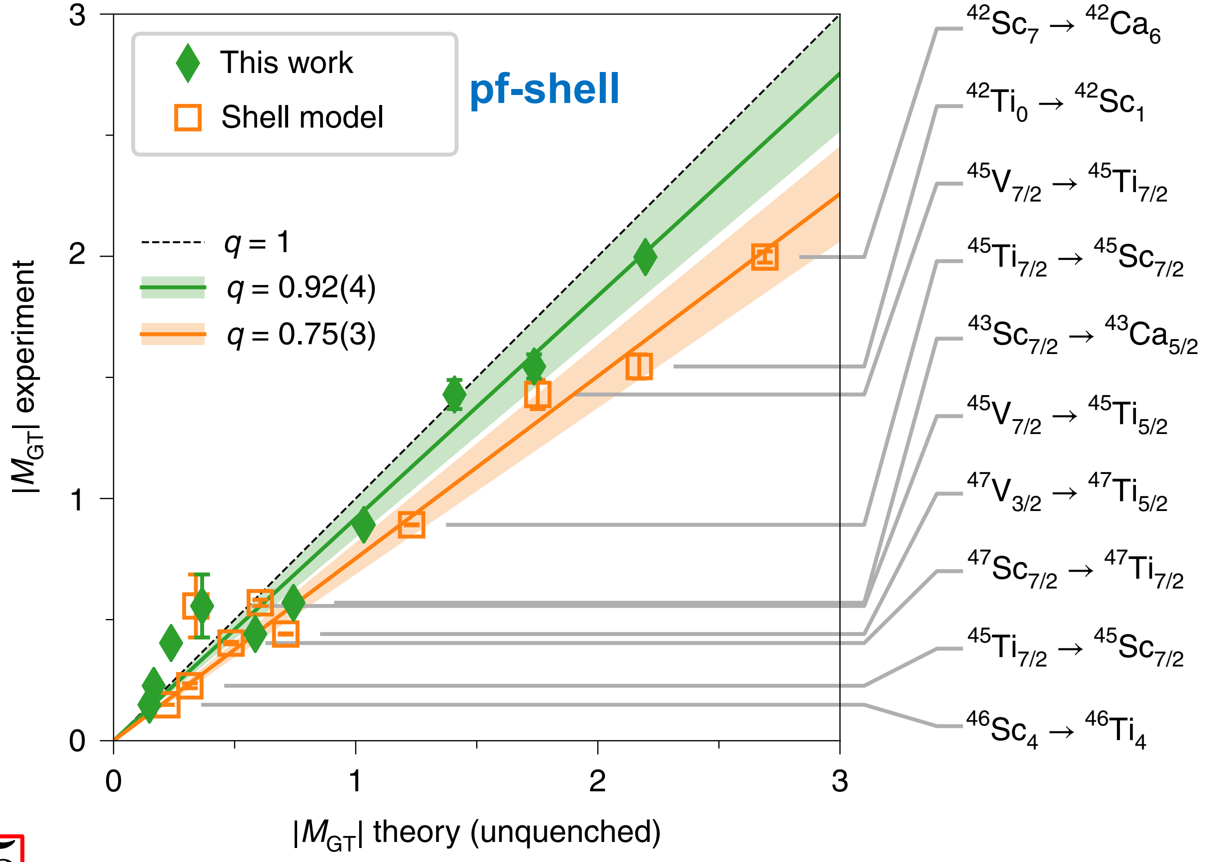


TRIUMF

Solution to g_A-Quenching Problem

VS-IMSRG calculations in regions from O → Ca (sd) and Ca→Ni (pf) shells





$$\boxed{g_A = 1.25}$$

Ab initio calculations across the chart explain data with unquenched g_A

Next up: explore **double**-beta decays…

Nature Physics **15**, 428 (2019)

TRIUMF

Milestone Result

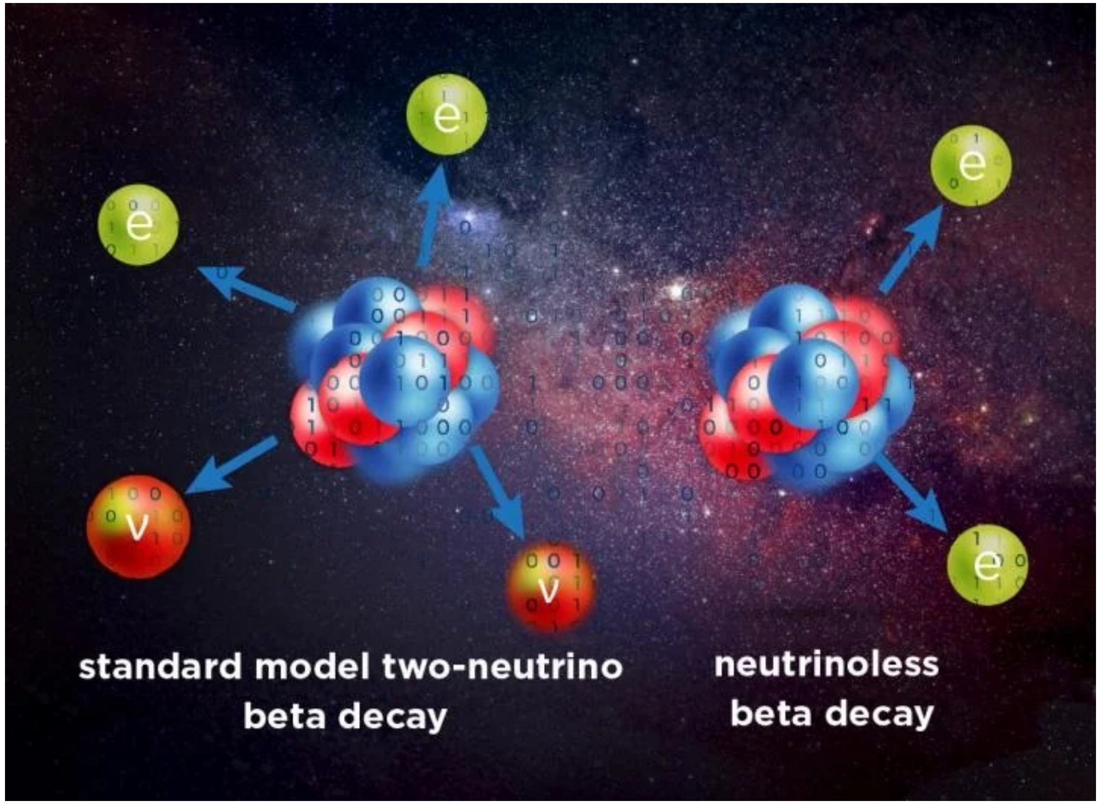
$0\nu\beta\beta$ Decay for All Major Players: ^{76}Ge ^{100}Mo, ^{130}Te, ^{136}Xe

Antoine Belley

Lotta Jokiniemi

Isabella Ginnett

Jack Pitcher



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

Ab initio uncertainty quantification of neutrinoless double-beta decay in Ge

Phys. Rev. Lett.

A. Belley, J. M. Yao, B. Bally, J. Pitcher, J. Engel, H. Hergert, J. D. Holt, T. Miyagi, T. R. Rodríguez, A. M. Romero, S. R. Stroberg, and X. Zhang

Physical Sciences - Article

Ab initio calculations of neutrinoless $\beta\beta$ decay refine neutrino mass limits

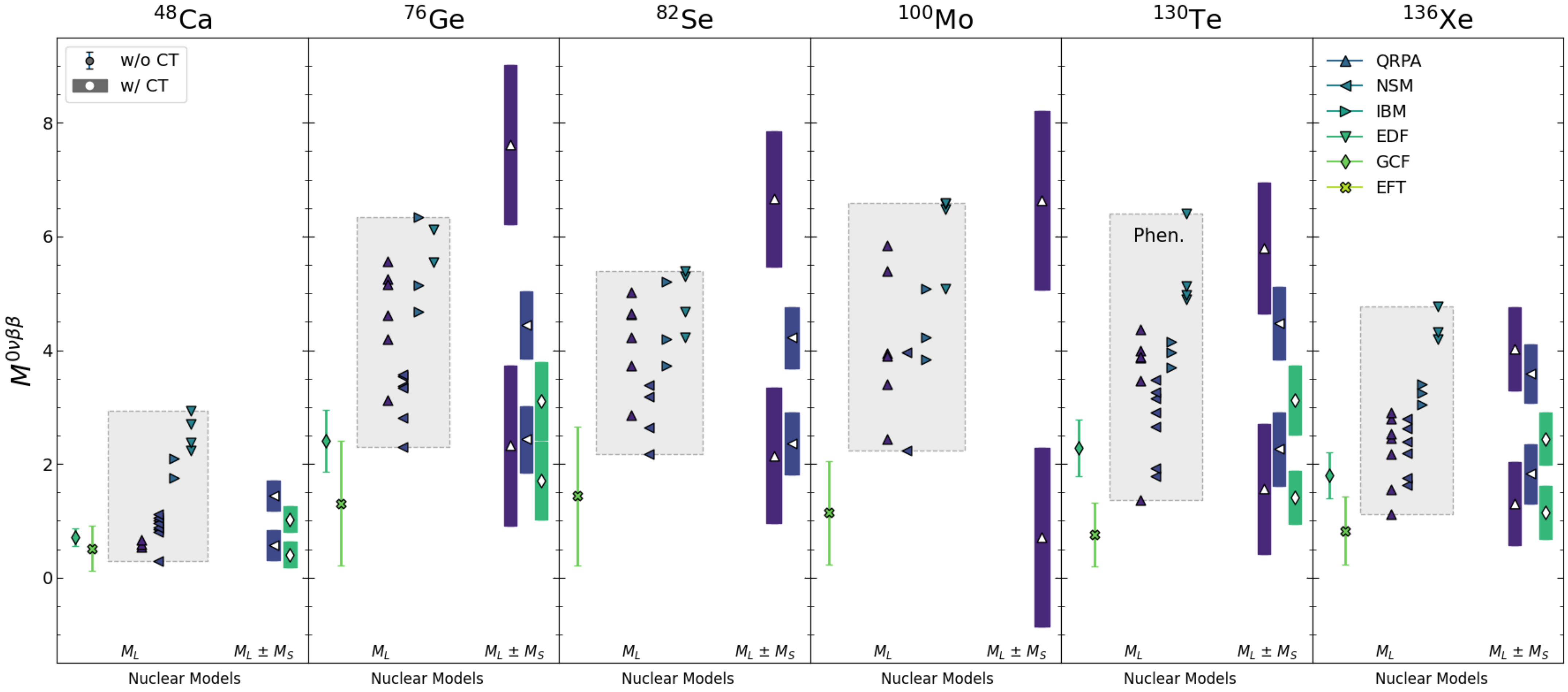
Status: Under Review

Jason Holt, Antoine Belley, Takayuki Miyagi, Steven Stroberg

nature portfolio

(More) Current Status of NMEs

Updated phenomenology w/ short-range contact Cirigliano et al. PRL (2018)

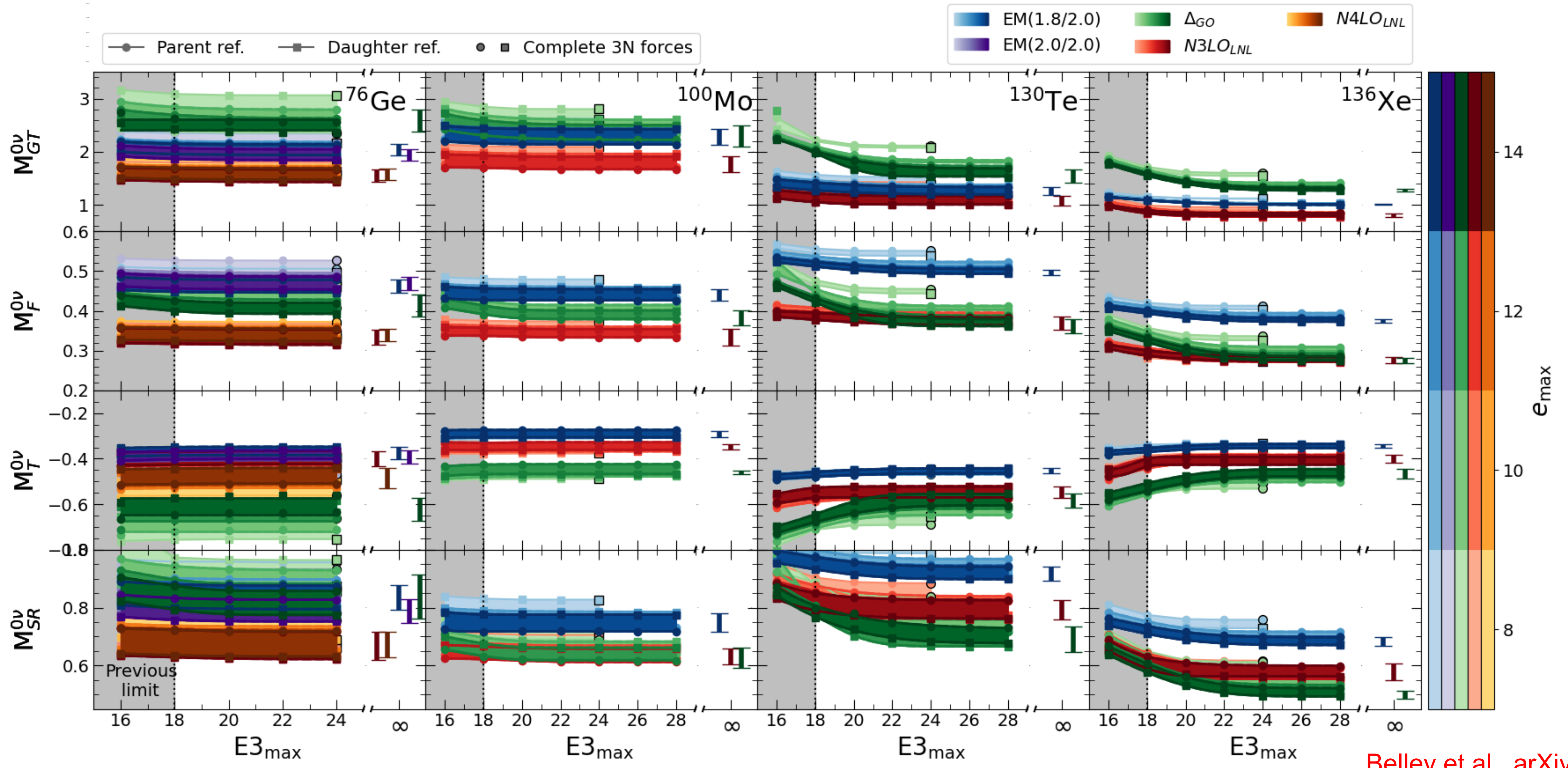


Uncertainty from **sign** of short-range term

New(er) results increase factors up to 10 uncertainty 😬 can ab initio help?

Ab Initio Strategy: Predict in Heavy Nuclei

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



Belley et al., arXiv:2307.15156
Nature (under review)

Ab Initio Strategy: Predict in Heavy Nuclei

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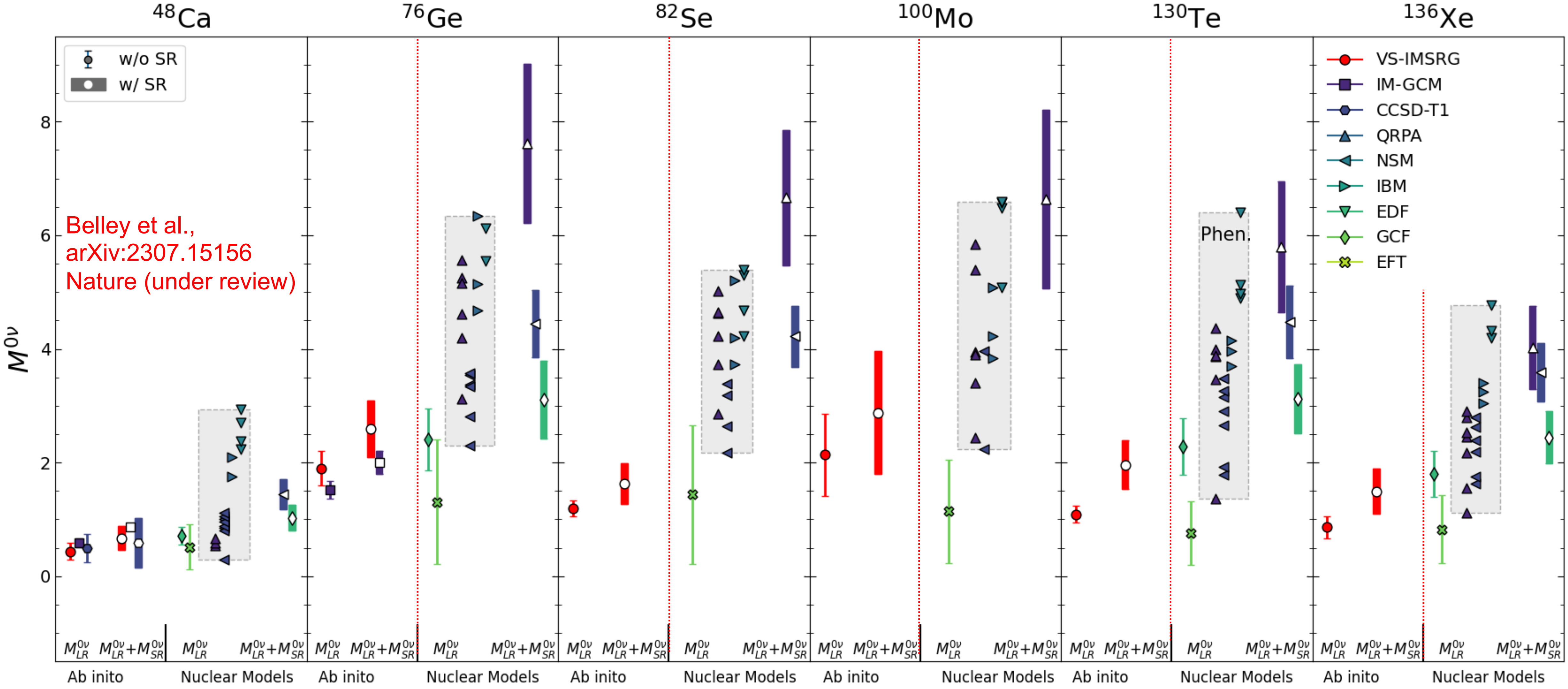
Ab initio results: differences from models; **large NMEs *strongly* disfavored**



Belley et al.,
arXiv:2307.15156
Nature (under review)

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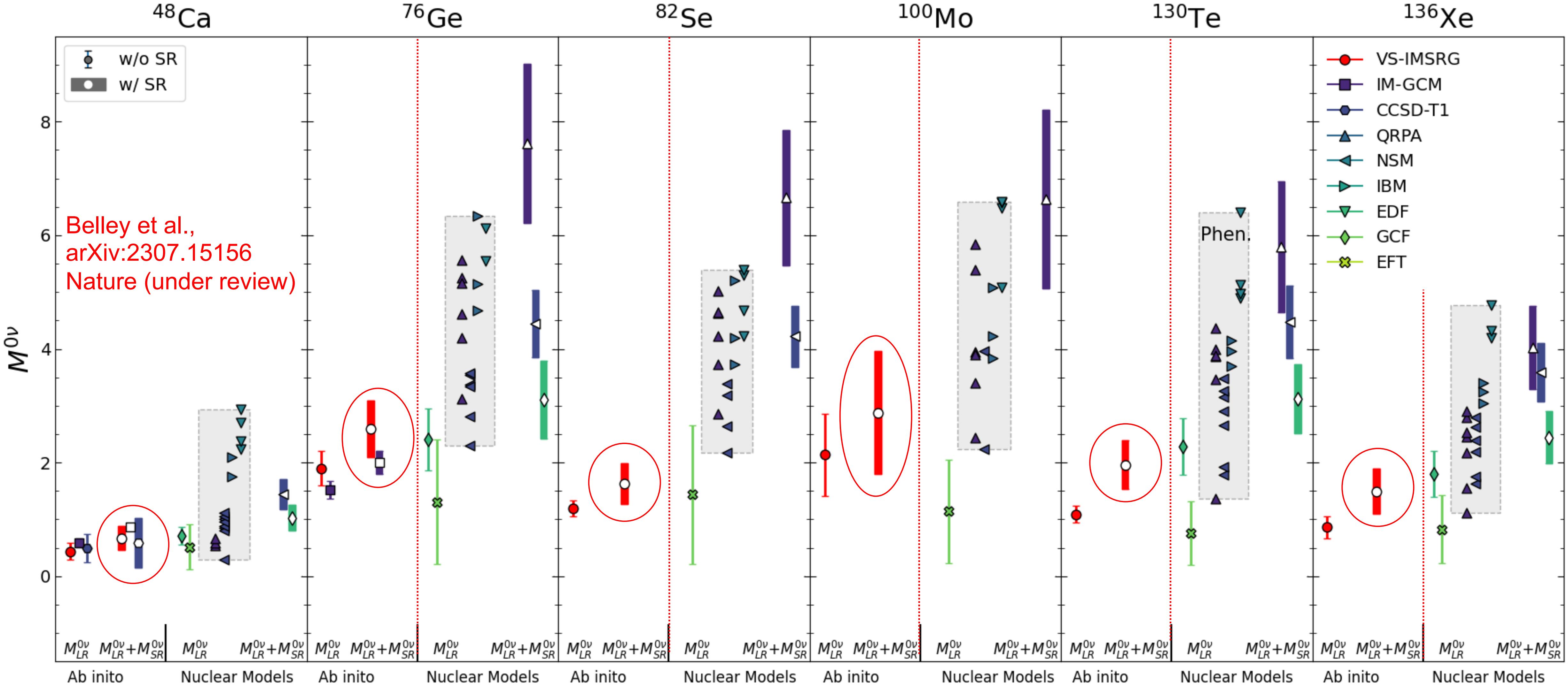
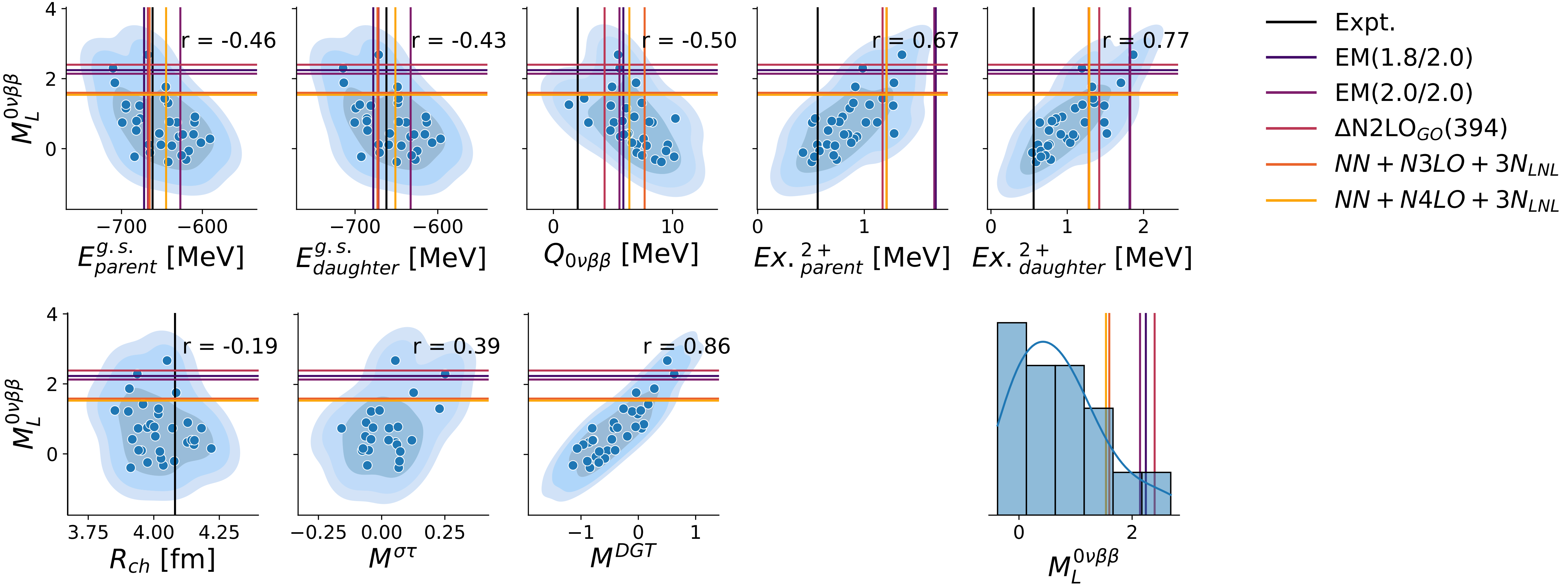


Ab Initio Strategy: Explore Correlations

^{76}Ge: Explore correlations with other observables from 34 interactions

No obvious correlations, except DGT



Use machine learning for further insights?

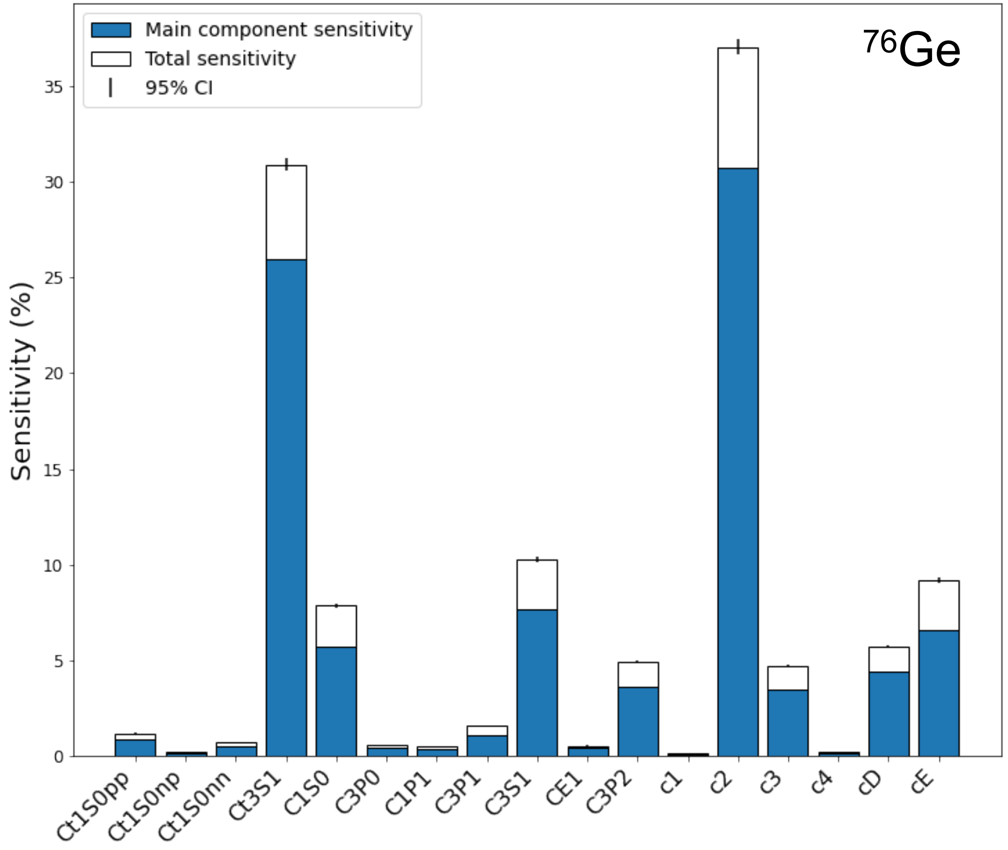
Belley et al., arXiV:2210.05809
Yao, Ginnett, Belley et al., PRC (2022)

MM-DGP Emulator for IMSRG: Sensitivity Analysis

Newly developed MM-DGP data-driven emulator

Sensitivity analysis: Connect energies to terms in chiral forces

Ground state energies



Sensitivity consistent with other complementary studies

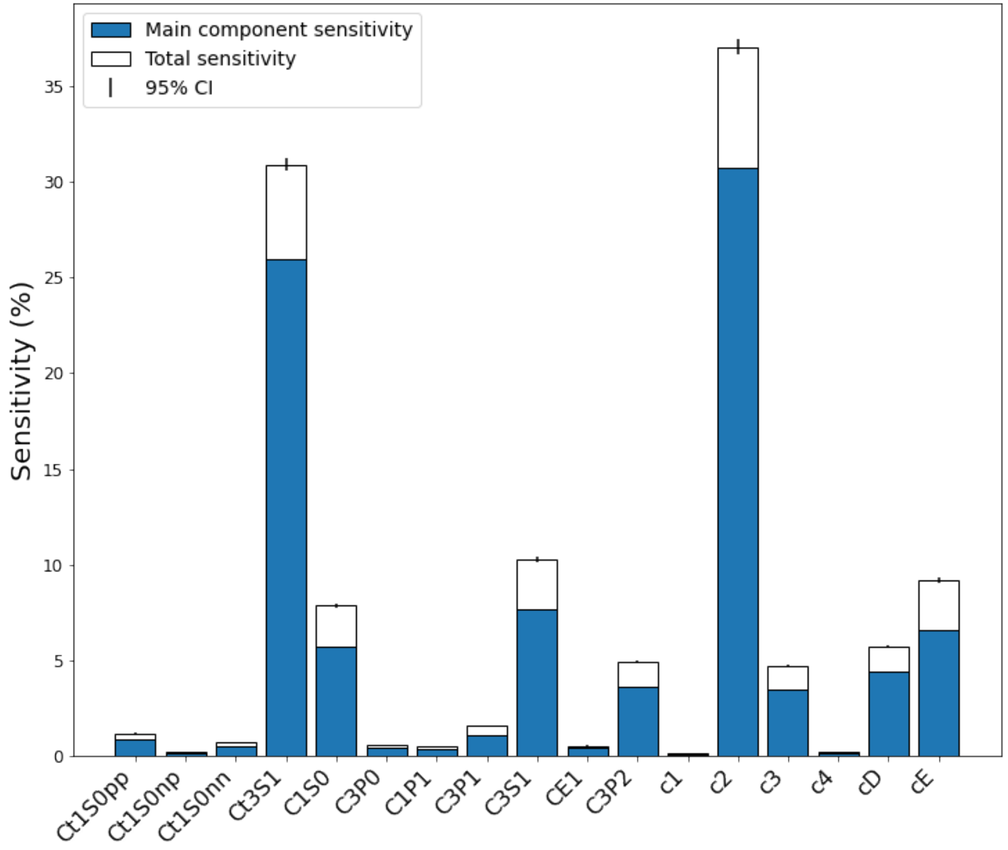
MM-DGP Emulator for IMSRG: Sensitivity Analysis

TRIUMF

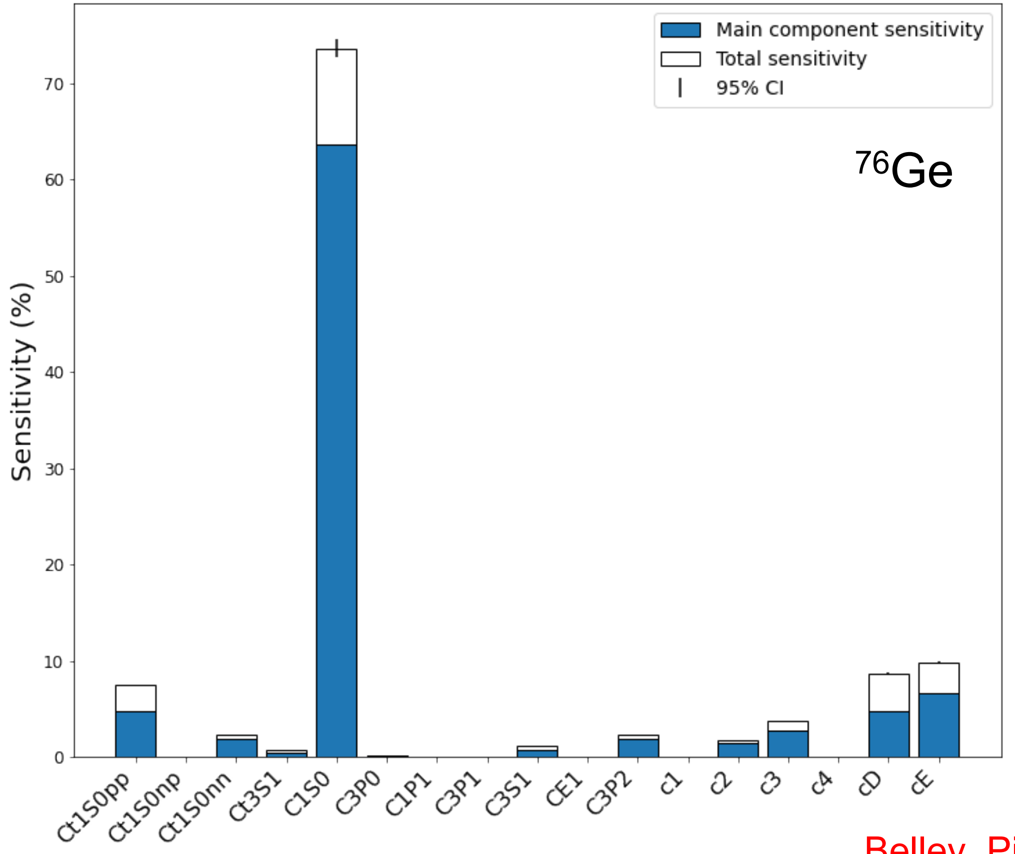
Newly developed MM-DGP data-driven emulator for VS-IMSRG

Sensitivity analysis: Connect $0\nu\beta\beta$ decay to terms in chiral forces

Ground state energies



$M_L^{0\nu}$



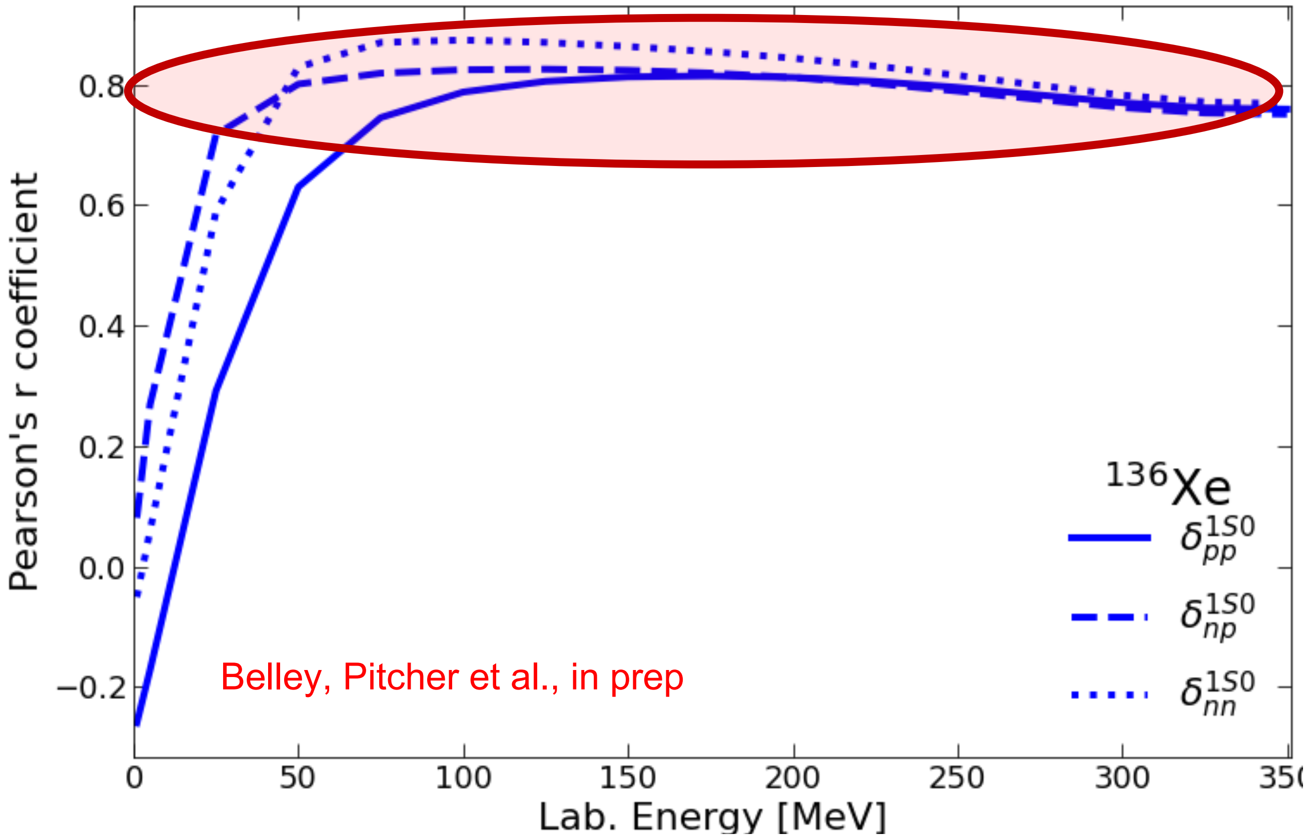
Belley, Pitcher et al., in prep

Highly sensitive to single constant "C1S0" – related to $^1S_0$ phase shift

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

Clear correlation with $^1S_0$ phase-shift

Strong correlation emerges for energies > 50MeV



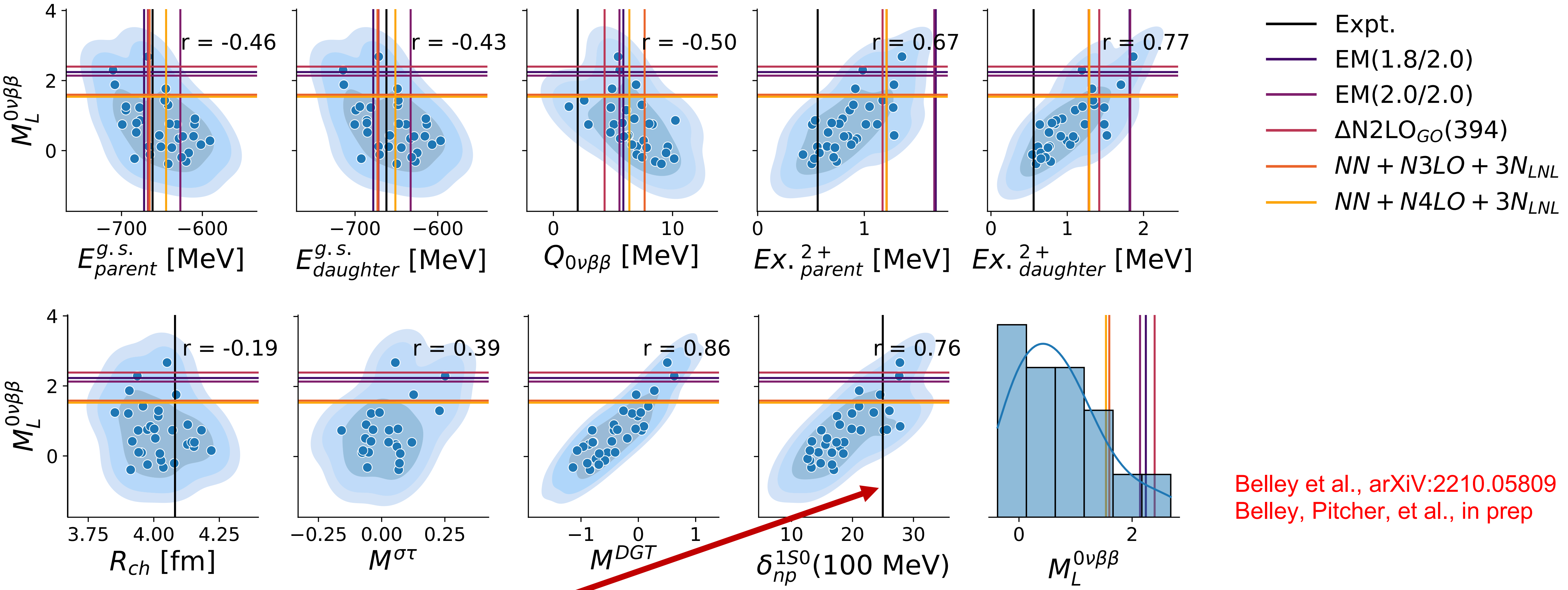
Constrained by part of interaction for the two nucleons when "close" to each other

TRIUMF

Ab Initio Strategy: Explore Correlations

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, Pitcher, et al., in prep

Novel correlation with **measured** $^1S_0$ phase shift!

Ab Initio Strategy: Rigorous Uncertainties

TRIUMF

Construct predictive posterior distribution for NME in ^{76}Ge

Consider *all* physics contributing to systematic error

$$y = y_{\mathrm{MM-DDGP}} + \epsilon_{\mathrm{emulator}} + \epsilon_{\mathrm{EFT}} + \epsilon_{\mathrm{many-body}} + \epsilon_{\mathrm{operator}}$$

Belley et al., Physical Review Letters (in press)

Use 8100+ samplings of NN+3N forces

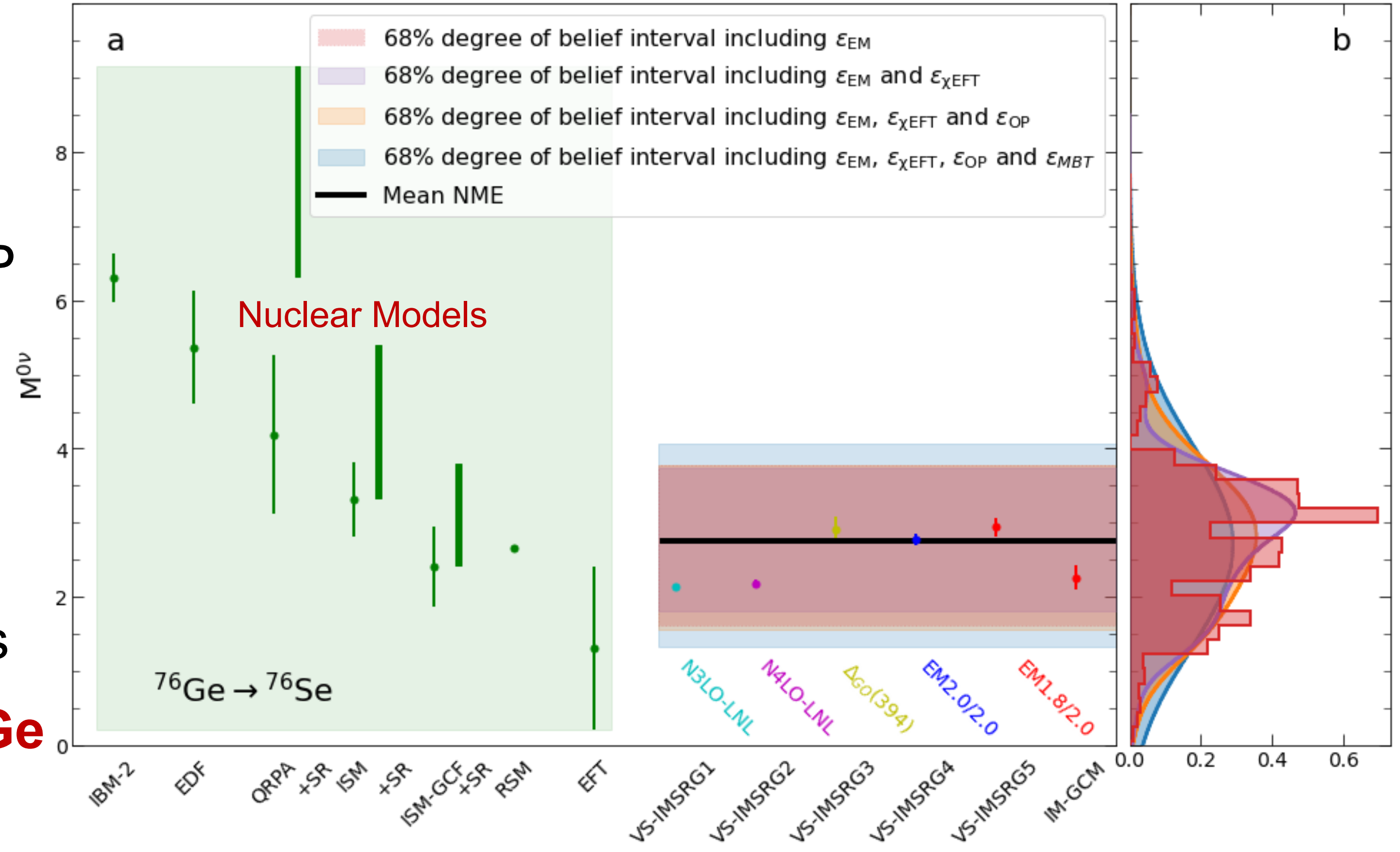
weight by quality of $^1S_0$ phase shift

"Solve" many-body problem with MM-DGP

Many-body error largest → IMSRG(3)

Mean NME validates previous interactions

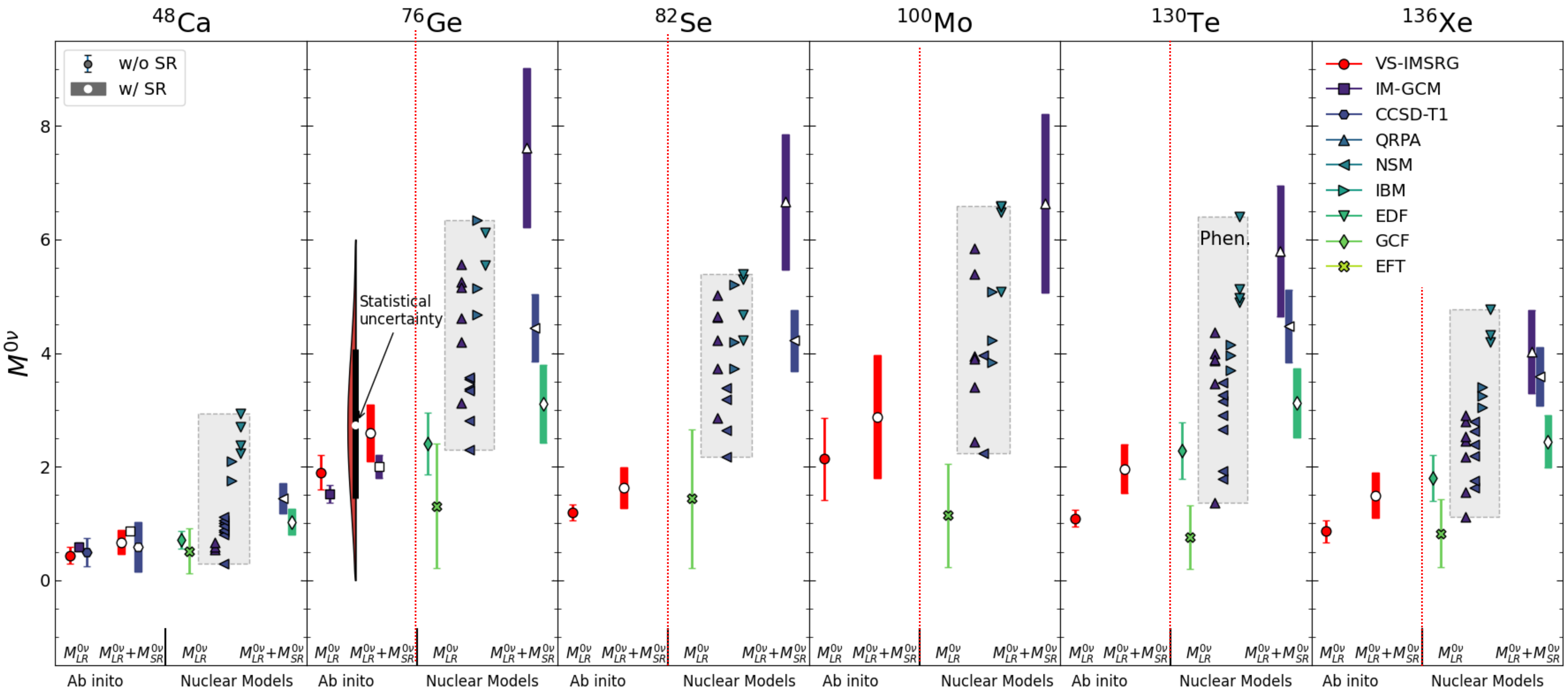
Dramatically reduced uncertainty in ^{76}Ge



Updated Predictions in Heavy Nuclei

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

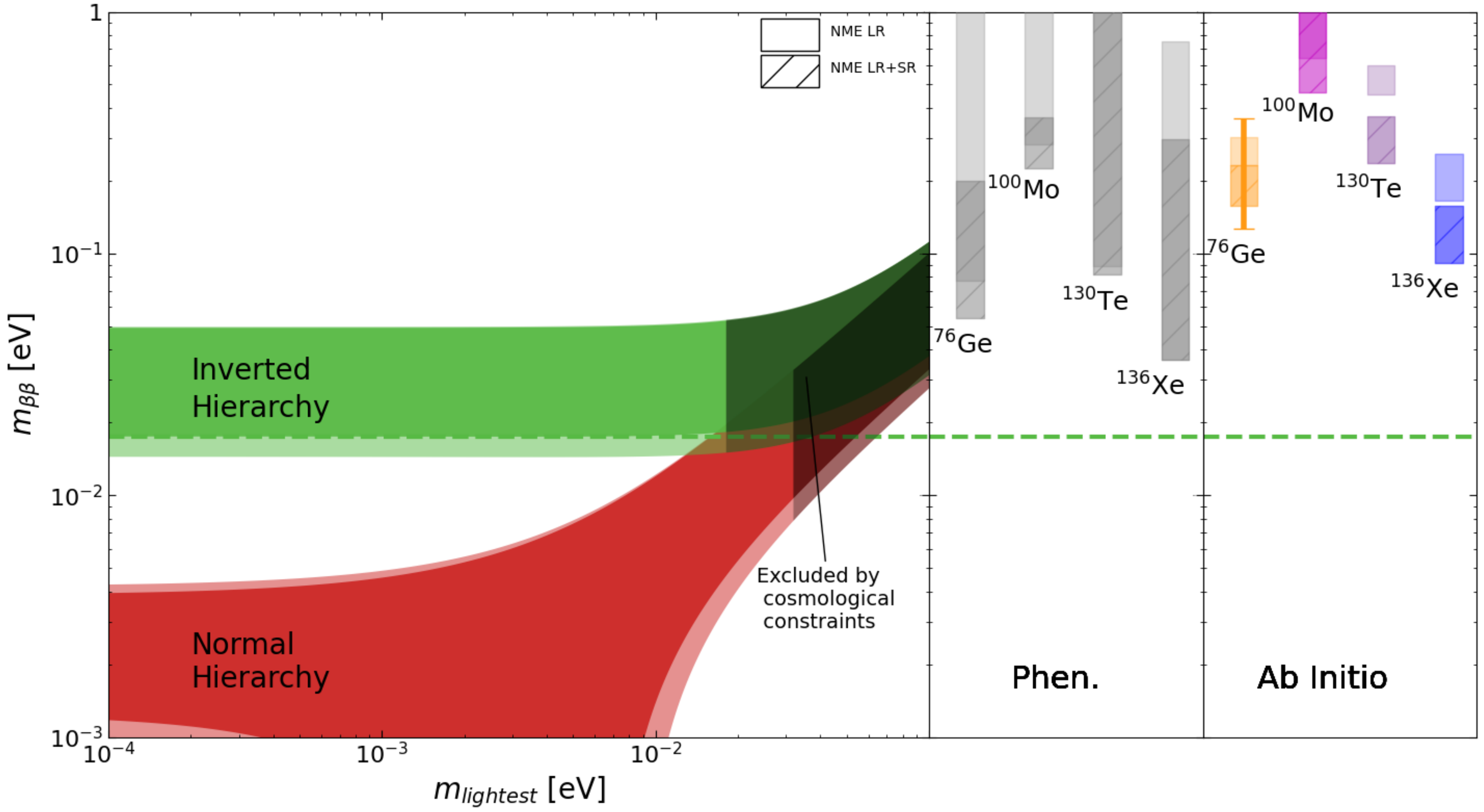
Independent PPD agrees with previous spread



Ab Initio Strategy: Impact on Worldwide Searches

Impact for current searches: large matrix elements disfavored, lowers expected rates

Current experimental reach – improved with effects of contact term



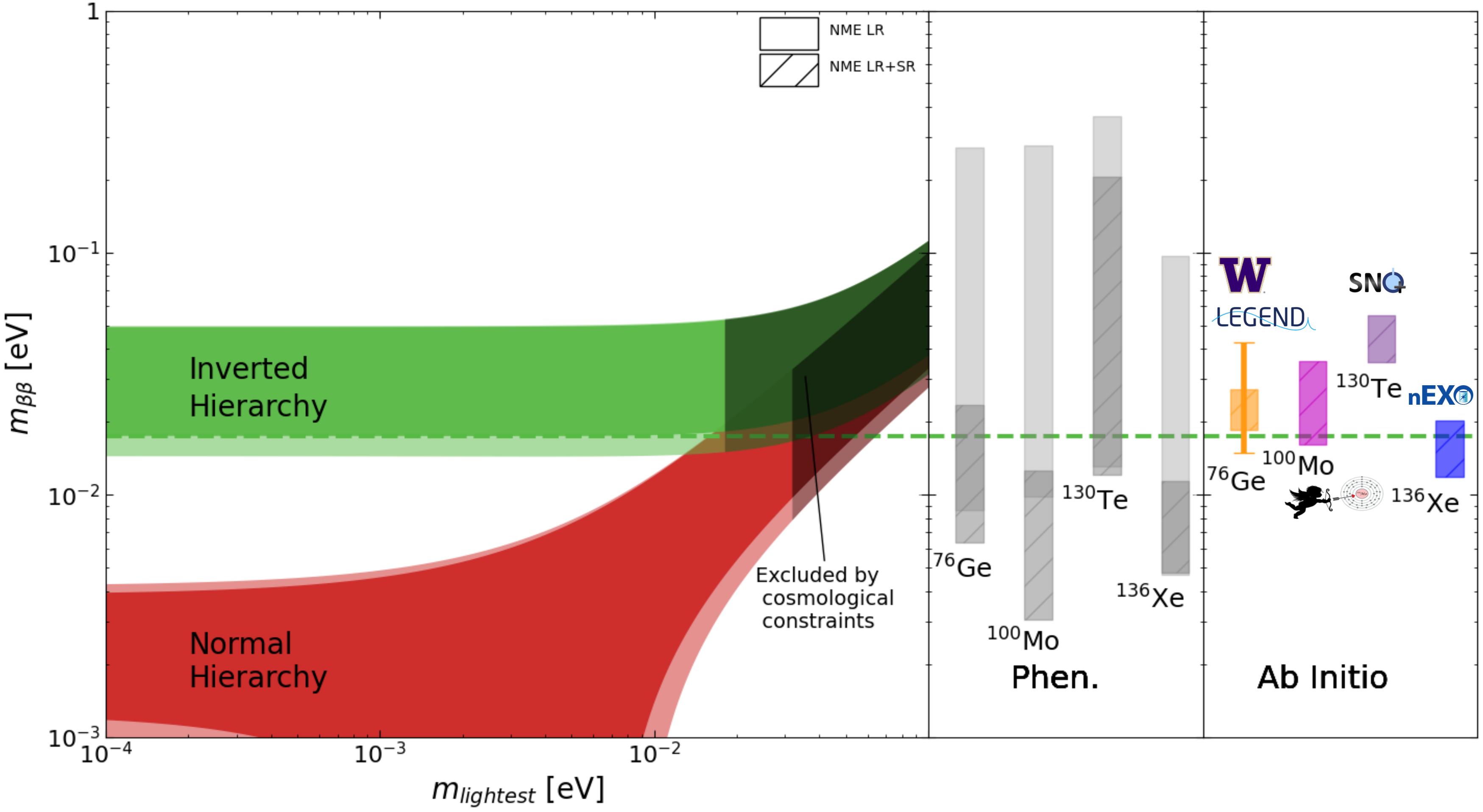
***Highly unlikely* inverted Hierarchy has been probed**

Belley et al, arXiv:2307.15156
Nature (under review)

Ab Initio Strategy: Impact on Ton-Scale Searches

Impact for next-generation searches: sensitivities from LEGEND, SNO+, nEXO, CUPID

Effect of short-range term improves experimental reach… **^{100}Mo now a major player**



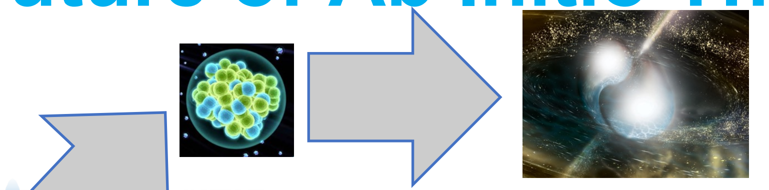
Uncertainty reduced by ***over one order of magnitude*!**

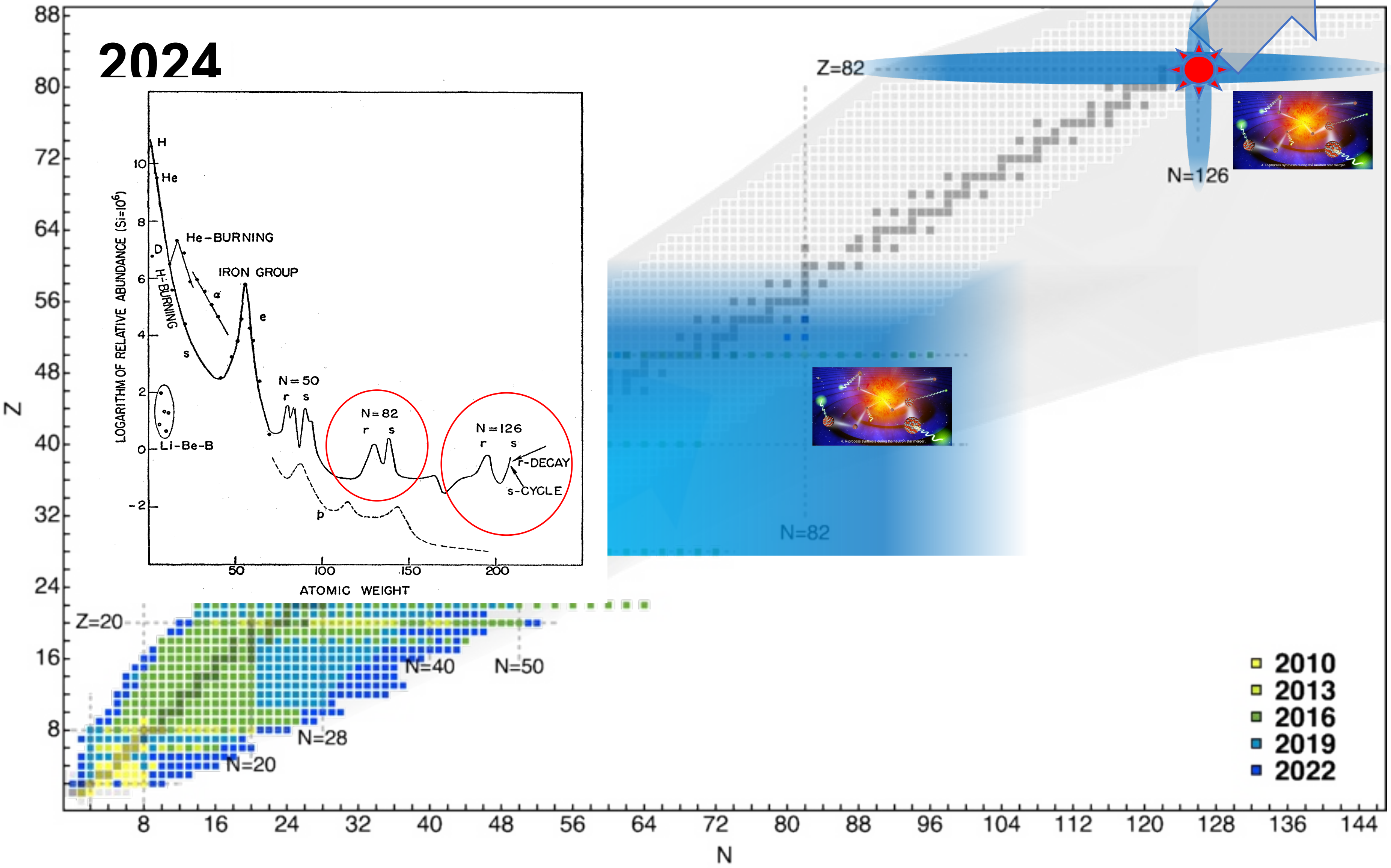
Belley et al, arXiv:2307.15156
Nature (under review)

TRIUMF

Act II Preview: Future of Ab Initio Theory

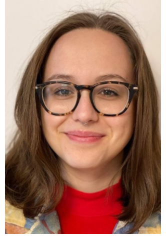
(Not so) Bold predictions: Five new directions in the next 5 years



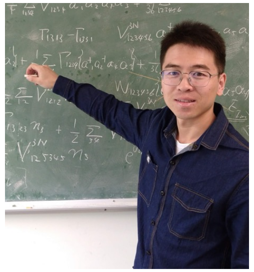


Nucleosynthesis

Ab initio input for r-process



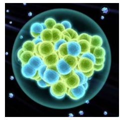
Nicole Vassh **Maude Larivière**

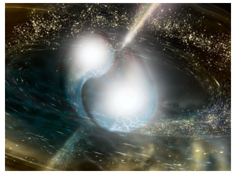


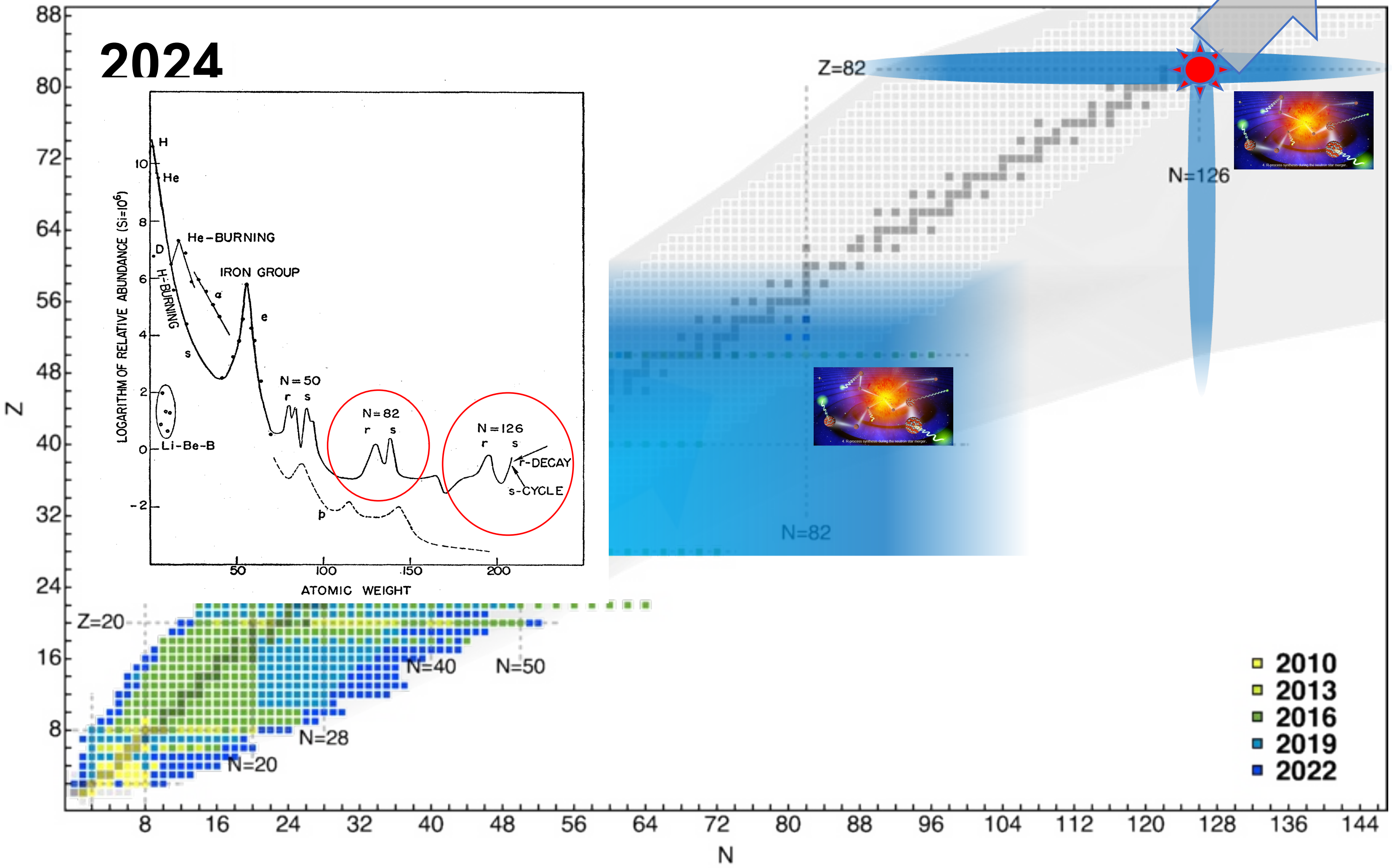
Baishan Hu

Act II Preview: Future of Ab Initio Theory

(Not so) Bold predictions: Five new directions in the next 5 years







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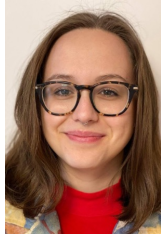
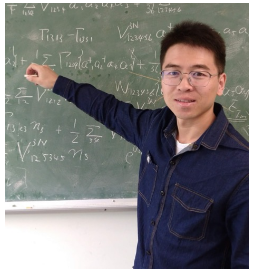
Ab initio input for r-process

Nicole Vassh



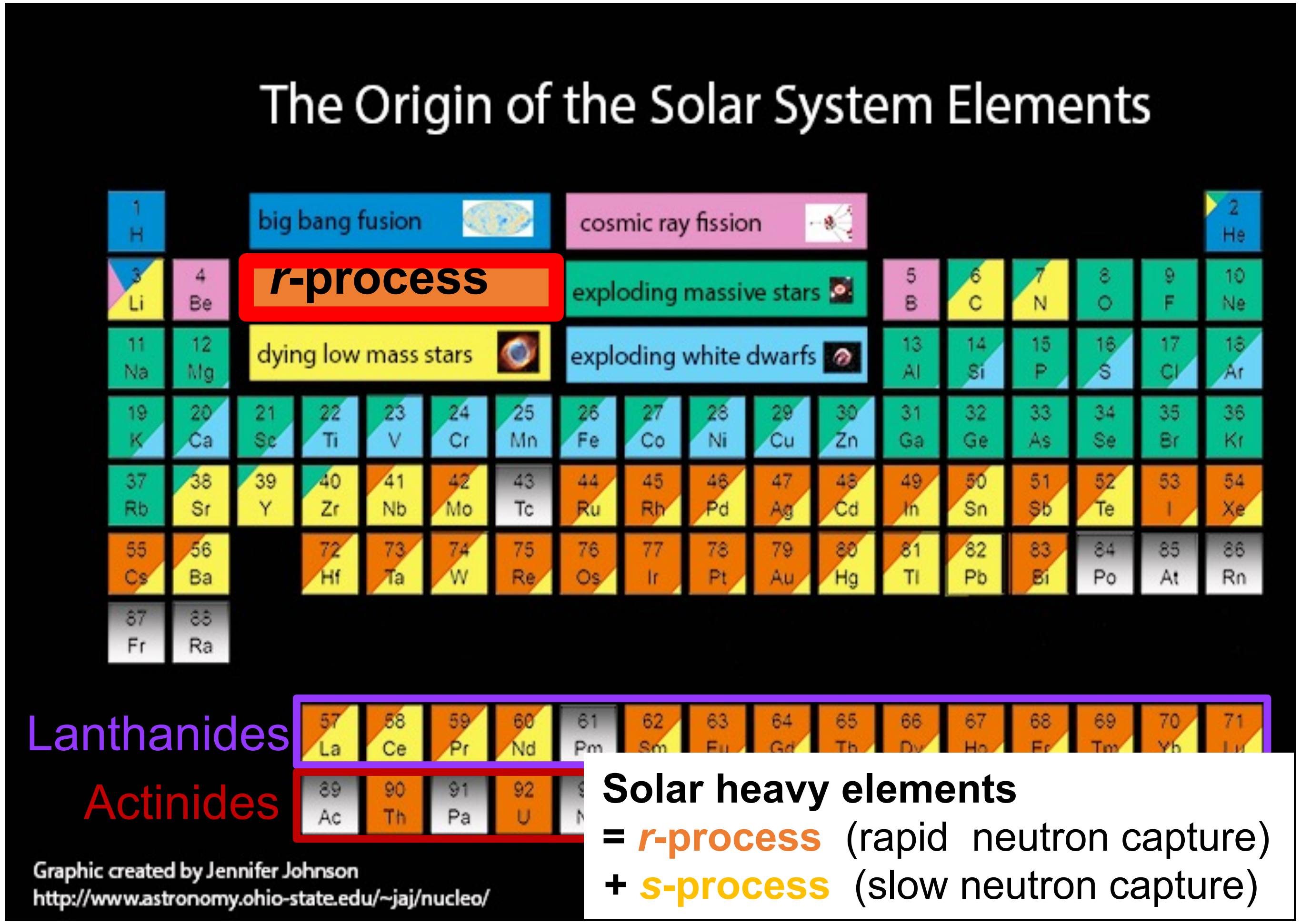
Maude Larivière



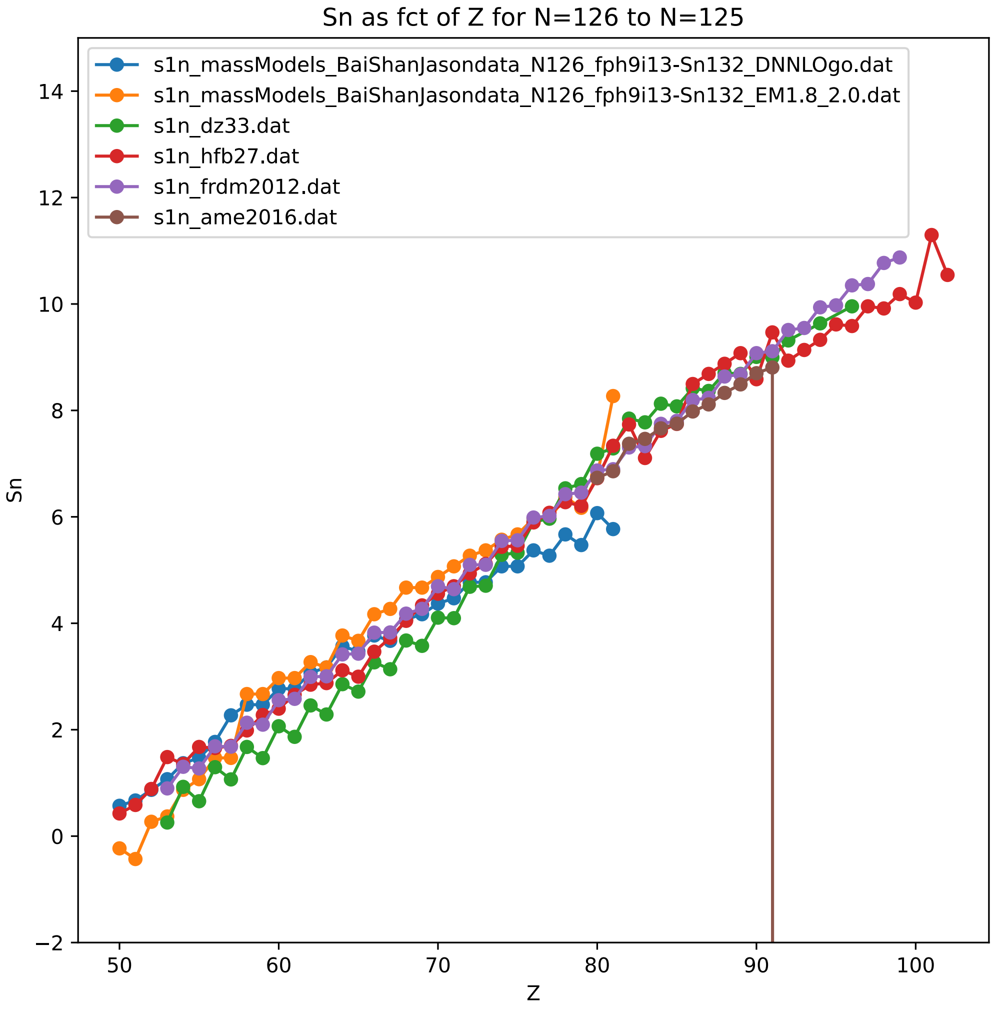
Baishan Hu

Next Big Discovery? Origin of Heavy Elements

Most heavy elements created via rapid-neutron capture process (r-process)



Solar heavy elements
= *r*-process (rapid neutron capture)
+ *s*-process (slow neutron capture)

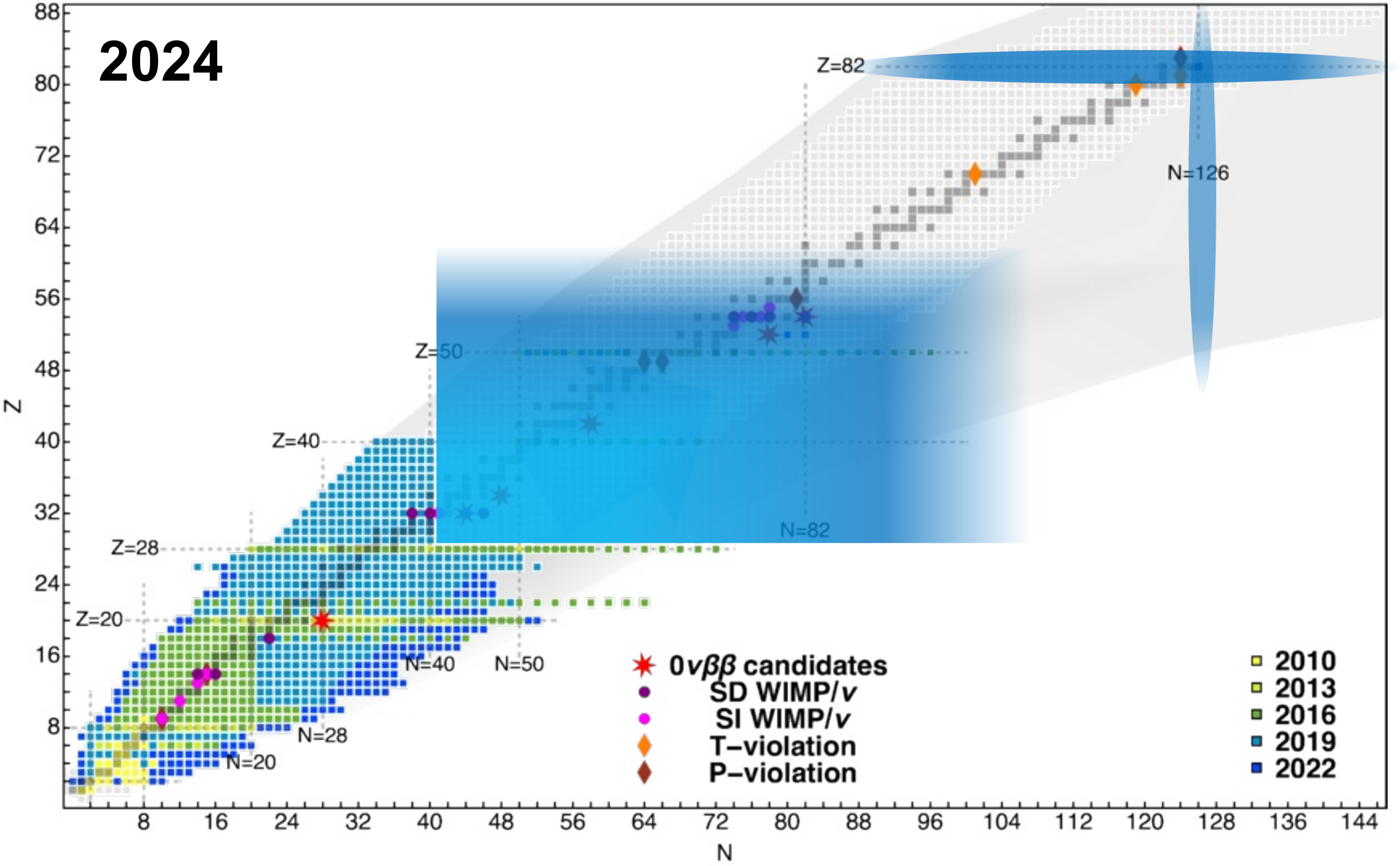


Theory input is crucial where no data exists

Act II Preview: Future of Ab Initio Theory

TRIUMF

(Not so) Bold predictions: Five new direction in the next 5 years

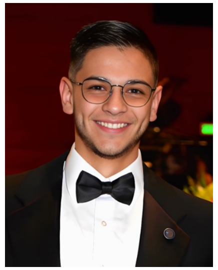


Nucleosynthesis
Ab initio input for r-process

Dark Matter/ν Scattering
Ab initio structure functions

CKM Unitarity (V_{ud})
Superallowed Fermi

Symmetry Violation
P/T-violating moments



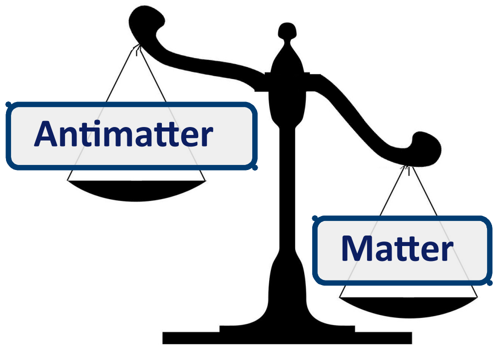
Antoine Belley Jose Munoz

The Magic of Molecules: CP Violation

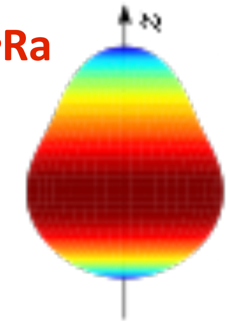
"One of the most compelling mysteries in all of science is how matter came to dominate over antimatter in the universe." – NSAC LRP

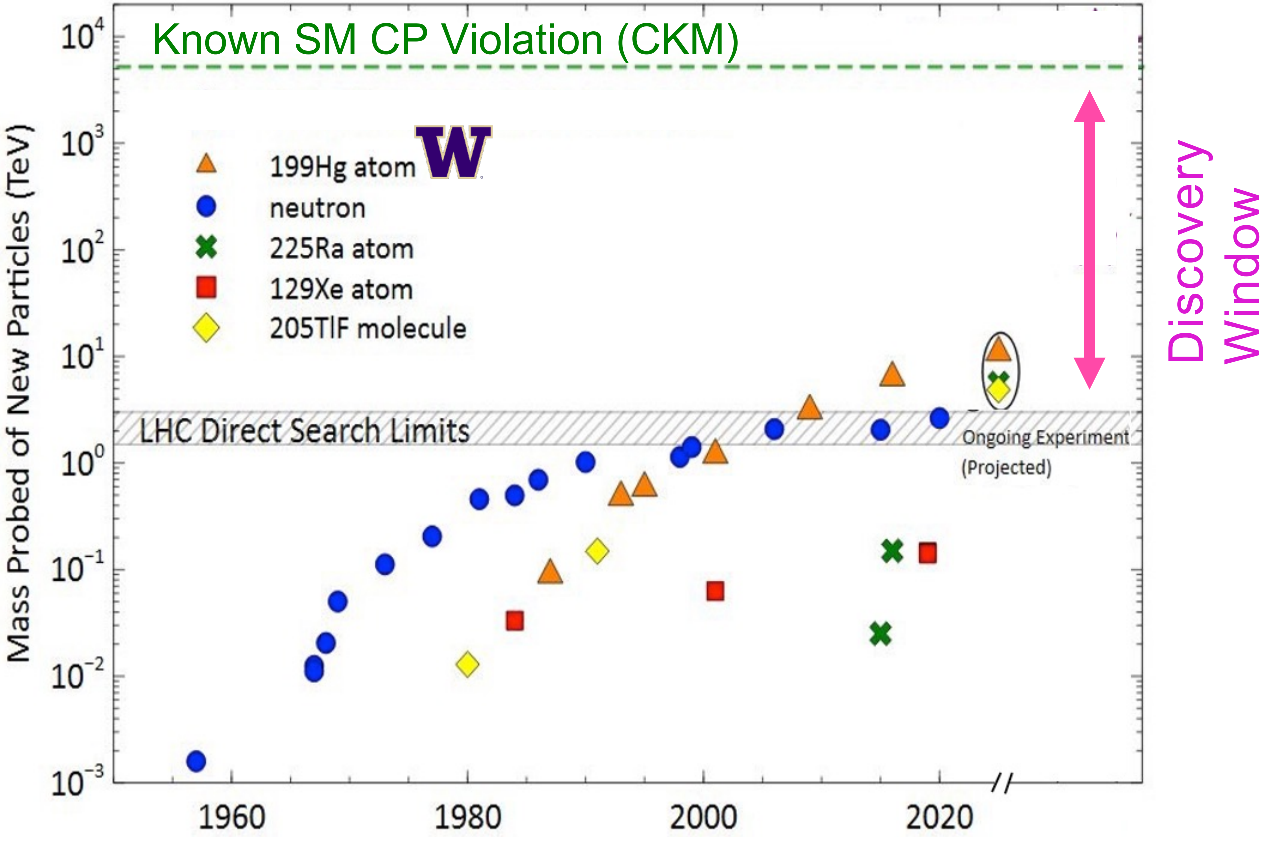
CP violation required beyond our current observations

Searches for CP violation ongoing for 50+ yr
neutron/atoms - ^{199}Hg EDM world leader



^{225}Ra





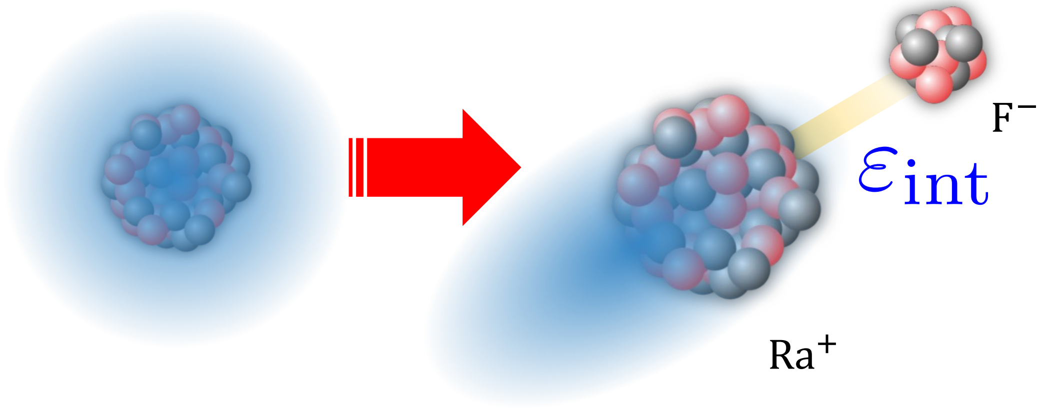
$$\sim \frac{Z A^{2/3} \beta_2 \beta_3^2}{E_+^N - E_-^N} \sim 10^3$$

Effects enhanced in:
Heavy systems, Octupole deformed

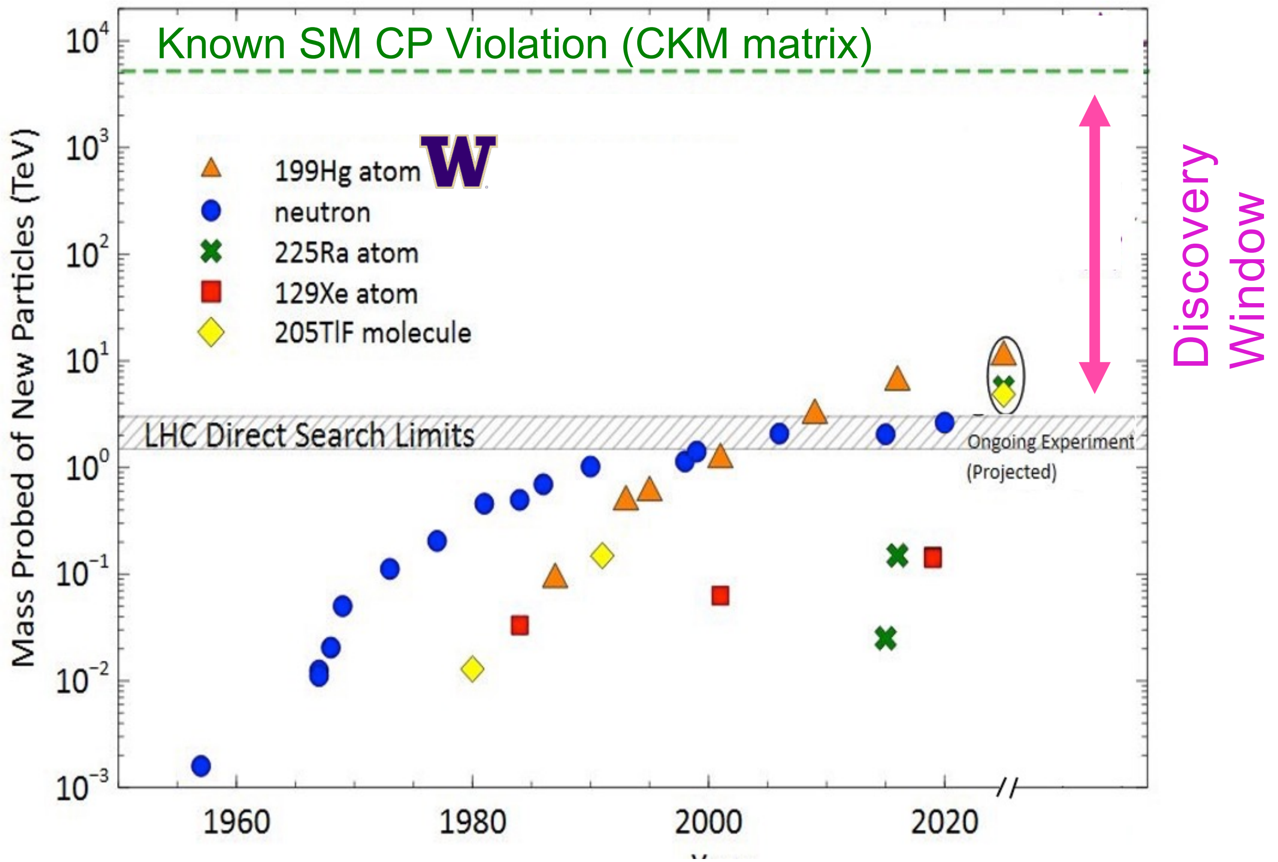
The Magic of Molecules: CP Violation

Worldwide race to exploit power of **Radioactive Molecules**

Generate internal fields **orders of magnitude** above lab possibilities



Enhancements in molecules vs atoms **>4000!**



The Magic of Molecules: CP Violation

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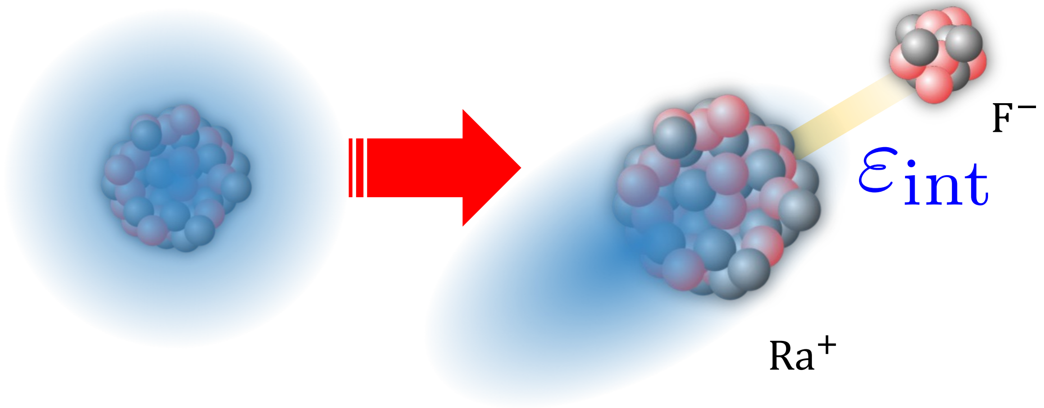
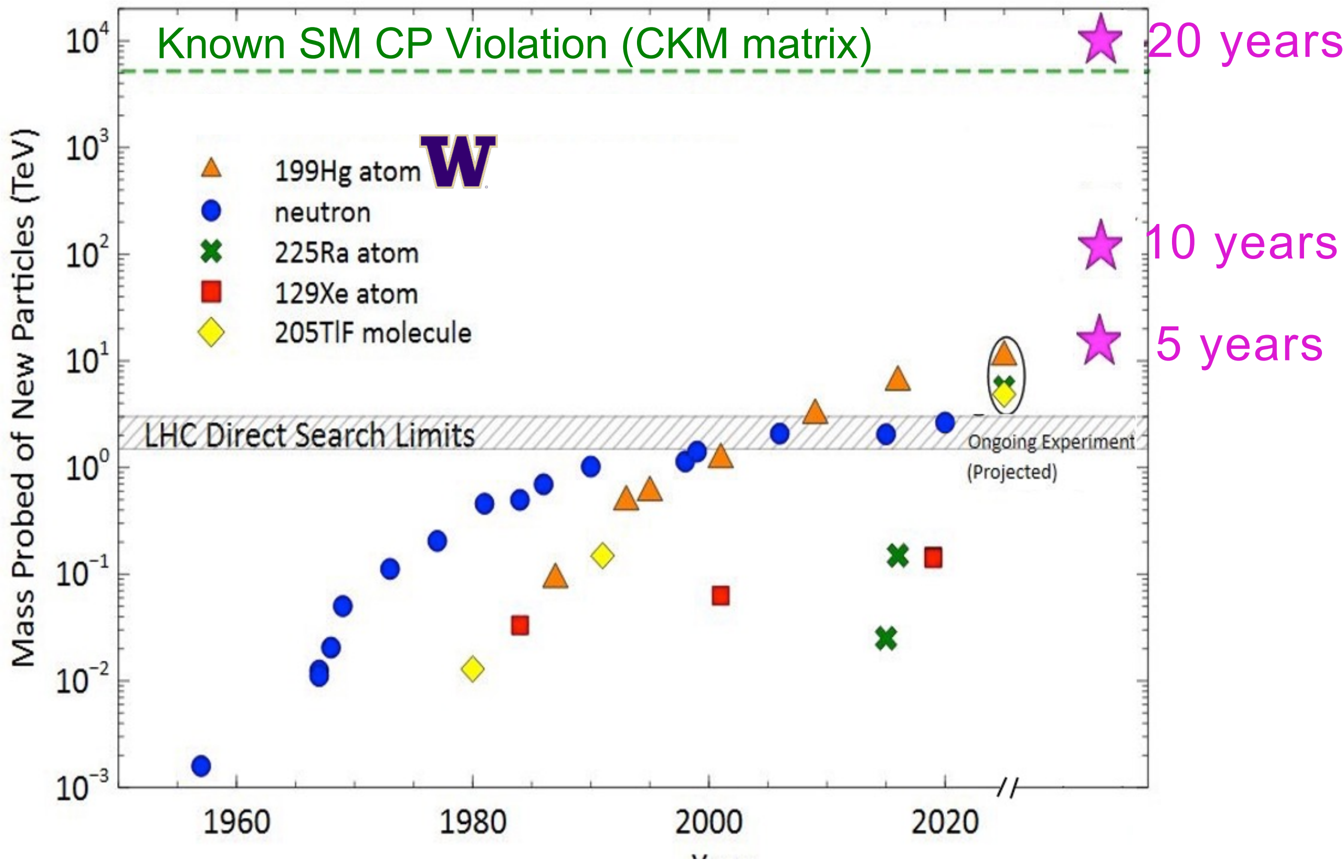




Enhancements in molecules vs atoms **>4000!**

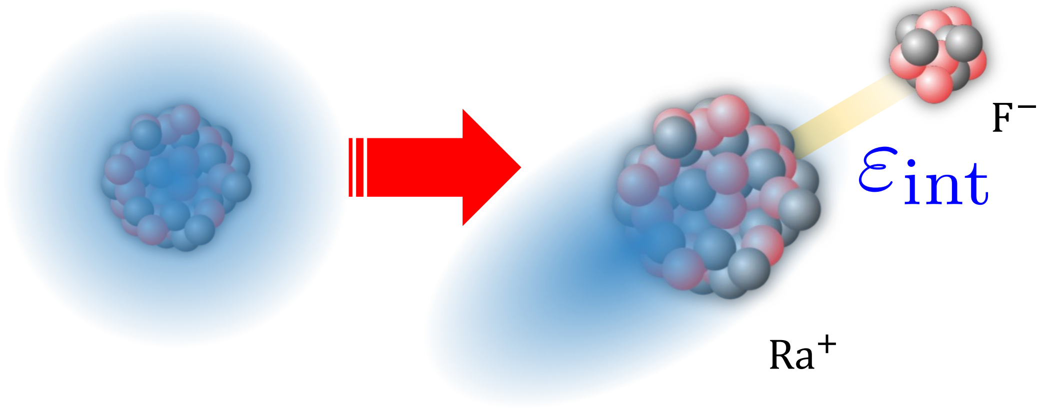
Probe **1000TeV** scale in our lifetimes

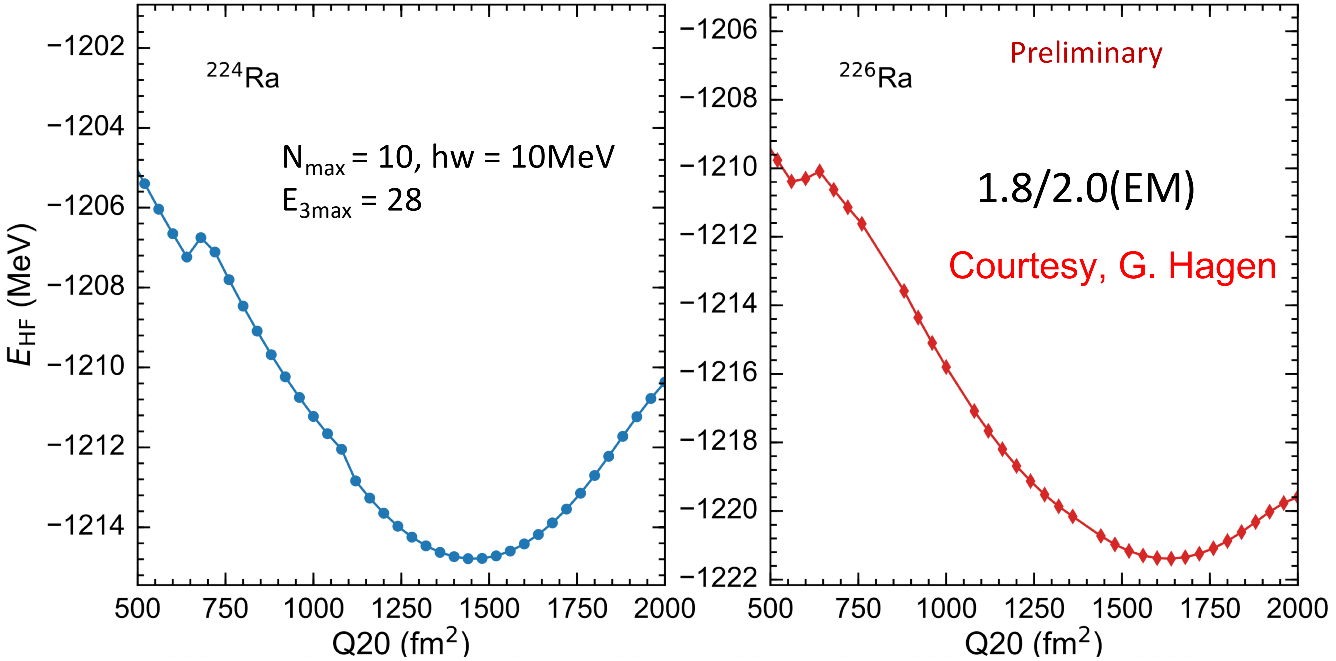
The Magic of Molecules: CP Violation

TRIUMF

Worldwide race to exploit power of **Radioactive Molecules**

Generate internal fields orders of magnitude above lab possibilities





Enhancements in molecules vs atoms **>4000**

Probe 1000TeV scale in our lifetimes

To date, no rigorous nuclear theory

Calculations for Ra, Hg underway!!

Measurement; Nuclear structure; P,T odd NN int

$$S = \langle \Psi_0 | S_z | \Psi_0 \rangle = \frac{\langle \Psi_+ | S_z | \Psi_- \rangle \langle \Psi_+ | V_{PT} | \Psi_- \rangle}{E_+ - E_-}$$

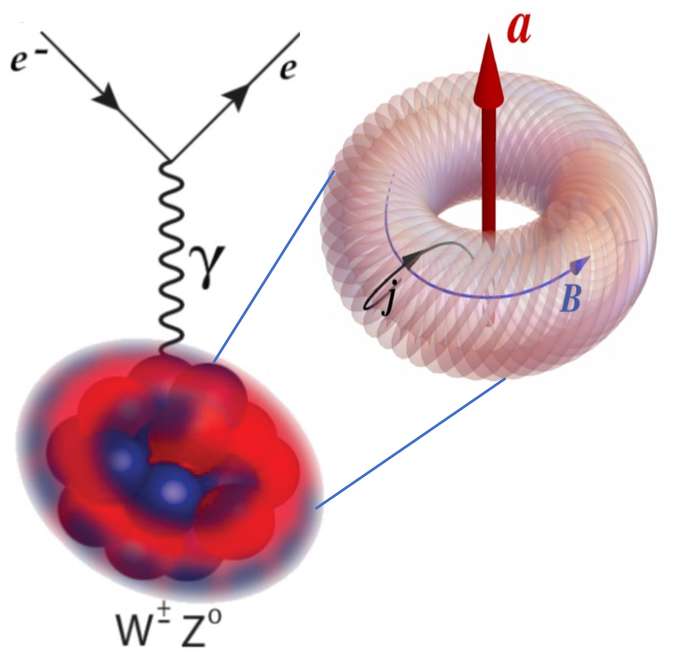
New physics

Experiment

The Magic of Molecules: Weak Structure of Nuclei

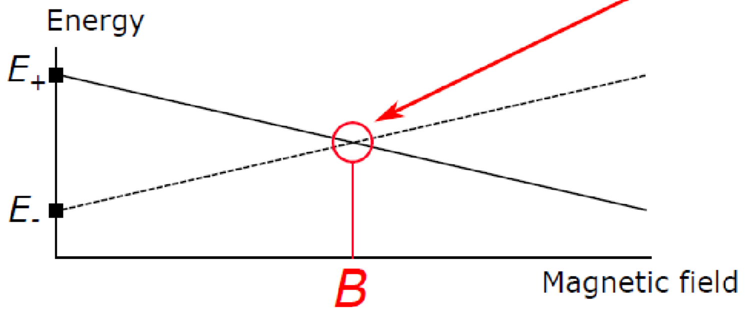
Hadronic P violation – probe the **weak structure** of the atomic nucleus!

W,Z exchange between nucleons generates **anapole moment**

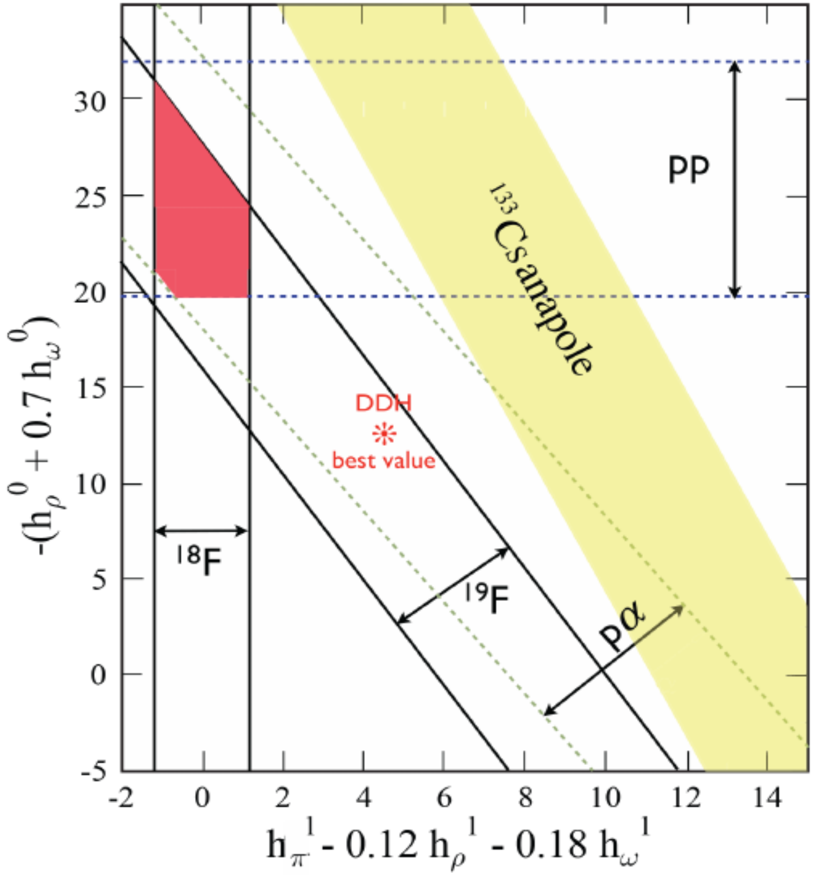


$$E_{PV} \sim \frac{\langle \psi_{\uparrow}^{+} | H_{\pm} | \psi_{\downarrow}^{-} \rangle}{\boxed{E_{-} - E_{+}}}$$

$>10^{11}$ molecular enhancement



Experimental tuning enhances $>10^{11}$



C. S. Wood et al., Science (80-.). 275, 1759 (1997).

RESEARCH ARTICLE

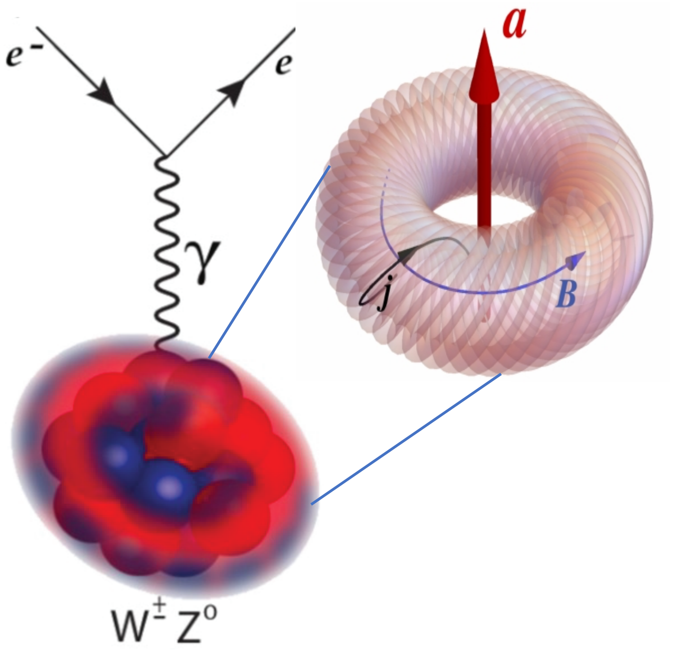
Measurement of Parity Nonconservation and an Anapole Moment in Cesium

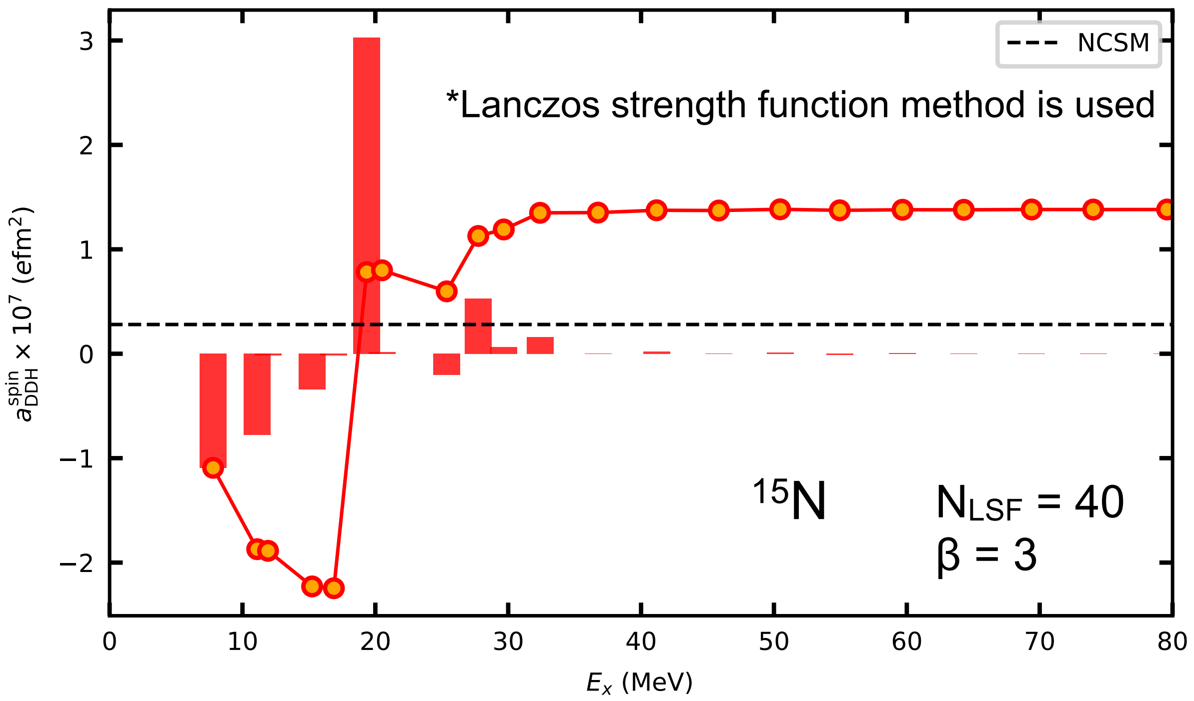
C. S. Wood, S. C. Bennett, D. Cho,* B. P. Masterson,†
J. L. Roberts, C. E. Tanner,‡ C. E. Wieman§

The Magic of Molecules: Weak Structure of Nuclei

Hadronic P violation – probe the weak structure of the atomic nucleus!

W,Z exchange between nucleons generates **anapole moment**





To date, no rigorous nuclear theory

^{133}Cs underway!

Nuclear structure   P-odd NN int

$$\langle IM|a_{10}^{\mathrm{pol}}|IM\rangle \sim \sum_n \frac{\langle I^\pi||a_1||I_n^{-\pi}\rangle\langle I_n^{-\pi}|V_{\mathrm{PV}}|I^\pi\rangle}{E_{\mathrm{g.s.}} - E_n}$$

Experiment

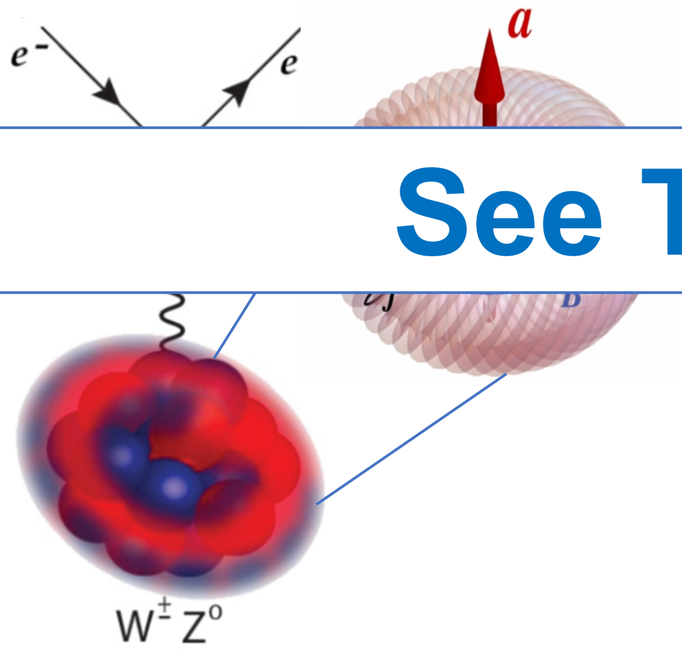
New P-violating physics

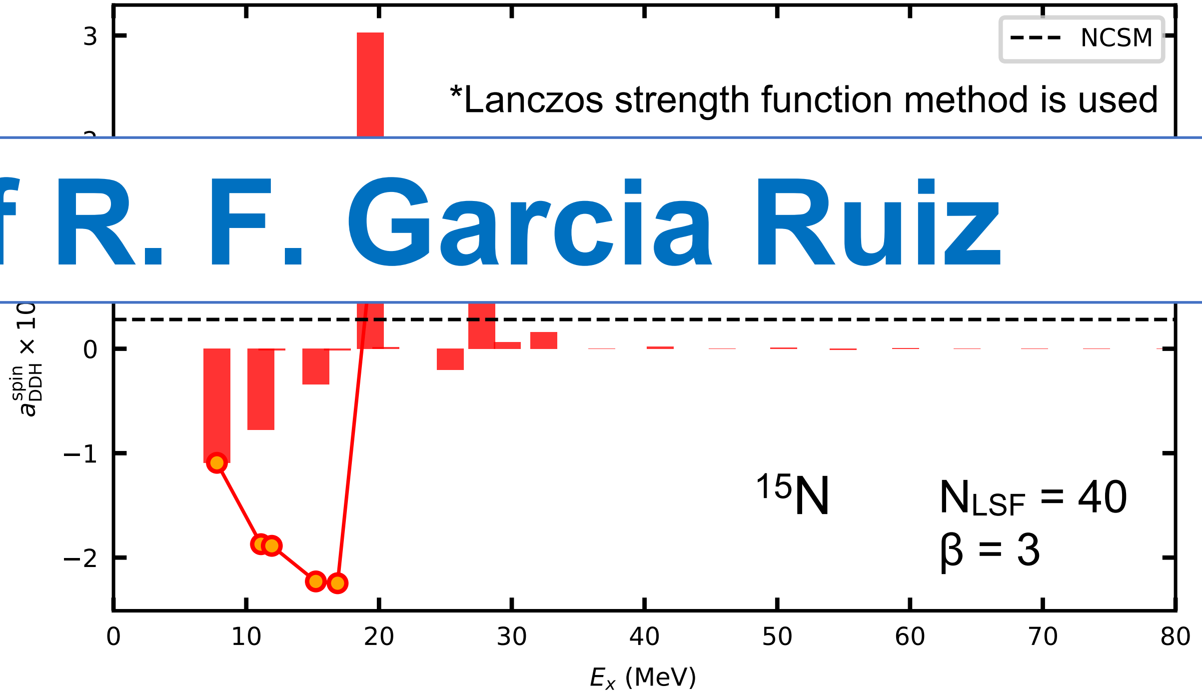
TRIUMF

The Magic of Molecules: Weak Structure of Nuclei

Hadronic P violation – probe the weak structure of the atomic nucleus!

W,Z exchange between nucleons generates **anapole moment**





See Talk of R. F. Garcia Ruiz

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Experiment

New P-violating physics

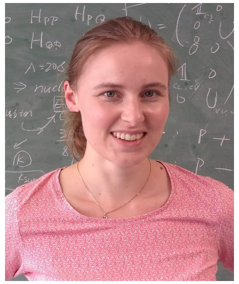
Act II Preview: Future of Ab Initio Theory

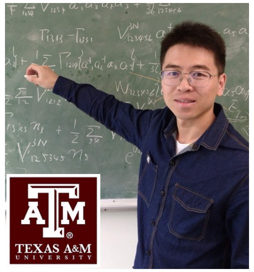
TRIUMF

(Former) Postdoctoral Fellows


Ragnar Stroberg

Takayuki Miyagi


Lotta Jokiniemi



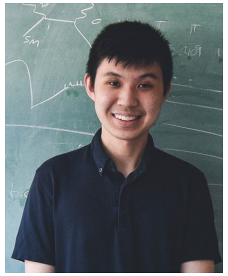
Baishan Hu

0νββ Decay

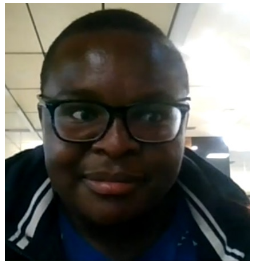
Antoine Belley

Isabella Ginnette


Anabelle Grimes


Michael Liudeng

Structure + Astrophysics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Maude Larivière

Symmetry Violation

Jose Munoz

Jack Pitcher

AI/Machine Learning

CKM Unitarity


Emily Love


Matt Martin

Atomic Systems

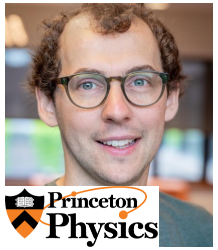
Gaurav Tenkila


Hrishi Patel


Vijay Chand

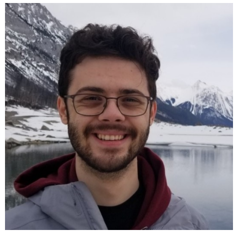
Just the beginning:
join our revolution!
jholt@triumf.ca

Dark Matter/ν Scattering



Sam Leutheusser

Jose Padua


Mathieu Bruneault

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Act II Preview: Future of Ab Initio Theory

(Former) Postdoctoral Fellows


Ragnar Stroberg


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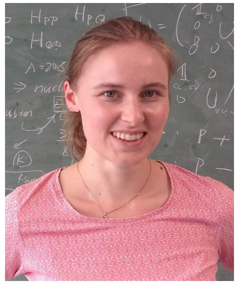
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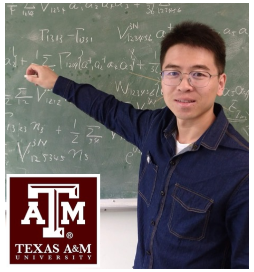
Baishan Hu

0νββ Decay


Antoine Belley


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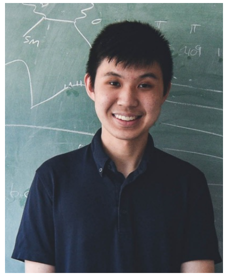
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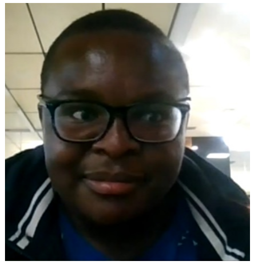
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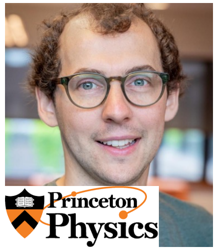
Just the beginning: join our revolution! jholt@triumf.ca

Dark Matter/ν Scattering


Sam Leutheusser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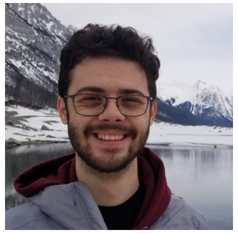
Mathieu Bruneault

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

T. Miyagi, B. S. Hu, L. Jokiniemi

TRIUMF — A. Belley, I. Ginnett, C. G. Payne, A. Grimes, J. Pitcher, D. Araujo

THE UNIVERSITY OF BRITISH COLUMBIA — M. Bruneault, J. Padua, S. Leutheusser

E. Love

McGill UNIVERSITY — K. Evidence, D. Kush

G. Tenkila, H. Patel, V. Chand

B. Wong, X. Cao

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

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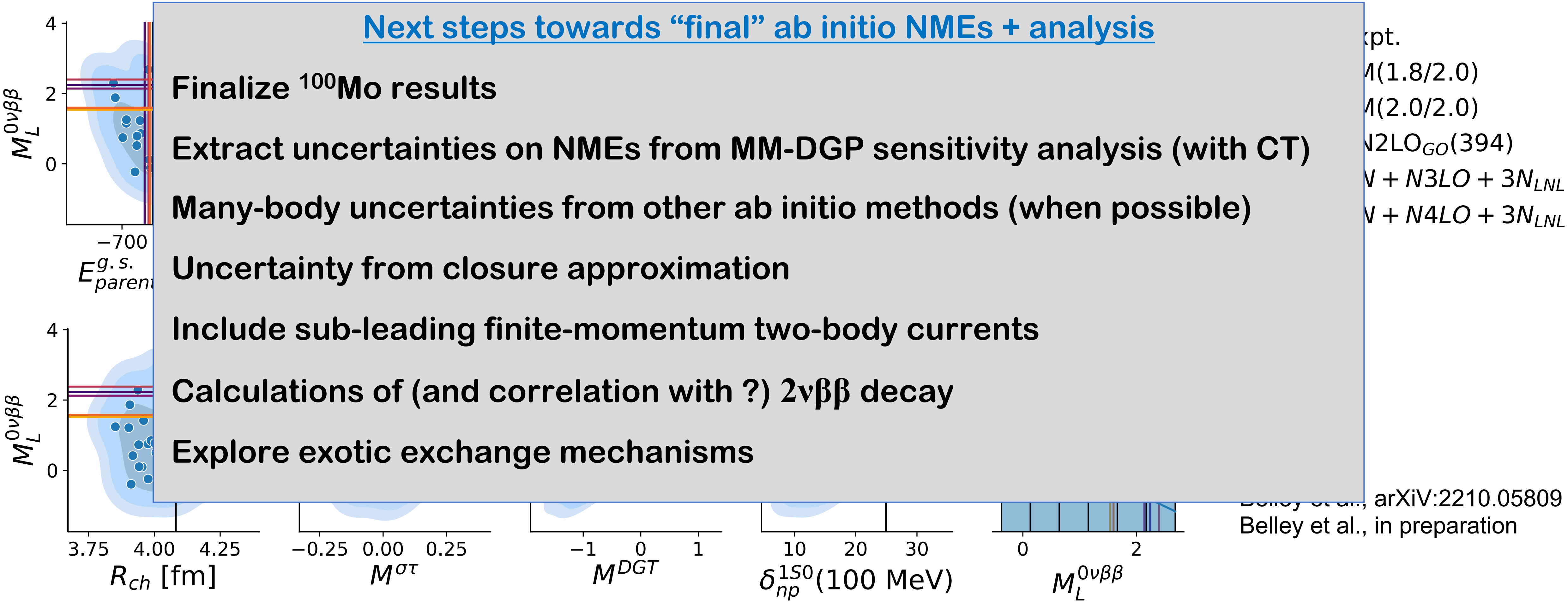
Strategy III: Correlation with Structure Observables

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

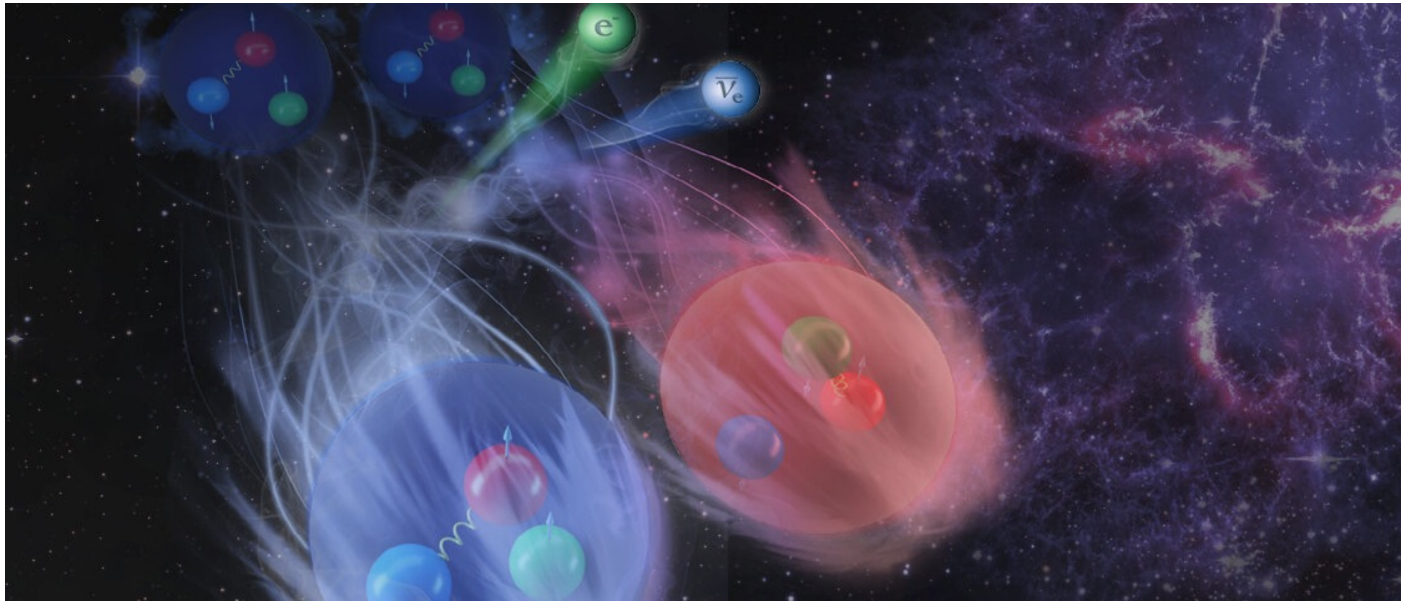
Calculations of (and correlation with ?) $2\nu\beta\beta$ decay

Explore exotic exchange mechanisms

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

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

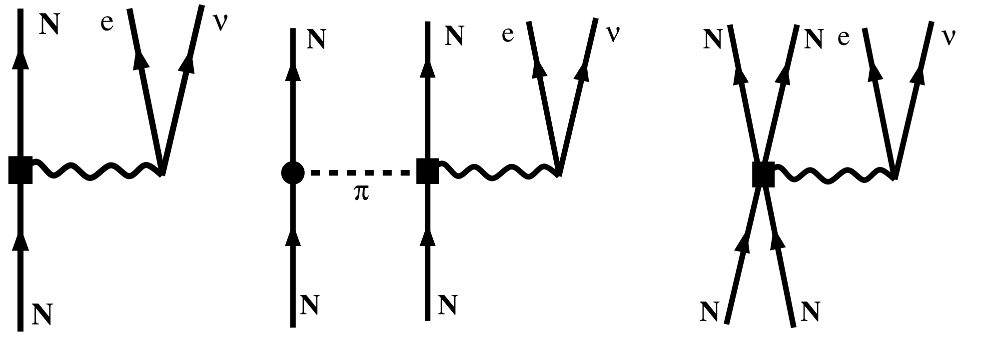
P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

TRIUMF

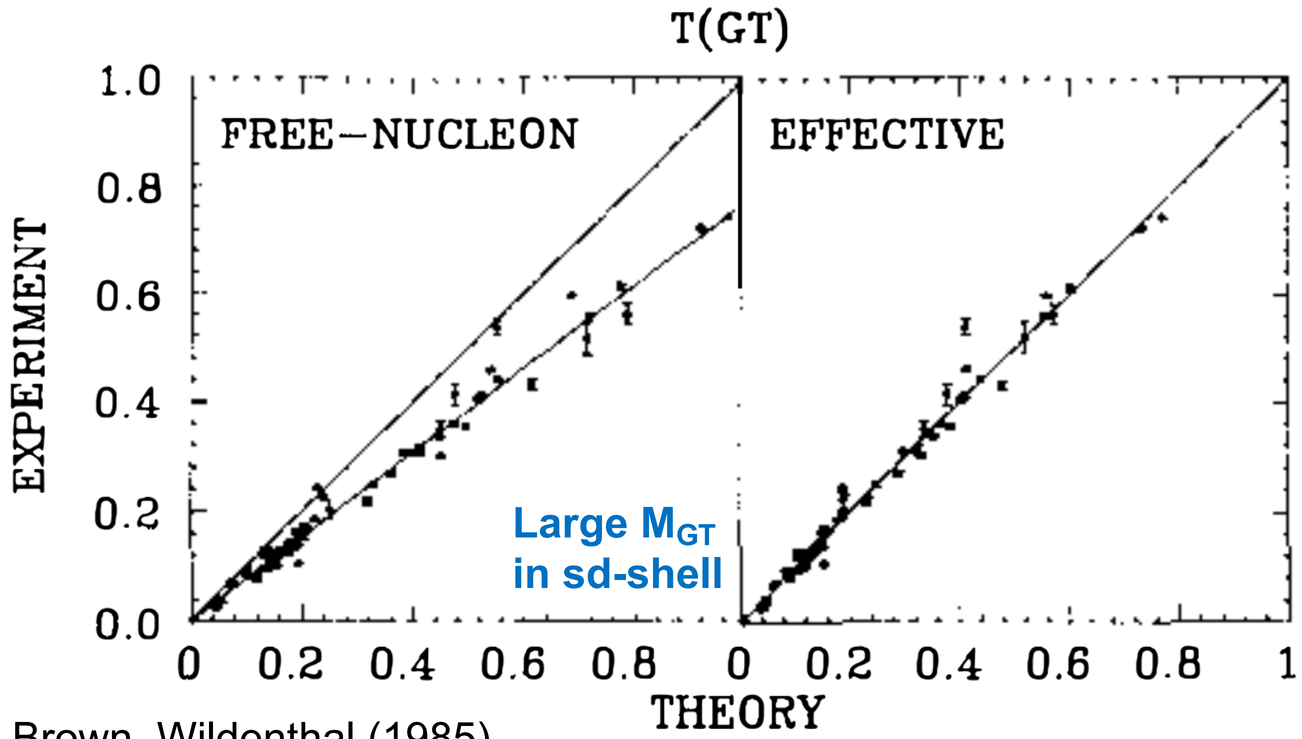
Beta-Decay "Puzzle": Quenching of g_A

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

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



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

Large-Scale Efforts for Ab Initio GT Transitions

TRIUMF

Calculate **large GT matrix elements**

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

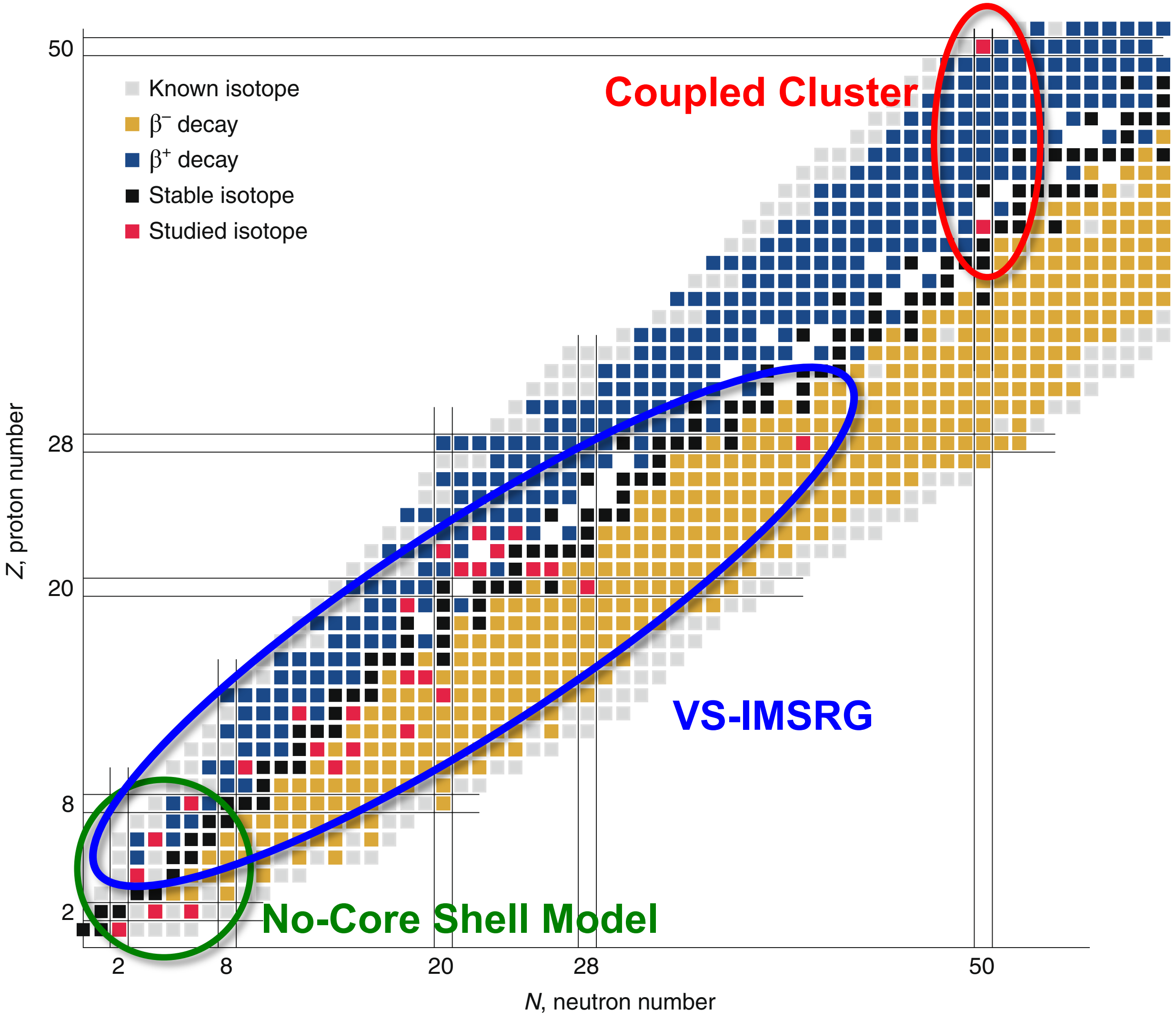
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

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

NUCLEAR PHYSICS

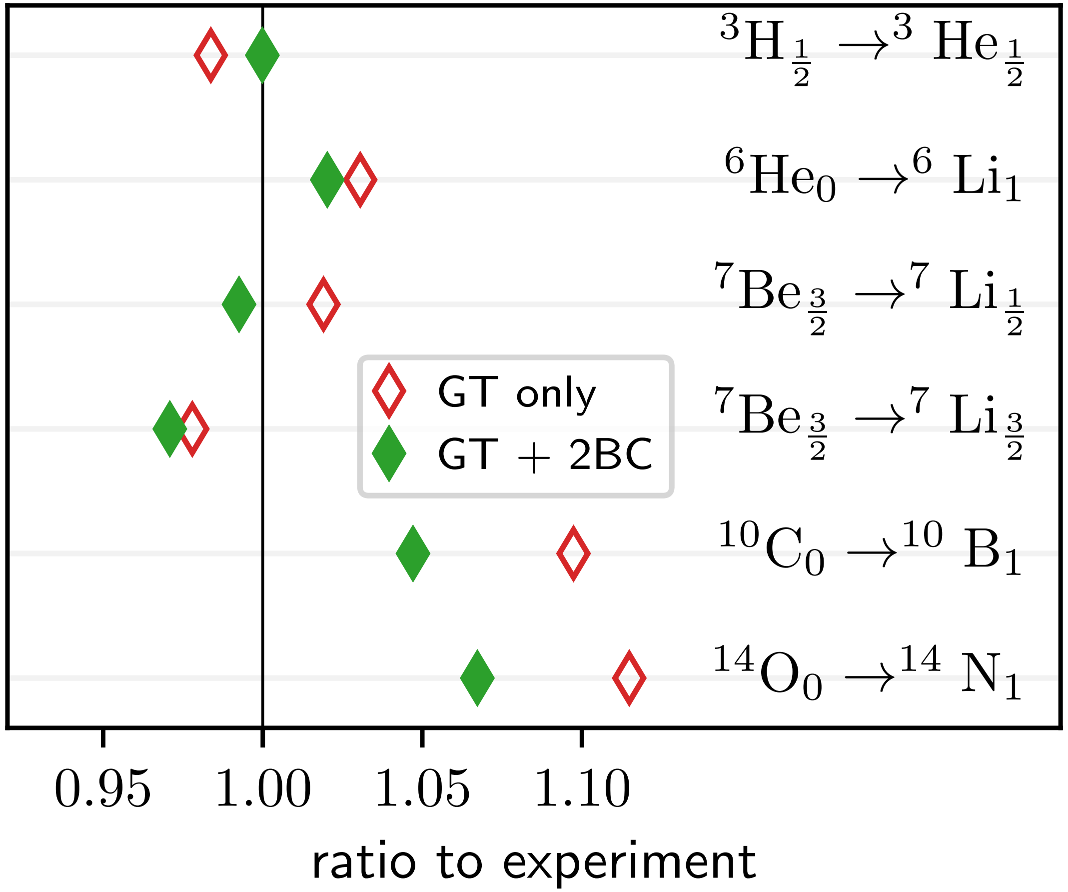
Beta decay gets the ab initio treatment

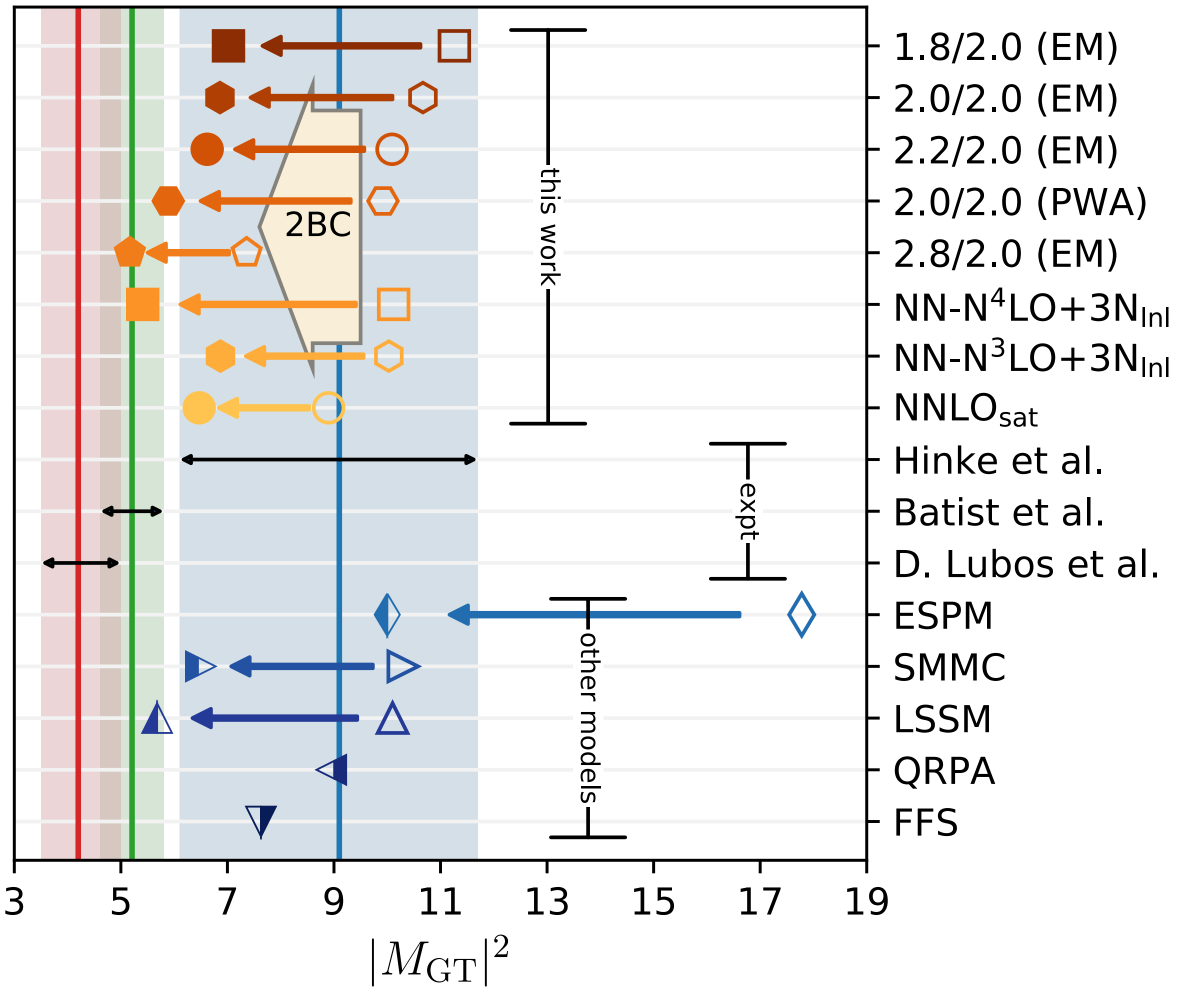
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.



GT Transitions in Light Nuclei + ^{100}Sn

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



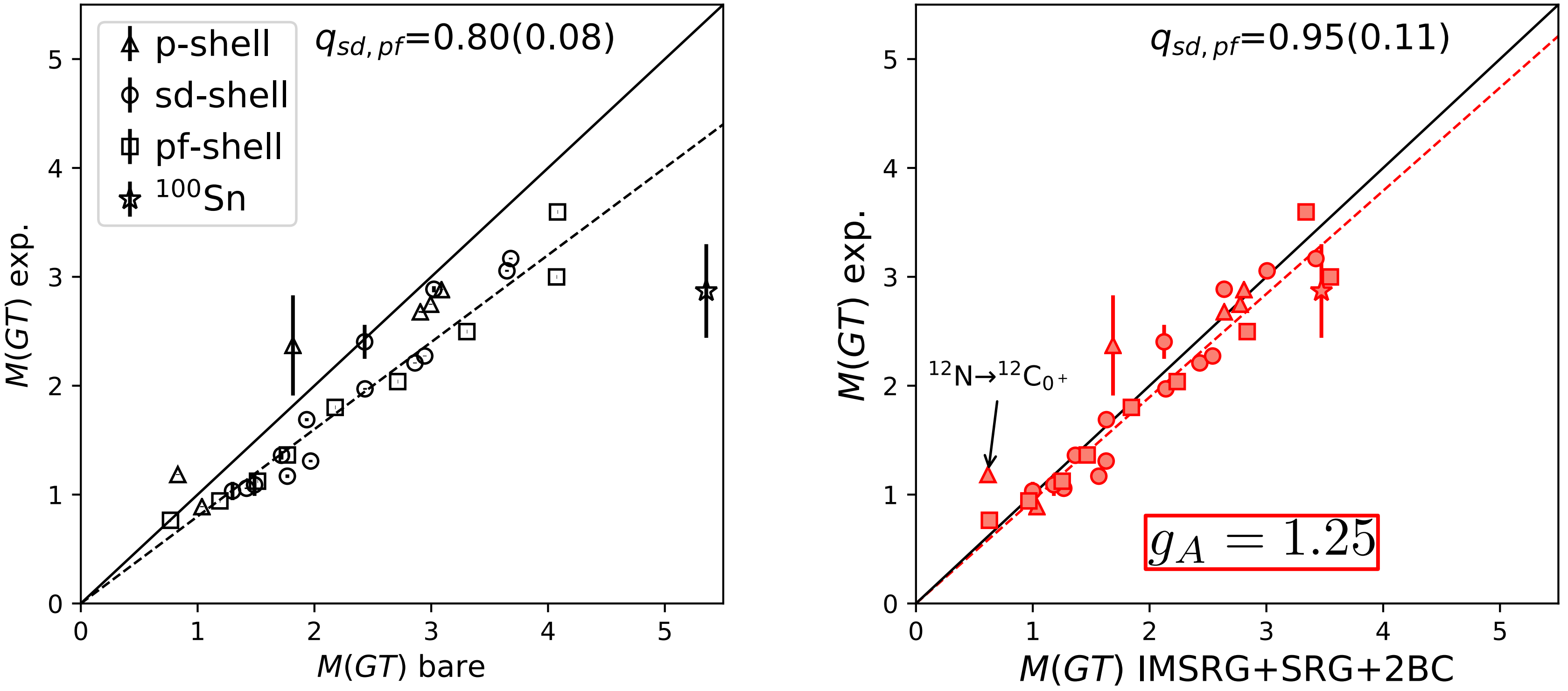


Large quenching from correlations in ^{100}Sn

Addition of 2BC further quenches; reduces spread in results

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)

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

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

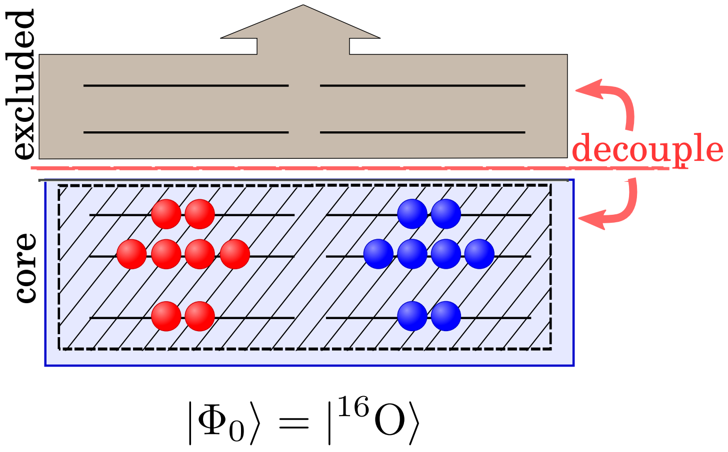
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

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

IMSRG(3) in progress

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

Step 1: Decouple core



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

Explicitly construct unitary transformation from sequence of rotations

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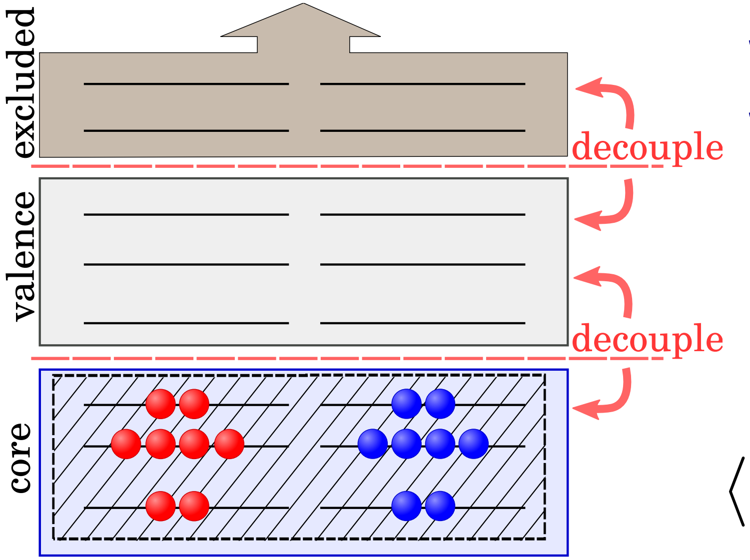
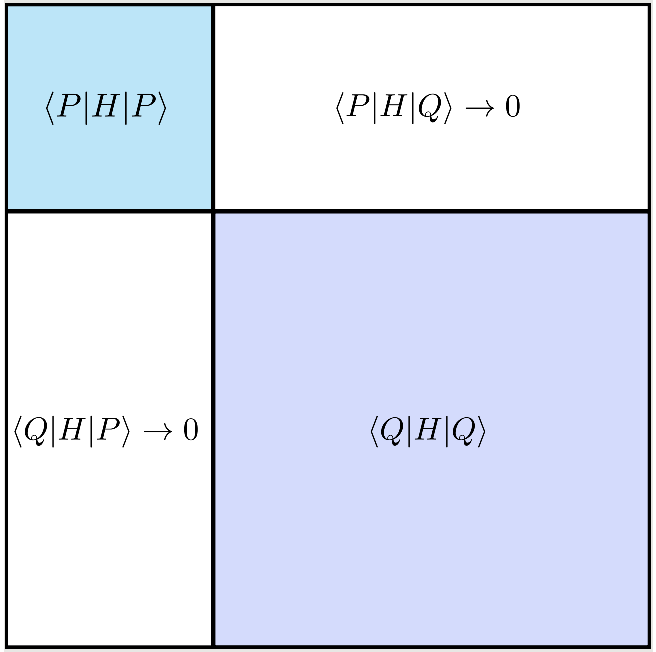


$|\Phi_0\rangle = |^{16}\mathrm{O}\rangle$

Step 1: Decouple core
Step 2: Decouple valence space

Can we achieve accuracy of large-space methods?

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



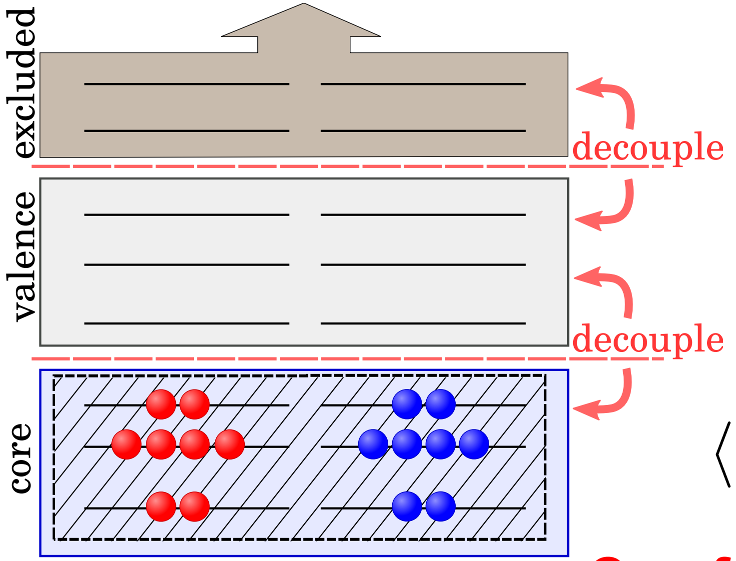
Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

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

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

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



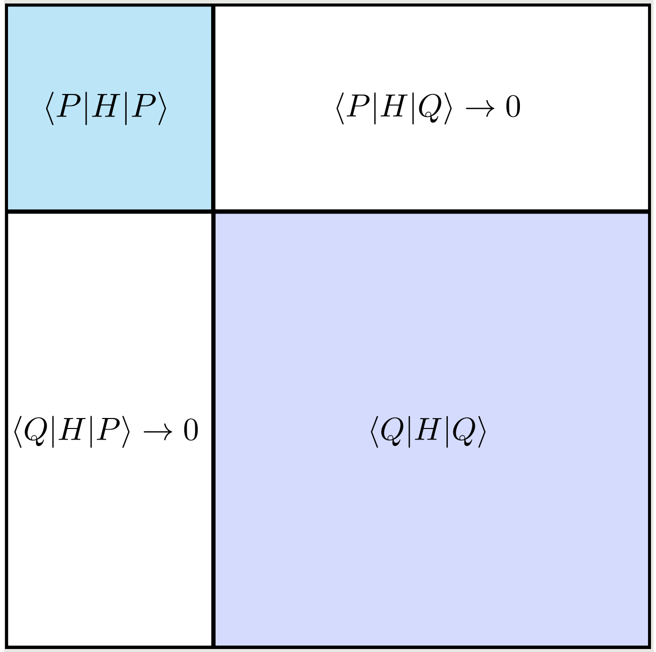
$|\Phi_0\rangle = |{}^{16}\mathrm{O}\rangle$

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

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

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

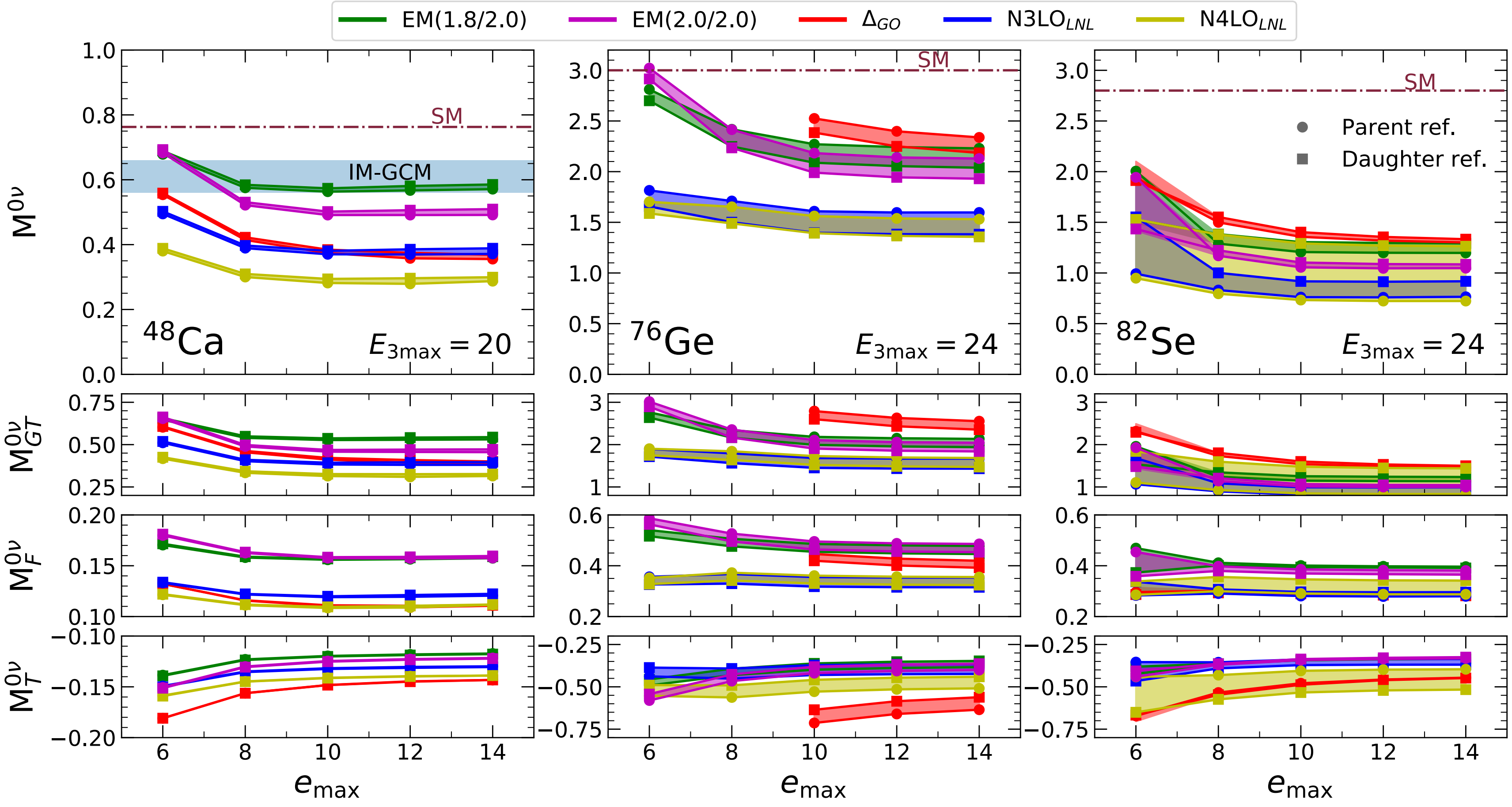
Careful benchmarking essential



Strategy II: "Uncertainties" from Input Forces

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

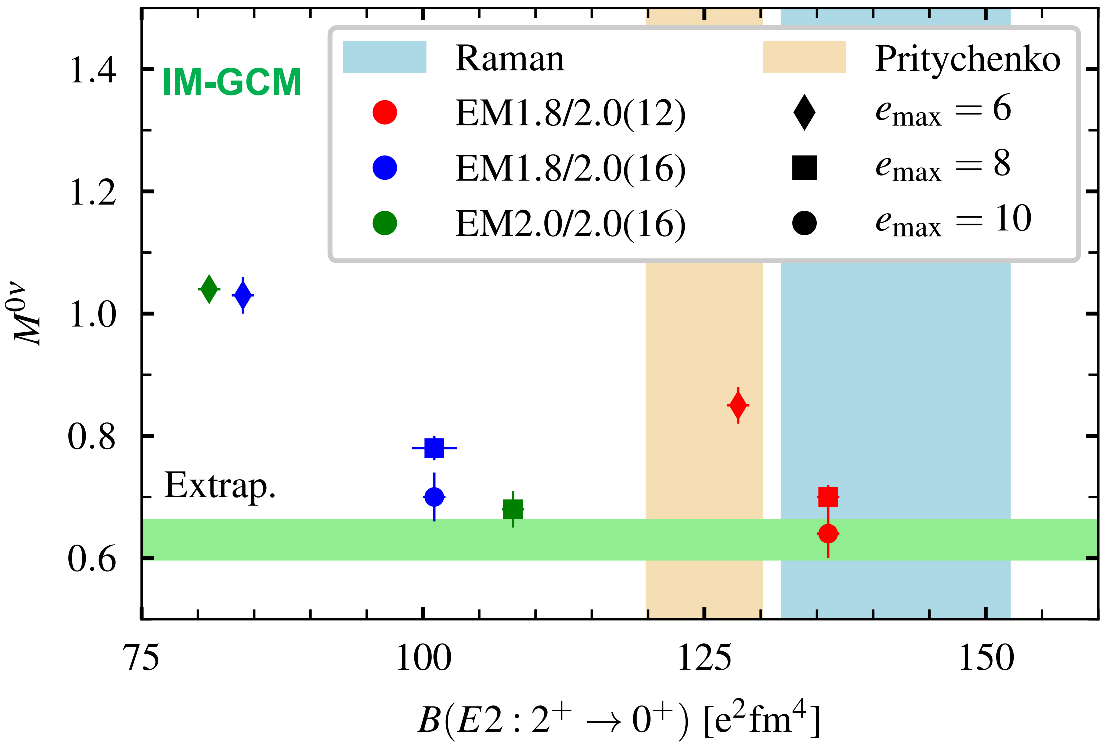
VS-IMSRG: clear convergence for ^{48}Ca, ^{76}Ge, ^{82}Se

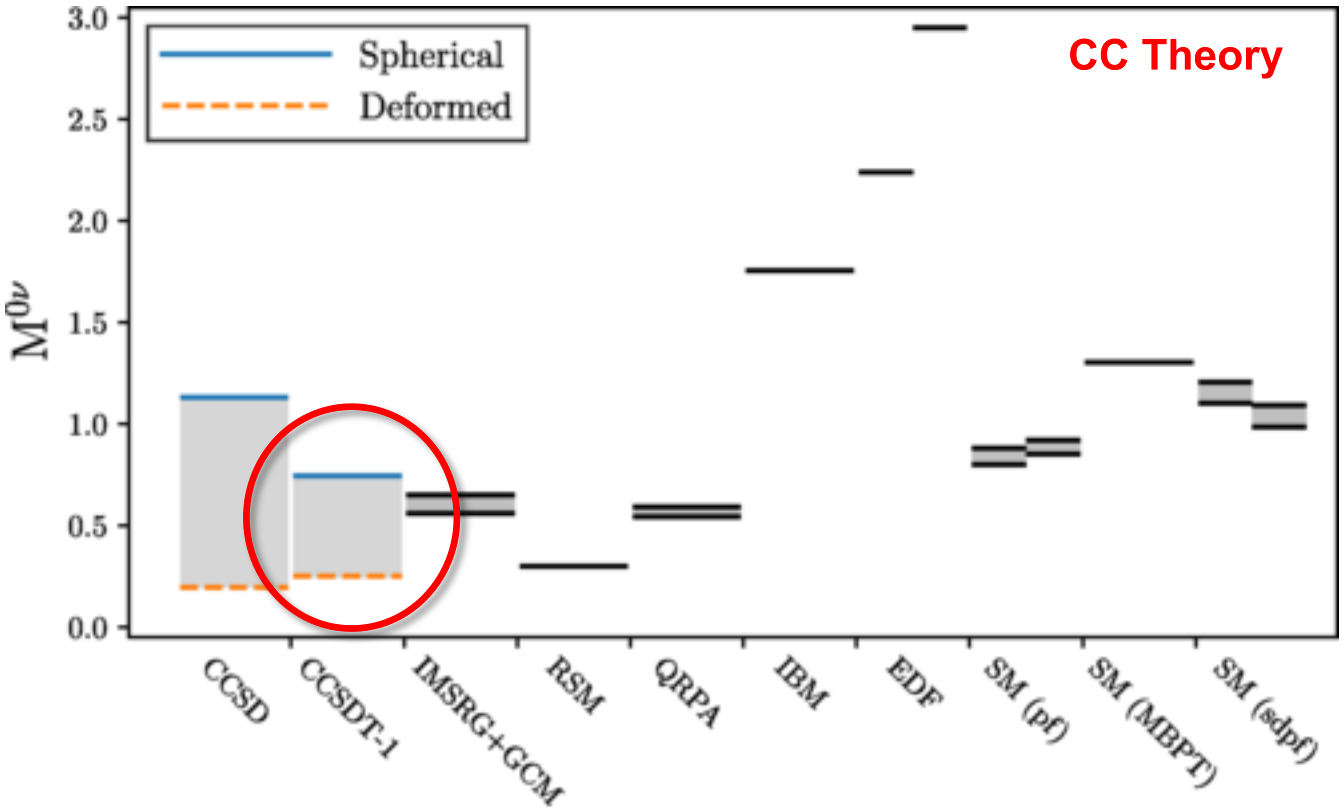


Strategy II: "Uncertainties" from Many-Body Methods

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

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





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

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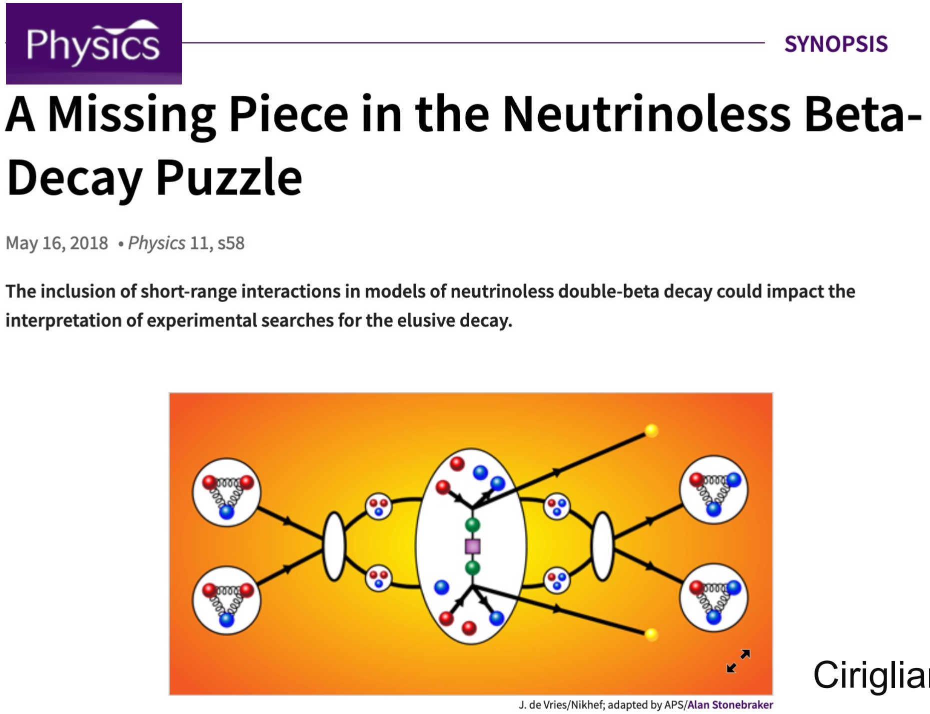
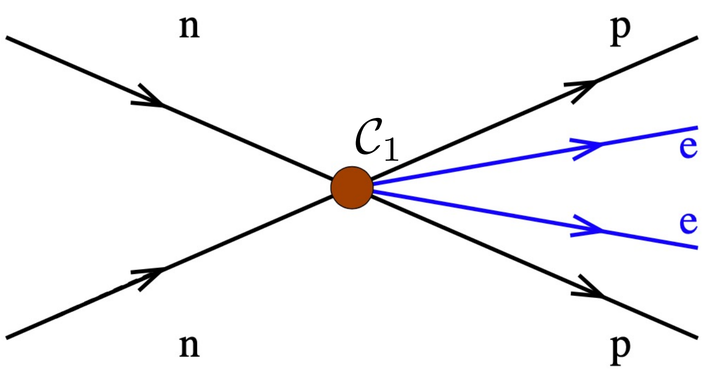
Proper renormalization requires short-range contact term at leading order



Cirigliano et al. PRL (2018)



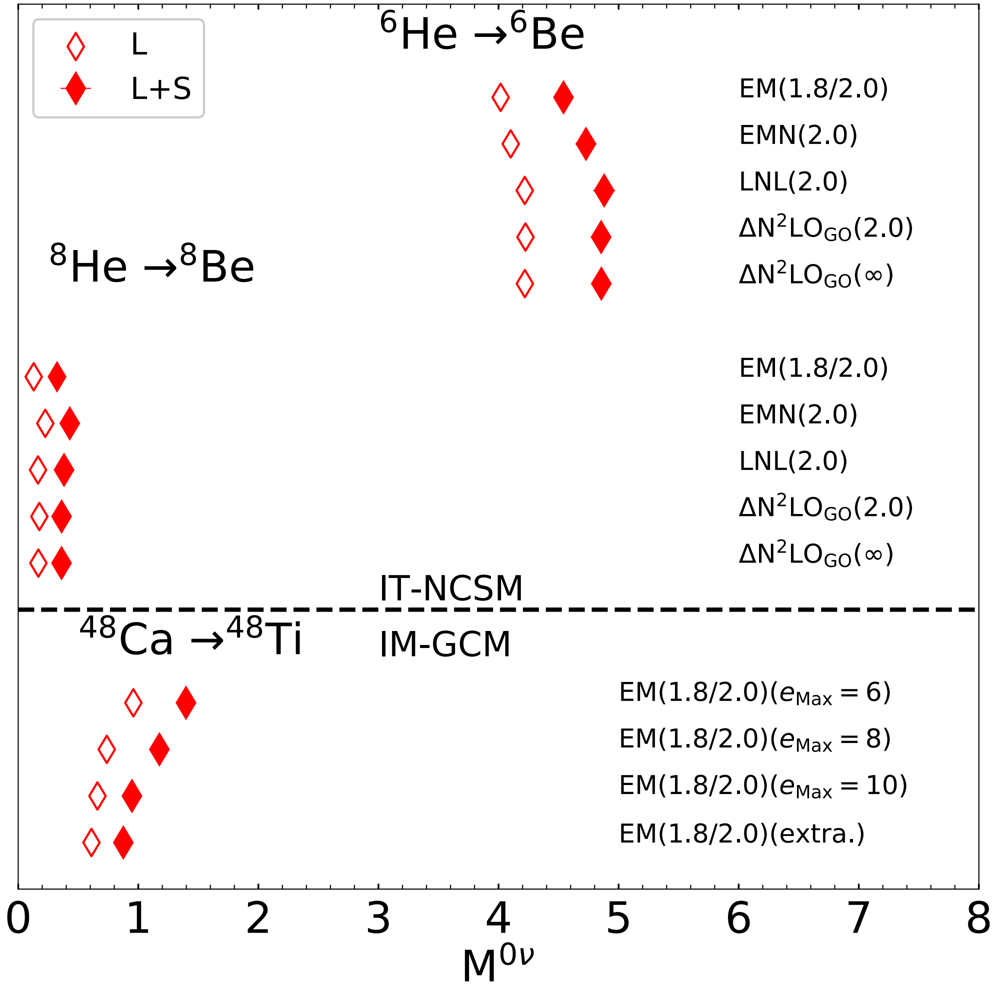
New physics inside blob:
High-energy ν exchange

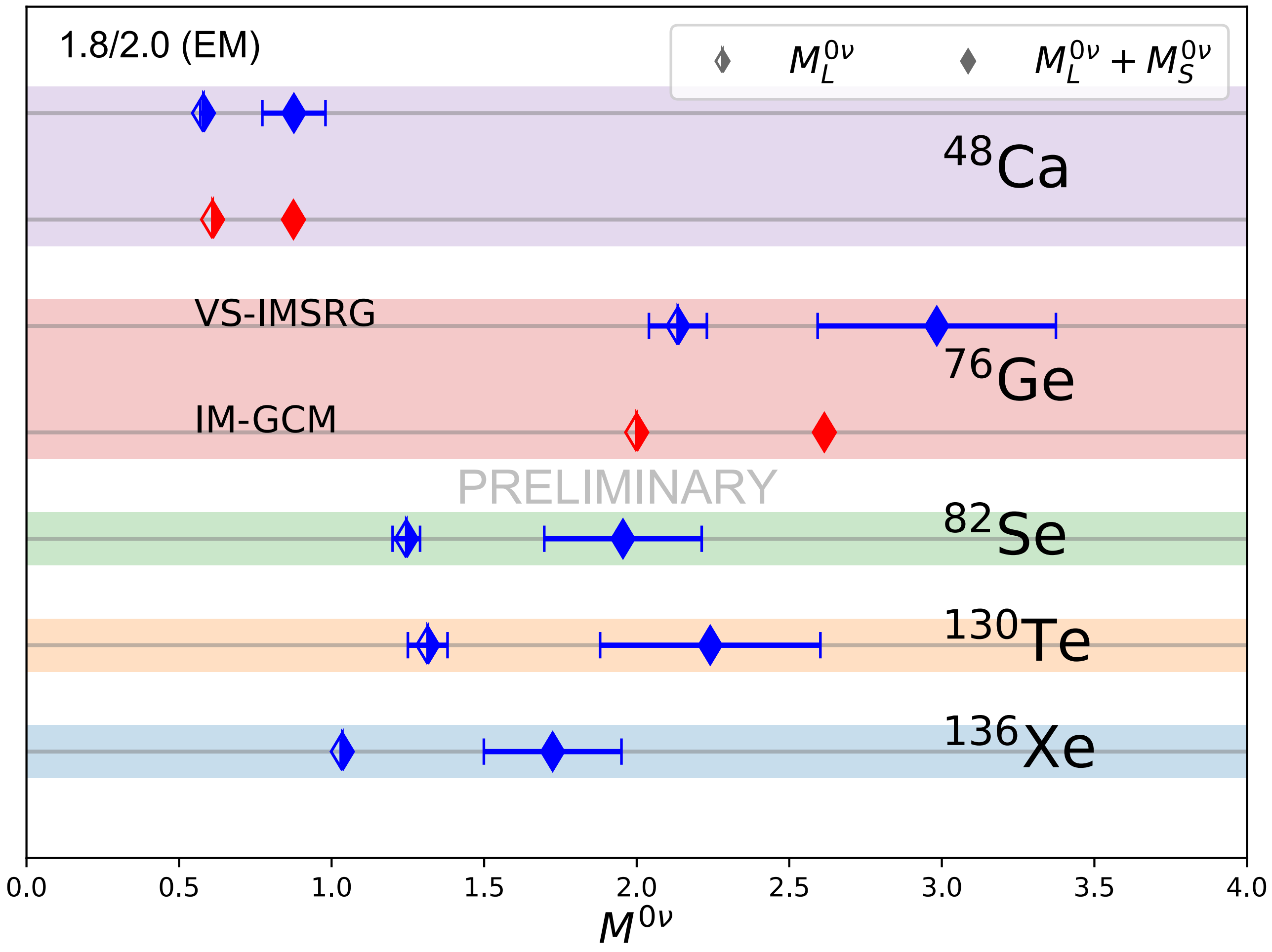
New paradigm for 0νββ decay: include long- and short-range terms

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

The Year We Regained Hope: Coupling Constant Fit

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



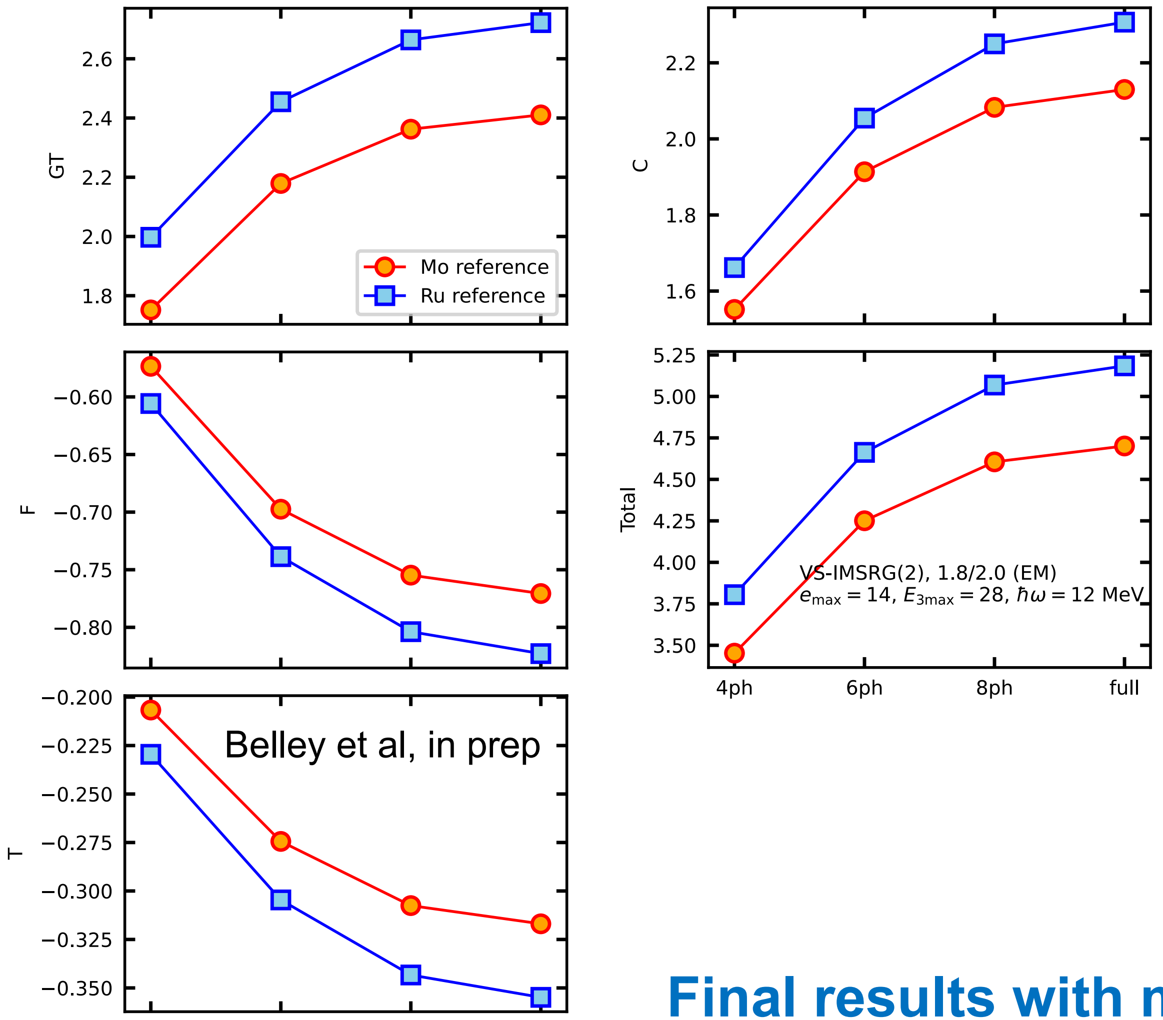


Increase of 40% (^{76}Ge) to 60% (^{130}Te/^{136}Xe)

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



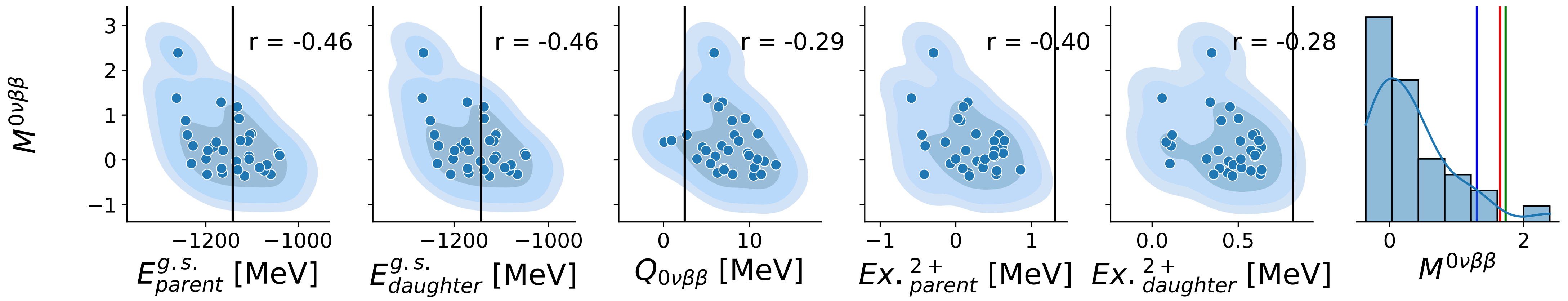
Final results with multiple NN+3N forces coming soon!

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

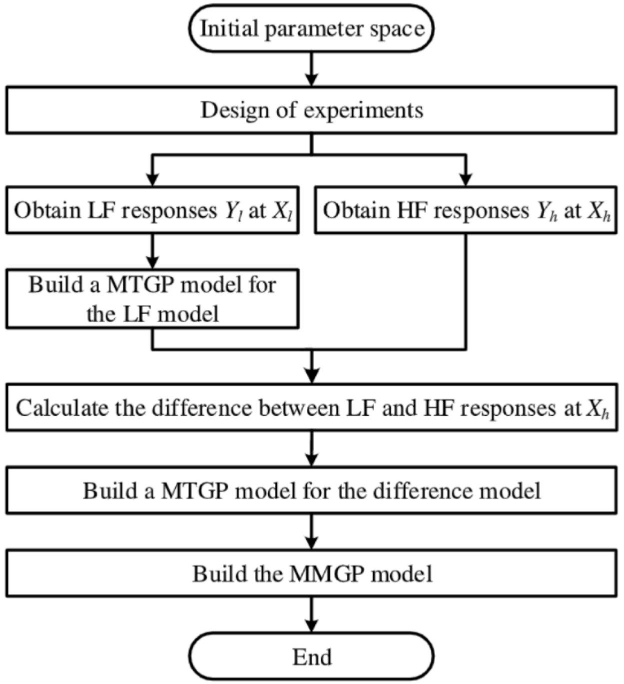
Explore dependence on chiral EFT LECs: requires many samples (as in ^{208}Pb)

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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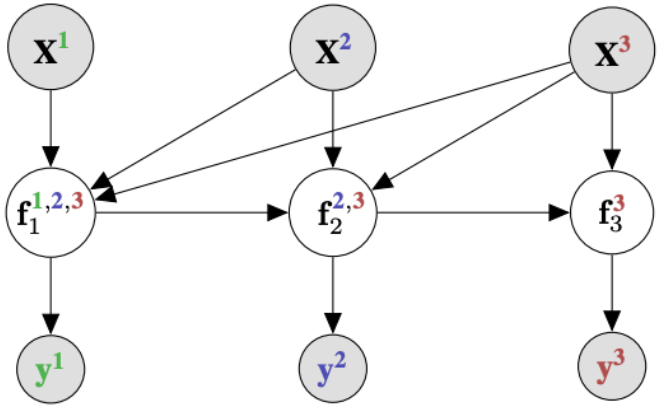
Deep Gaussian Process: Neural network links multiple GP



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

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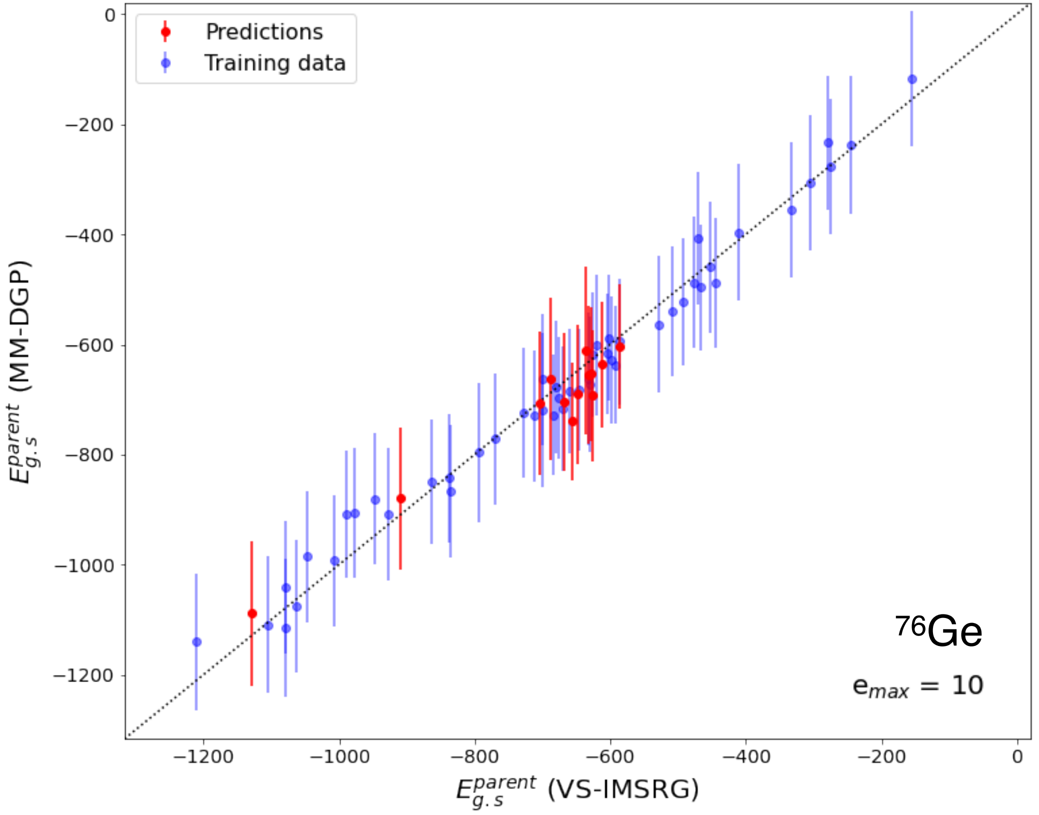
MM-DGP Emulator: Ground-State Energies

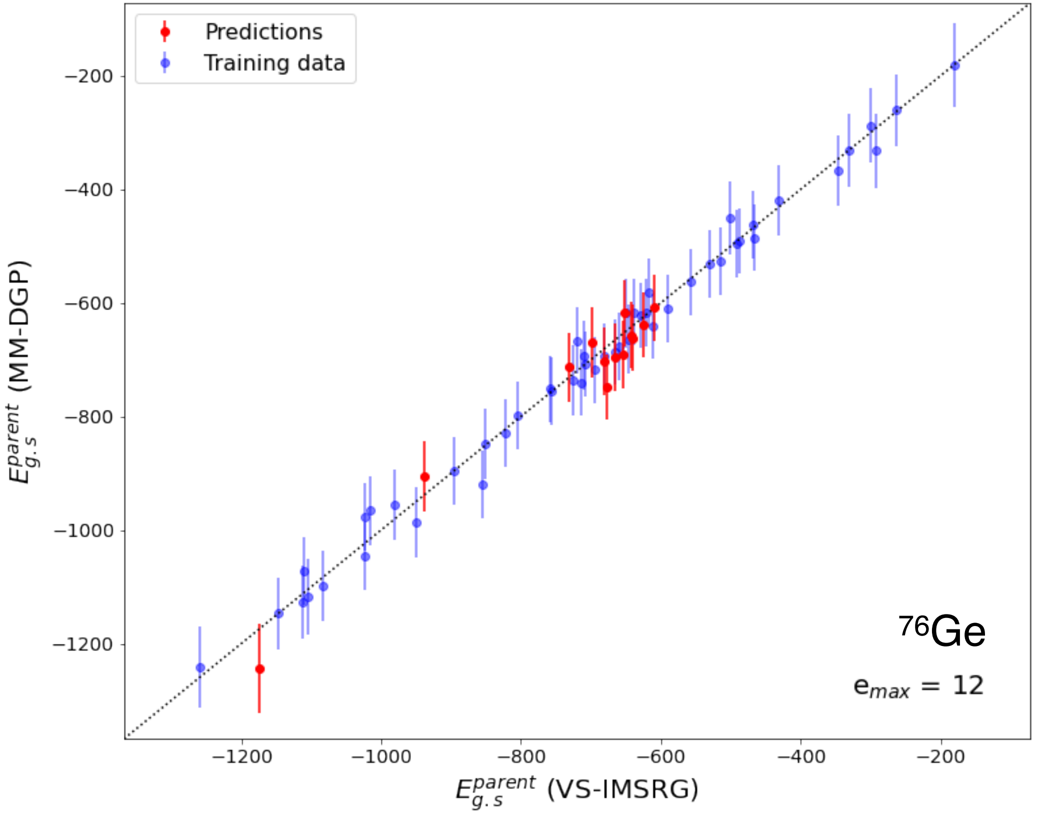
Testing MM-DGP: use delta-full chiral EFT at N2LO

Improved energy predictions with high-fidelity training points

Low-Fidelity



High-Fidelity



Belley, Pitcher et al. in prep.

TRIUMF

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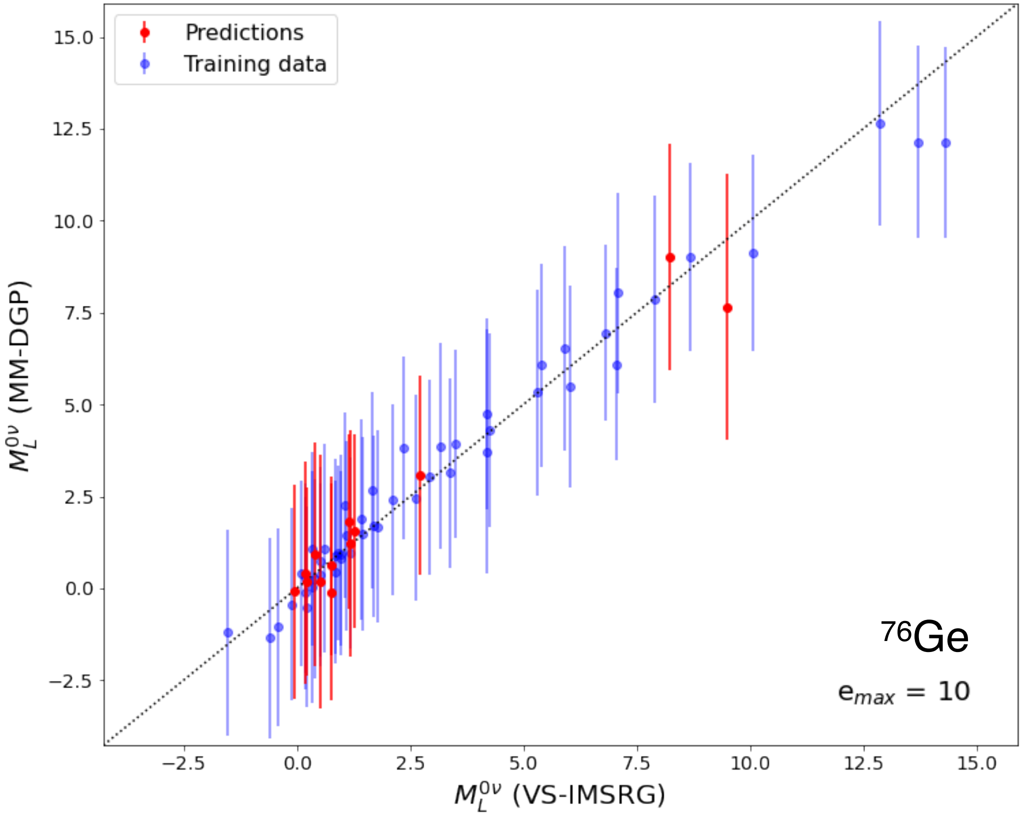
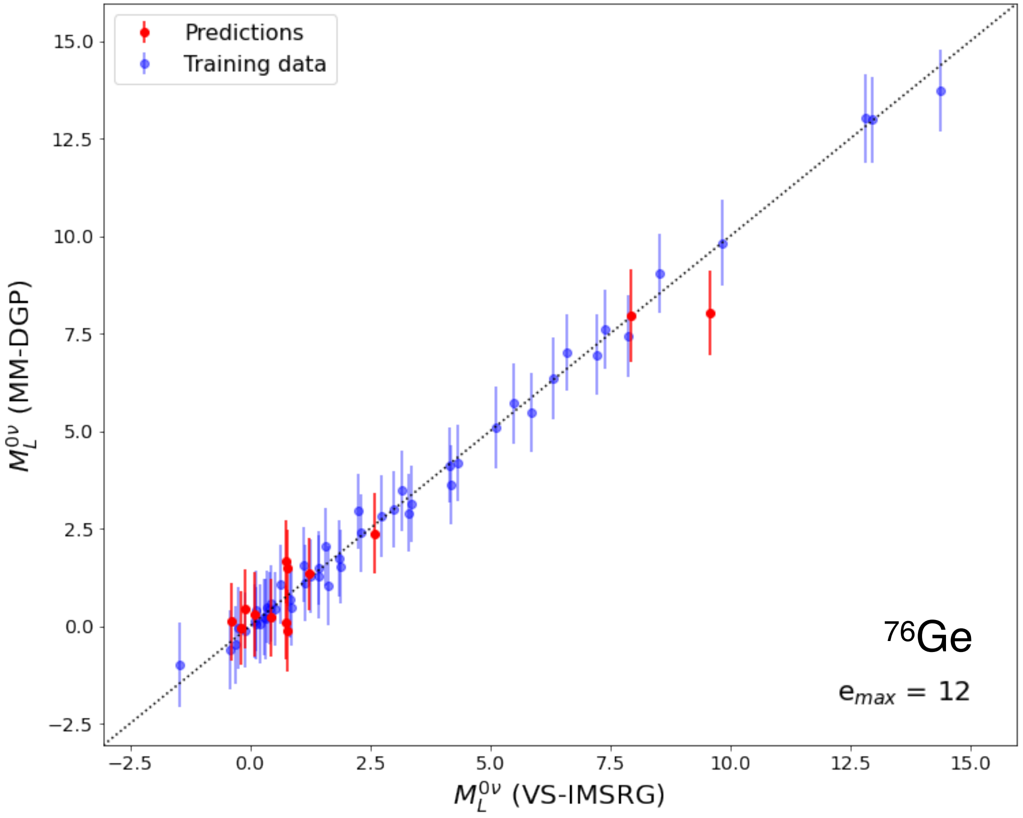


High-Fidelity



Belley, Pitcher et al. in prep.