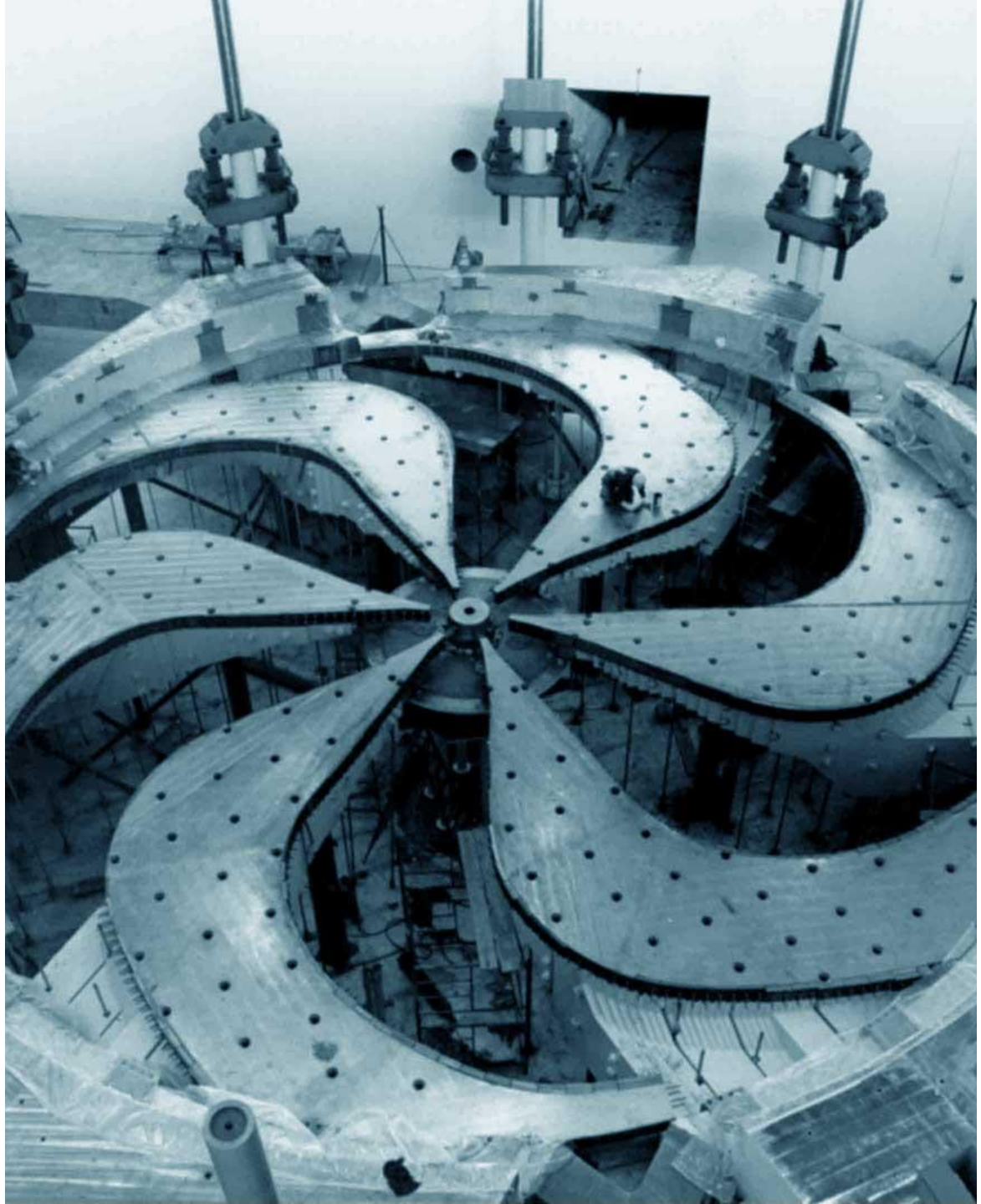
First-Principles Theory for Nuclear Structure, Astrophysics, and New Physics Searches

Jason D. Holt
TRIUMF, McGill University
CAP Congress
Saskatoon, SK; June 10, 2025

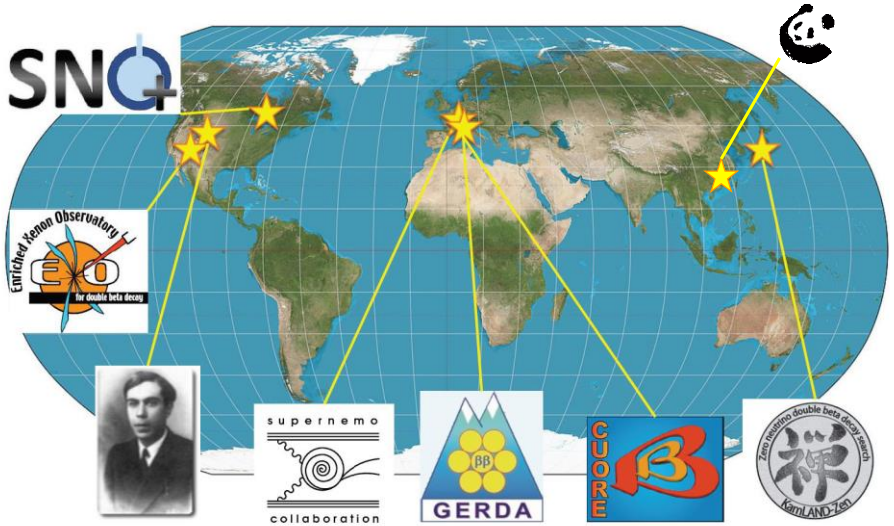


Discovery, accelerated

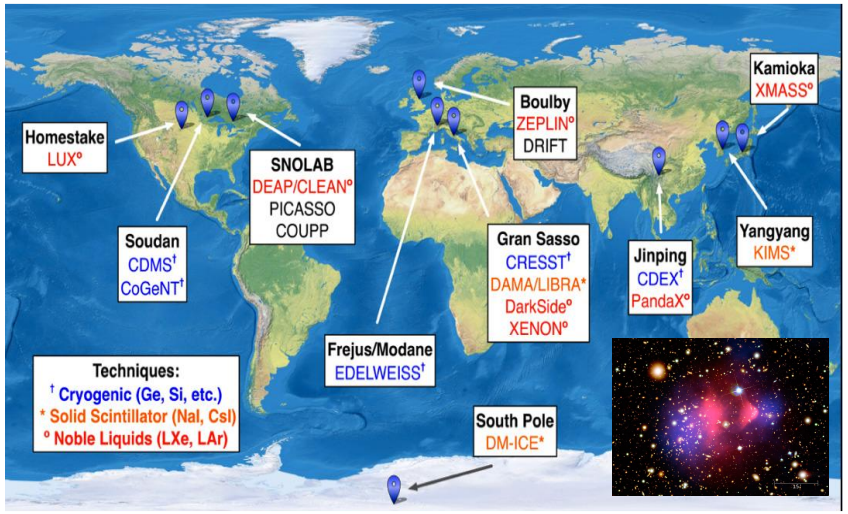
Major BSM Searches Worldwide

Worldwide search for BSM physics w/ neutrinos, dark matter, and radioactive molecules!

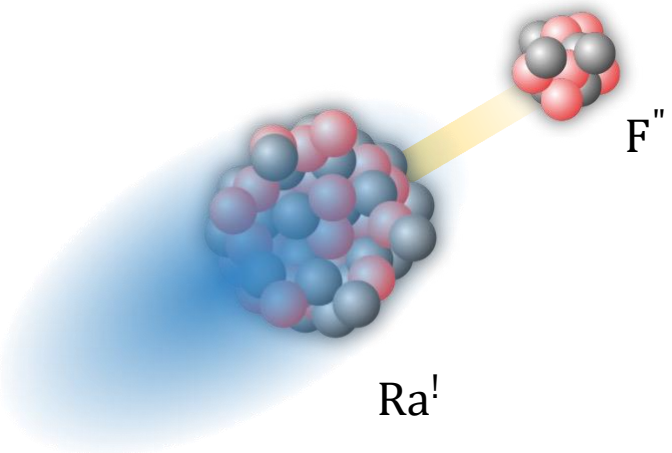
0νββ Decay



Dark Matter Direct Detection



Symmetry Violation



Billions invested worldwide – theory of the nucleus is essential

Strategic planning for discovery (**motivation**) + **interpretation**

Atomic Nucleus Drives New Physics Discoveries

Nuclear theory vital for SIX of eight key science drivers: Canadian SAP-LRP

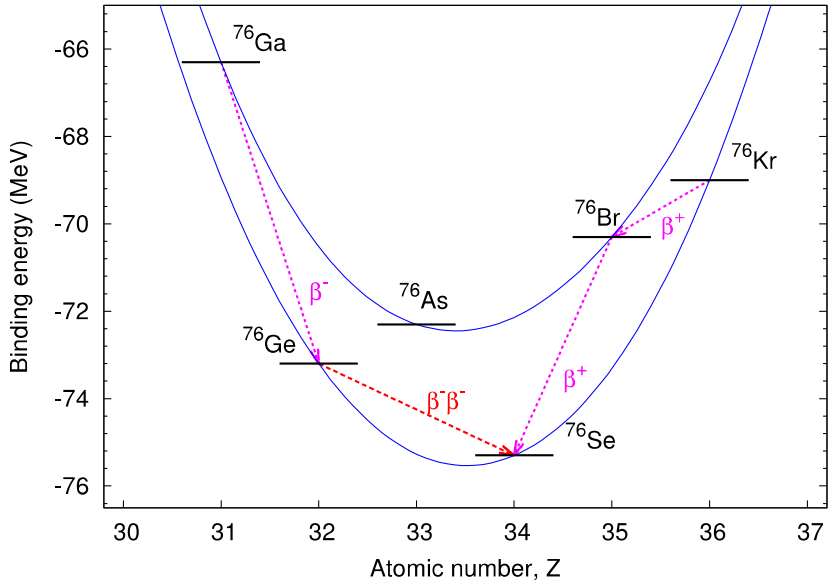
SUBATOMIC PHYSICS
is a fundamental science that seeks to understand the basic building blocks of the universe and the laws that explain the behaviour of those constituents.

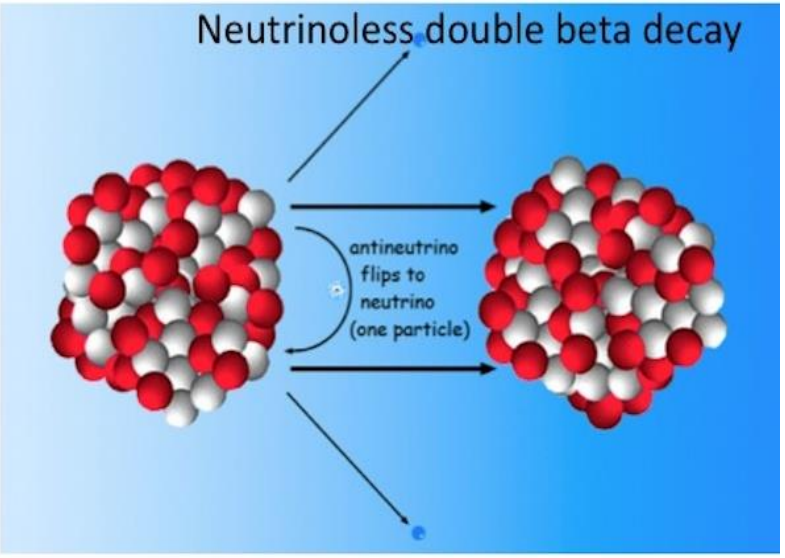
Canadian science priorities similar to those of US (but valued at 0.736)

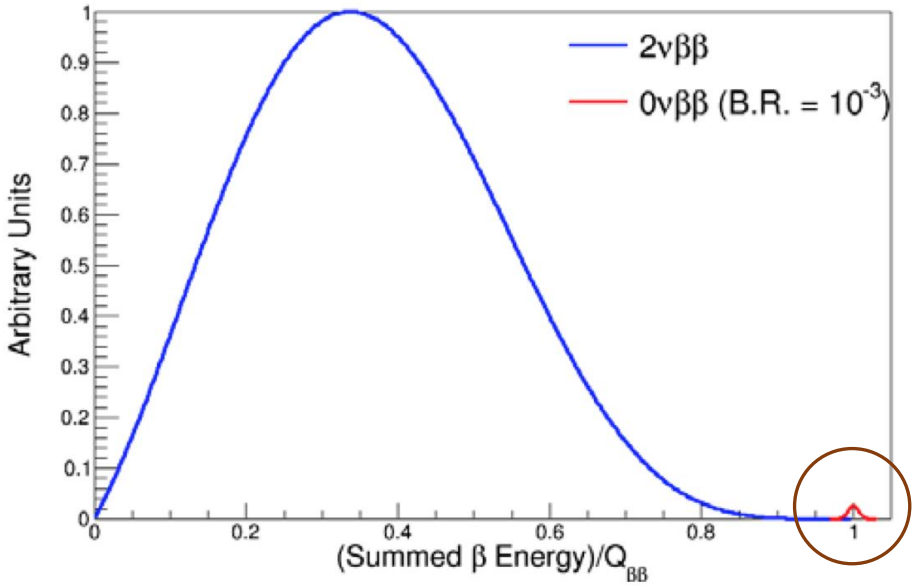
- Nuclear Structure
- Cosmic Formation of Nuclei
- **Dark Matter Detection**
- **Electroweak Scale and Beyond**
- **Fundamental Symmetries: anti/matter asymmetry**
- **Neutrino Properties**
- **New Connection: Hadron Properties and Phases**

Neutrino-less (0ν) Double-Beta (ββ) Decay

Neutrino own antiparticle $\Longleftrightarrow$ 0νββ decay







Tremendous impact on BSM physics

Lepton-number violation

Majorana character of neutrino

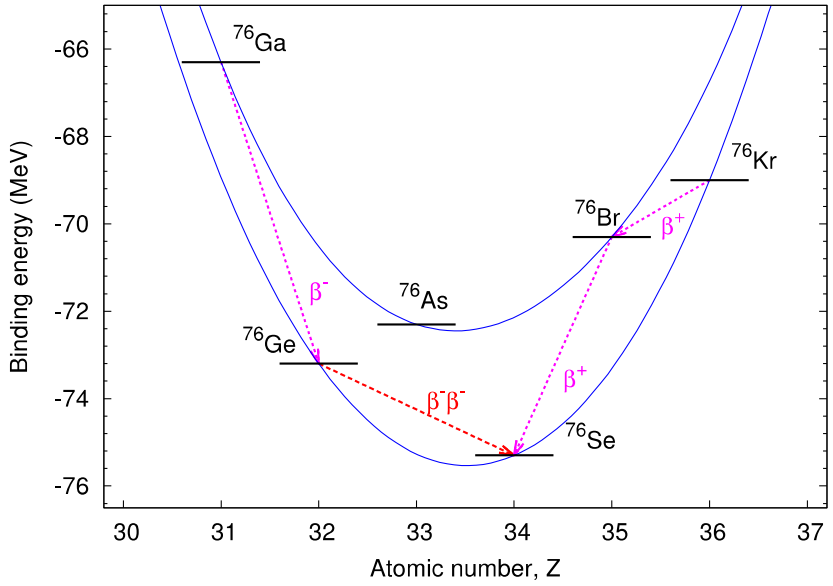
Matter/antimatter asymmetry

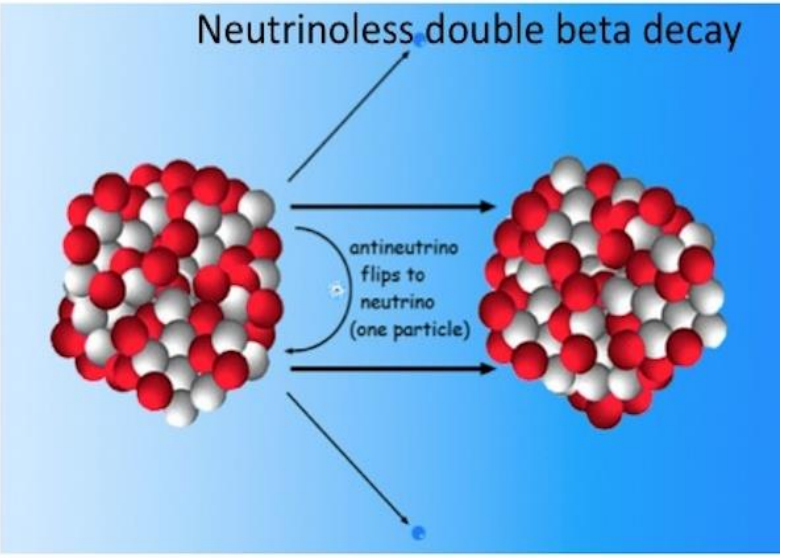
Absolute neutrino mass scale

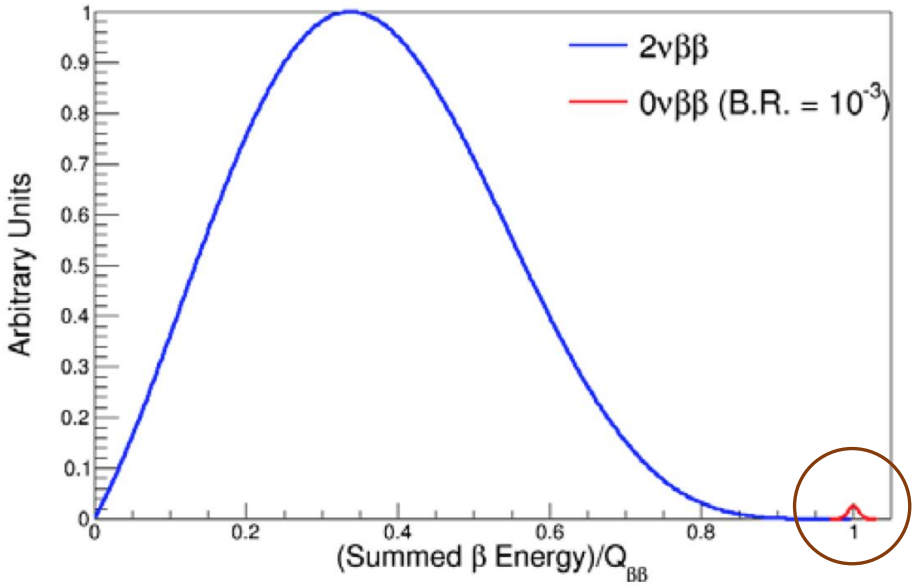
$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu}\left|M^{0\nu}\right|^2 \langle m_{\beta\beta}\rangle^2 \quad \langle m_{\beta\beta}\rangle = \left|\sum_{i=1}^{3} U_{ei} m_i\right|$$

Neutrino-less (0ν) Double-Beta (ββ) Decay

Neutrino own antiparticle $\Longleftrightarrow$ 0νββ decay







Tremendous impact on BSM physics

Lepton-number violation/matter creation

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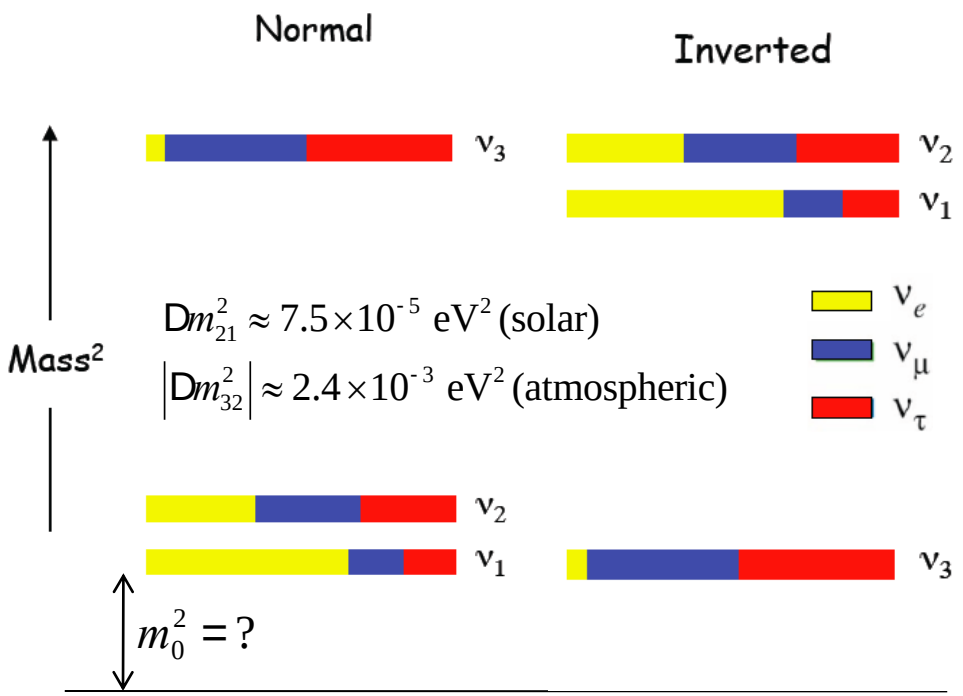
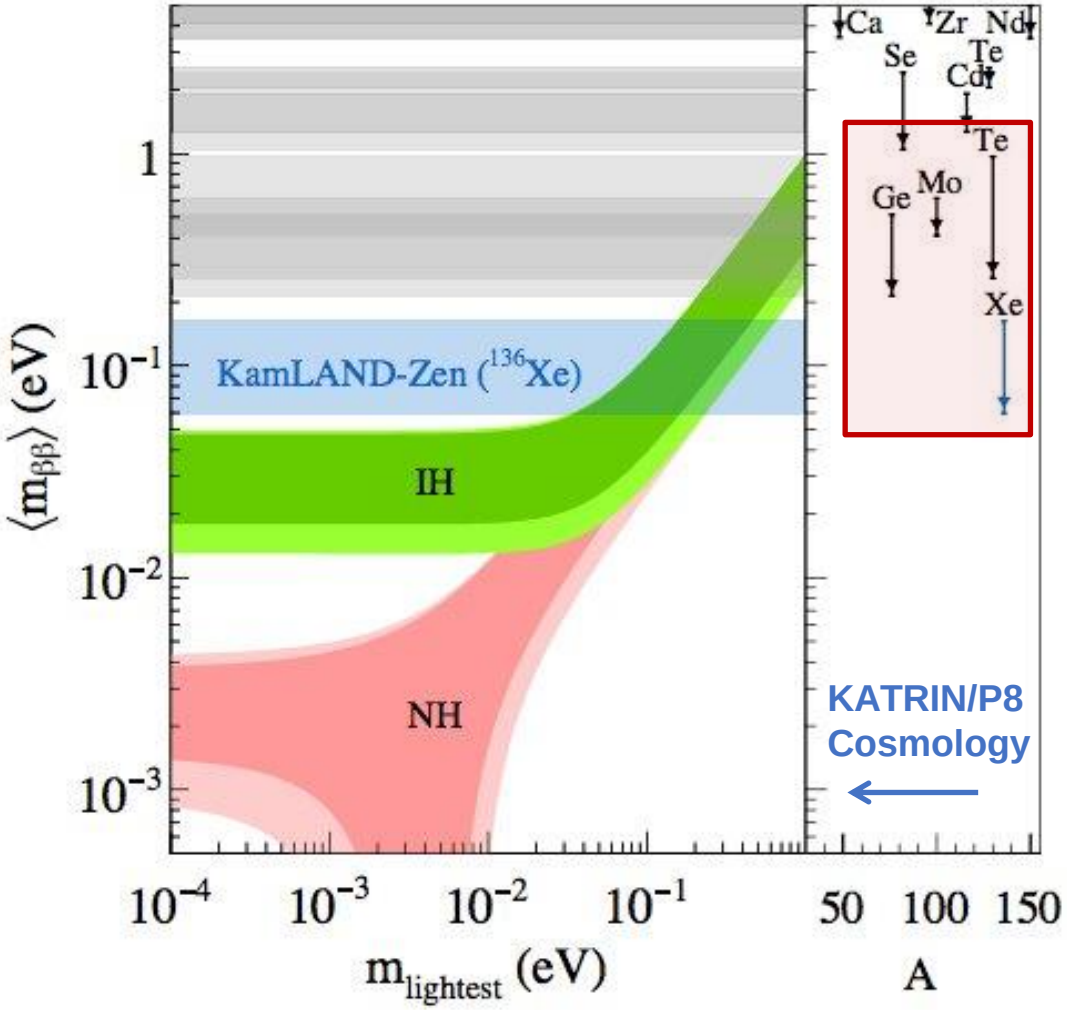
NME not observable: must be calculated

Nature of Neutrino: 0νββ Decay

Next-generation searches probe **Inverted Hierarchy**



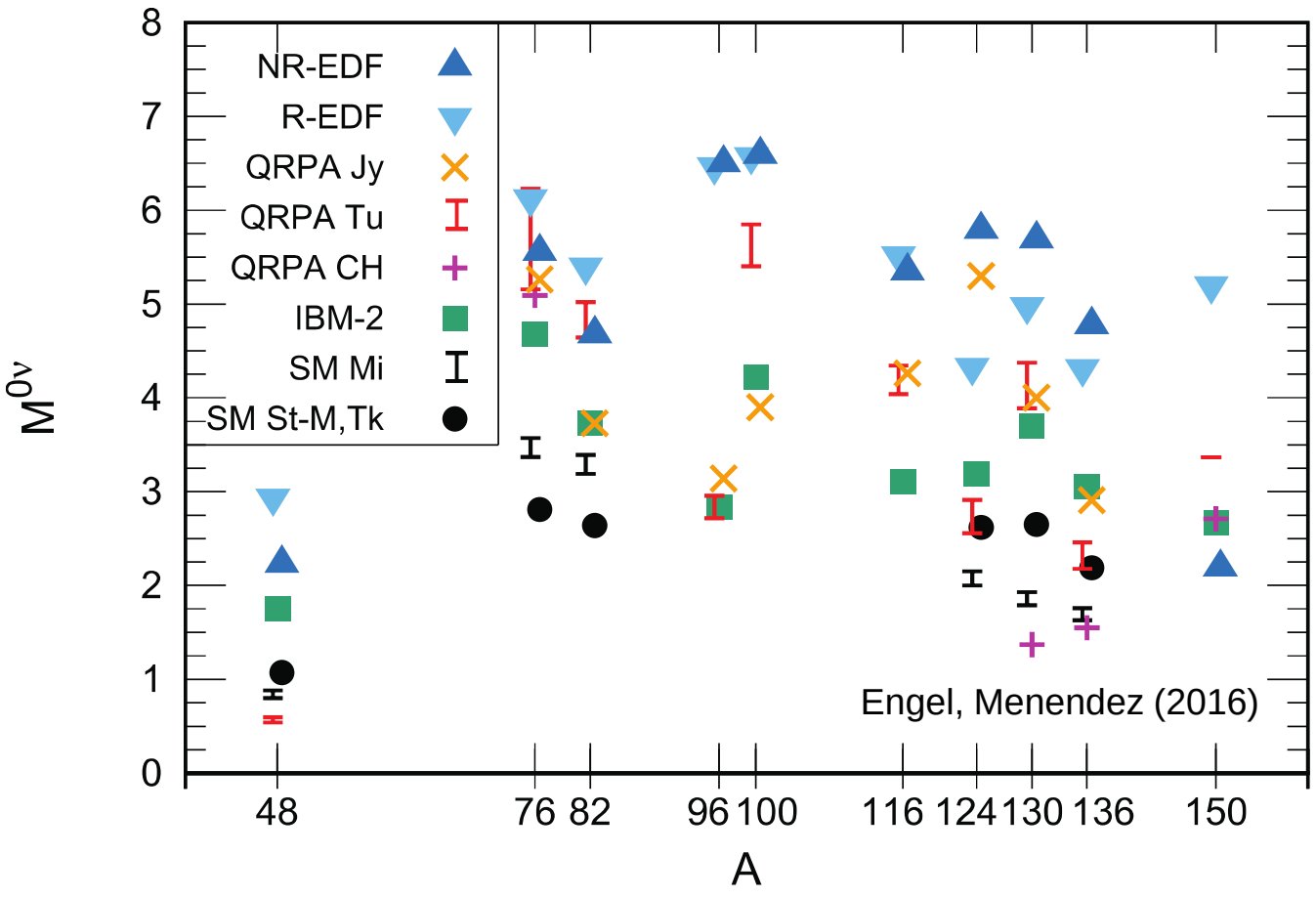


$$\left(T^{0\nu\beta\beta}_{1/2}\right)^{-1} = G^{0\nu}\left|M^{0\nu}\right|^2 \langle m_{\beta\beta}\rangle^2 \quad \langle m_{\beta\beta}\rangle = \left|\sum_{i=1}^{3} U_{ei} m_i\right|$$

Spread from **Nuclear Matrix Element**; bands **do not** represent rigorous uncertainties

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

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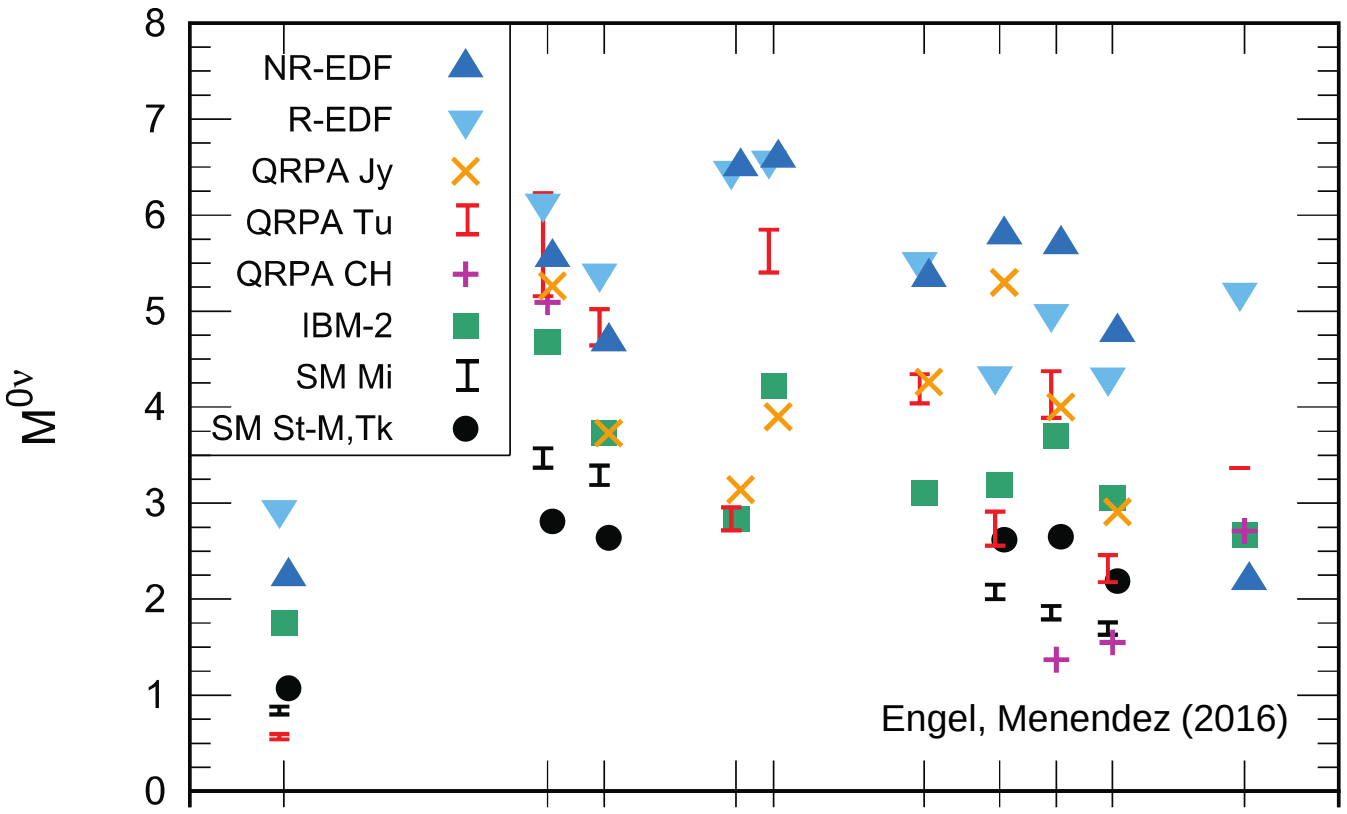
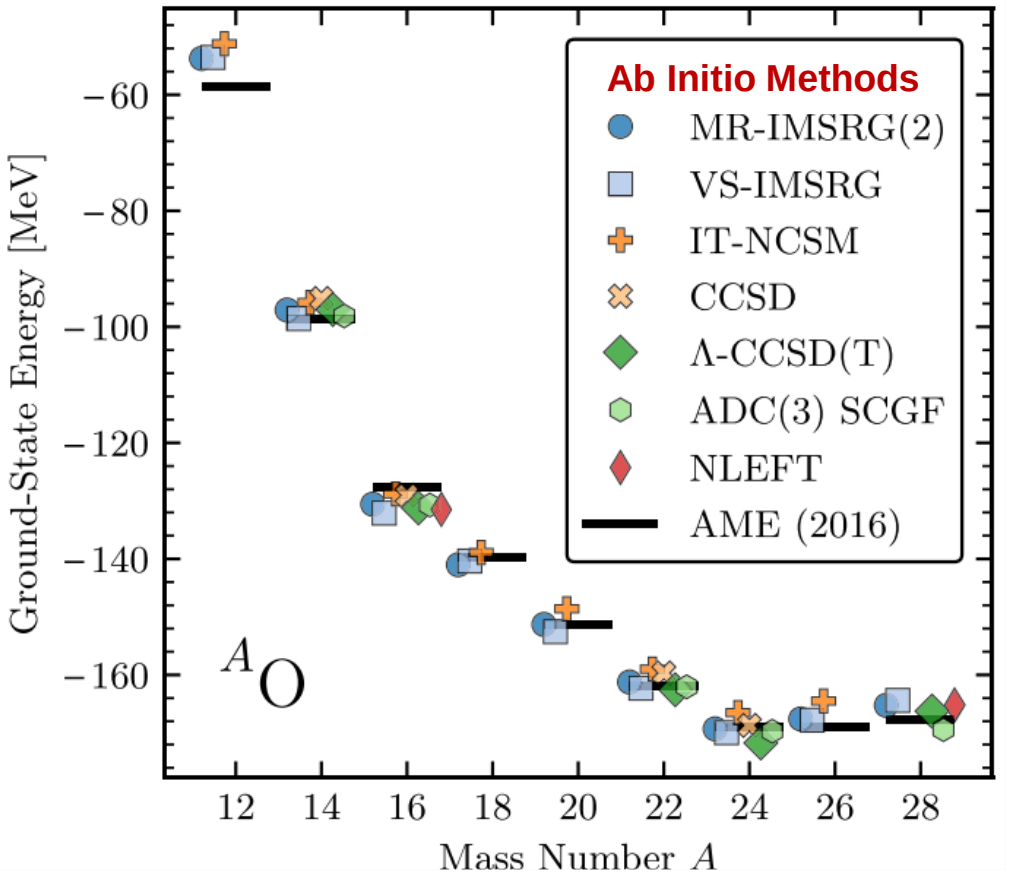




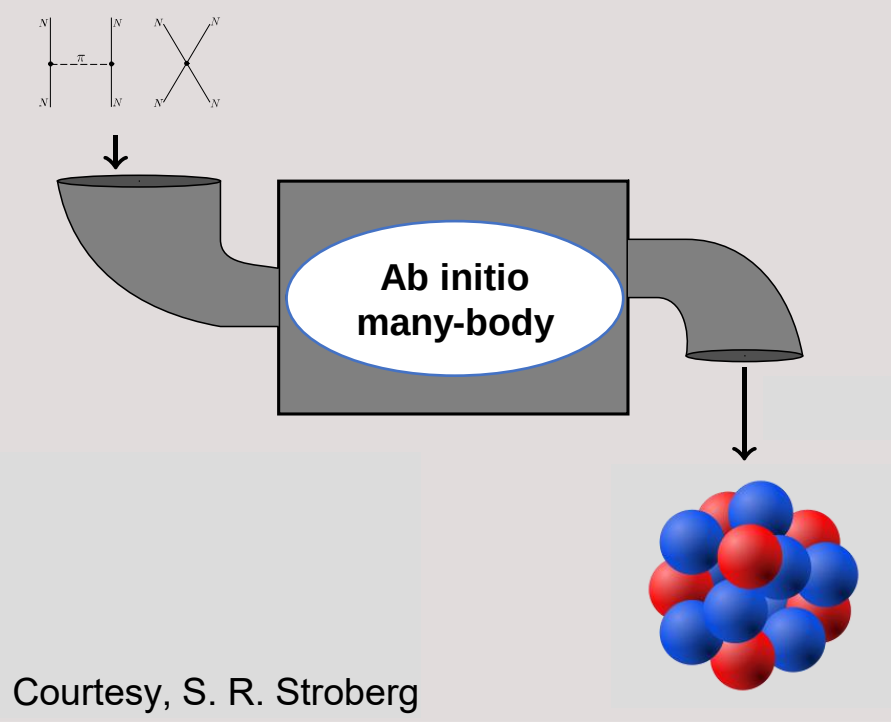
New approach to NME calculations: **ab initio theory** consistent results when extrapolated

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

$$H\psi_n = E_n\psi_n$$



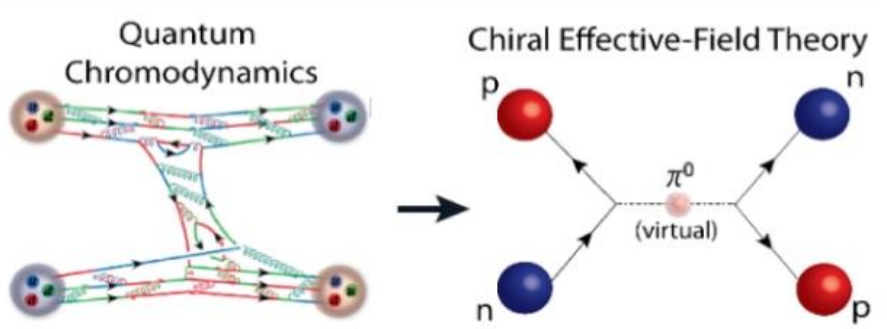
Courtesy, S. R. Stroberg

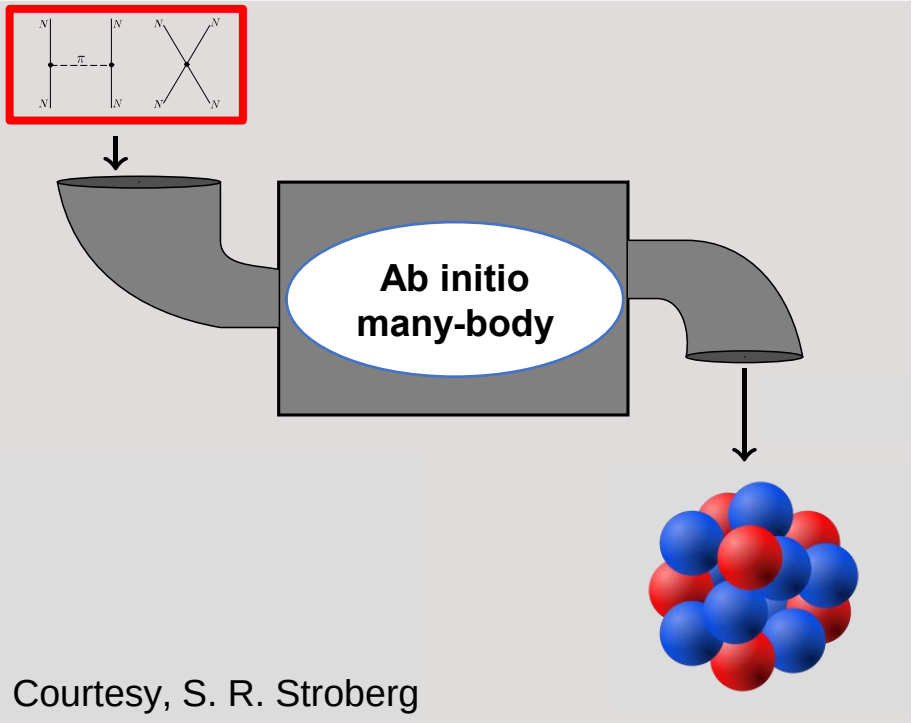
Ingredient I: Nuclear Forces

Chiral Effective Field Theory: low-energy expansion of QCD, nucleons + pions

High-energy information encoded in contact terms

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





Courtesy, S. R. Stroberg

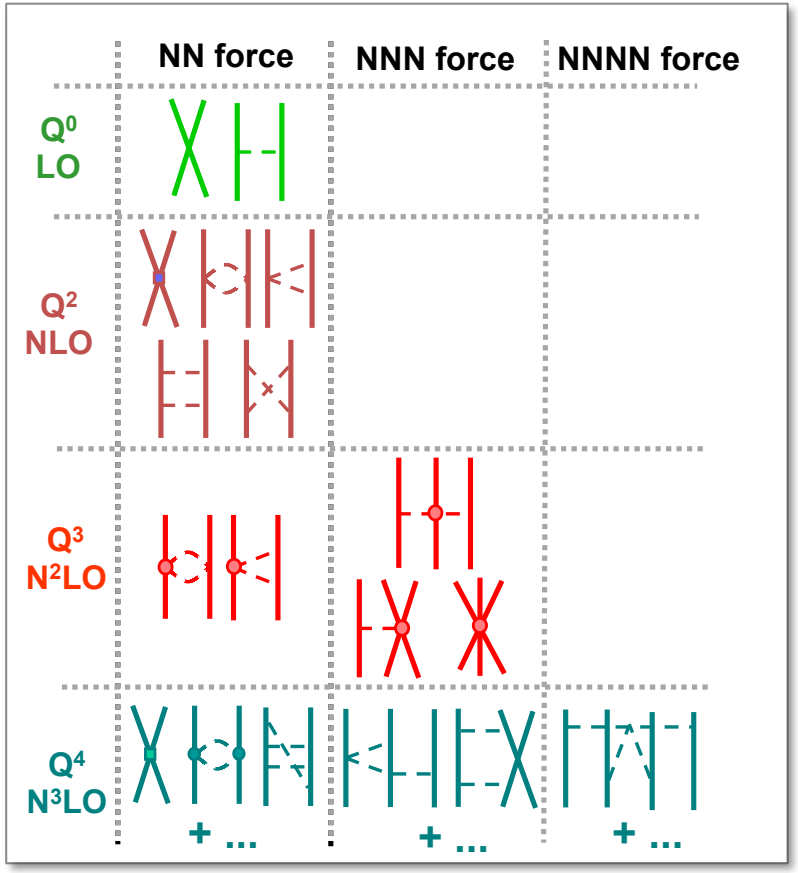
Chiral Effective Field Theory

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

Quantifiable uncertainties

Interactions

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



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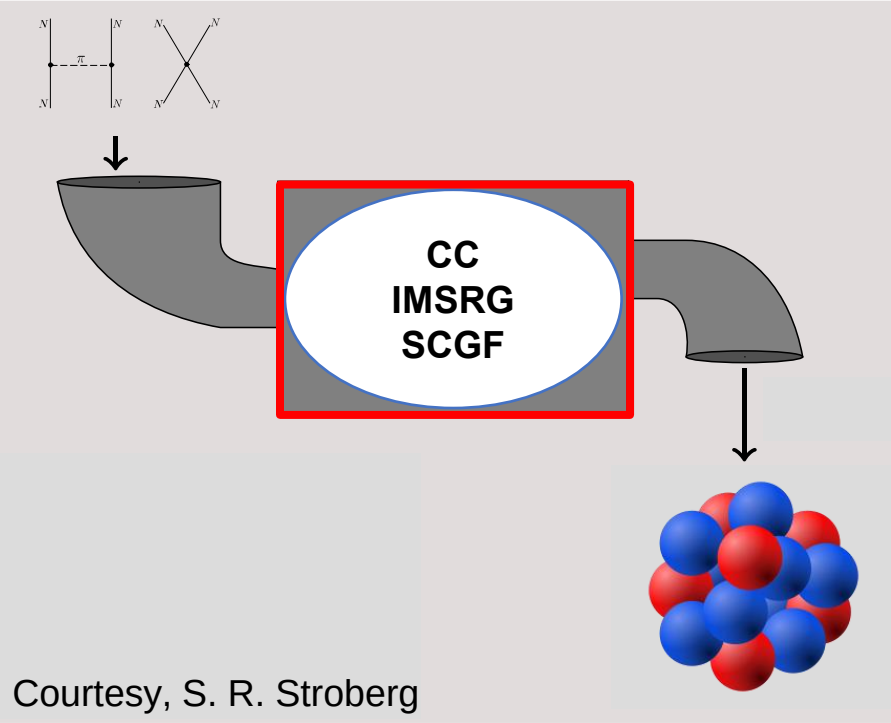
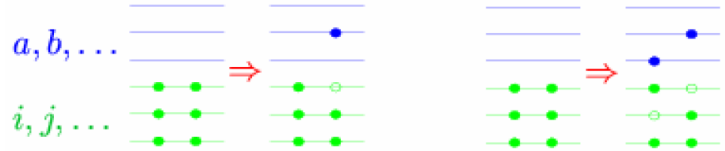


Courtesy, S. R. Stroberg

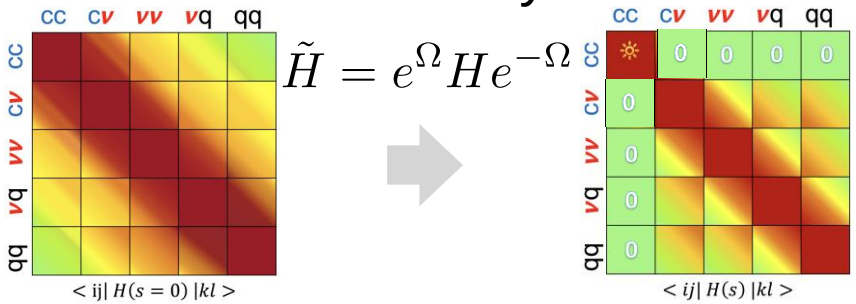
Ab Initio Cheat Sheet (polynomial scaling methods)

CC: Coupled cluster theory

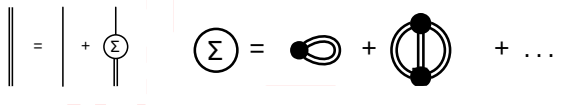


$$\begin{aligned} E &= \langle\Phi|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\ \overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c \end{aligned}$$

IMSRG: In-medium similarity renormalization group



SCGF: Self-consistent Green's function

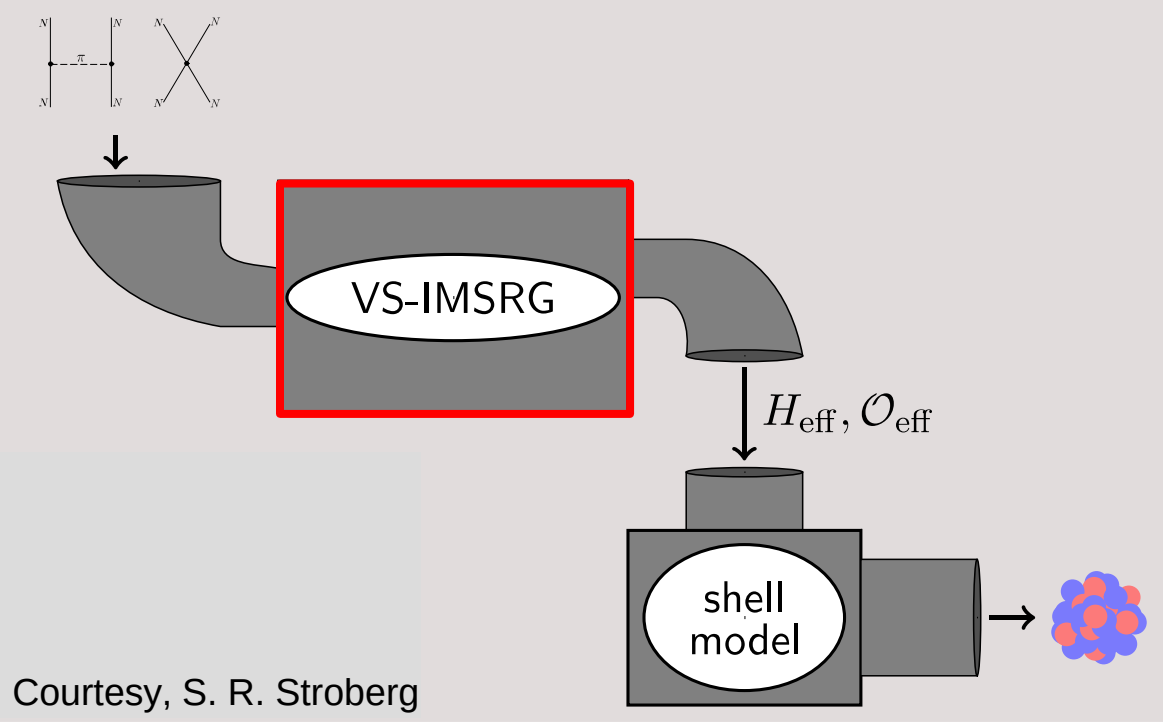


Key Advance Valence-Space Approach

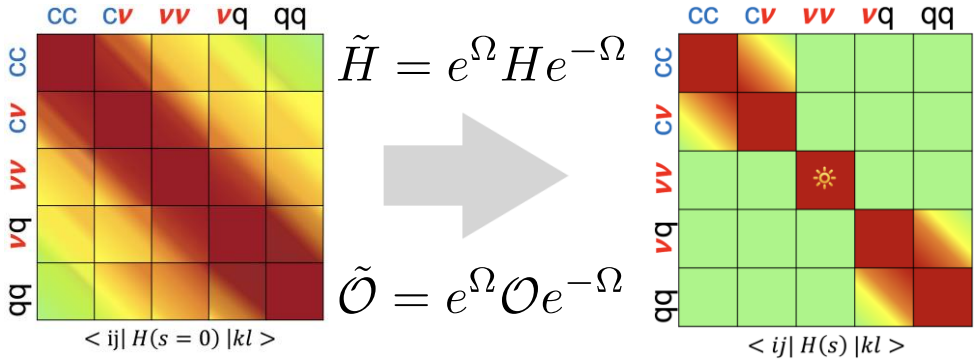
Polynomially scaling methods tailored for doubly magic, semi-magic chains

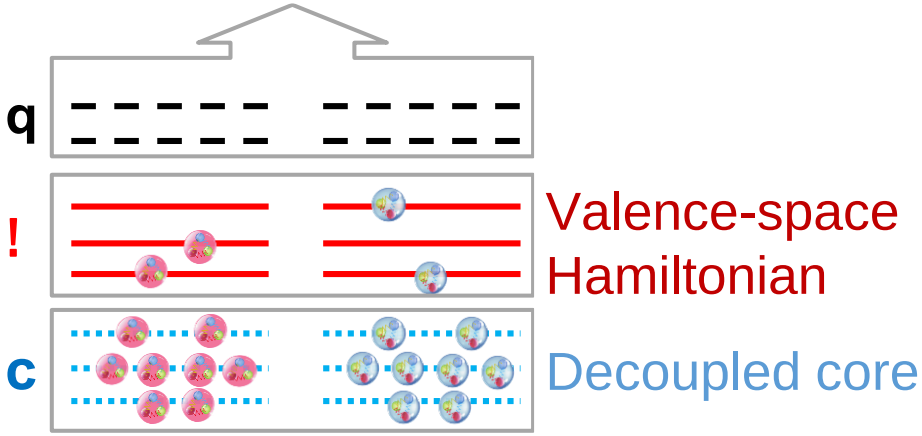
Valence-space IMSRG: Novel approach for all open-shell nuclei

$$H\psi_n = E_n\psi_n$$



Courtesy, S. R. Stroberg





Ragnar Stroberg

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

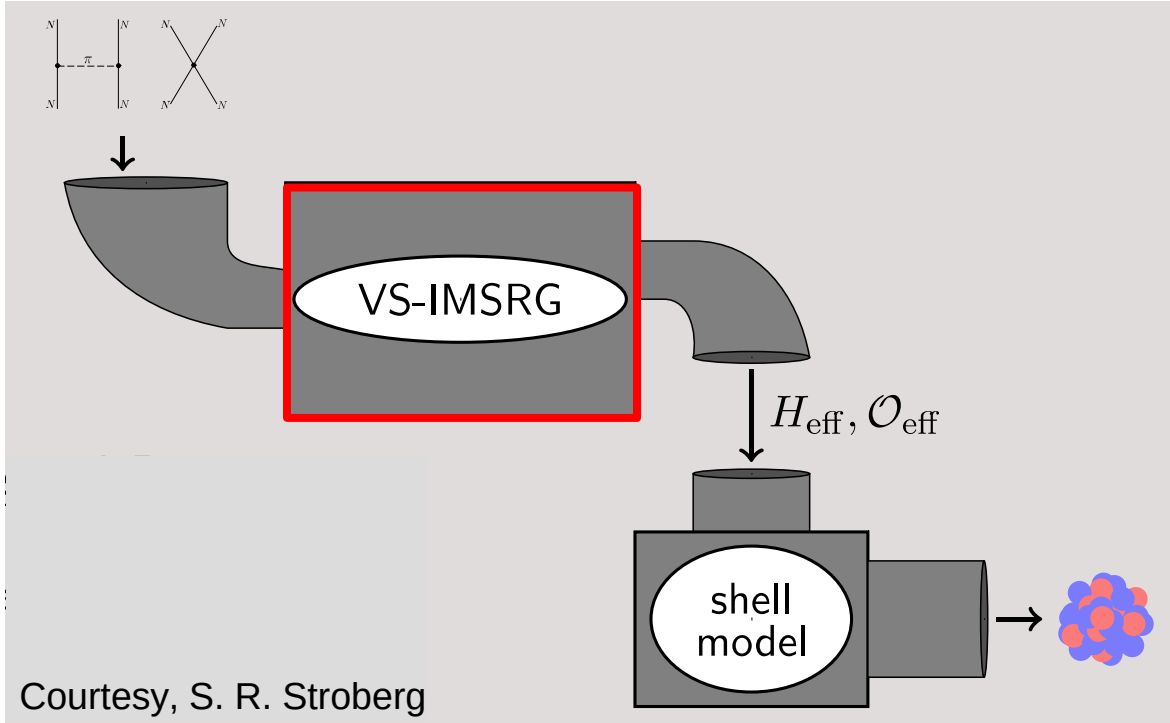
Ab initio → scope of nuclear shell model

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

$$H\psi_n = E_n\psi_n$$



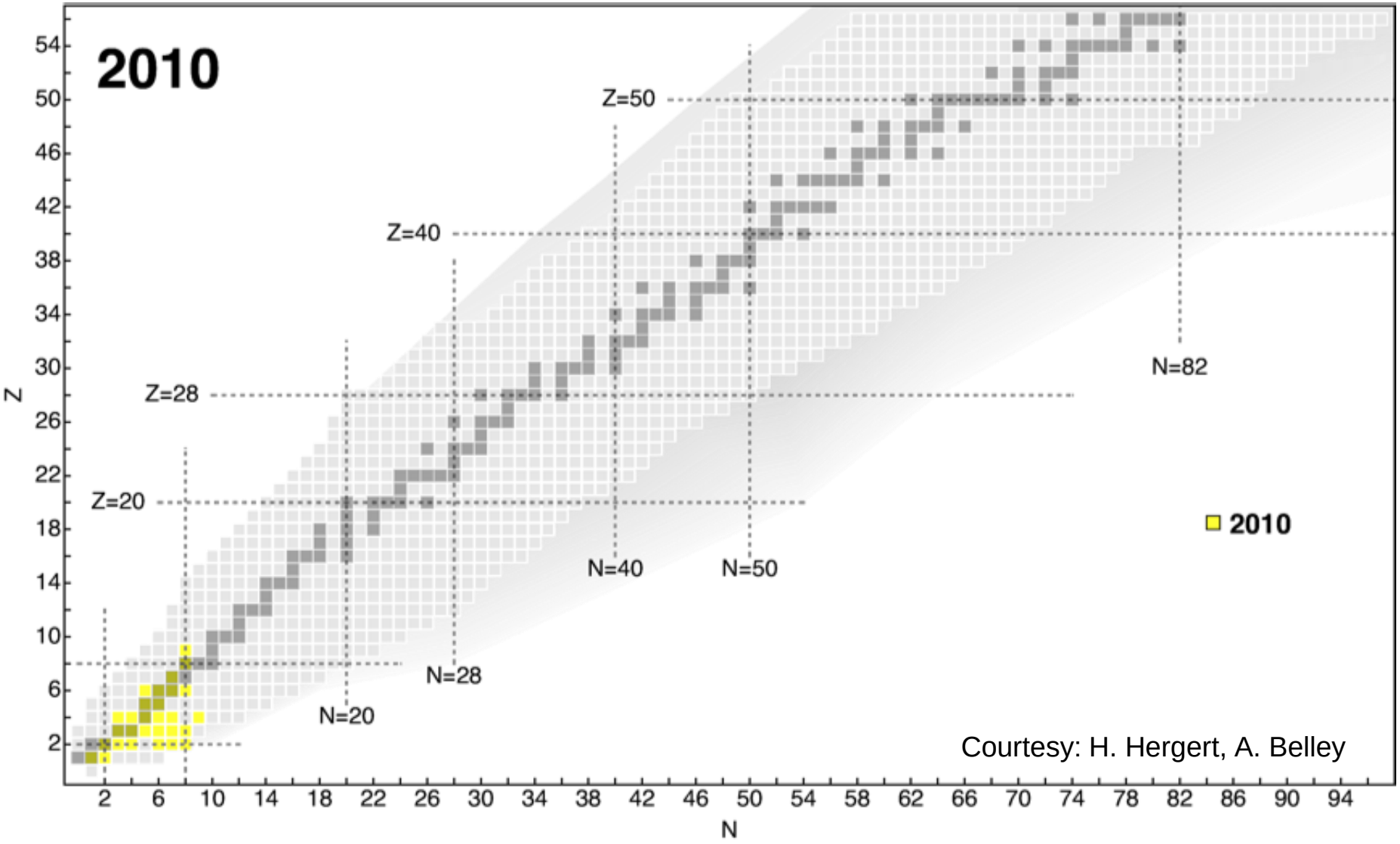
Courtesy, S. R. Stroberg

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

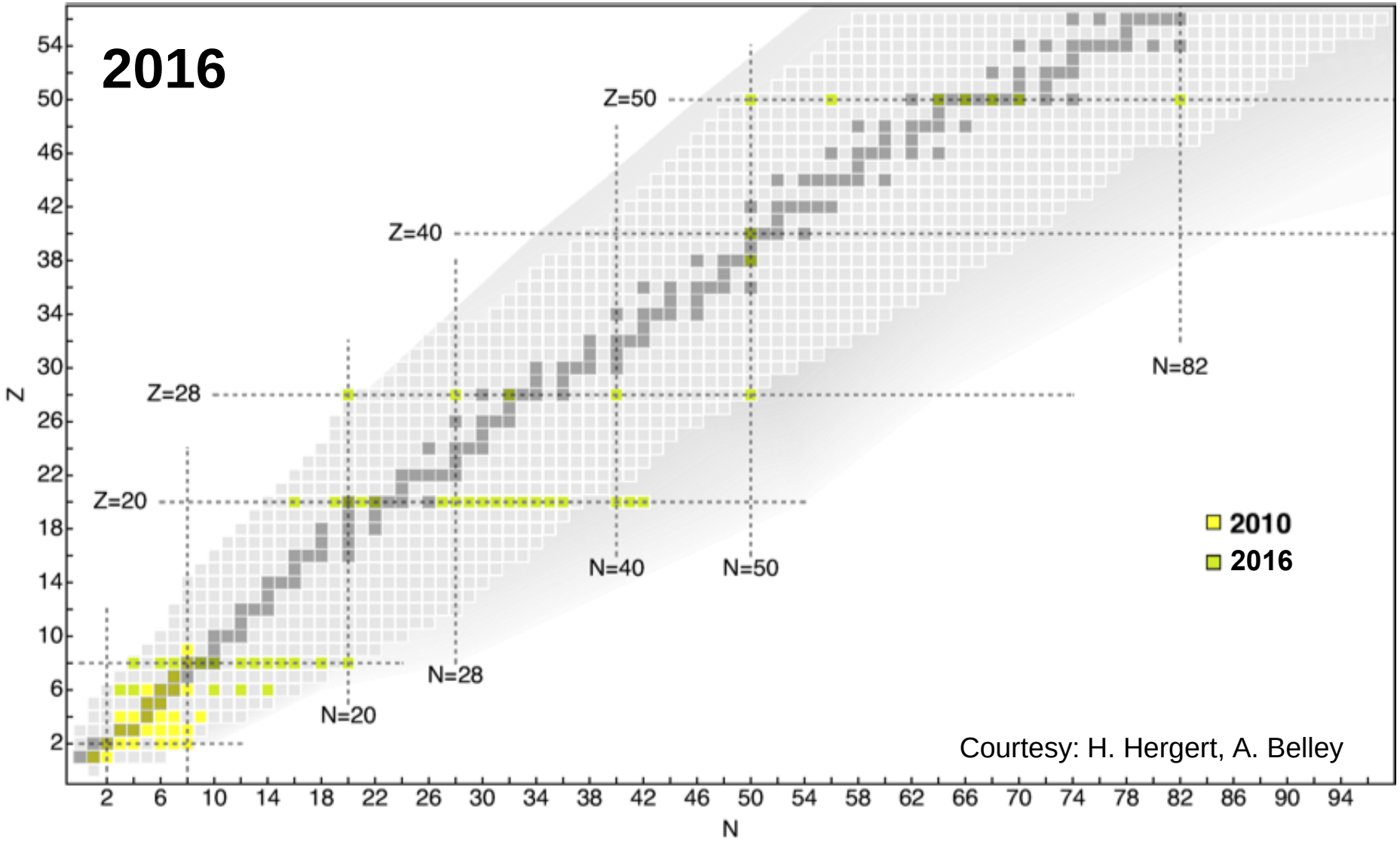
2010 Quasi-exact methods for light nuclei (^{16}O); limited capability for 3N forces



Ab Initio 2016

2016 Polynomially scaling methods (Coupled Cluster, IMSRG)

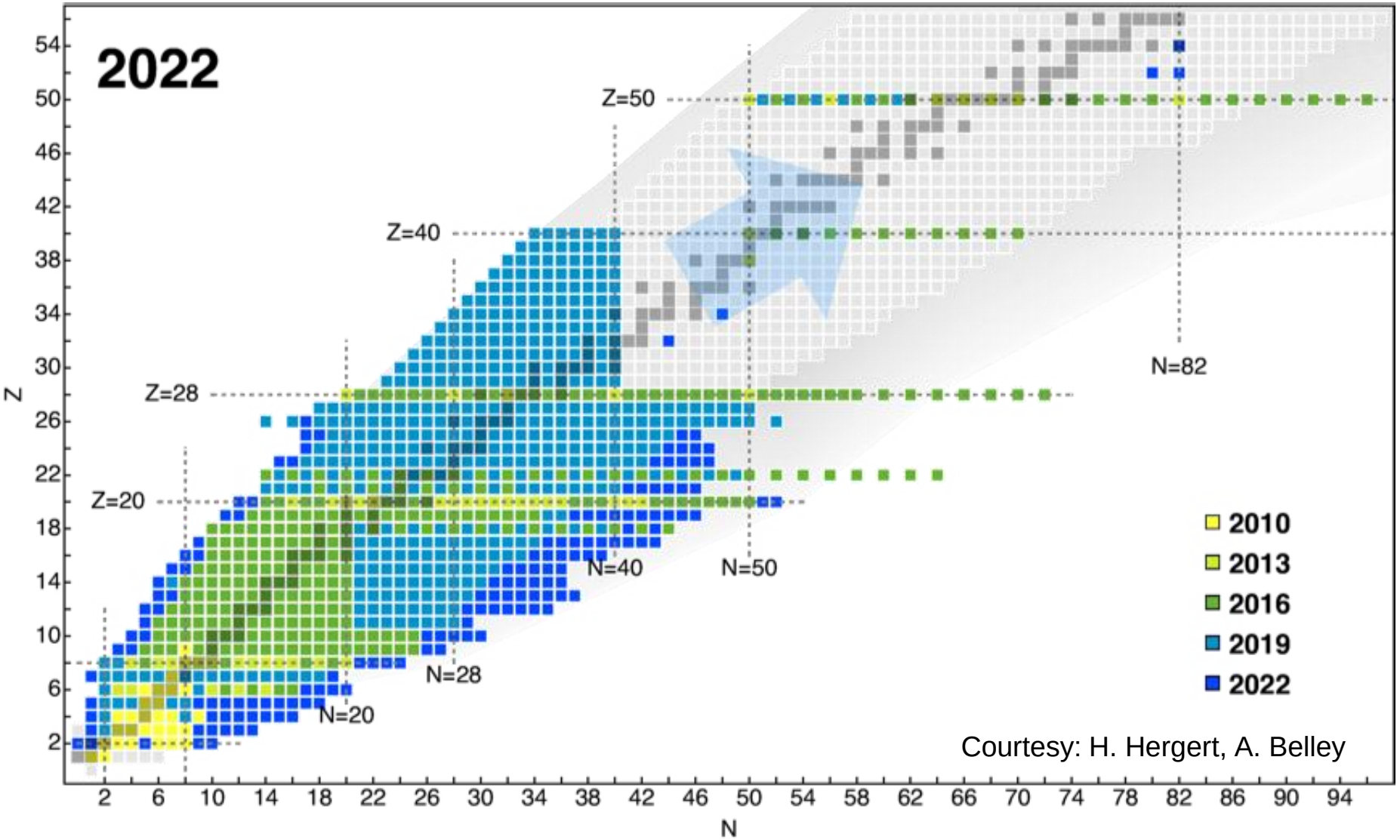
Progress to doubly magic $^{56/78}$Ni + semi-magic chains



The 5-Year Revolution: 2022

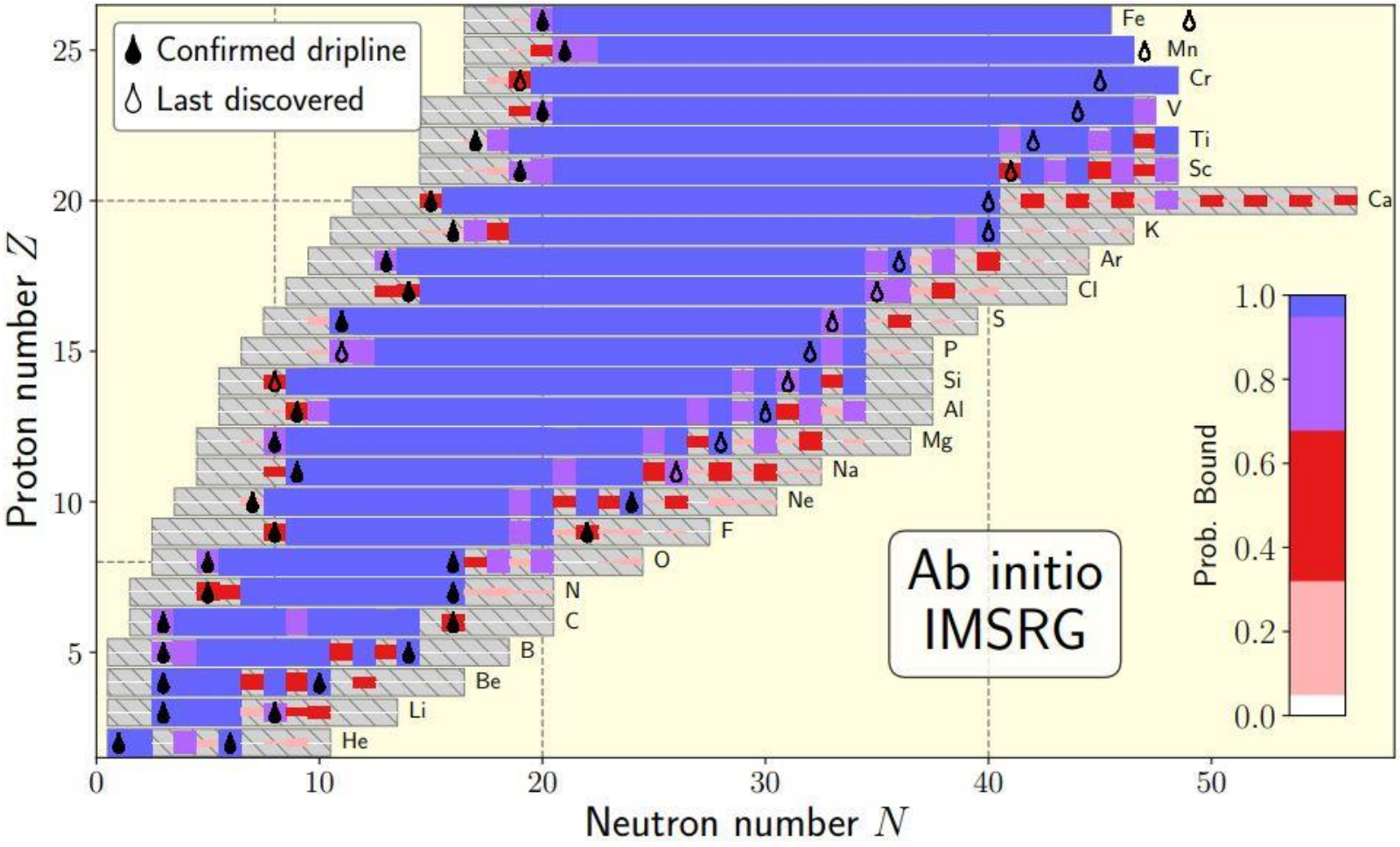
2022 Valence-space approach: essentially *all* properties of *all* nuclei

What can we do with this advance?

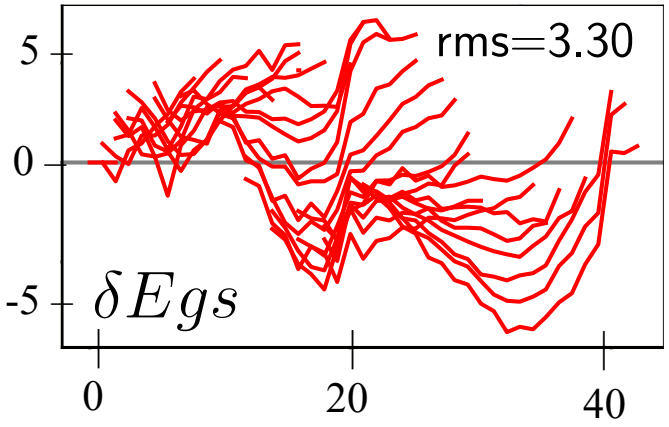


Limits of Existence in Medium-Mass Region

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

Ragnar Stroberg

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

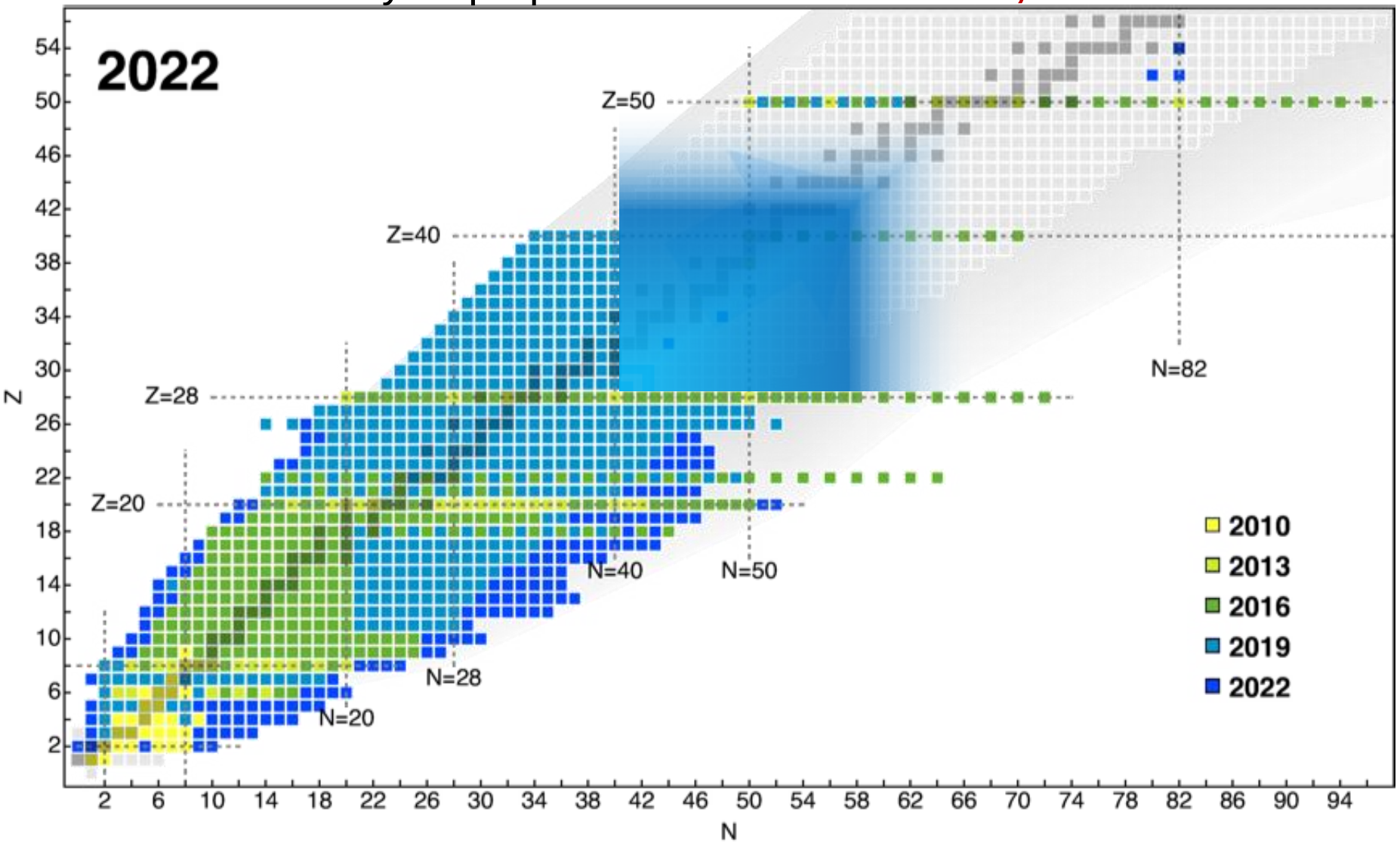
Known drip lines predicted within uncertainties

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… **to N, Z ~ 50**



Key Limitation

3NF matrix element storage

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

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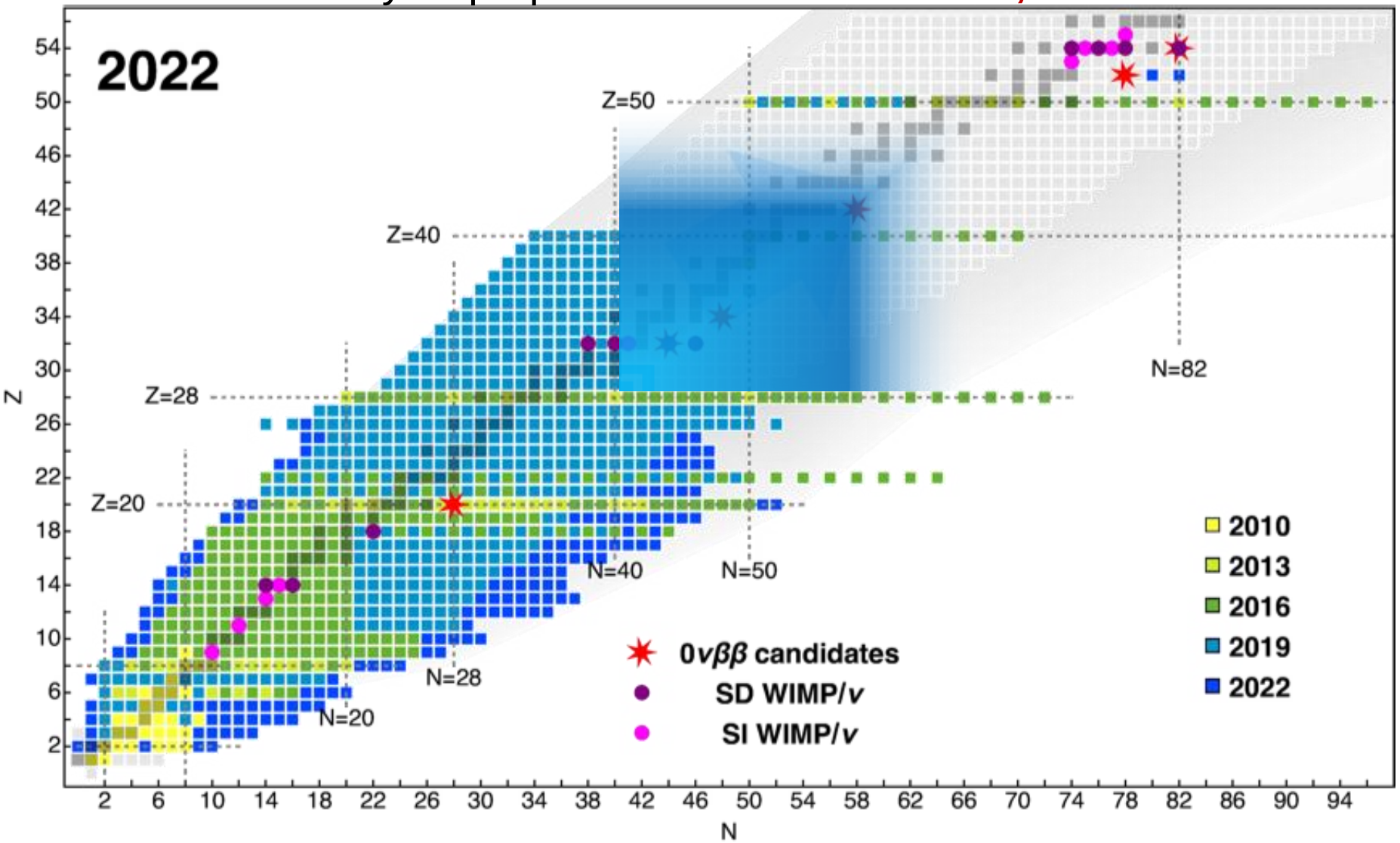

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TRIUMF

KEY ADVANCE

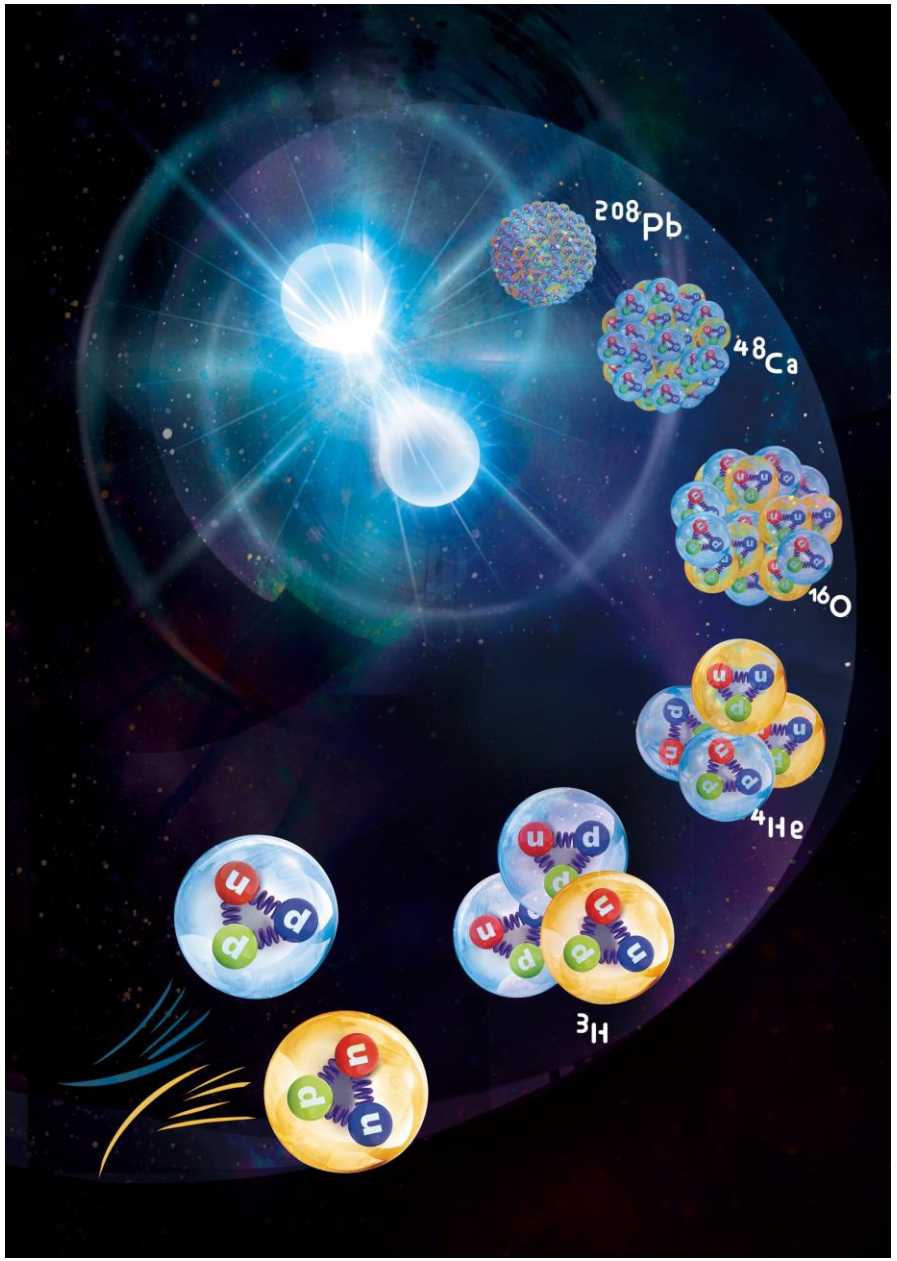
Converged Calculations of Heavy Nuclei

筑波大学
University of Tsukuba

Takayuki Miyagi

Converged *ab initio* calculations of heavy nuclei

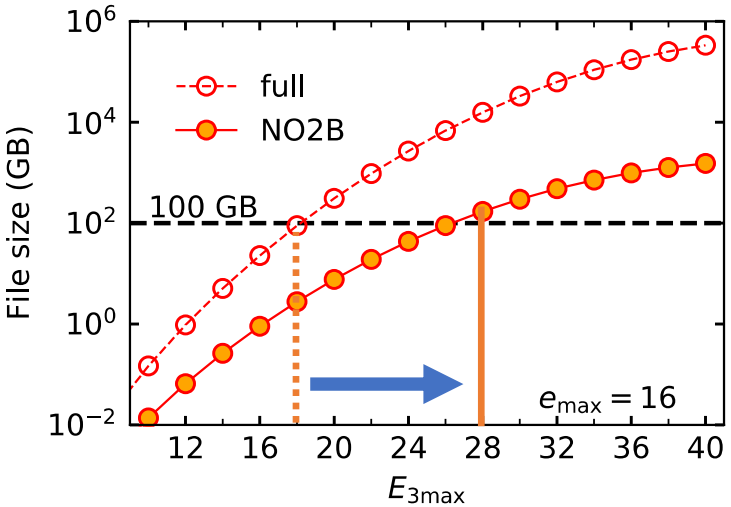
T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt
Phys. Rev. C **105**, 014302 – Published 3 January 2022

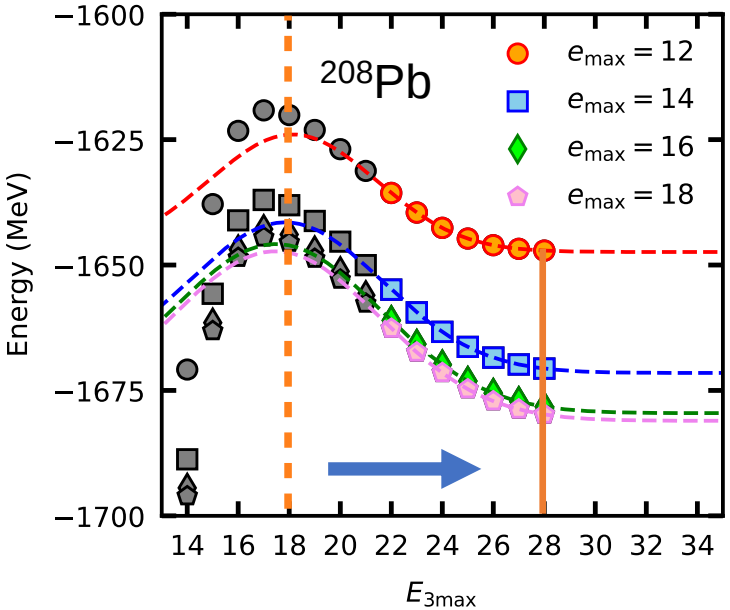


Ab Initio Calculations of Heavy Nuclei

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

Clever storage reduces needs: TB → GB





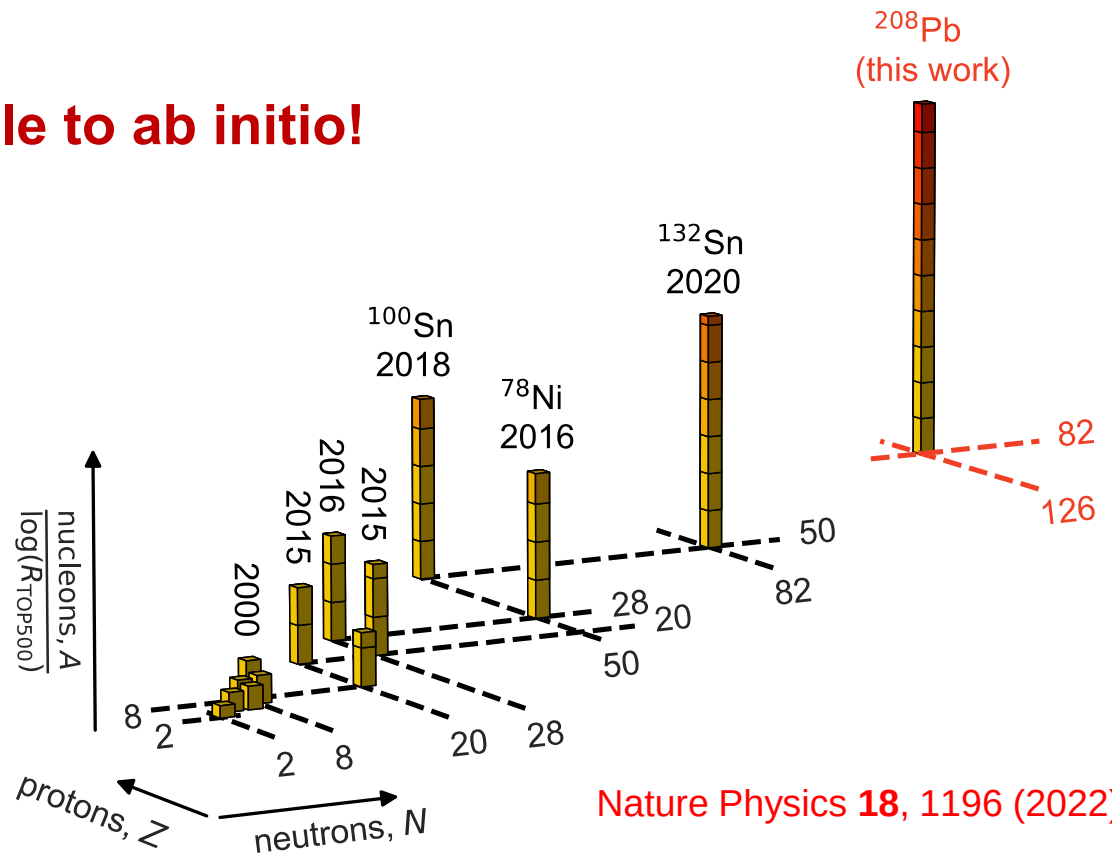
^{208}Pb now straightforward:

Solving the Schrödinger equation for 200+ nucleons!

(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

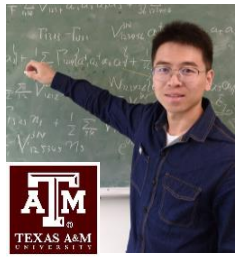
OPEN

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

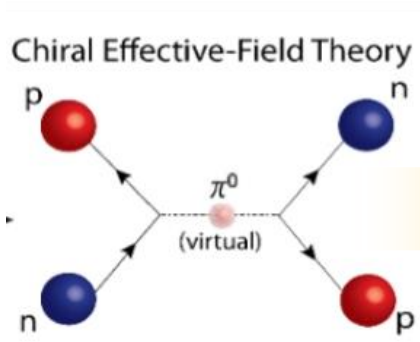
280

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]

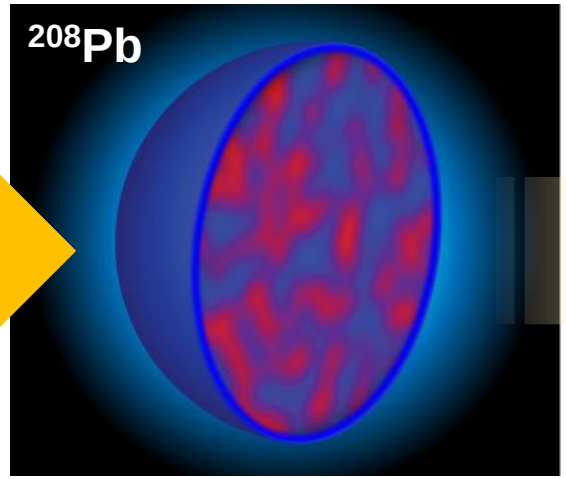
Takayuki Miyagi



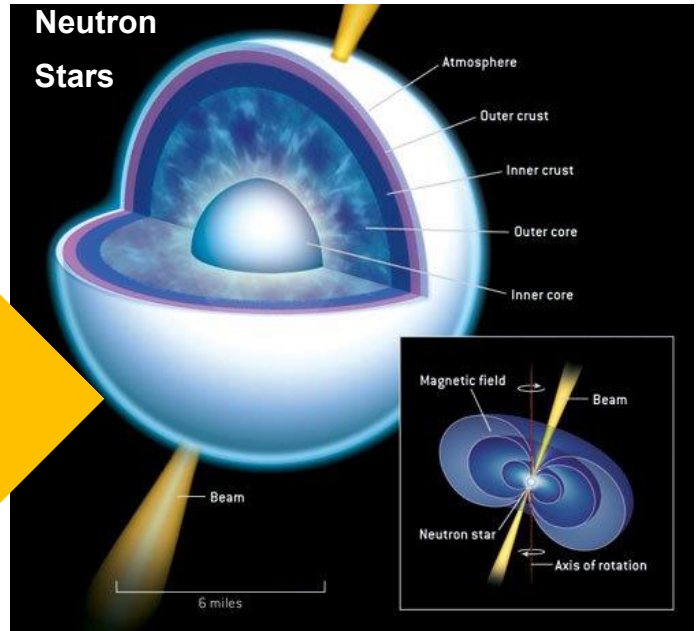
Baishan Hu



Ab Initio



Nuclear EOS



Ab Initio Neutron Skin of ^{208}Pb

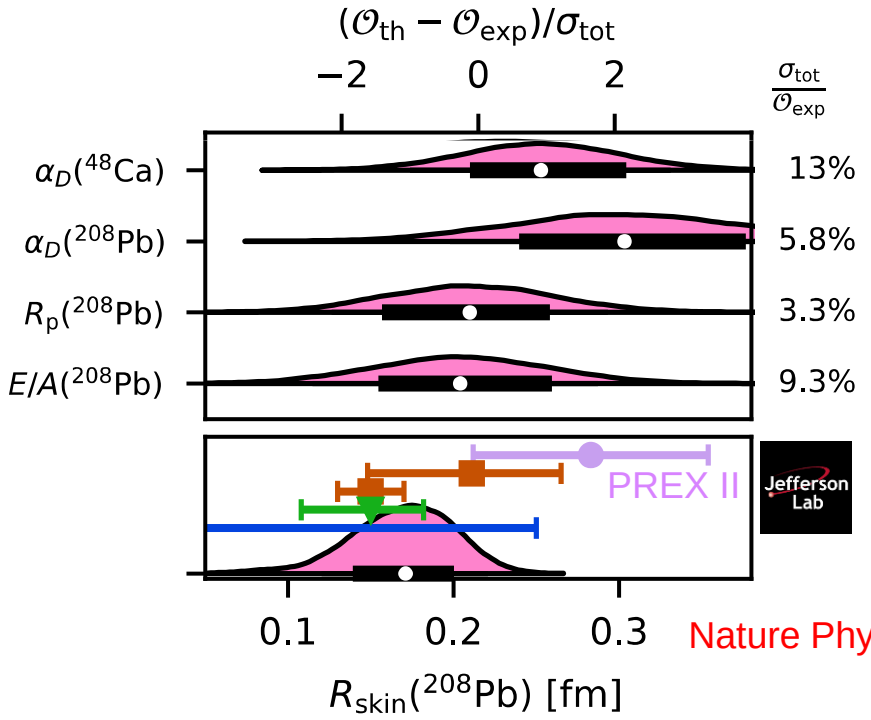
Combine ab initio + machine learning advances

I: History Matching: 34 “non-implausible” interactions

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

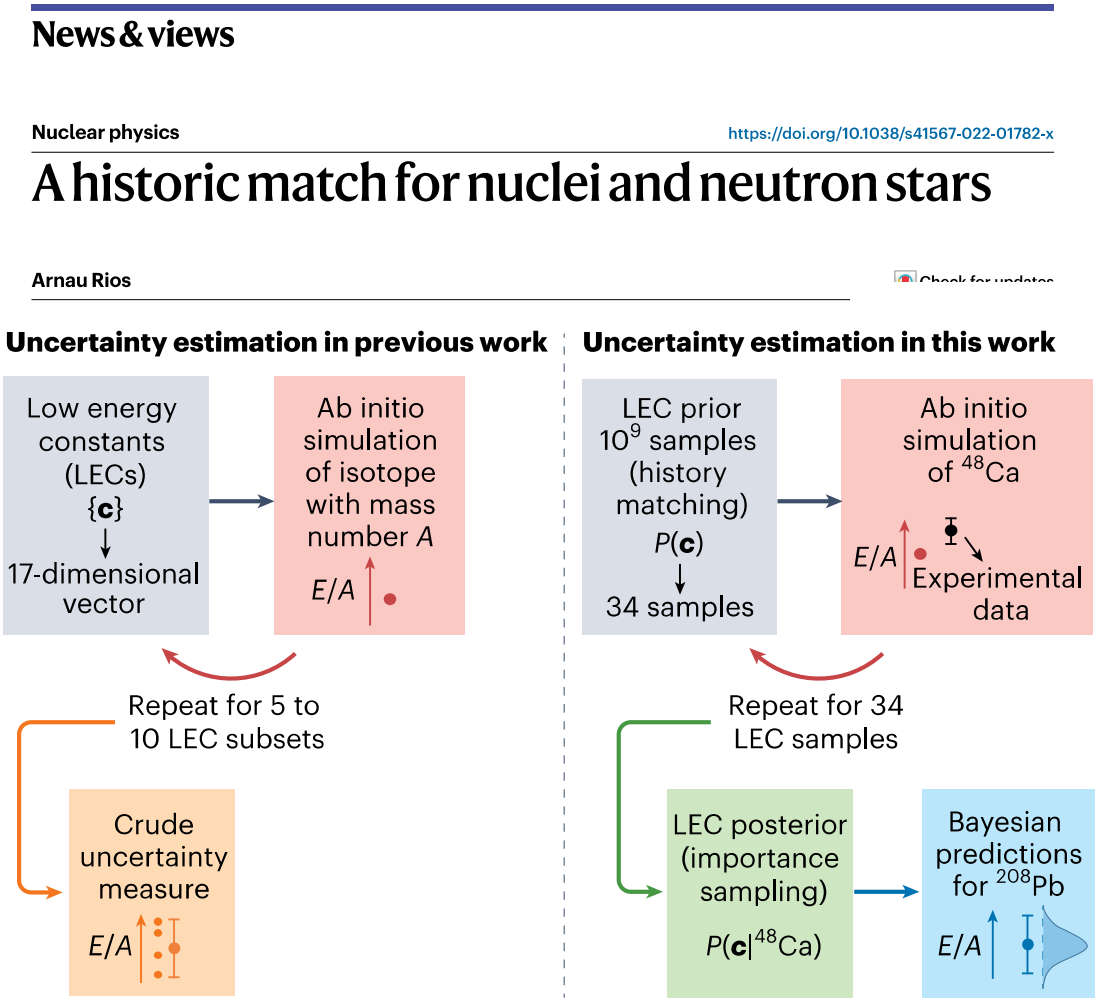
III: Validation: ^{208}Pb properties from ab initio

IV: Prediction: PPD for neutron skin



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

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

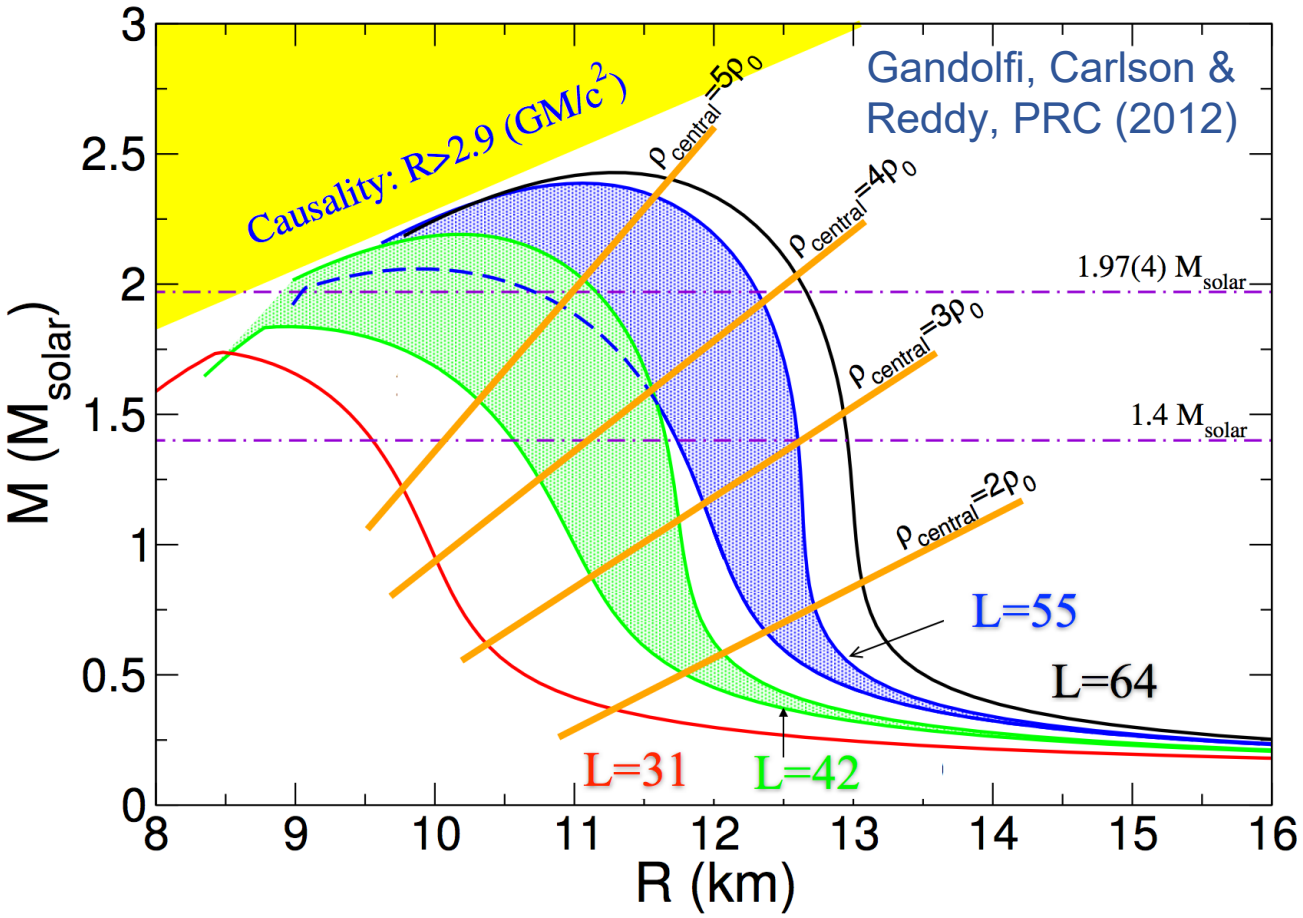


Neutron Skin of ^{208}Pb and Nuclear EOS

Slope of symmetry energy (**L**) related to NS pressure

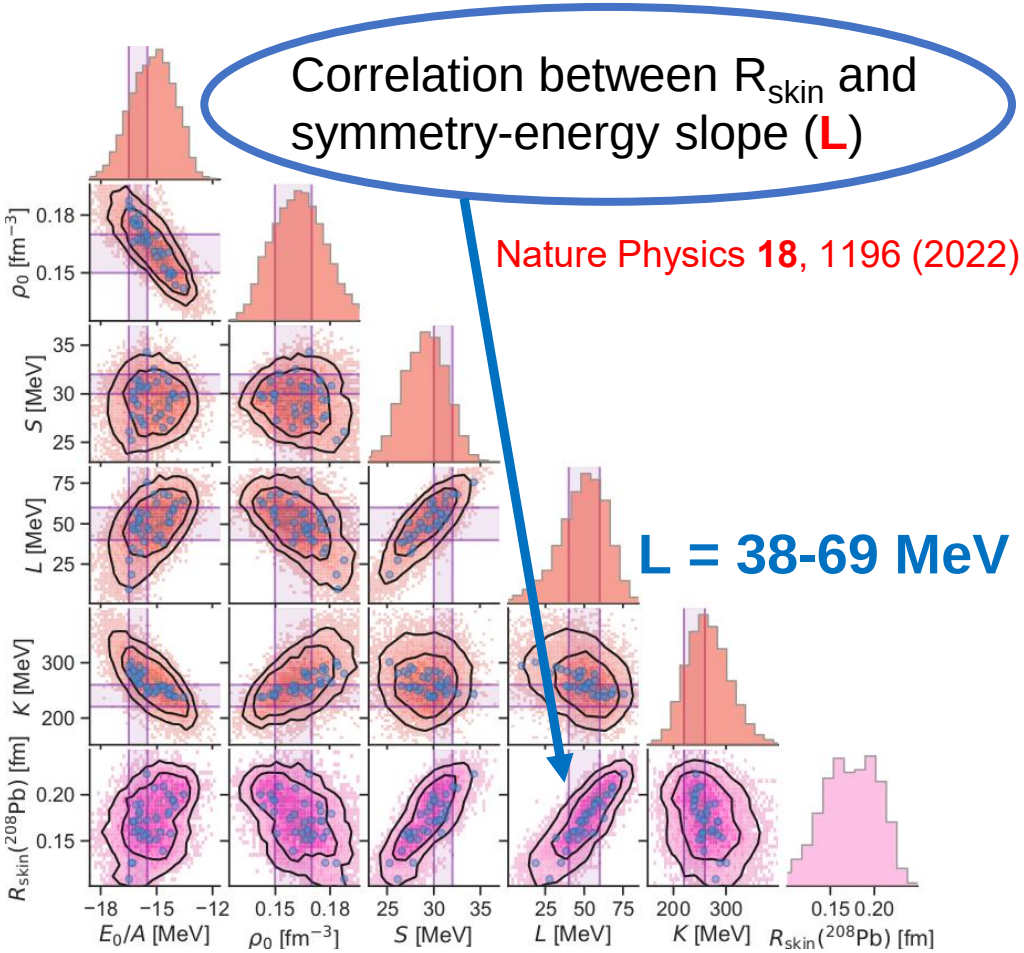
Crucial for mass-radii relationship

$$P = \rho^2 \frac{\partial(E/A)}{\partial\rho}$$



Mirror charge radii, dipole/quadrupole polarizabilities

Correlations from ab initio ^{208}Pb



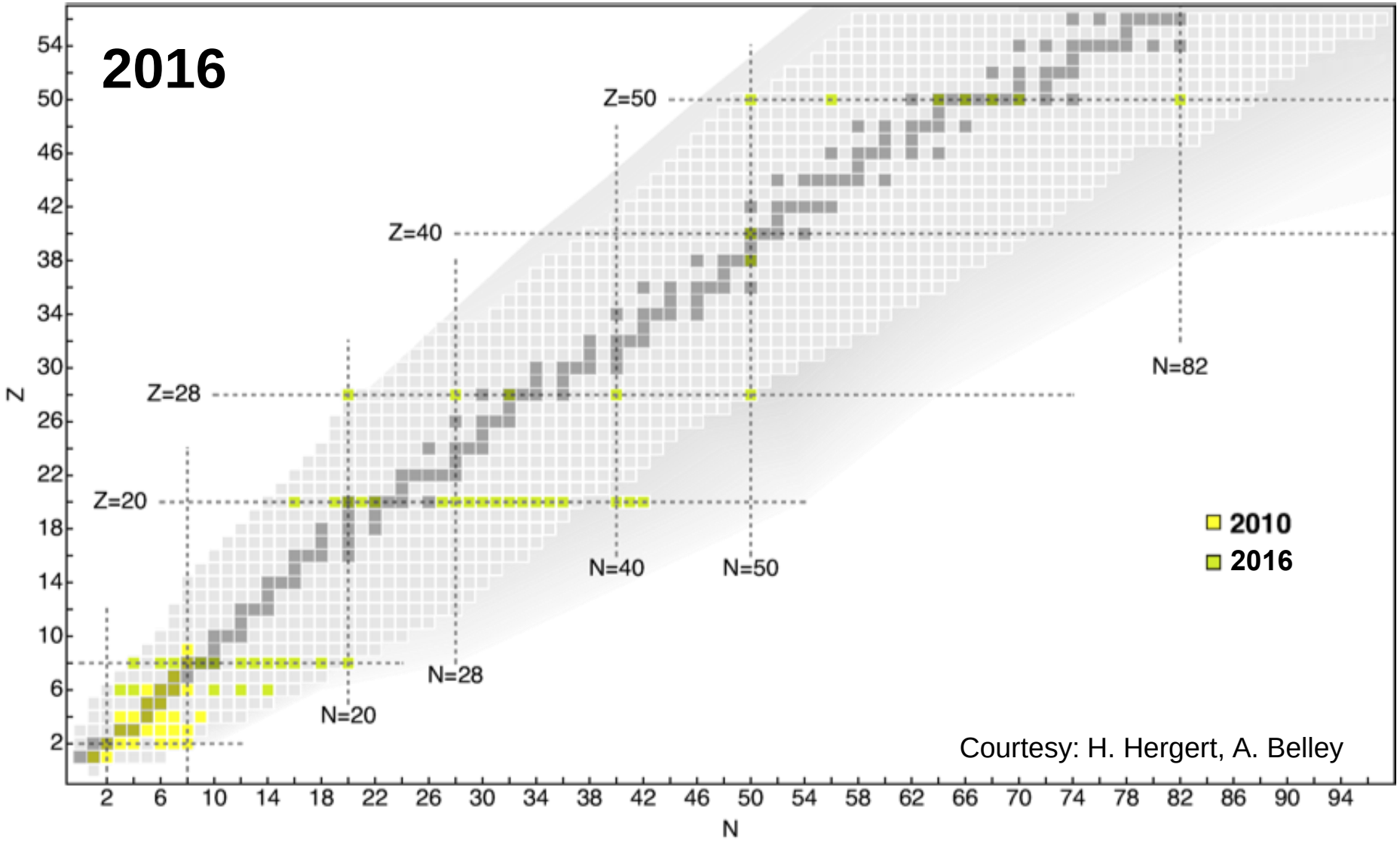
Potentially constrain nuclear forces:

Neutron star radii/mergers

Ab Initio 2016

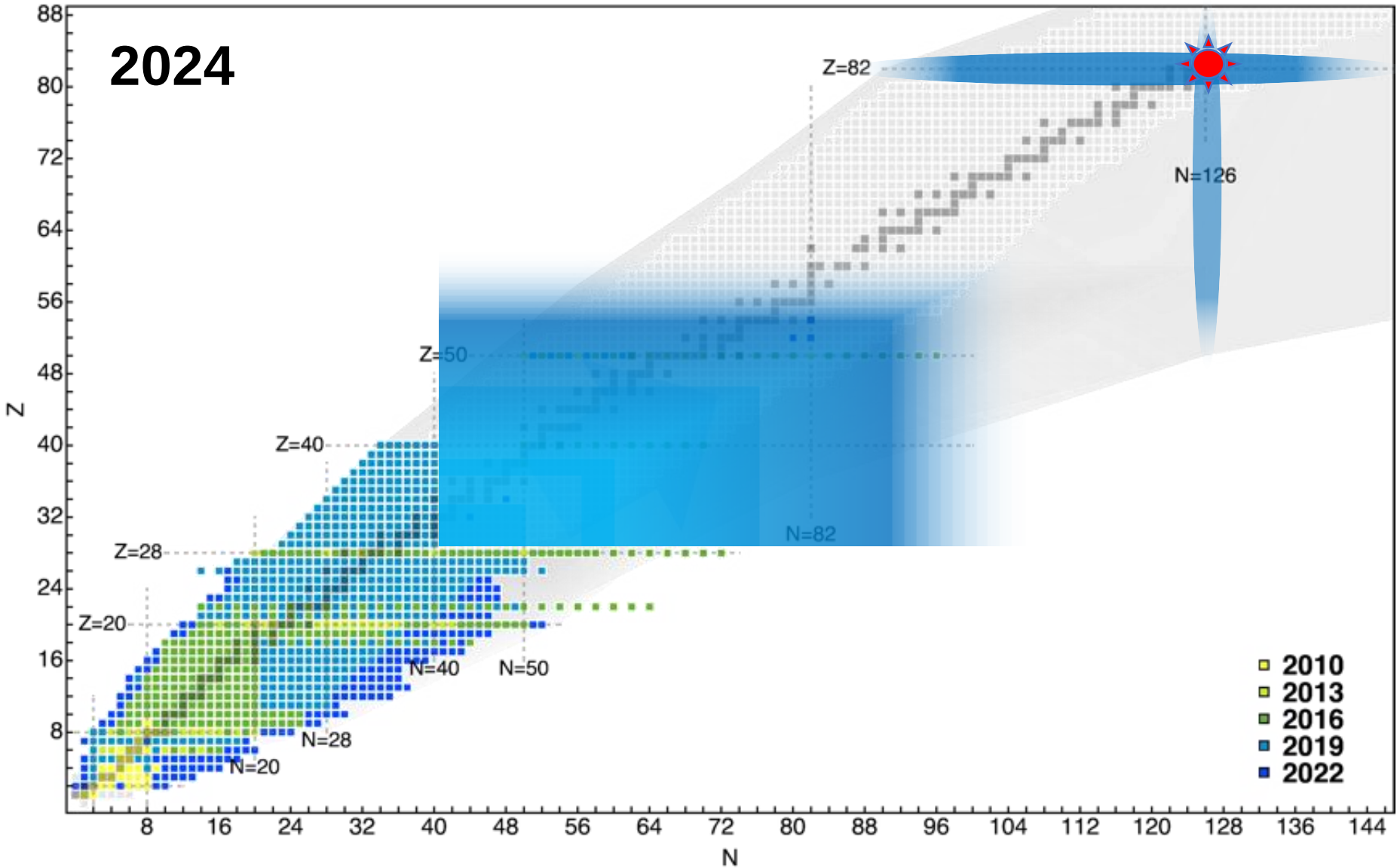
2016 Polynomially scaling methods (Coupled Cluster, IMSRG)

Progress to doubly magic $^{56/78}$Ni + semi-magic chains



New Scope of Ab Initio Theory

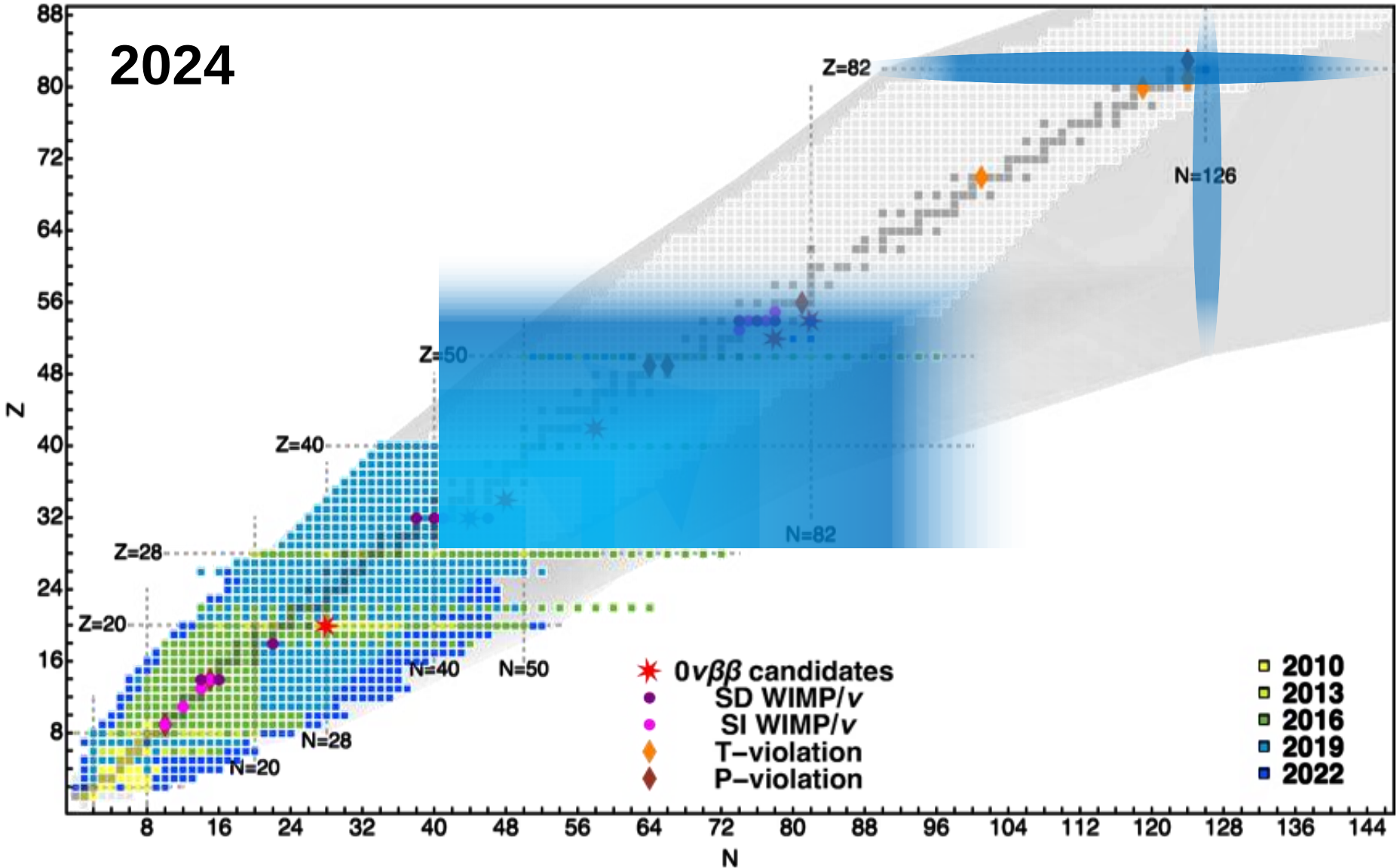
Rapid progress in ab initio reach: **global + heavy**



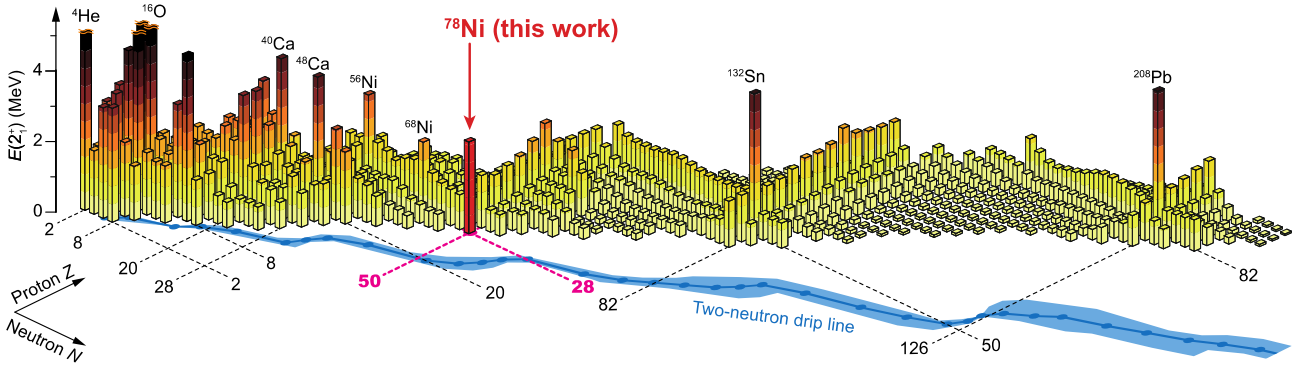
New Scope of Ab Initio Theory

Rapid progress in ab initio reach: **global + heavy**

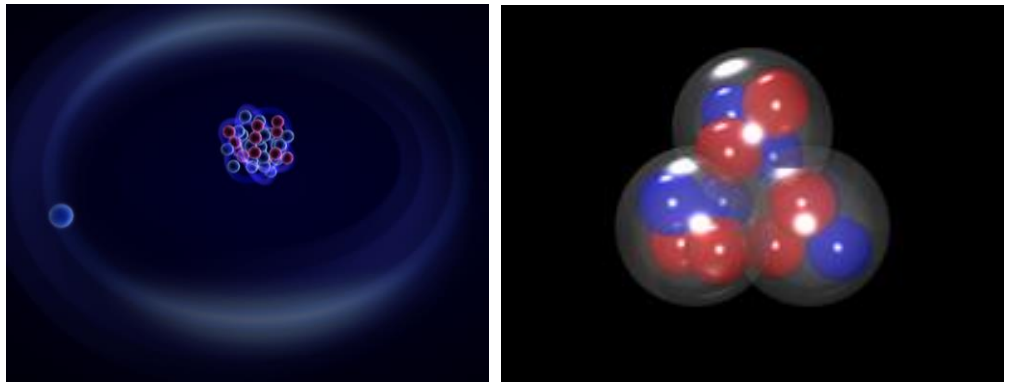
Exciting applications to searches for BSM physics!



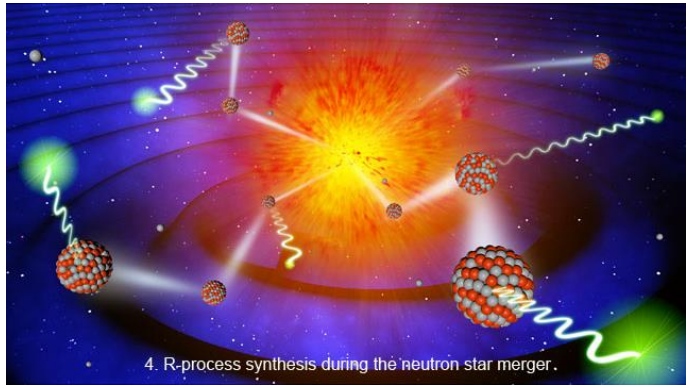
Major Questions in Nuclear Structure/Astrophysics



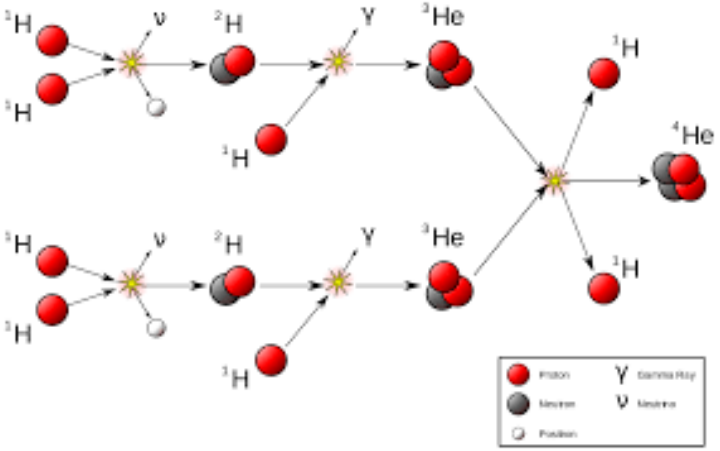
Limits of existence + formation/evolution of magic numbers



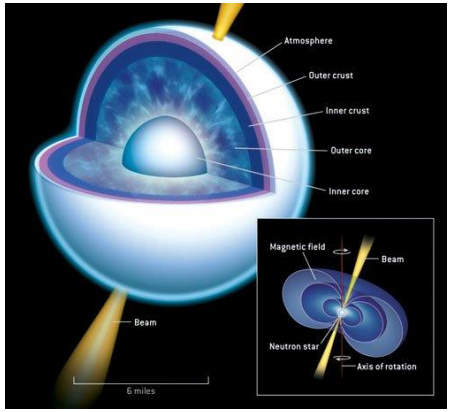
Nuclear skins/halos/clusters



Heavy Element Nucleosynthesis



Continuum and nuclear reactions



Infinite matter/Neutron stars

Ab Initio VS-IMSRG Campaign: Masses and Charge Radii

Extensive campaign for nuclear structure, nuclear astrophysics, and searches for physics beyond the standard model

Neutron skin of ^{208}Pb
B. Hu *et al.*,
Nature Physics **18**, 1196

N=124-128: Ab initio masses for r-process nucleosynthesis
B. Hu *et al.* (in preparation)

N=50-82 Sn charge radii
P.F. Gustaffson *et al.*, Phys. Rev. Lett (under review)

In – Ag masses for structure of ^{100}Sn
M. Mougeout *et al.*, Nature Phys. 17, 1099 (2021)
L. Nies *et al.*, Phys. Rev. Lett. 131, 022502 (2023)
Z. Ge *et al.*, Phys. Rev. Lett. 133, 132503 (2024)

$^{132-140}$Sn masses for r-process nucleosynthesis
A. Mollaebrahimi *et al.*, Phys. Rev. Lett. XXX, yyyyy (2025)

Reduced size of excited state isomer in ^{129,131}In
A. Vernon et al., Phys. Rev. Lett. (under review)

$^{74-76}$Sr masses for IMME/superallowed Fermi
Z. Hockenberry *et al.,* Phys. Rev. C 111, 014327 (2025)

Masses of Cd isotopes for N=82 shell closure
V. Manea et al., Phys. Rev. Lett. 124, 092502 (2020)

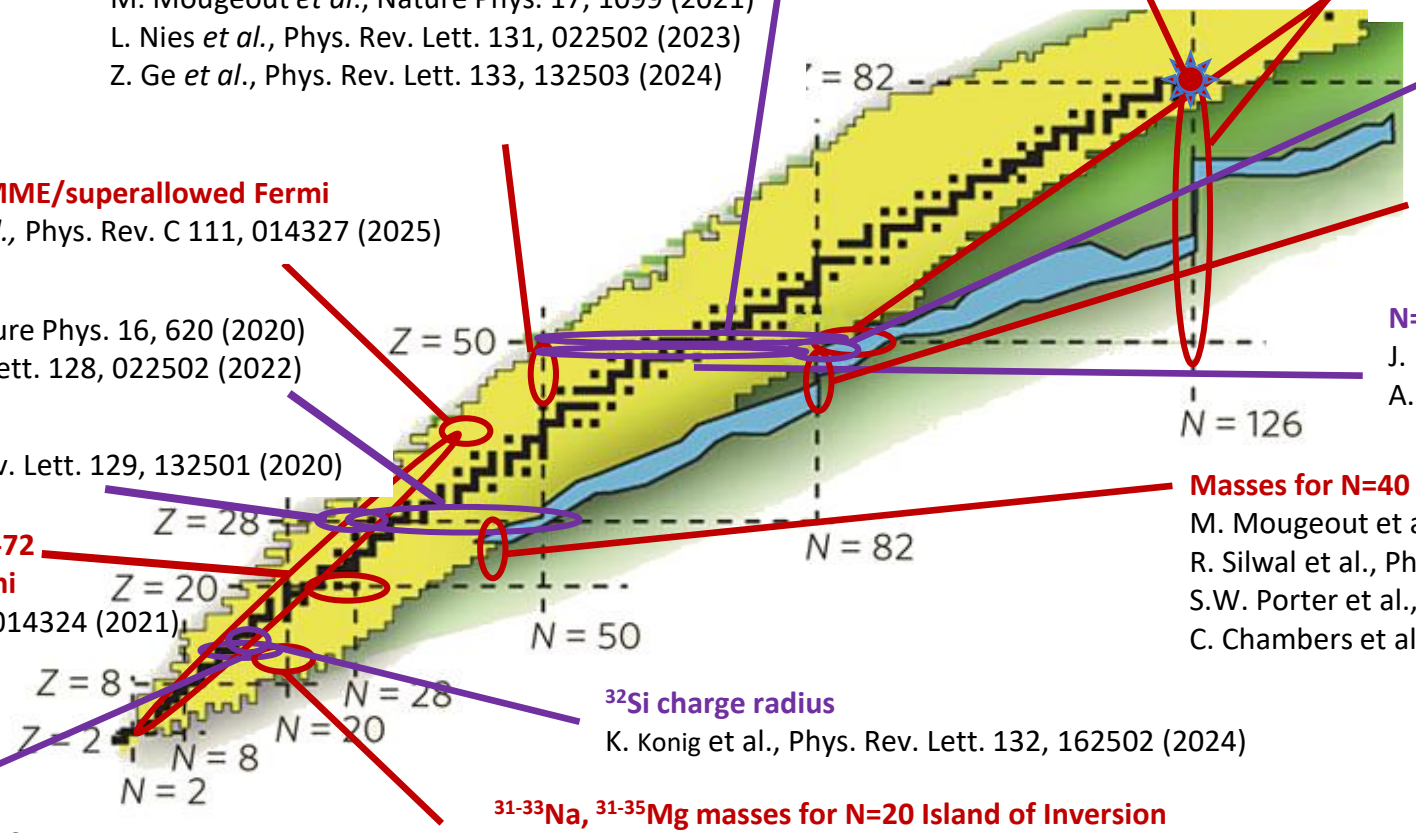
N=28-50 Ni and Cu radii
R.P. de Groote *et al.*, Nature Phys. 16, 620 (2020)
S. Malbrunot Phys. Rev. Lett. 128, 022502 (2022)

N=50-82 In radii for structure of ^{100}Sn
J. Karthein *et al.,* Nature Phys. 20, 1719 (2024)
A. R. Vernon et al., Phys. Rev. C XXX, yyyyyy (2025)

^{55,56}Ni radii
F. Sommer *et al.*, Phys. Rev. Lett. 129, 132501 (2020)

Masses for N=40 Island of Inversion
M. Mougeout et al., Phys. Rev. Lett. 120, 232501 (2018)
R. Silwal et al., Phys. Lett. B 833, 137288 (2022)
S.W. Porter et al., Phys Rev C 105, L041301 (2022)
C. Chambers et al., Phys. Rev. C XXX, yyyyyy (2025)

Isospin triplets from A=10-72 for ISB/Superallowed Fermi
M. Martin *et al.*, PRC 104, 014324 (2021)



^{32}Si charge radius
K. Konig et al., Phys. Rev. Lett. 132, 162502 (2024)

$^{27-32}$Al radii
H. Heylen *et al.*, Phys. Rev. C 103, 014318 (2021)

$^{31-33}$Na, $^{31-35}$Mg masses for N=20 Island of Inversion
E.M. Lykiardopoulou et al., Phys. Rev. Lett. 134, 052503 (2025)

Ab Initio VS-IMSRG Campaign: Spectra and EM Moments

Extensive campaign for nuclear structure, nuclear astrophysics, and searches for physics beyond the standard model

Magnetic moments from O to Bi
T.Miyagi *et al.*, Phys. Rev. Lett 104, 014324 (2021)

Spectroscopy of $^{126\text{-}136}$Sn and ^{129}Cd
T. Miyagi *et al.,* Phys. Rev. C 105, 014302 (2022)

0^+ states in ^{90}Kr
D. Walter *et al.,* Phys. Lett. B 862, 139352 (2025)

Spectroscopy of ^{132}Sn, ^{132}In and ^{131}Sb
K. Whitmore *et al.,* Phys. Rev. C 102, 024327 (2020)

EM Moments of 47,49Sc
S.W. Bai *et al.*, Phys. Lett B 829, 137064 (2022)

Reduced size of excited state isomer in ^{129,131}In
A. Vernon et al., Phys. Rev. Lett. (under review)

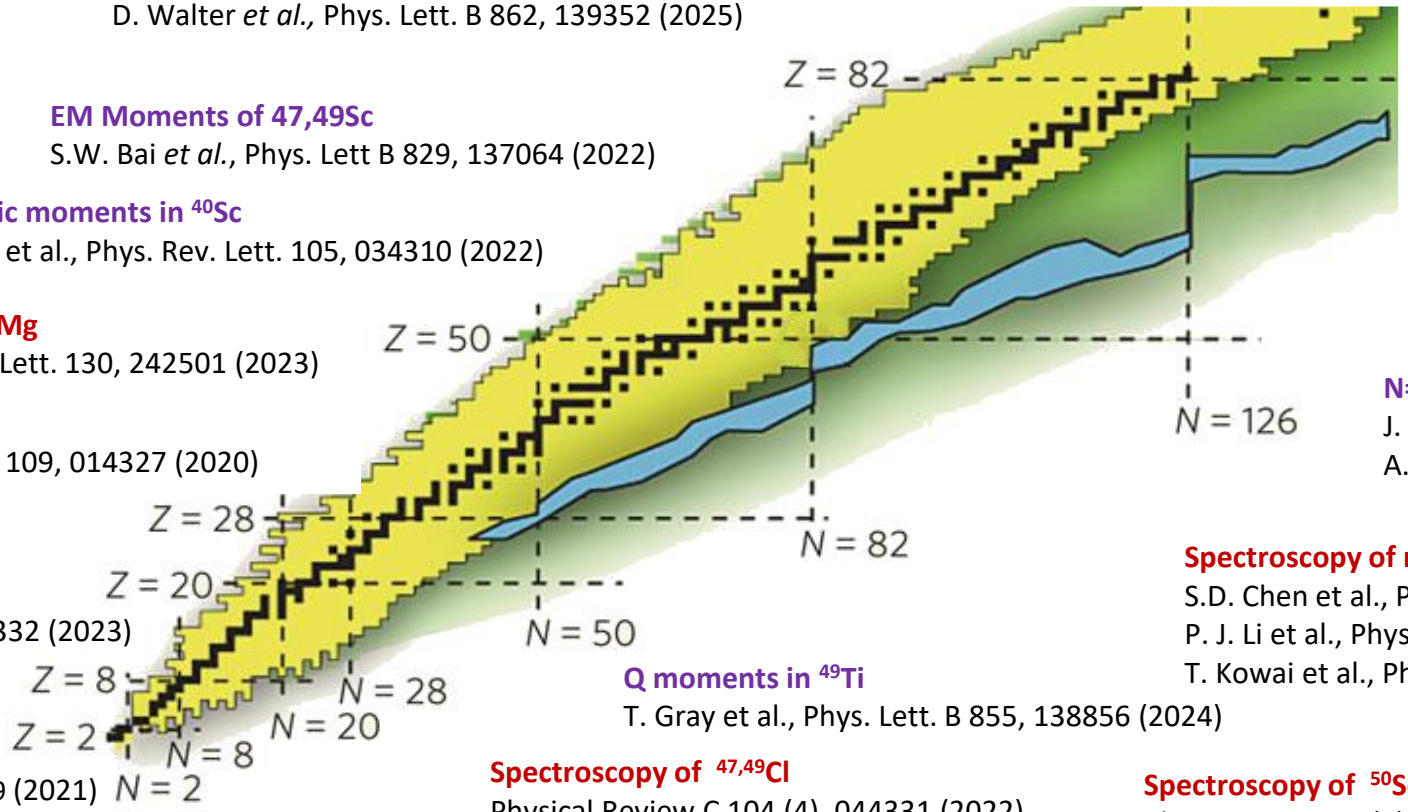
Magnetic moments in ^{40}Sc
R Powel et al., Phys. Rev. Lett. 105, 034310 (2022)

EM moments of neutron-rich Sb isotopes
S. Lecher *et al.,* Phys. Lett. B 847, 138278 (2024)

Microsecond Isomer in ^{32}Mg
T.J. Gray *et al.*, Phys. Rev. Lett. 130, 242501 (2023)

N=50-82 In EM moments
J. Karthein *et al.,* Nature Phys. 20, 1719 (2024)
A. R. Vernon et al., Phys. Rev. C (under review)

Q moments of ^{32}Si
J. Heery *et al.*, Phys. Rev. C 109, 014327 (2020)



Spectroscopy of neutron-rich Ca isotopes
S.D. Chen et al., Phys. Lett. B 843 138025 (2023)
P. J. Li et al., Phys. Lett. B 855, 138828 (2024)
T. Kowai et al., Phys. Lett. B 827, 136952 (2022)

B(E2) in ^{23}Mg
Physical Review C 105, 034332 (2023)

Q moments in ^{49}Ti
T. Gray et al., Phys. Lett. B 855, 138856 (2024)

Spectroscopy of ^{42}Sc
Physics Letters B 819, 136439 (2021)

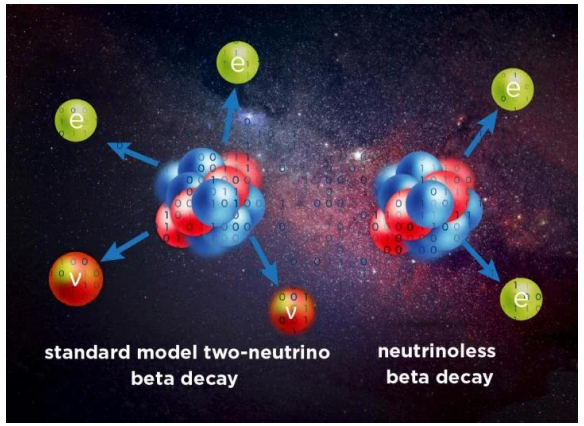
Spectroscopy of ^{47,49}Cl
Physical Review C 104 (4), 044331 (2022)

Spectroscopy of ^{50}Sc and ^{50}Ti
Phys. Revi. C 104 (2), 024314 (2021)

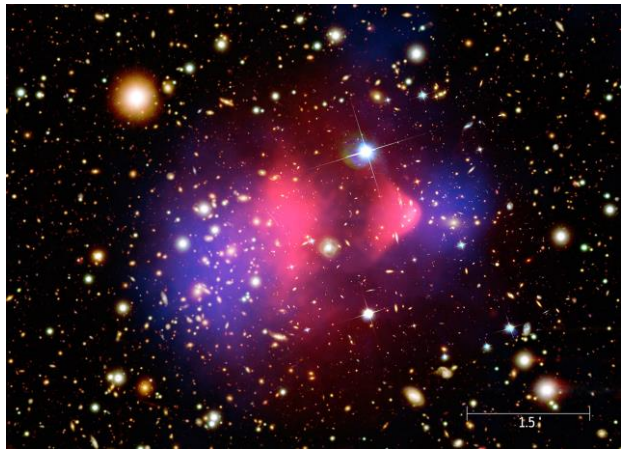
Spectroscopy of ^{23}F
H. Crawford *et al.*, Phys. Rev. C 103, L061303 (2022)

Spectroscopy of ^{49,50}Ar for N=32
B.D. Linh et al., Phys. Rev. C 109, 043312 (2024)
Physical Review C 102 (6), 064320 (2020)

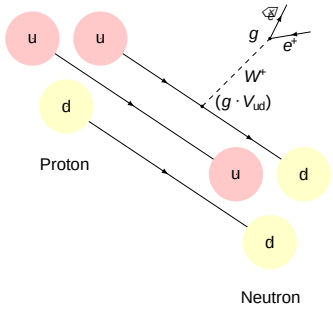
Searches for BSM Physics



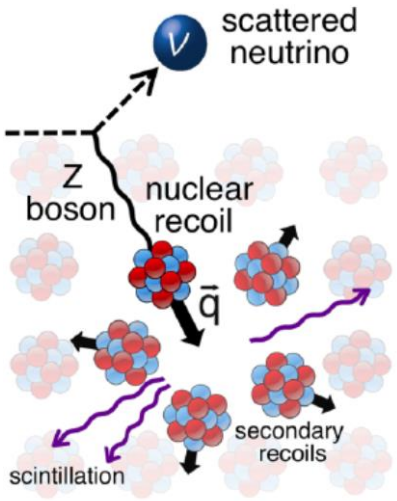
Neutrinoless double-beta decay



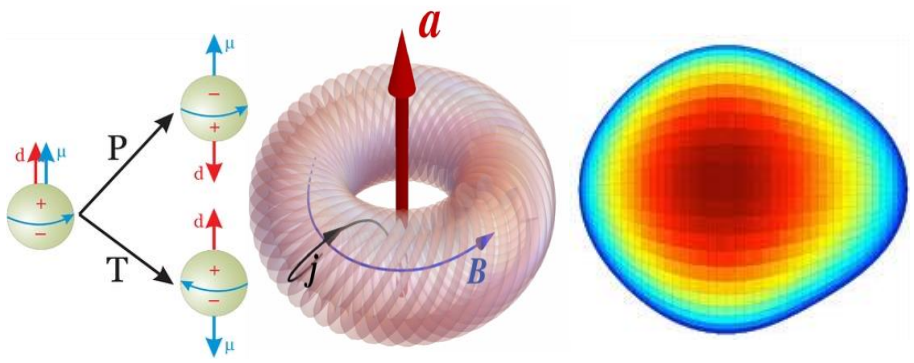
Dark matter direct detection



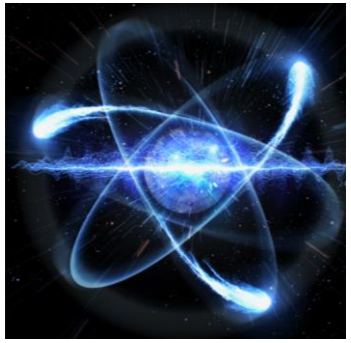
Superallowed Fermi transitions



Neutrino scattering



Symmetry-violating moments

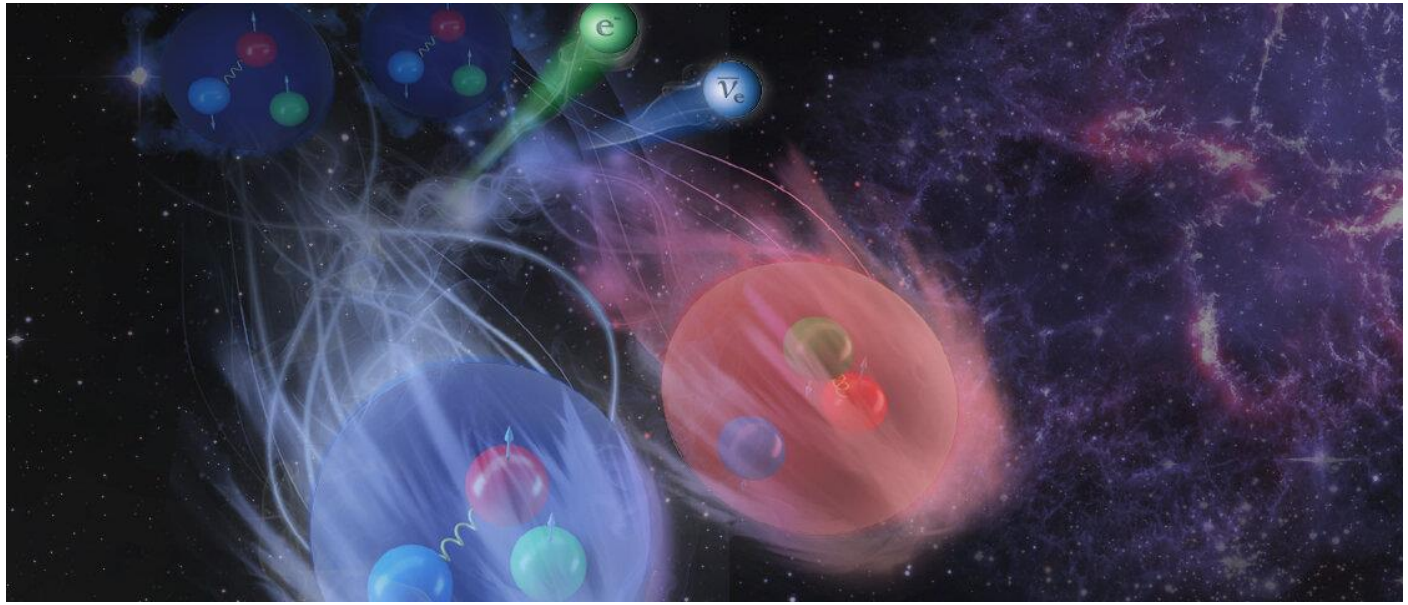


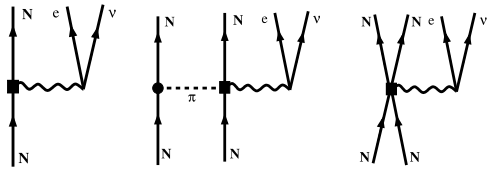
Atomic theory

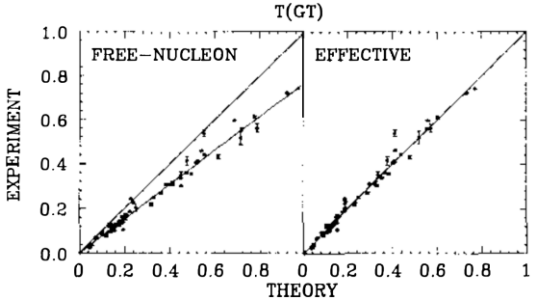
TRIUMF

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

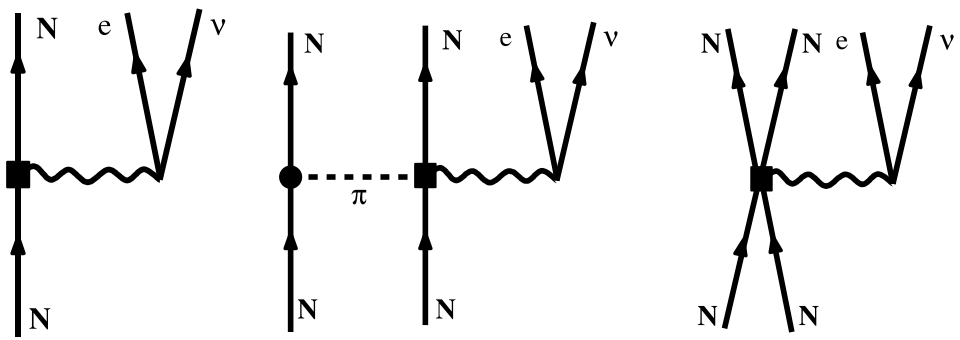
P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

Large-Scale Ab Initio GT Transitions

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

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

2BC: Coupling of weak force to two nucleons



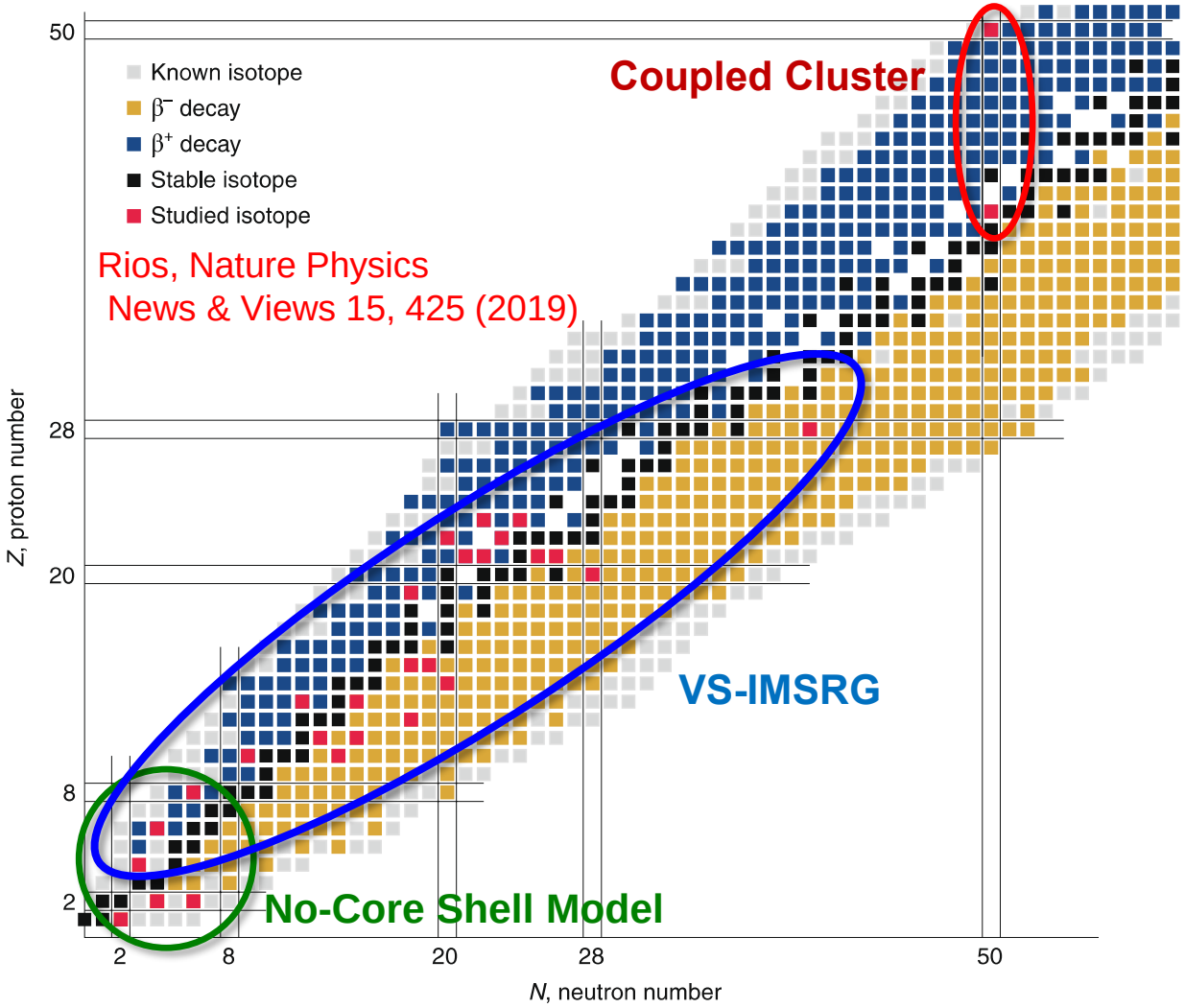
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

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

NUCLEAR PHYSICS news & views

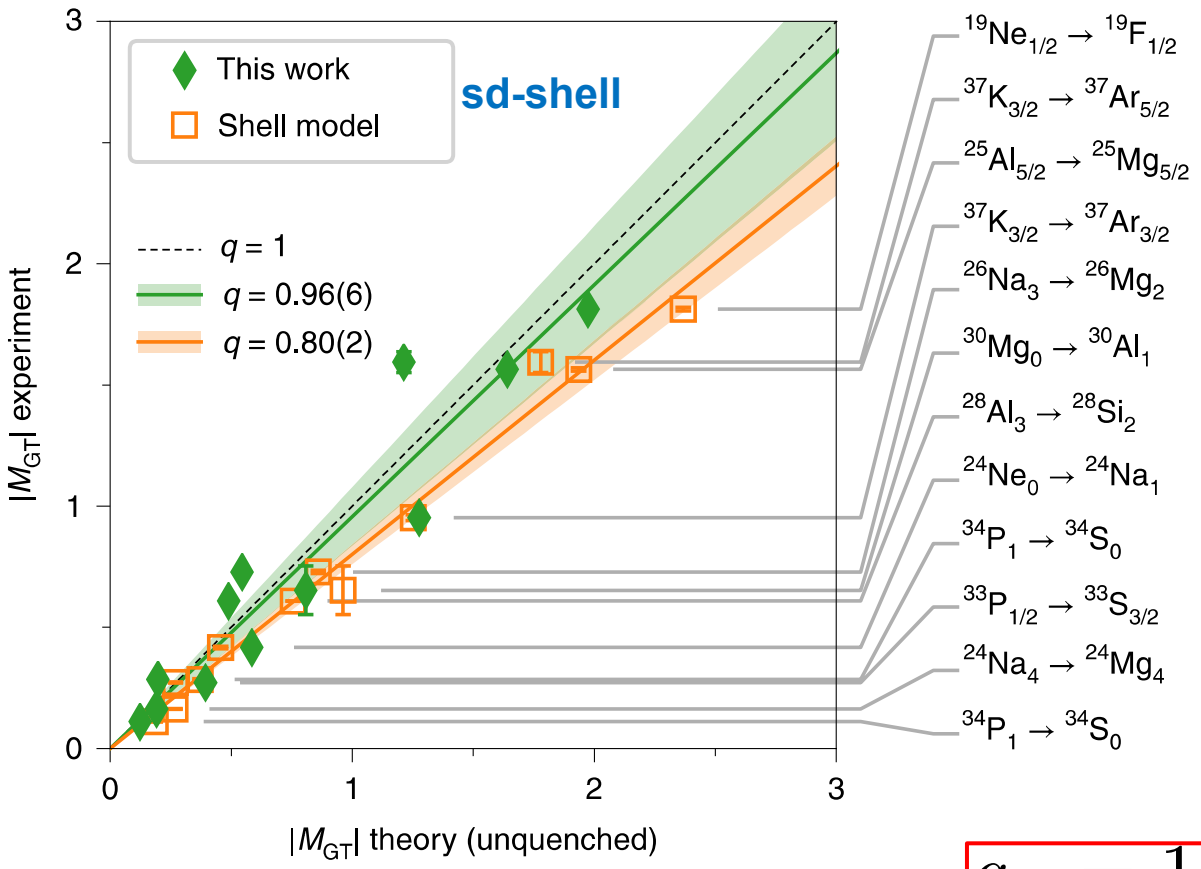
Beta decay gets the ab initio treatment

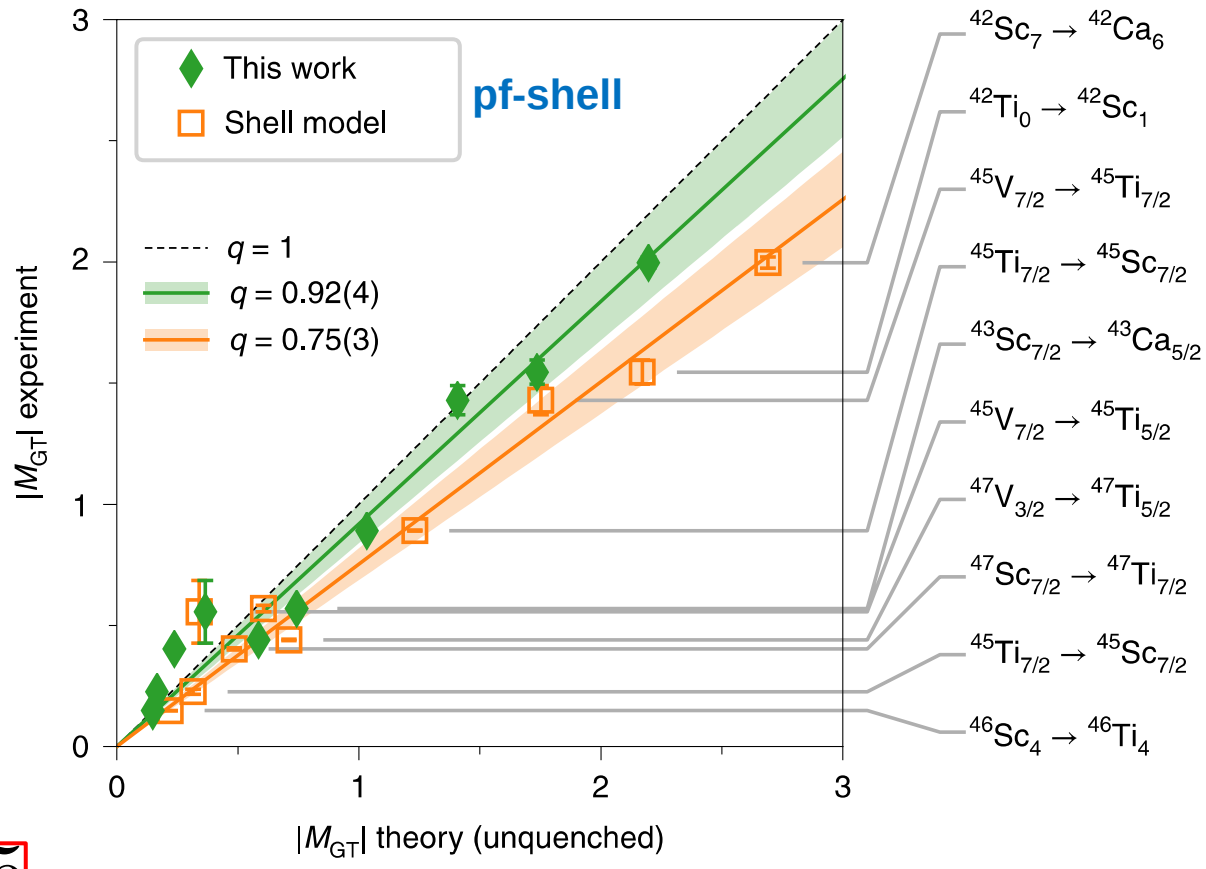
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.



Solution to g_A-Quenching Problem

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





$$g_A = 1.25$$

Ab initio calculations across the chart explain data with unquenched g_A

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

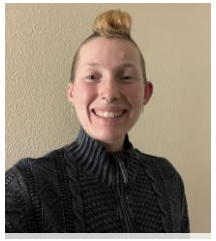
Nature Physics **15**, 428 (2019)

TRIUMF

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

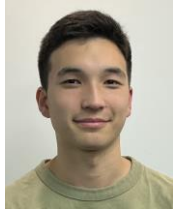
A. Belley

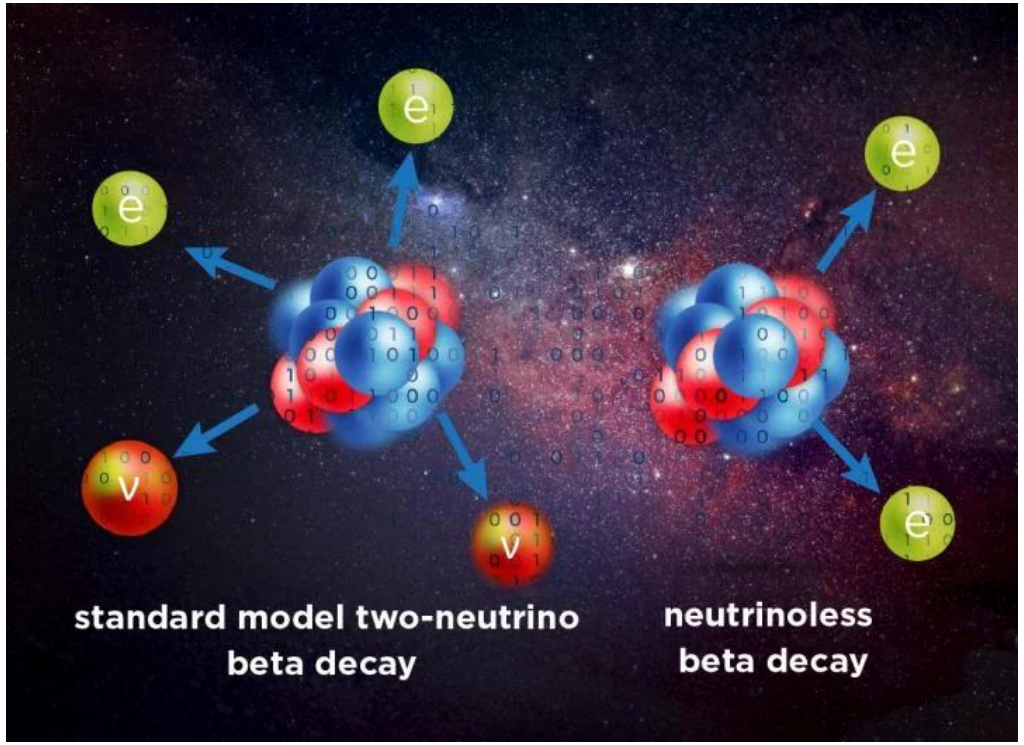
L. Jokiniemi


I. Ginnett

J. Pitcher

A. Todd


T. Shickele



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

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

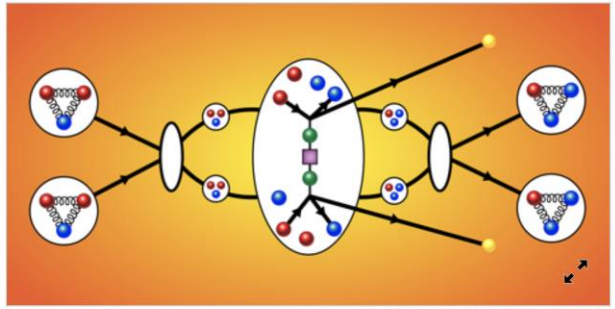
Proper renormalization requires short-range contact term at leading order

Physics — SYNOPSIS

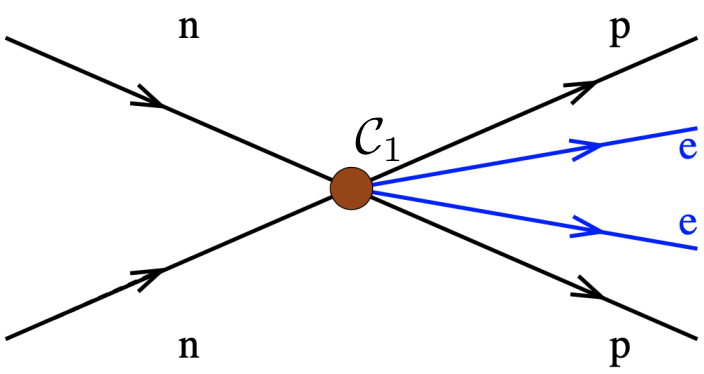
A Missing Piece in the Neutrinoless Beta-Decay Puzzle

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

V. Cirigliano et al. PRL (2018), PRL (2022)

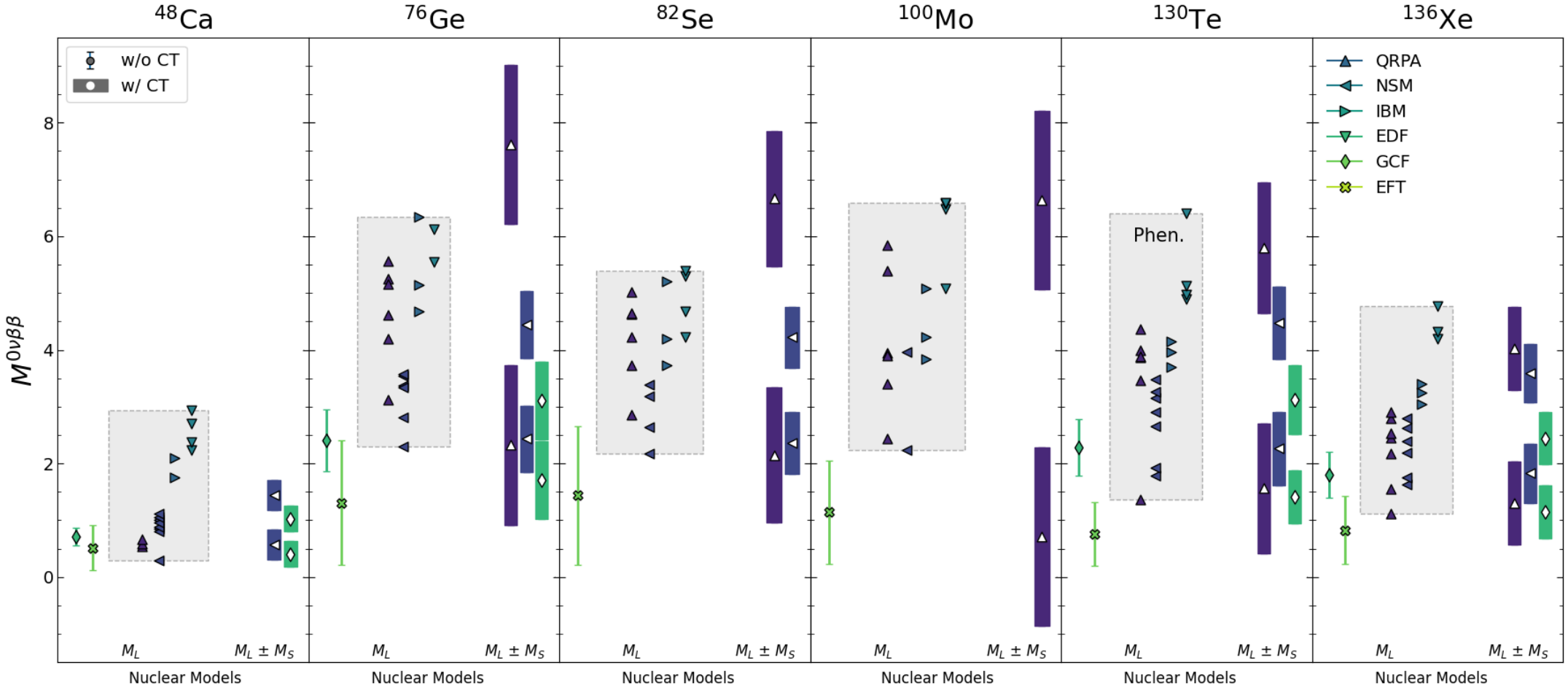
New paradigm for $0\nu\beta\beta$ decay: include long- and short-range terms

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

Estimated to ~30% - no consistent way to assess with phenomenology

(More) Current Status of NMEs

Updated phenomenology w/ short-range contact

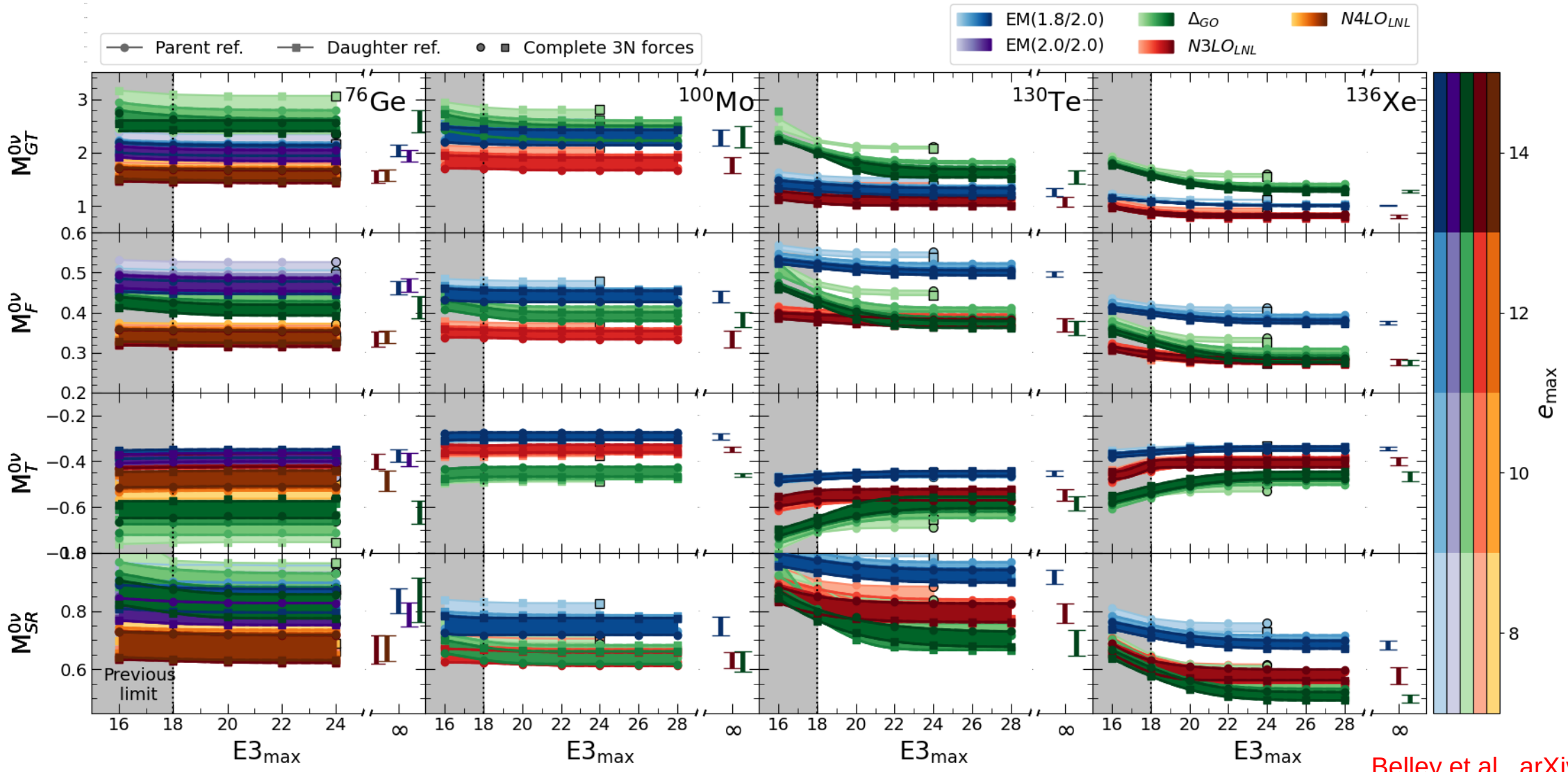


Uncertainty from **sign** of short-range term

New(er) results increase factors up to >10 uncertainty 😬 can we do better?

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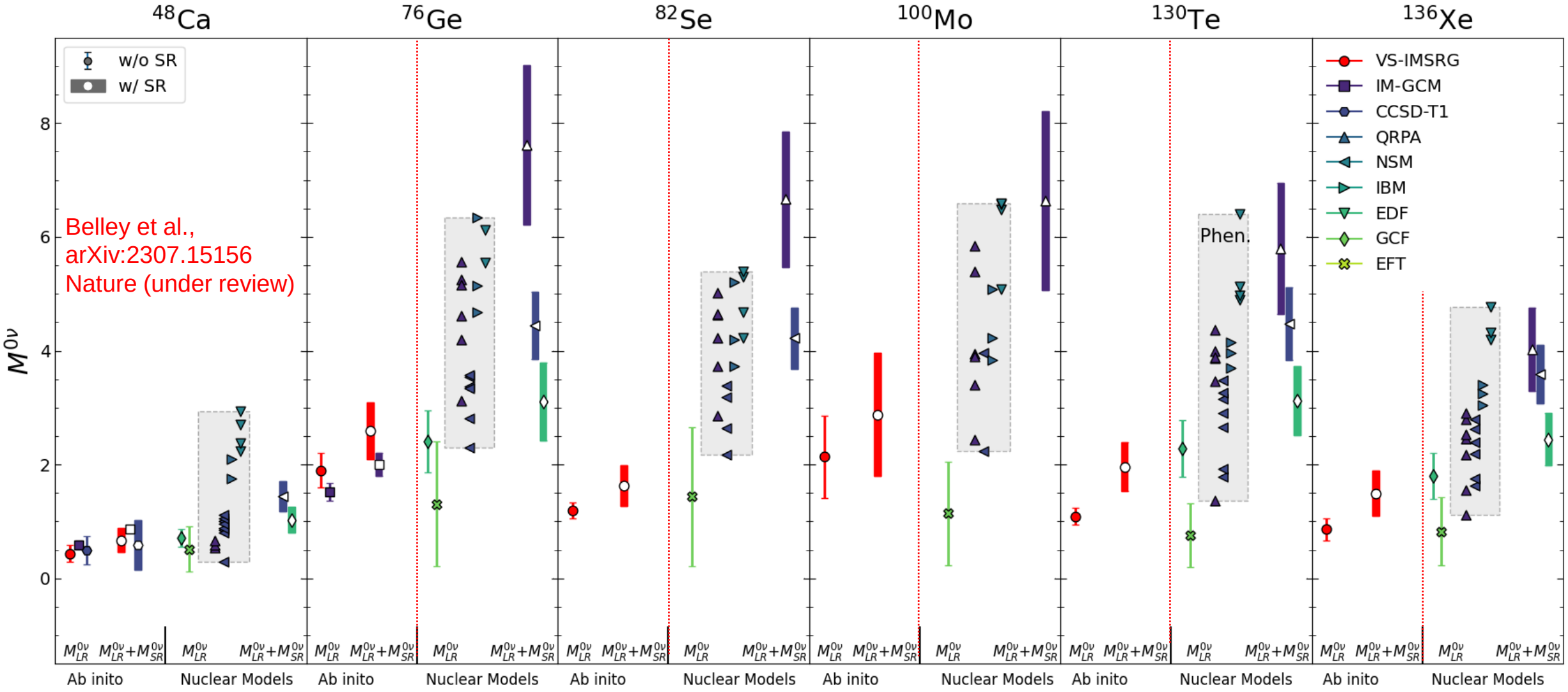
Ab initio results: differences from models; **large NMEs *strongly* disfavored**



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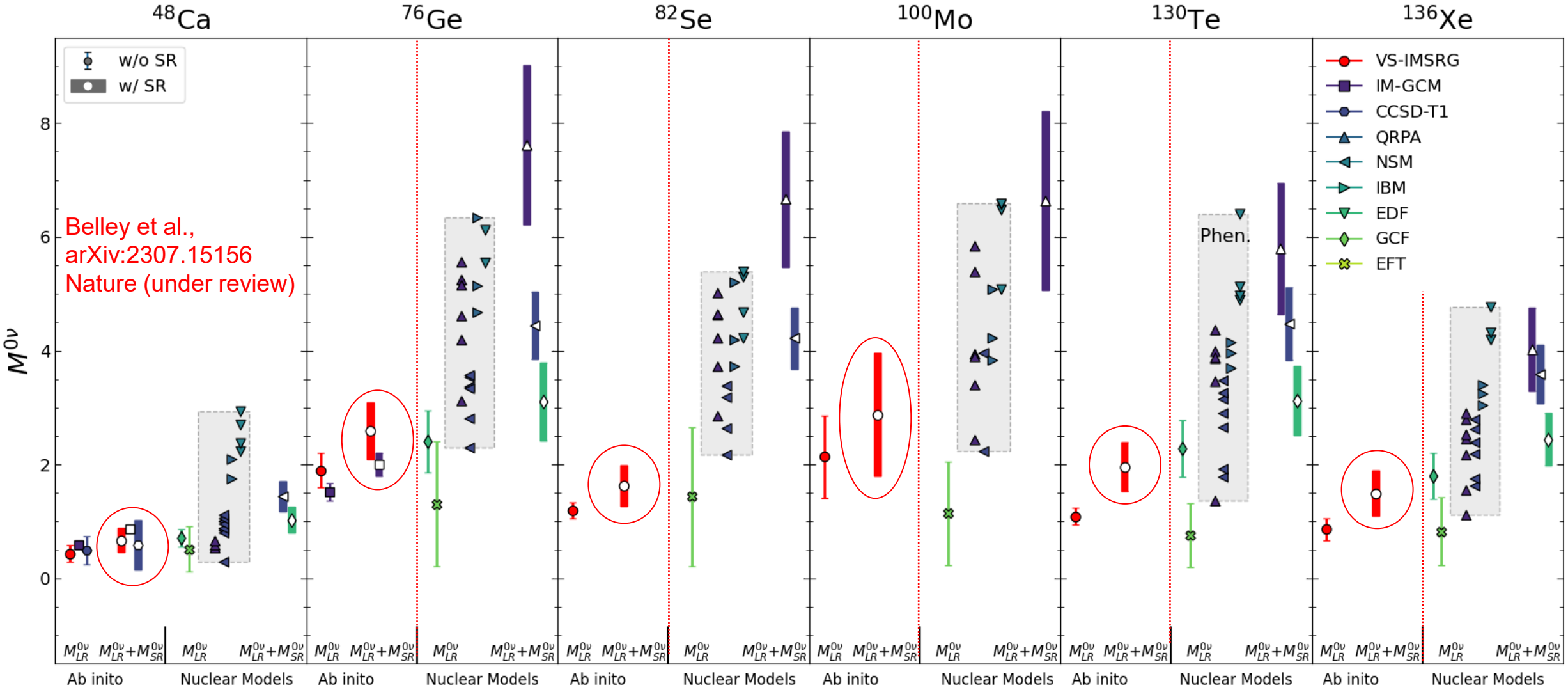
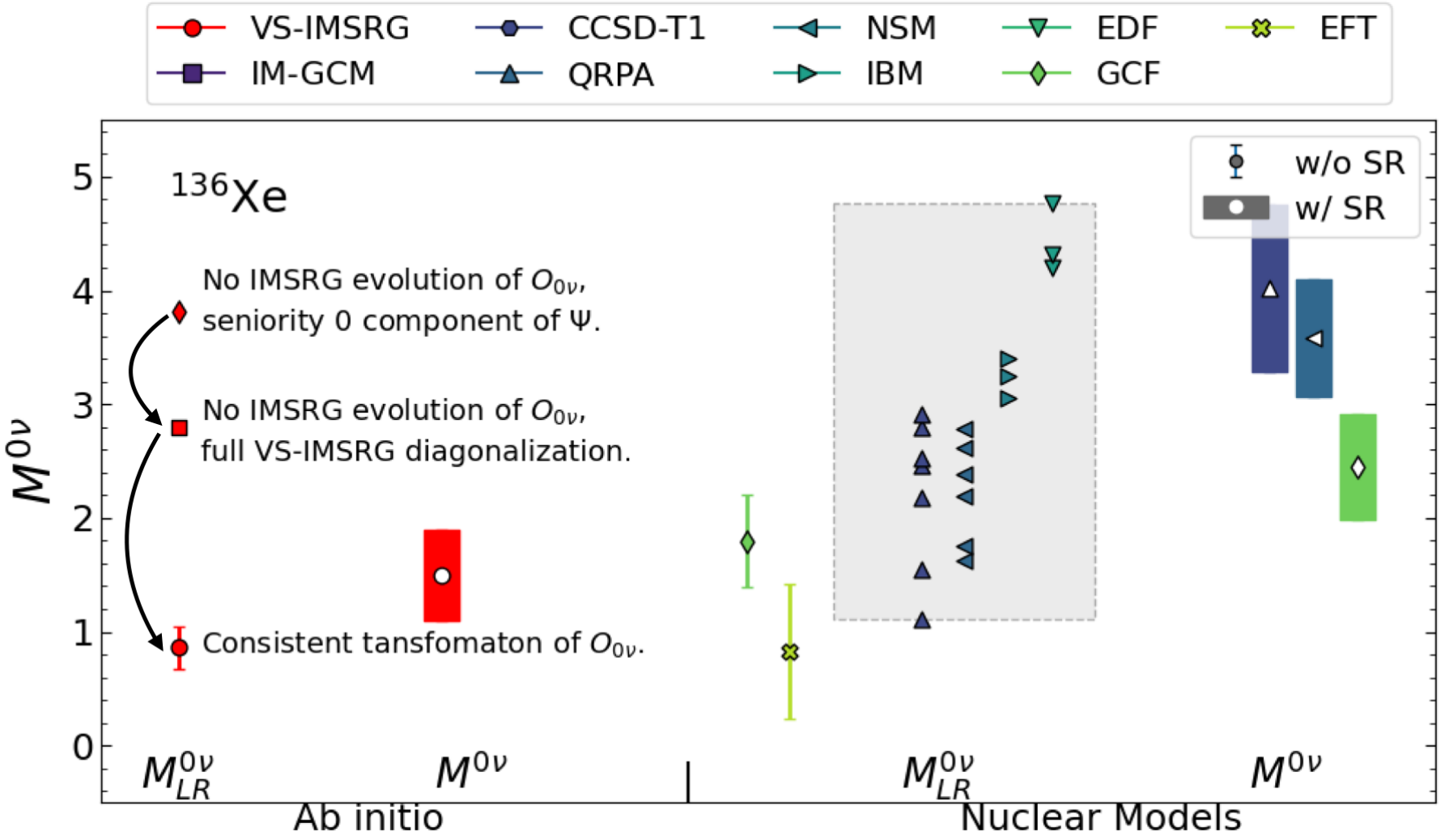


Why Small Matrix Elements?

Correlations in wavefunction and operator drive small NMEs

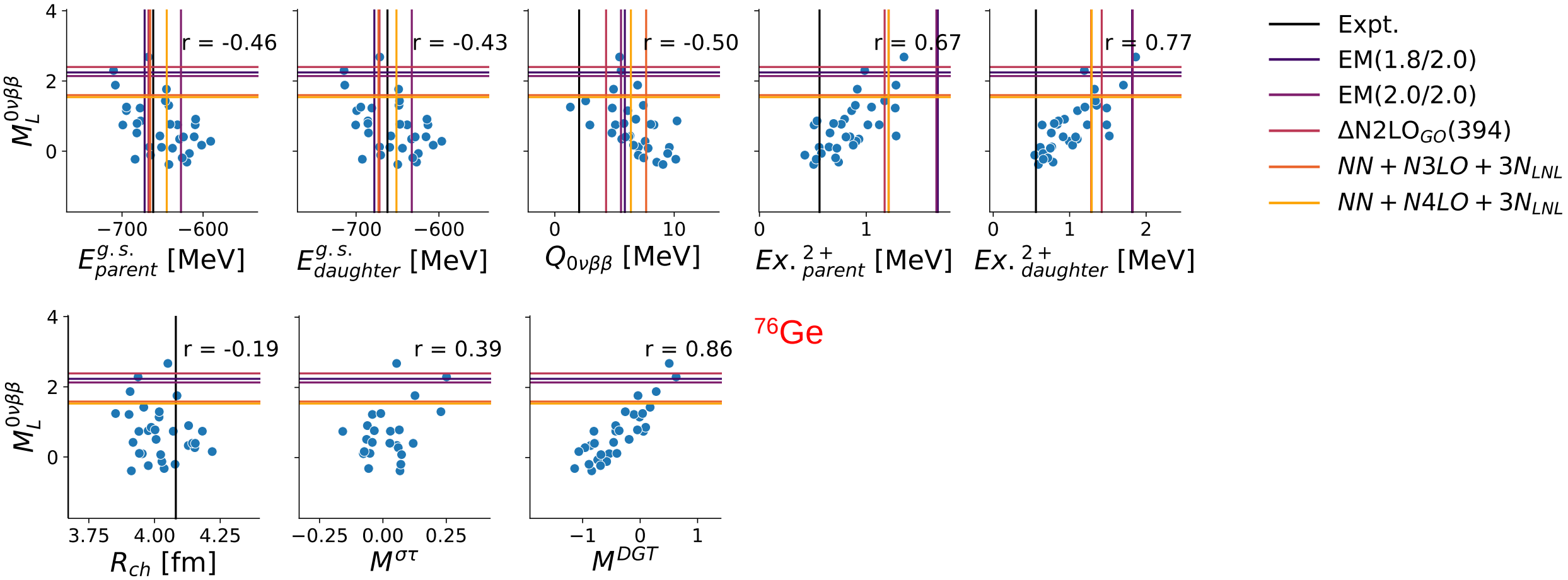
Ab initio results: differences from models; **large NMEs *strongly* disfavored**



Ab Initio Strategy: Explore Correlations

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

No ab initio correlations, except DGT



Use machine learning for further insights?

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

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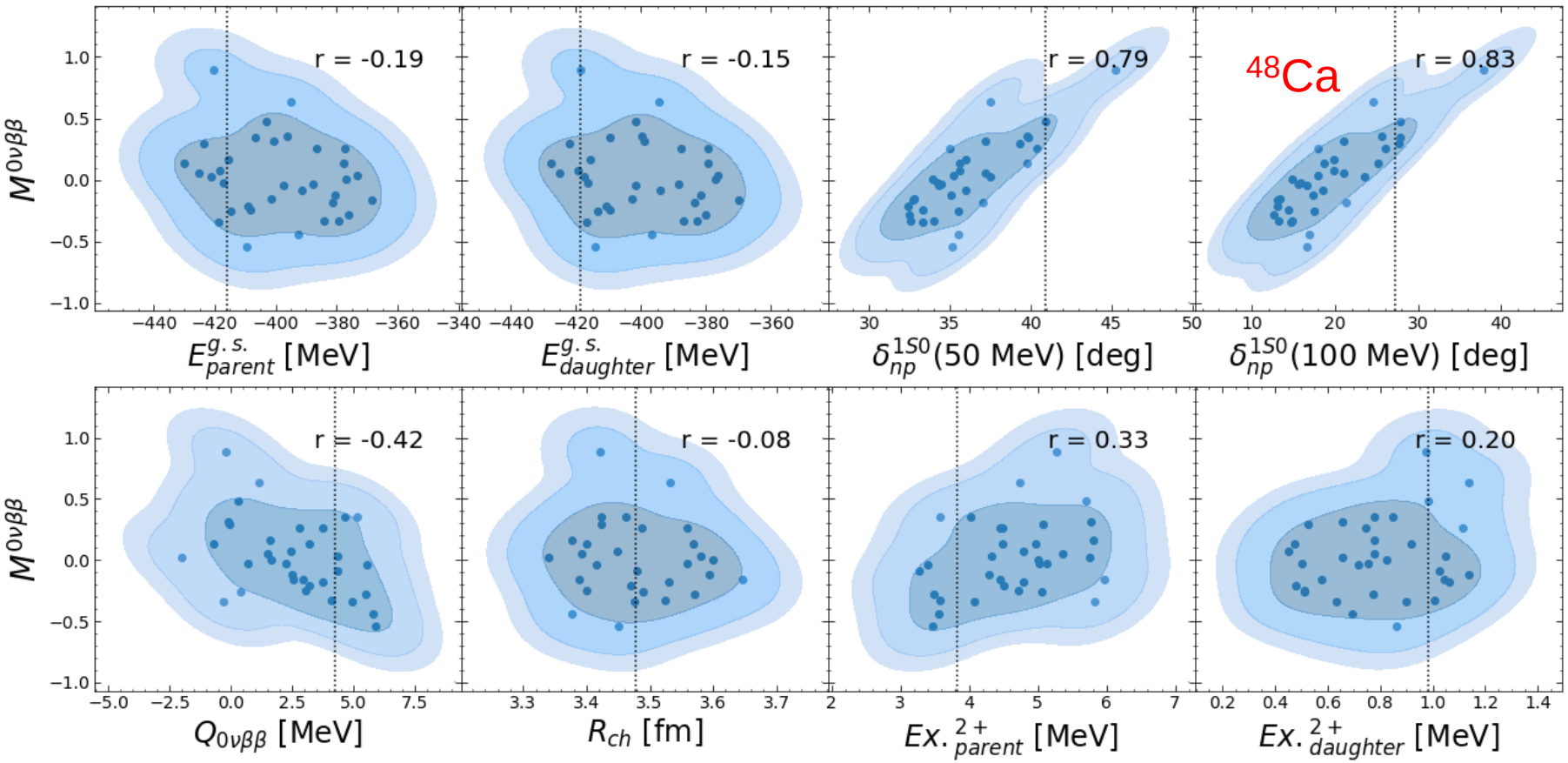

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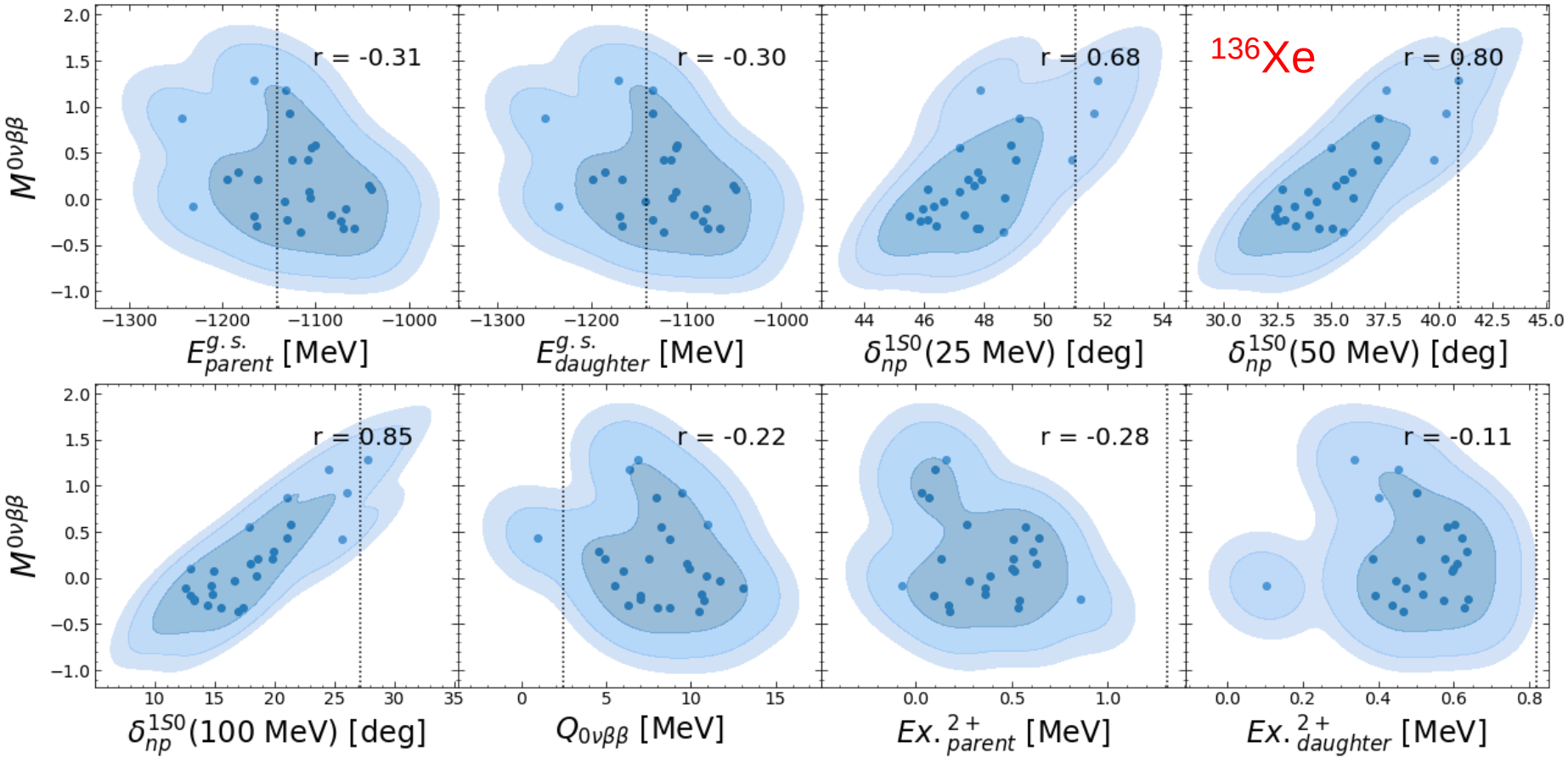


Use machine learning for further insights?

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

Machine Learning for Sensitivity Analysis

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

Use gaussian processes as an emulator

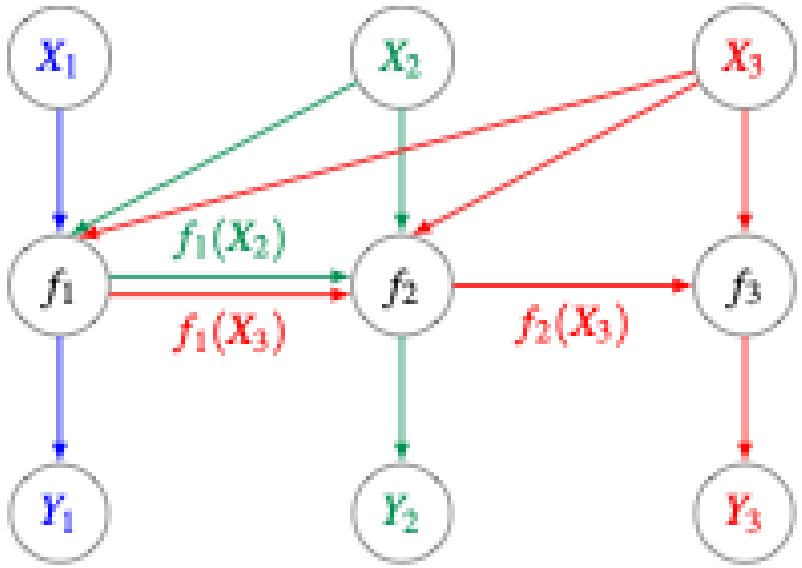
Multi-Fidelity Gaussian Process: connects few (complicated) high-fidelity data points (e.g., full IMSRG) w/ many low-fidelity data points (HF, low e_{max}, etc)

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)

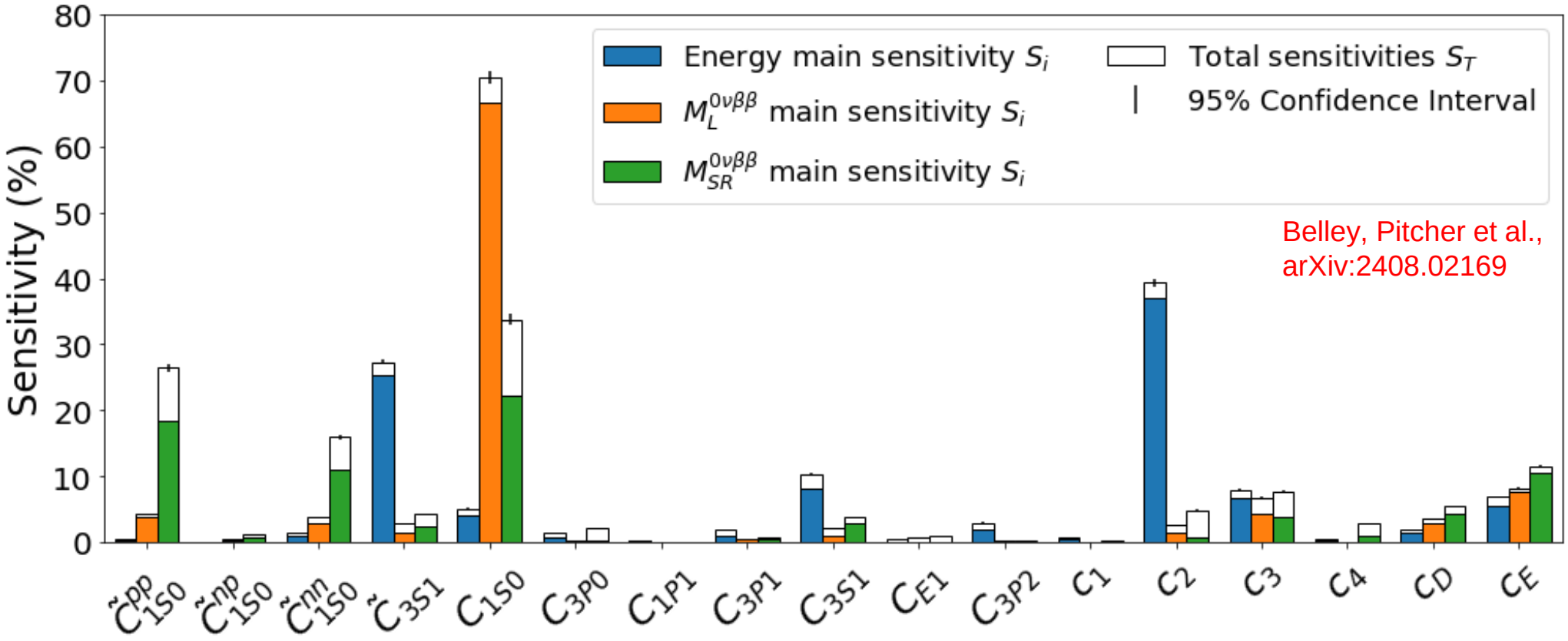


Belley, Pitcher et al., in preparation

MM-DGP Emulator for IMSRG: Sensitivity Analysis

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

Sensitivity analysis: **Connect long-range 0νββ decay to terms in nuclear forces**

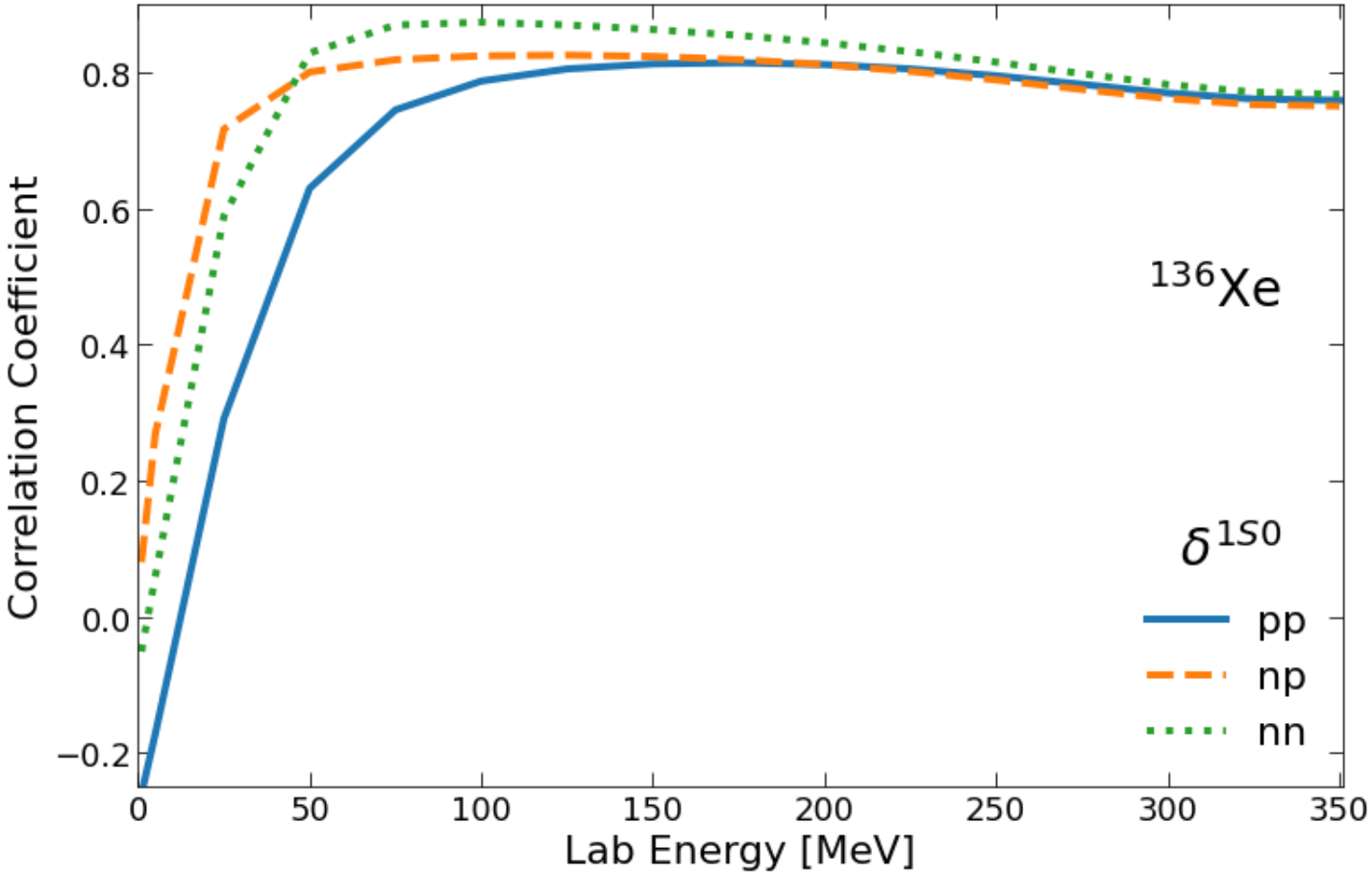


Highly sensitive to single constant "C1S0" – related to $^1S_0$ phase shift

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

Clear correlation with $^1S_0$ phase-shift

Strong correlation emerges for energies > 50MeV



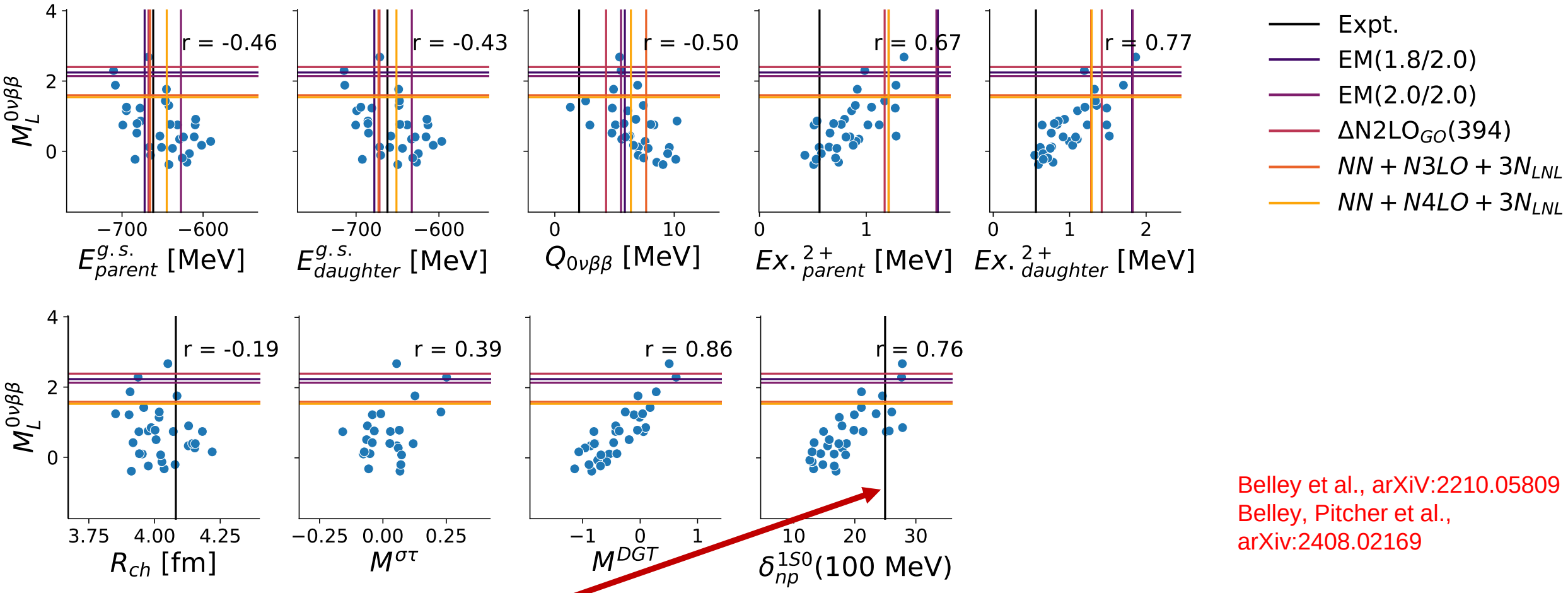
Belley, Pitcher et al., arXiv:2408.02169

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

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., arXiv:2408.02169

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

Rigorous Ab Initio Uncertainties for ^{76}Ge

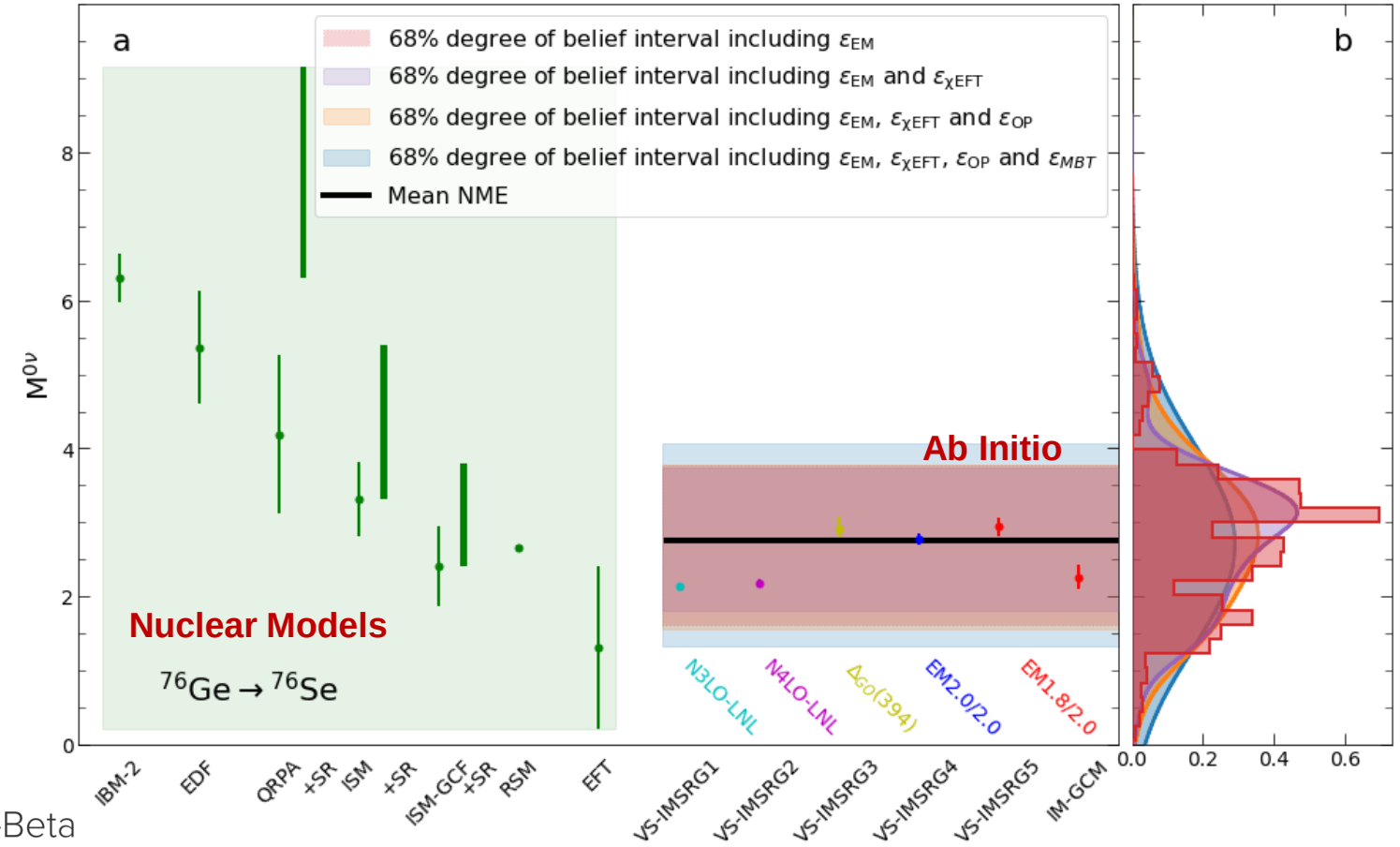
Consider *all* physics contributing to theoretical error in $0\nu\beta\beta$ decay

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

Nuclear many-body problem treated w/ newly developed ML emulators

Construct PPD for NME in ^{76}Ge

Dramatically reduced uncertainty compared to nuclear models



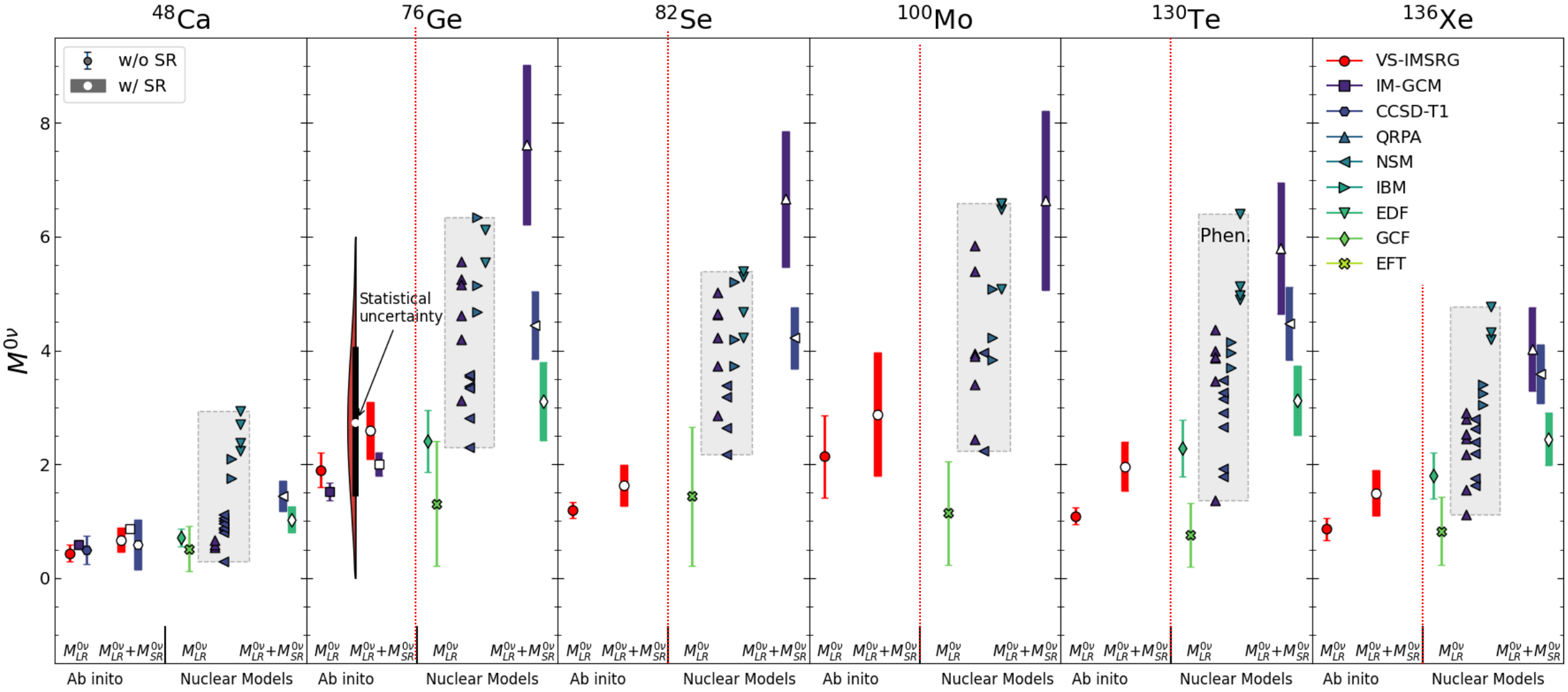
Ab Initio Uncertainty Quantification of Neutrinoless Double-Beta Decay in ^{76}Ge

A. Belley, J. M. Yao (尧江明), 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 (张馨)
Phys. Rev. Lett. **132**, 182502 – Published 30 April 2024

Updated Predictions in Heavy Nuclei

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

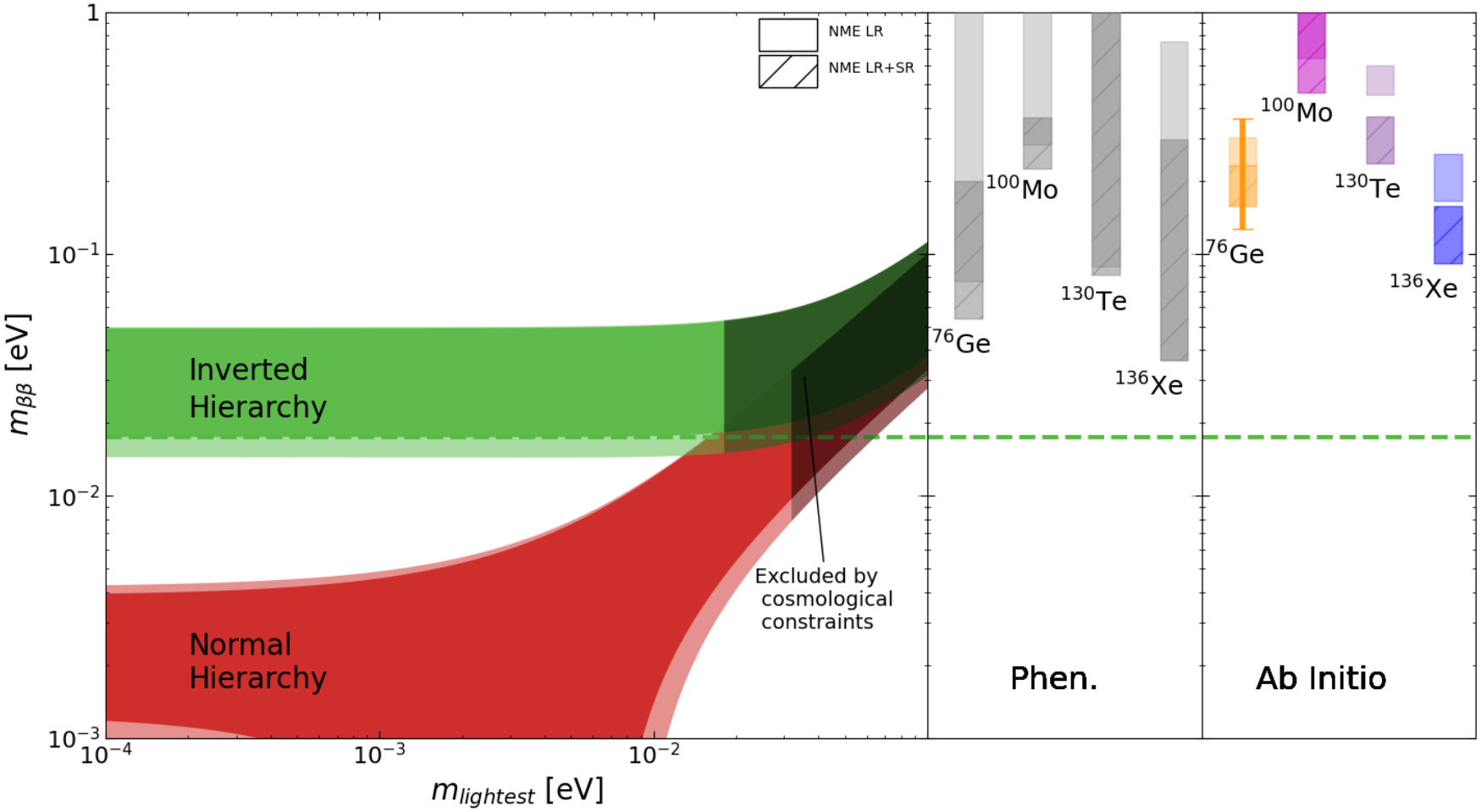
Independent PPD agrees with previous spread



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



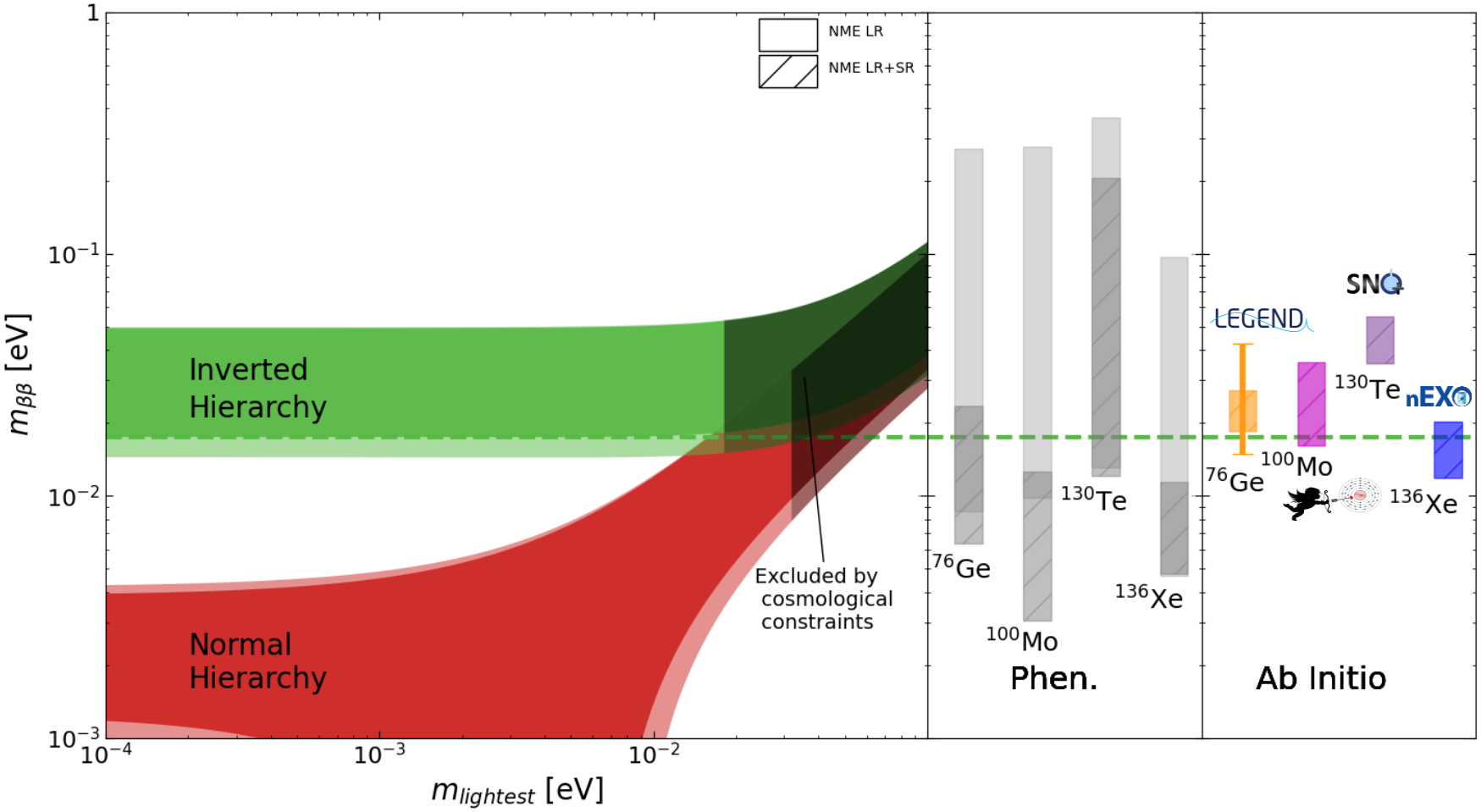
Highly unlikely **inverted Hierarchy has been probed**

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*!**

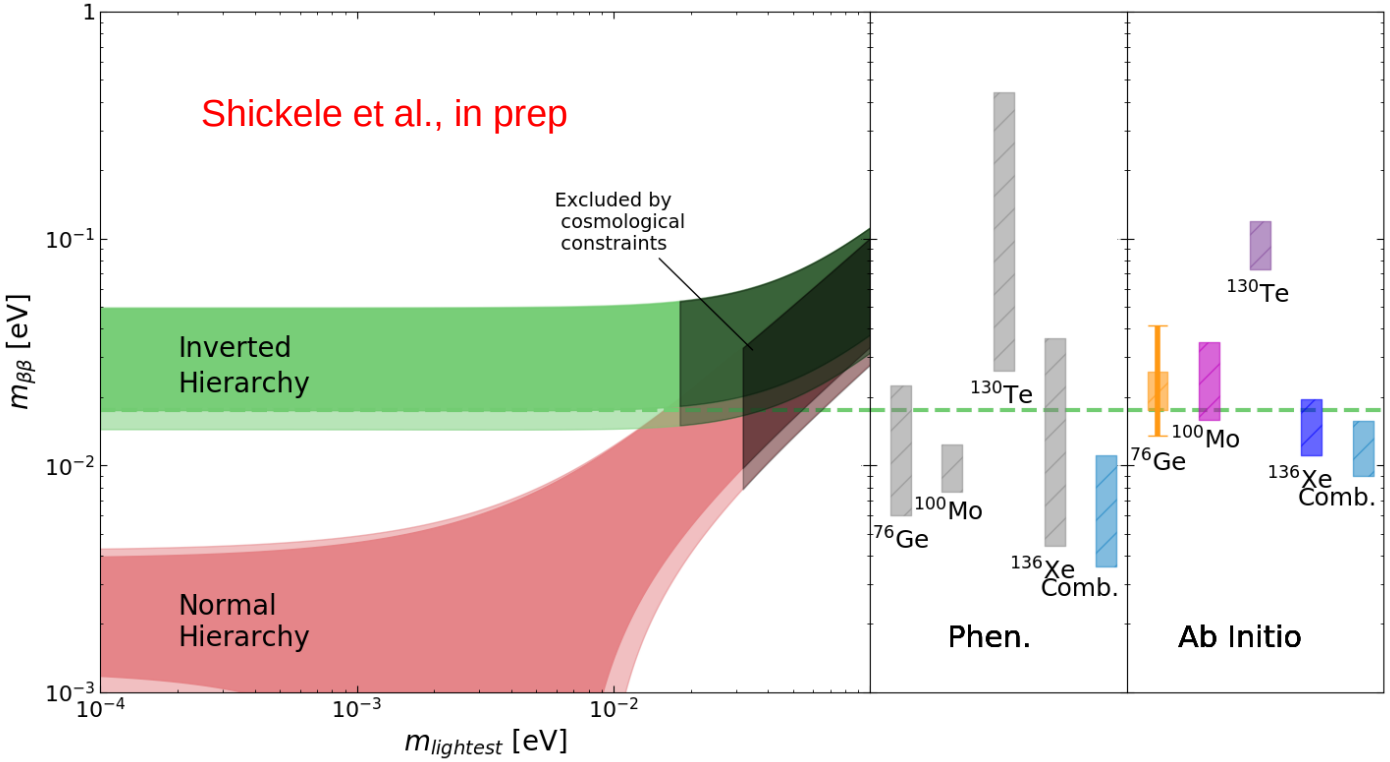
Belley et al, arXiv:2307.15156
Nature (under review)

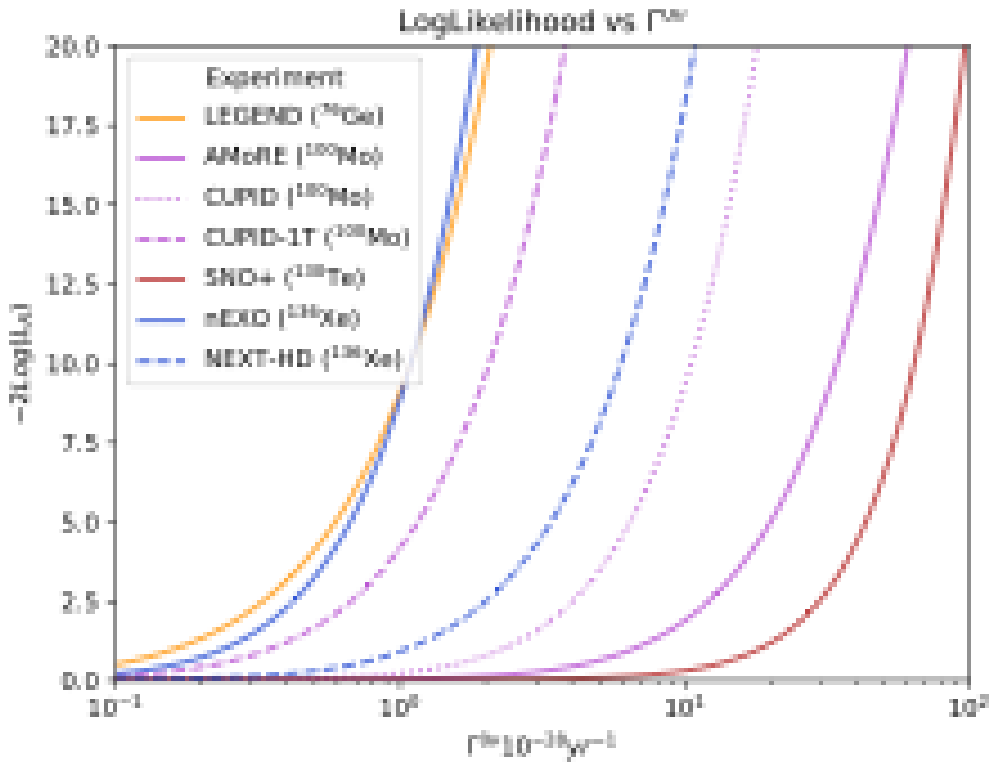
Combined Limits: Likelihood Functions

Obtain likelihood functions from experiments – convert decay rates to $m_{\beta\beta}$

$$m_{\beta\beta} = \frac{m_e}{g_A^2 |M^{0\nu}|} \sqrt{\frac{\Gamma^{0\nu}}{G^{0\nu} \log 2}}$$

Likelihoods allow combined limit via Bayes' Theorem



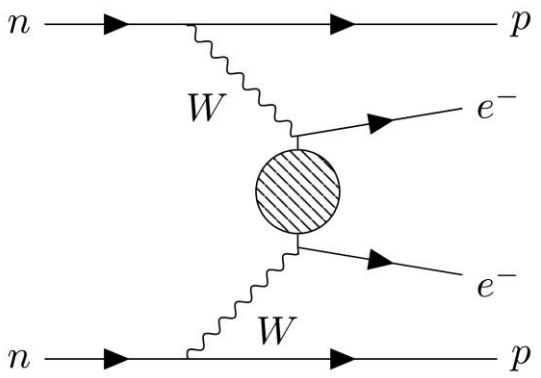


Analysis based on S. Biller PRD (2021)

Combined limits indicate IH will be probed!

NMEs for Heavy Sterile Neutrino Exchange

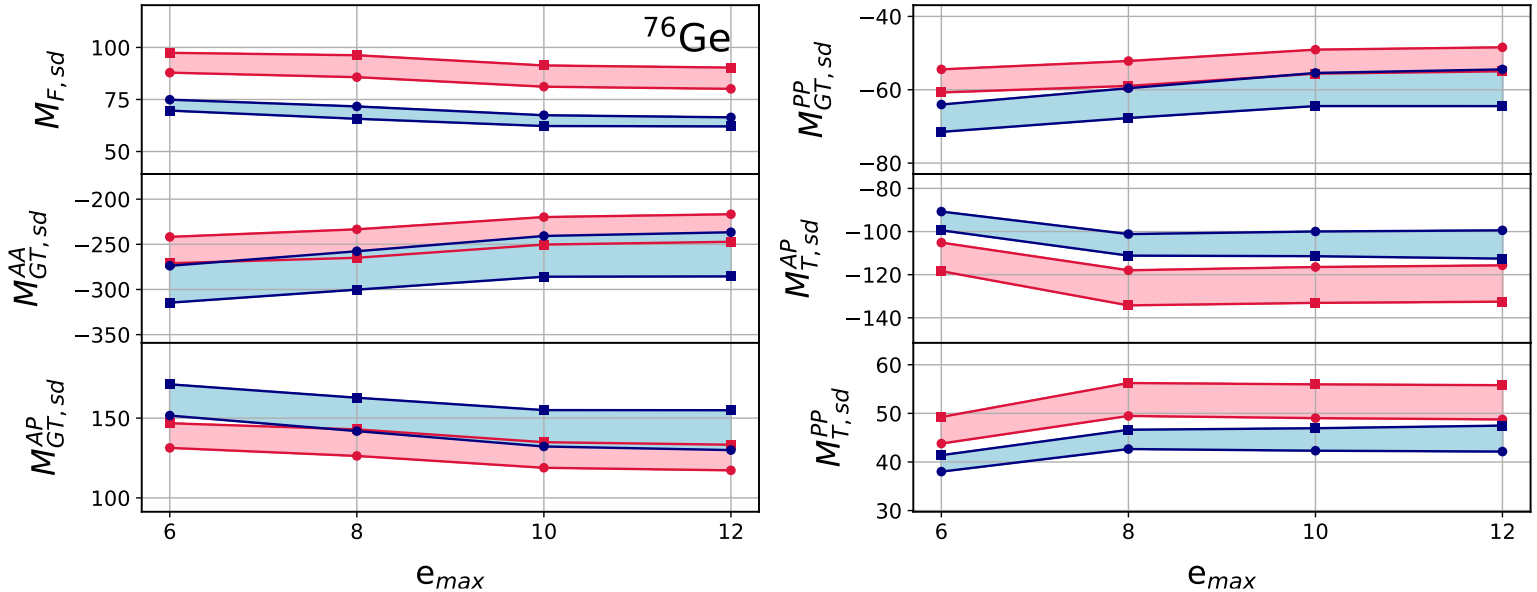
Explore other possible exchange mechanisms: heavy sterile neutrinos



$$\frac{1}{T^{0\nu}_{1/2}} = g_A^4 G^{0\nu} \left(|M_L^{0\nu}| \frac{m_{\beta\beta}}{m_e} + |M_H^{0\nu}| \frac{m_p}{M_{\beta\beta}} \right)^2$$

V. Cirigliano et al. J. High Energ. Phys. (2018)

Complicated operator structures (15); now implemented in ab initio theory

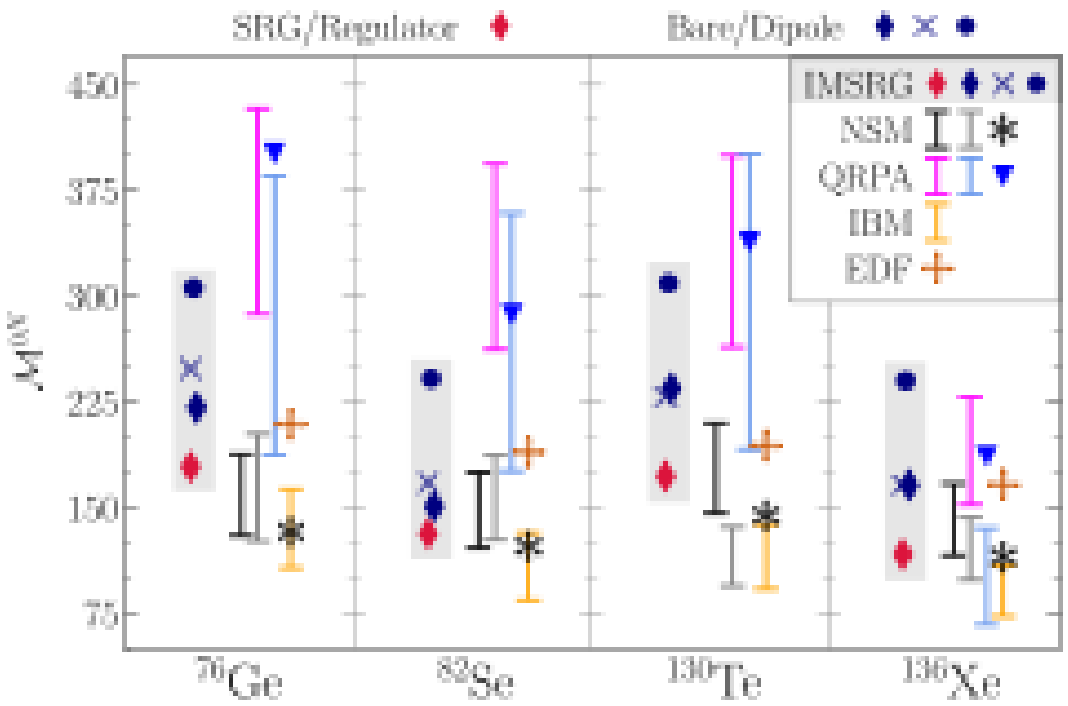


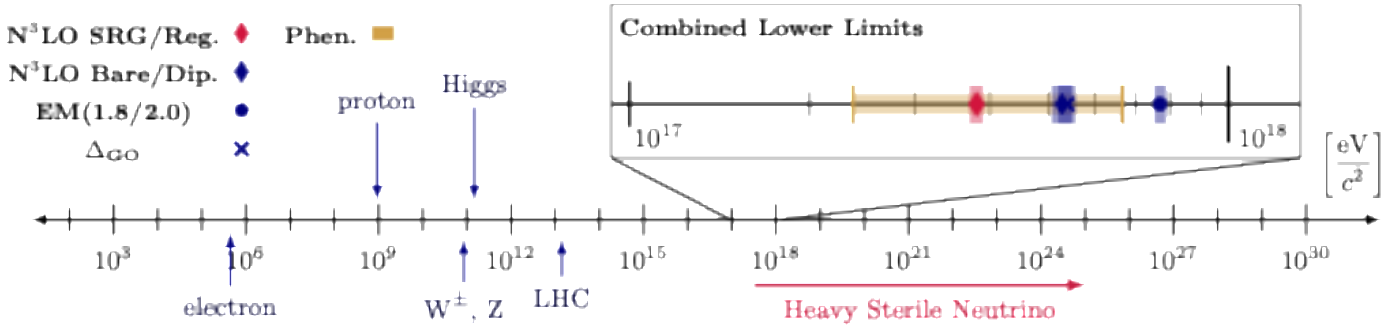
Todd, Shickele et al., in prep.

NMEs for Heavy Sterile Neutrino Exchange

Converged heavy NMEs for all major candidates

Generally smaller values (and spread) than nuclear models





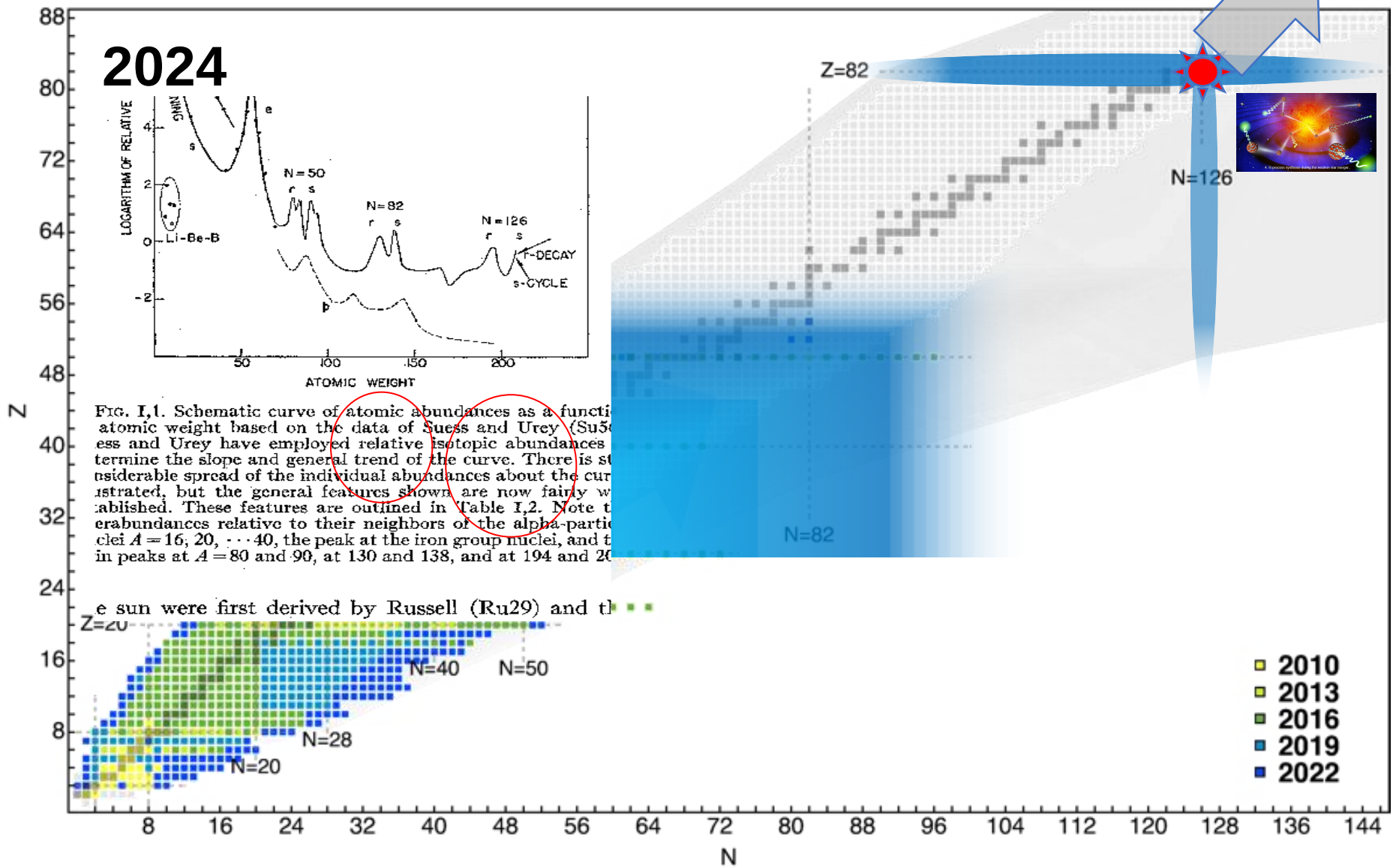
Todd, Shickele et al. in prep.

Use $0\nu\beta\beta$ limits to obtain combined lower limit for heavy neutrino mass

Results probe particle masses beyond the LHC: new collaborations w/ particle theory @TRIUMF

Future of Ab Initio Theory

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

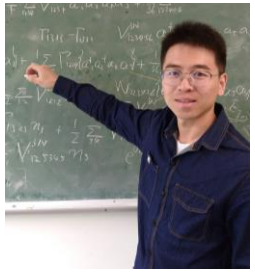


Nucleosynthesis

Ab initio input for r-process

Nicole Vassh

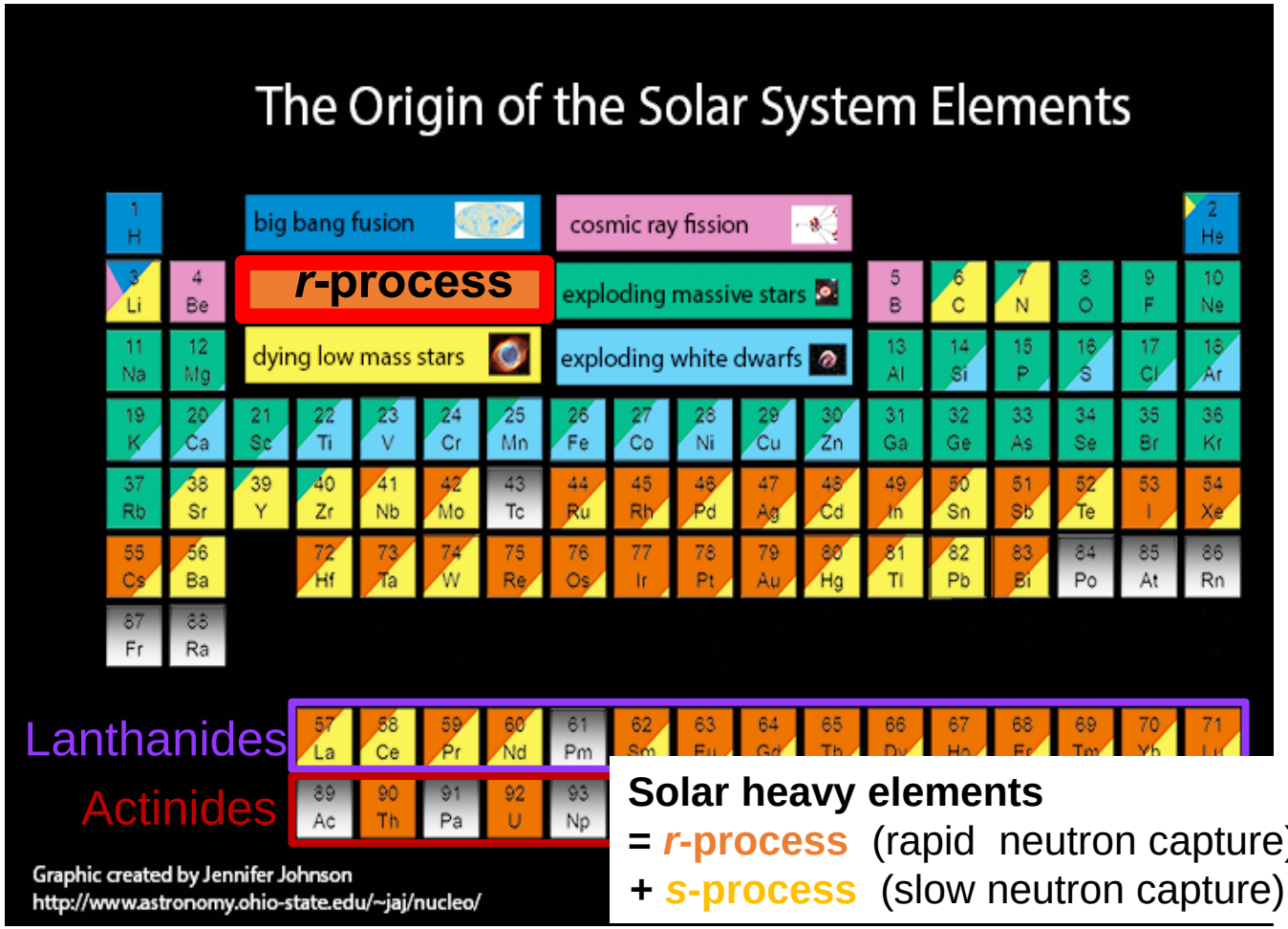
Maude Larivière



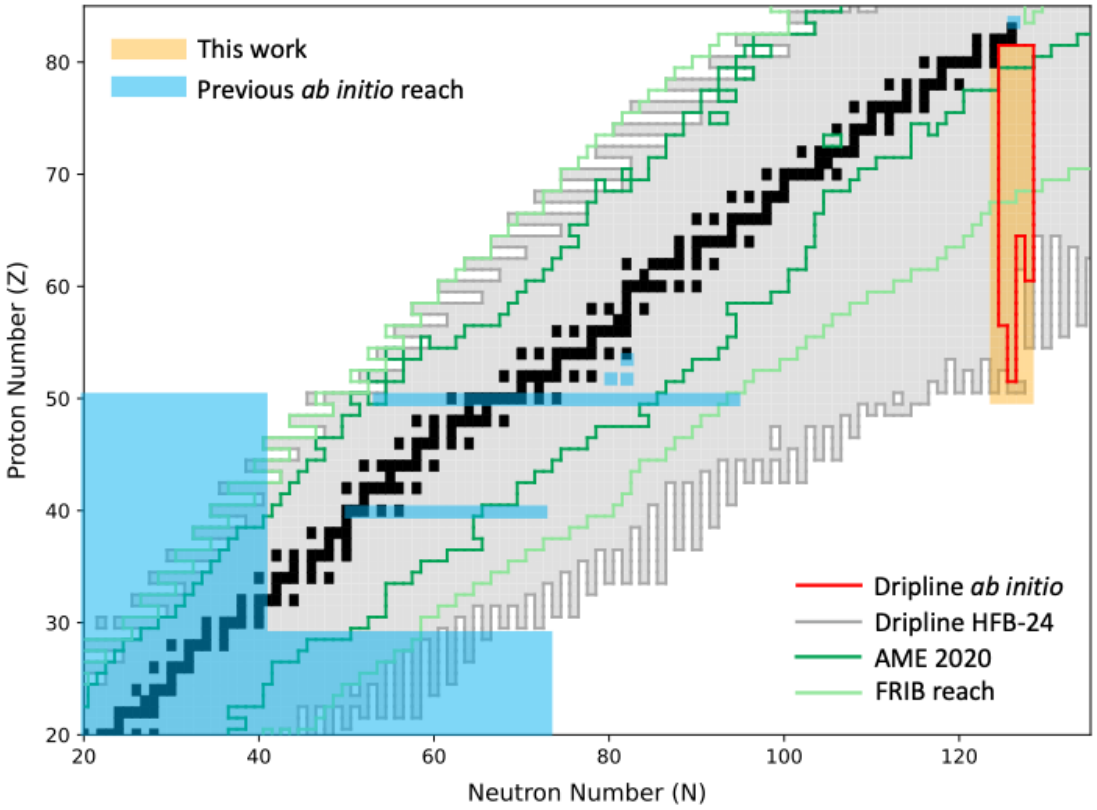
Baishan Hu

Ab Initio Theory for Origin of Heavy Elements

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



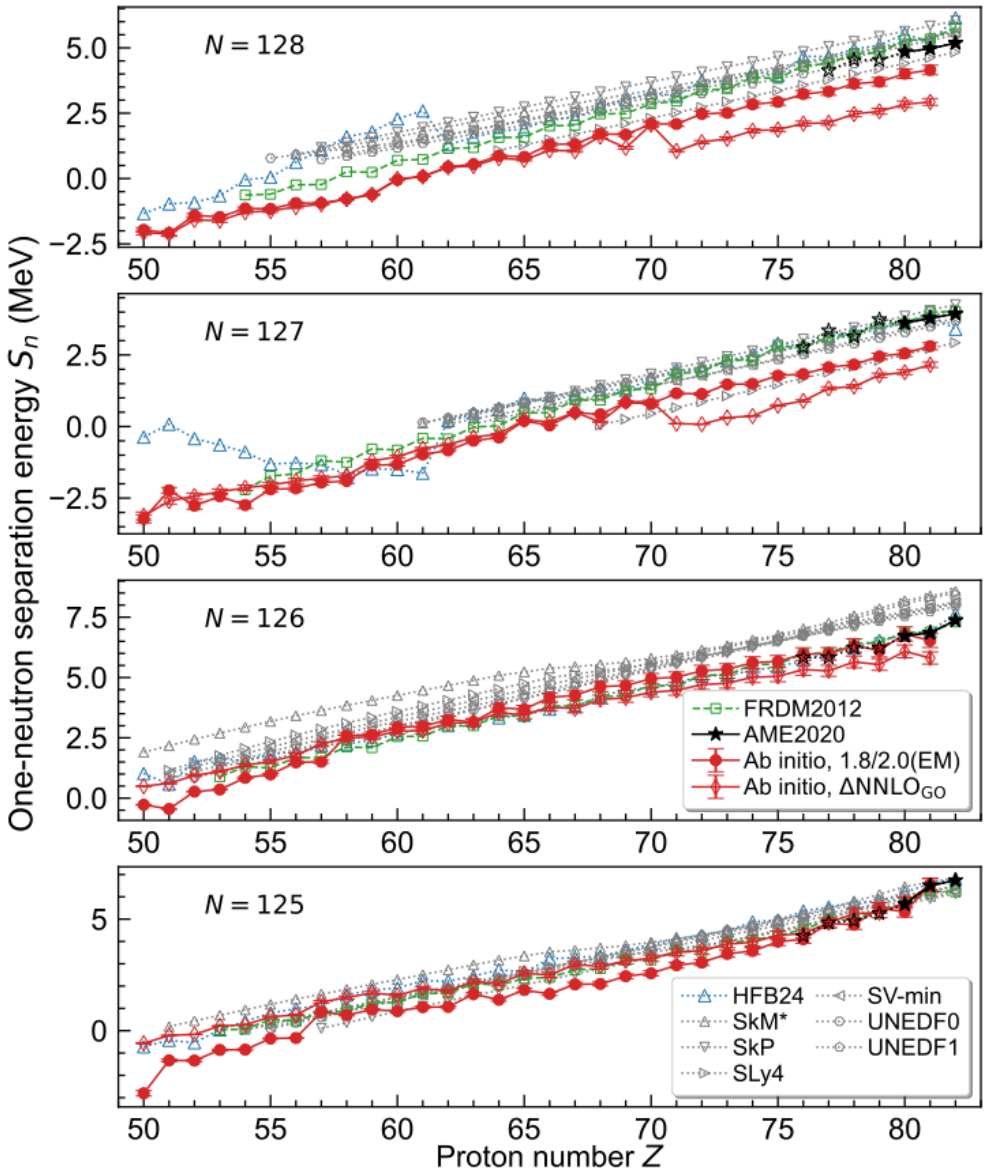
Solar heavy elements
= ***r*-process** (rapid neutron capture)
+ ***s*-process** (slow neutron capture)

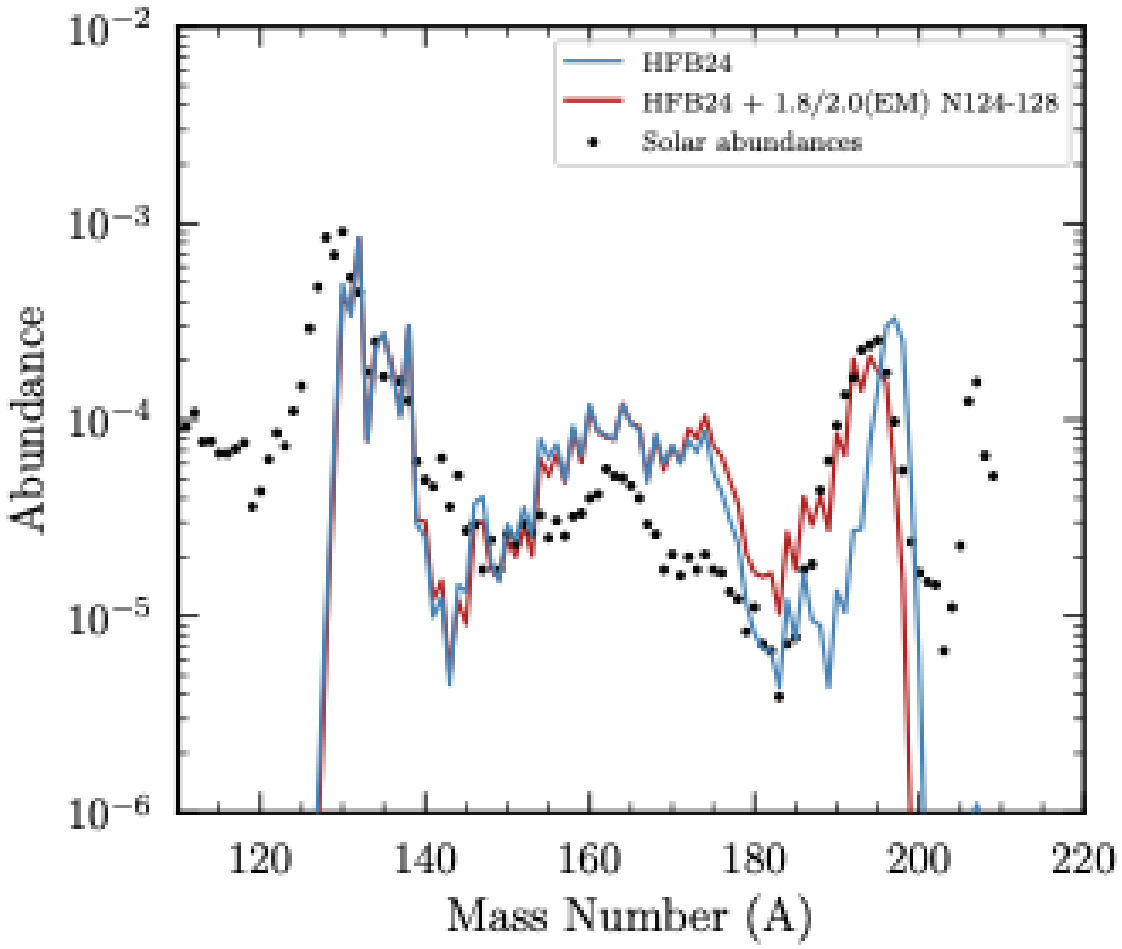


Theory input is crucial where no data exists – little known "south" of ^{208}Pb

Ab Initio Impact on r-Process Simulations

Separation energies, Q-values calculated to N=12x driplines for r-process inputs

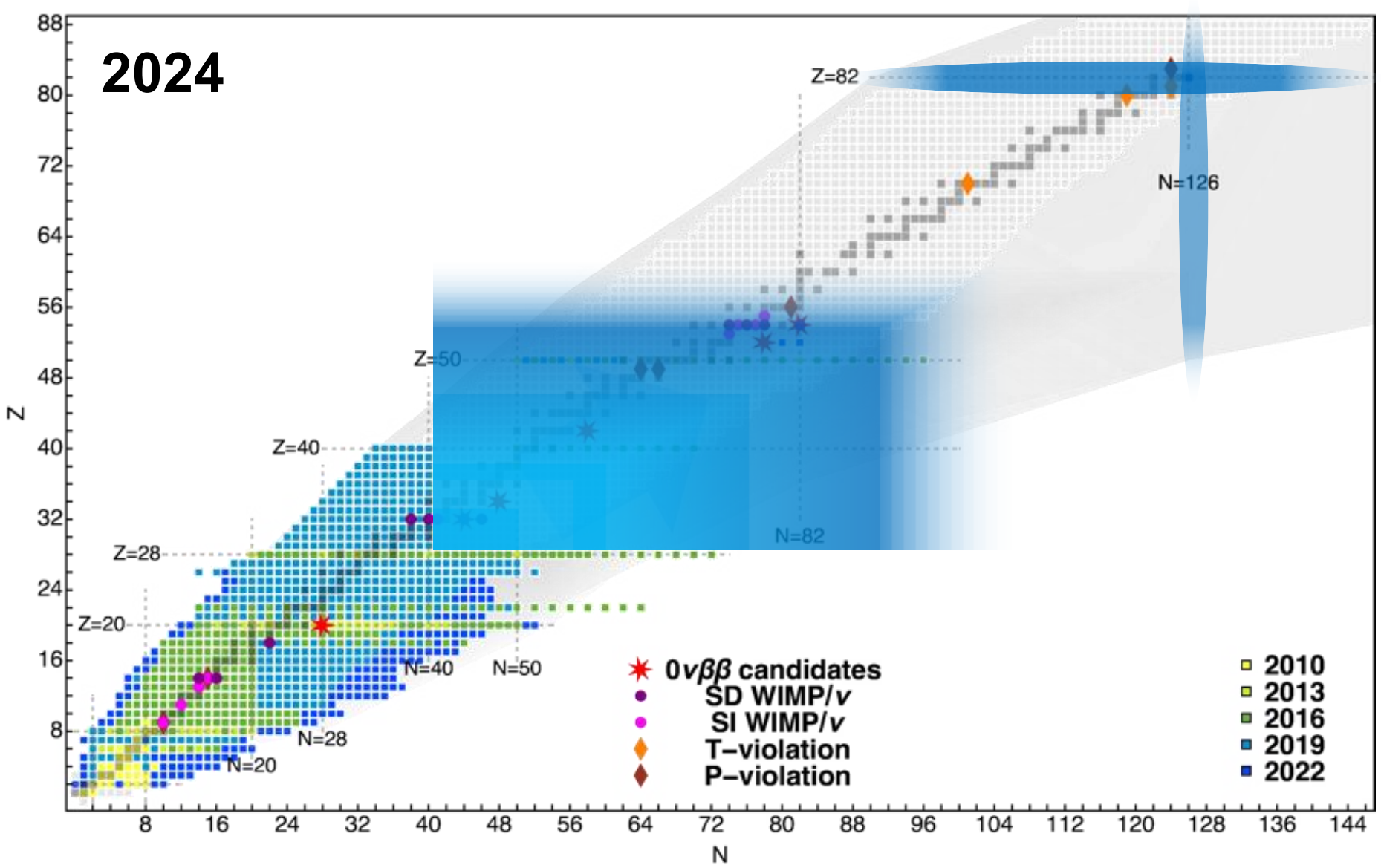




Significant improvement in 3rd abundance peak!

Future of Ab Initio Theory

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

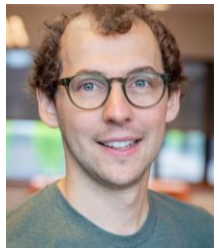


Nucleosynthesis

Ab initio input for r-process

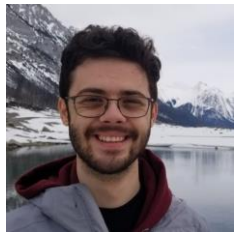
Dark Matter/ν Scattering

Ab initio structure functions

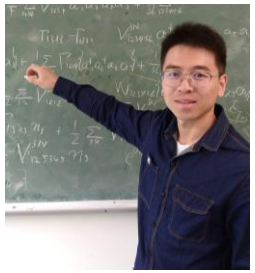


Sam Leutheusser

Jose Padua



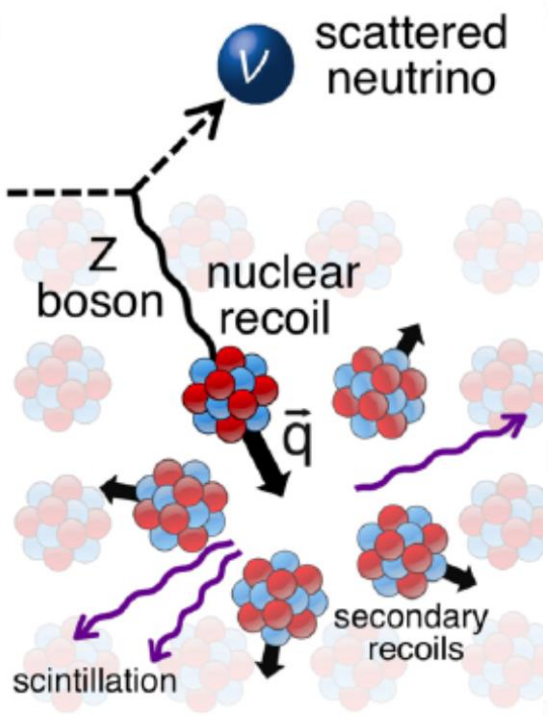
Mathieu Bruneault

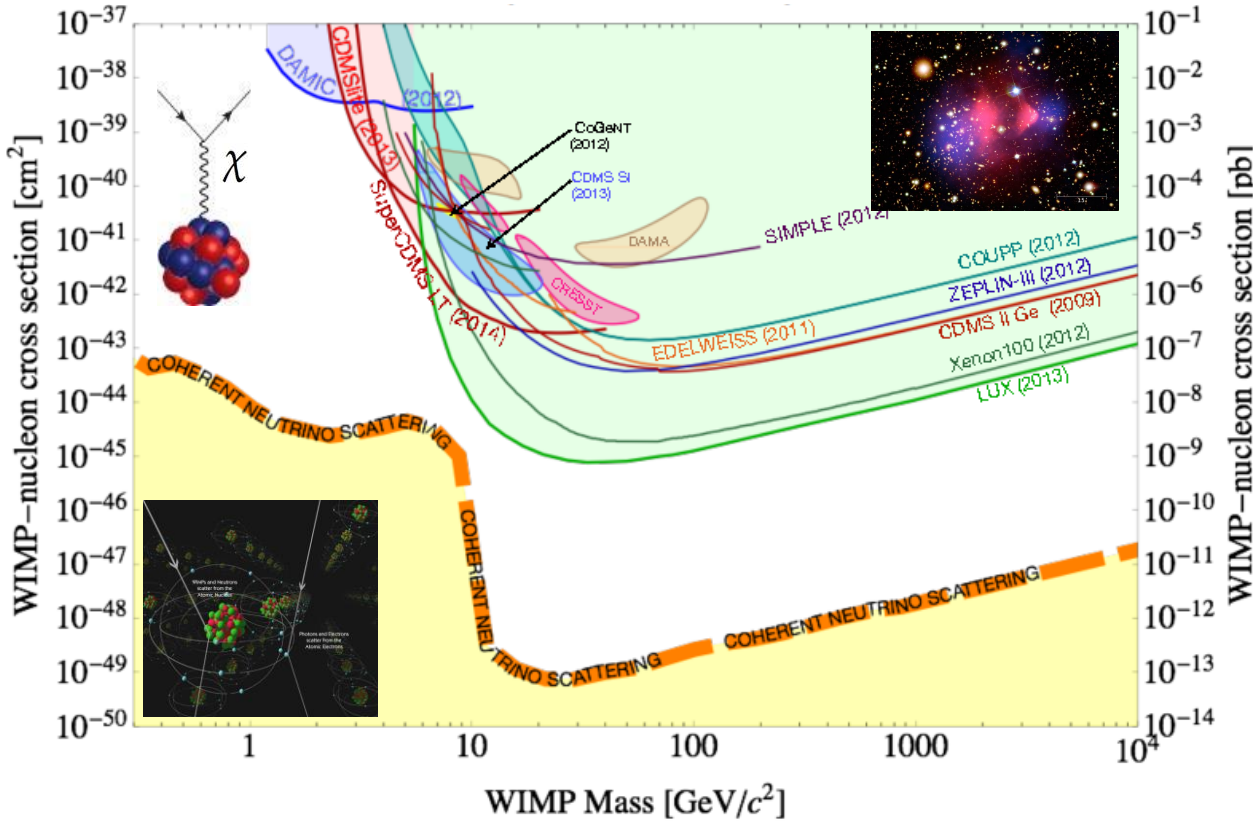


Baishan Hu

Nuclear Theory for BSM Searches

Dark matter direct detection and CEνNS require similar ab initio theory





Differential cross section, well-defined in SM

$$\frac{\mathrm{d}\sigma_A}{\mathrm{d}T}(E_\nu, T) = \frac{G_F^2 M_A}{4\pi}\left(1 - \frac{M_A T}{2E_\nu^2} - \frac{T}{E_\nu}\right) Q_{\mathrm{w}}^2 \left|F_{\mathrm{w}}(\mathbf{q}^2)\right|^2 + \frac{G_F^2 M_A}{4\pi}\left(1 + \frac{M_A T}{2E_\nu^2} - \frac{T}{E_\nu}\right) F_A(\mathbf{q}^2)$$

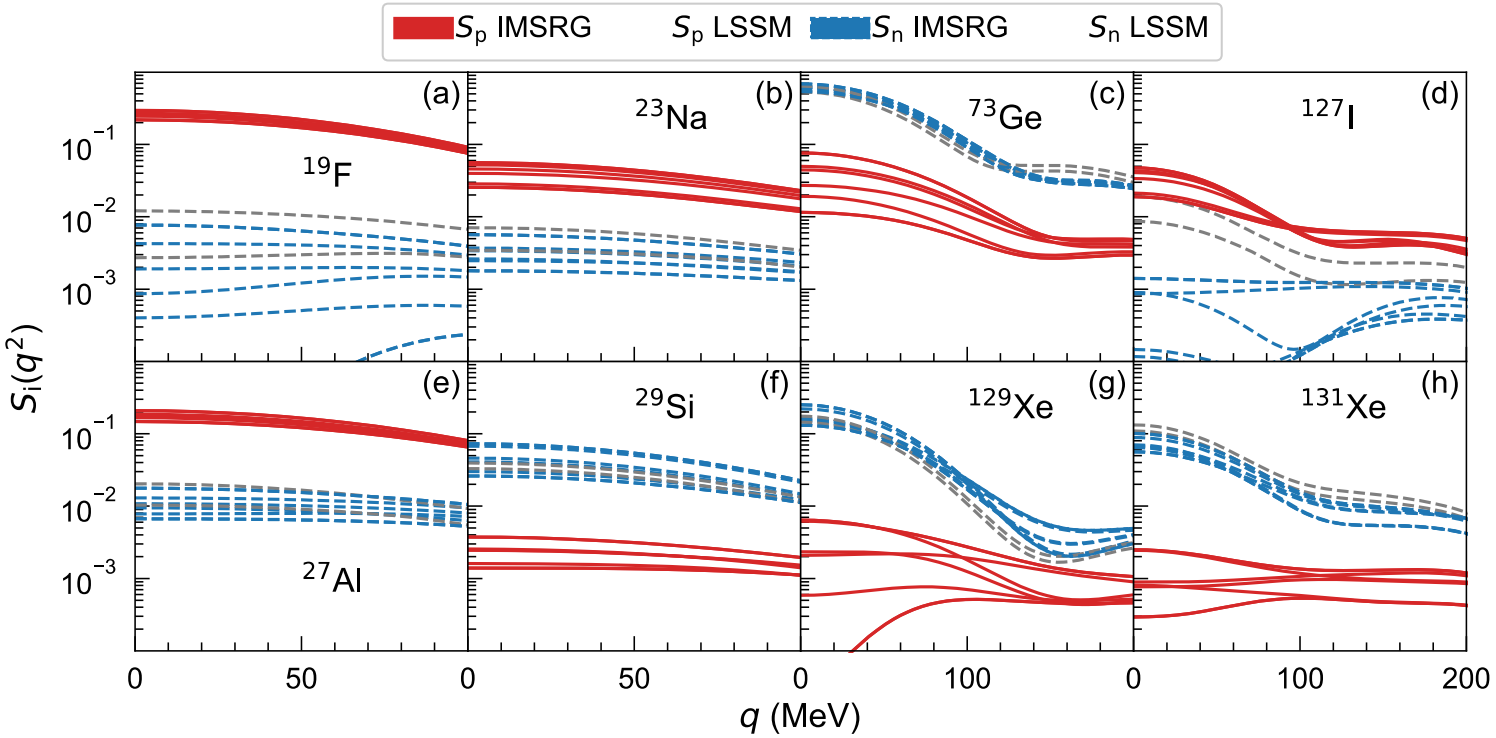
$$\frac{d\sigma}{dq^2} = \frac{8G_{\mathrm{F}}^2}{(2J+1)v^2} S_A(\mathbf{q}^2)$$

Weak/Axial form factors from nuclear theory

Ab Initio SD WIMP-Nucleus Response Overview

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

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



Provide ab initio structure functions for all SD direct-detection candidates

Ab Initio Structure Factors for Spin-Dependent Dark Matter Direct Detection

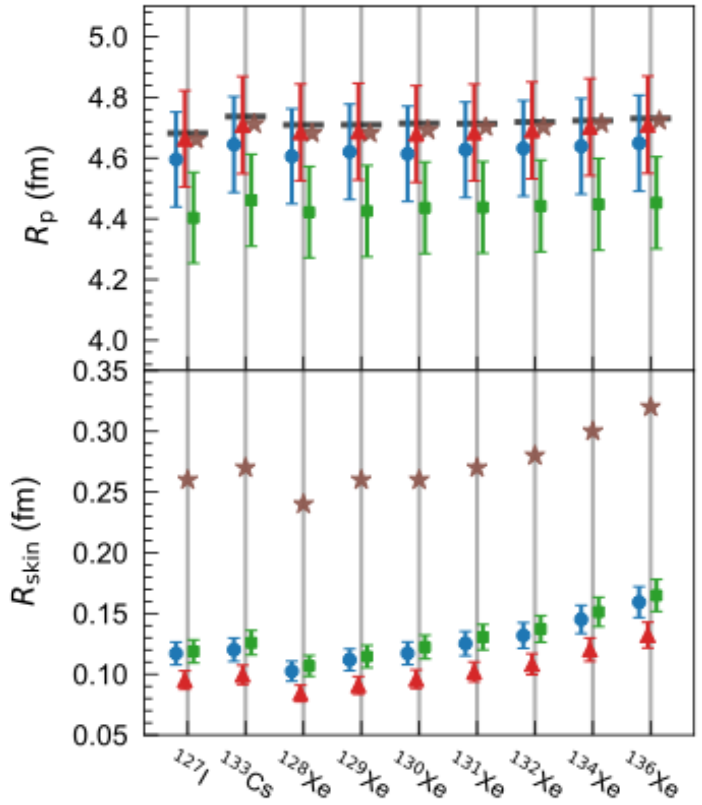
B. S. Hu, J. Padua-Argüelles, S. Leutheusser, T. Miyagi, S. R. Stroberg, and J. D. Holt
Phys. Rev. Lett. **128**, 072502 – Published 17 February 2022

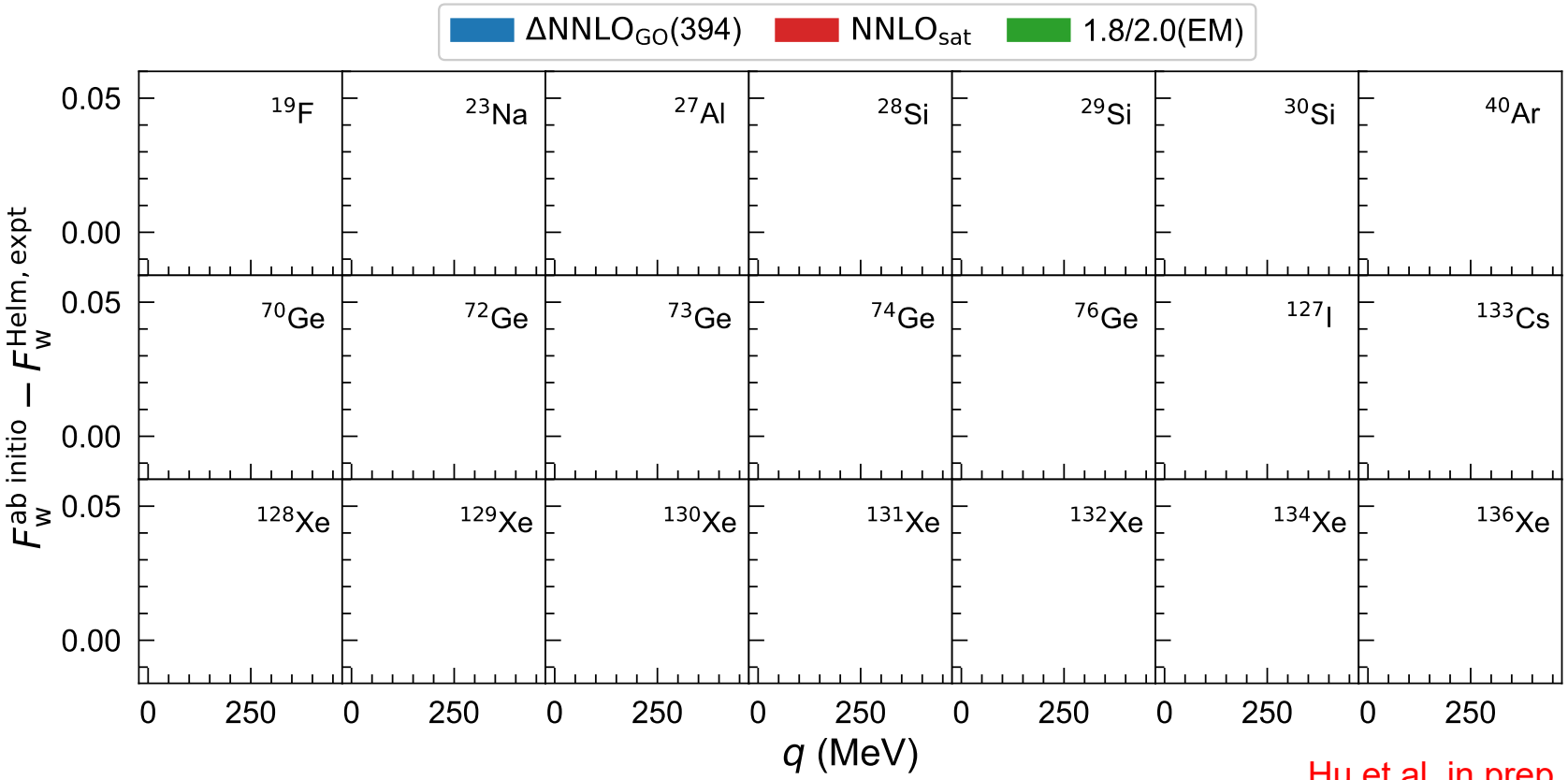
Ab Initio WIMP/ν-Nucleus Responses

Structure functions for dark matter direct detection and CEνNS

Typically use phenomenological form factors (Helm, etc.) same for p/n

CE} NS sensitive to neutron distribution in nuclei – use neutron skin calculations to refine



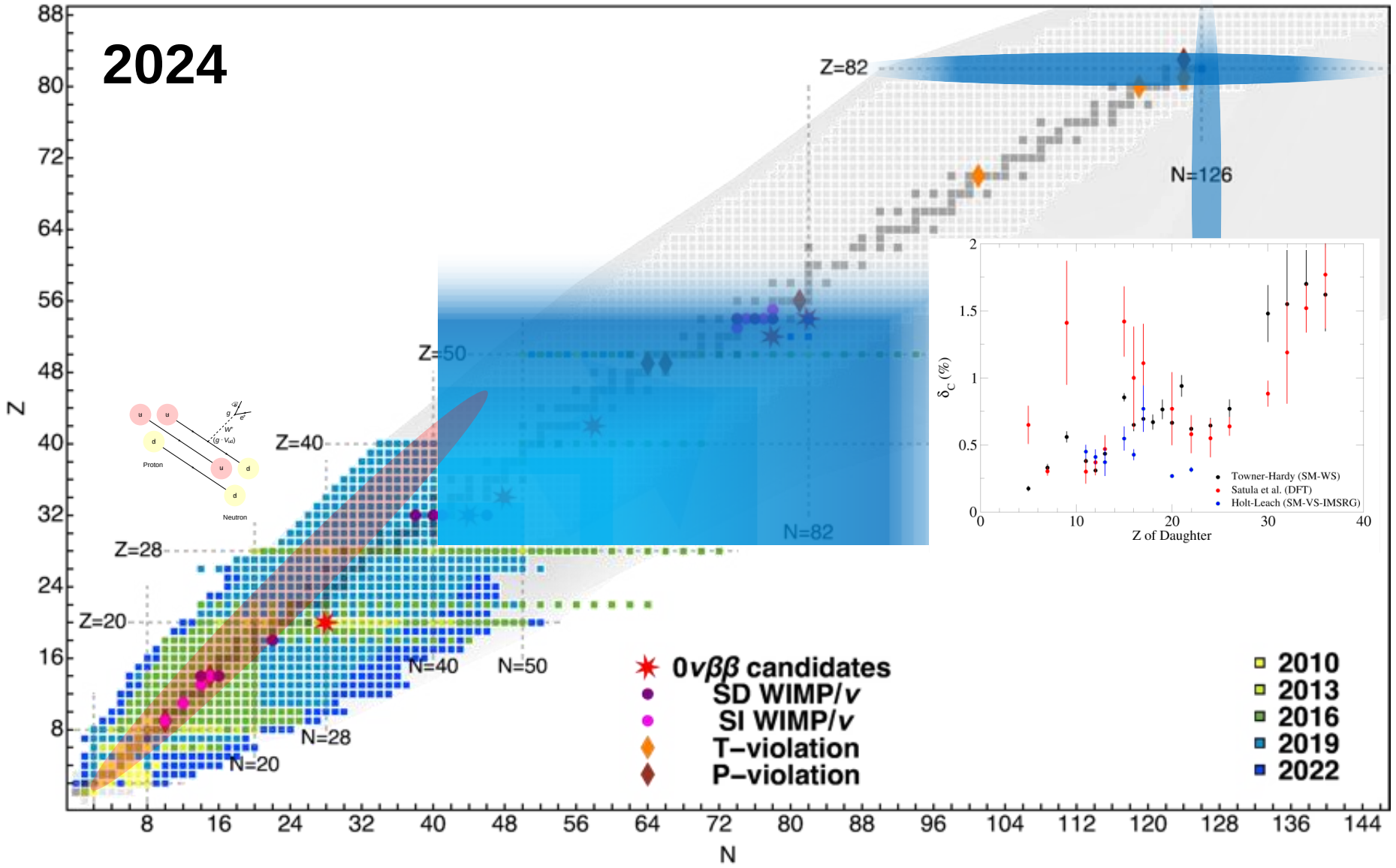


Hu et al. in prep.

Comparison with ab initio calculations shows refined Helm well reproduced

Future of Ab Initio Theory

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



Nucleosynthesis

Ab initio input for r-process

Dark Matter/ν Scattering

Ab initio structure functions

Heavy Ion Collisions

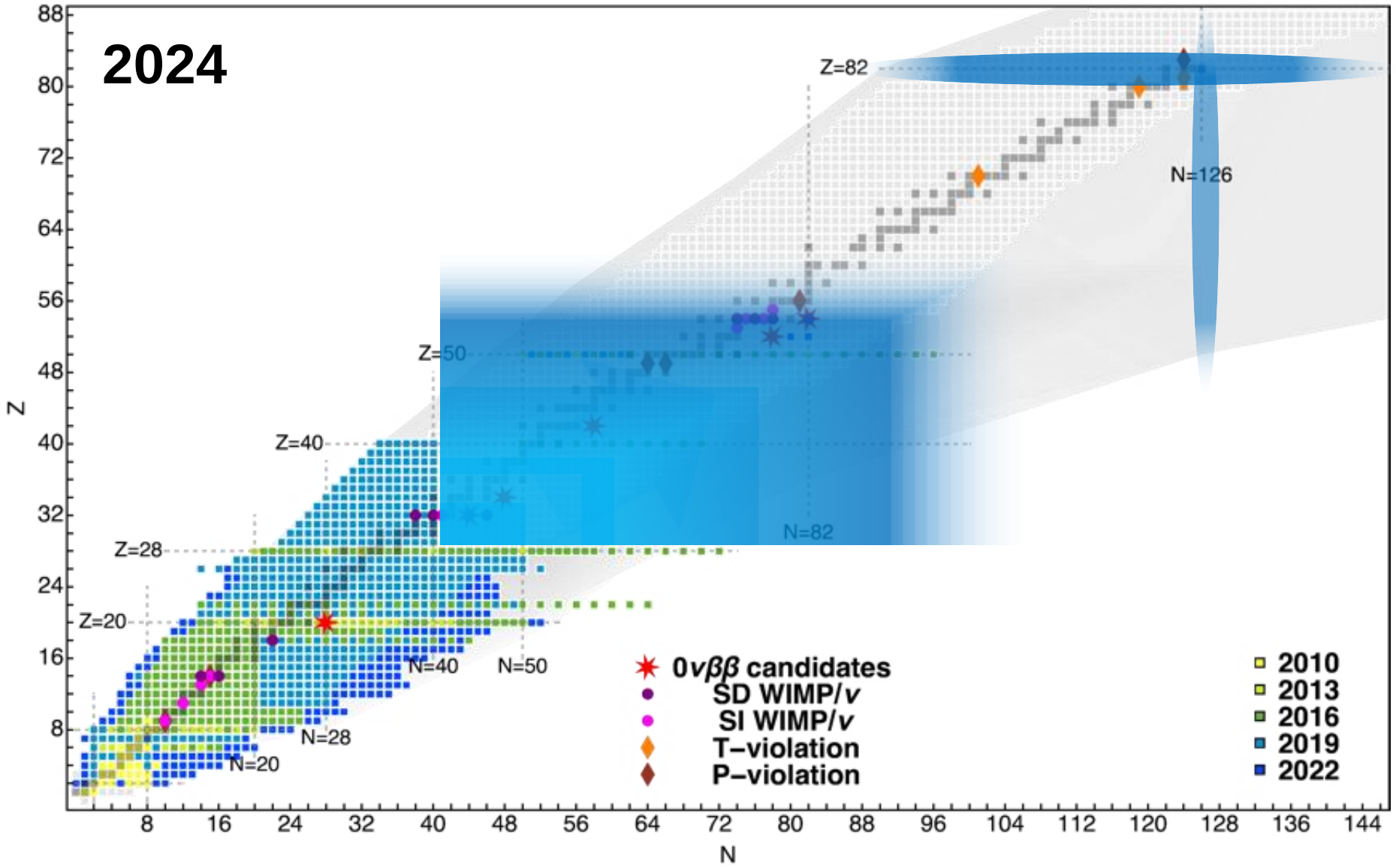
Nuclear structure/NMEs

CKM Unitarity (V_{ud})

Superallowed Fermi

Future of Ab Initio Theory

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



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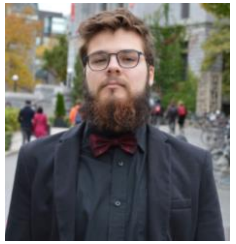
Symmetry Violation

P/T-violating moments

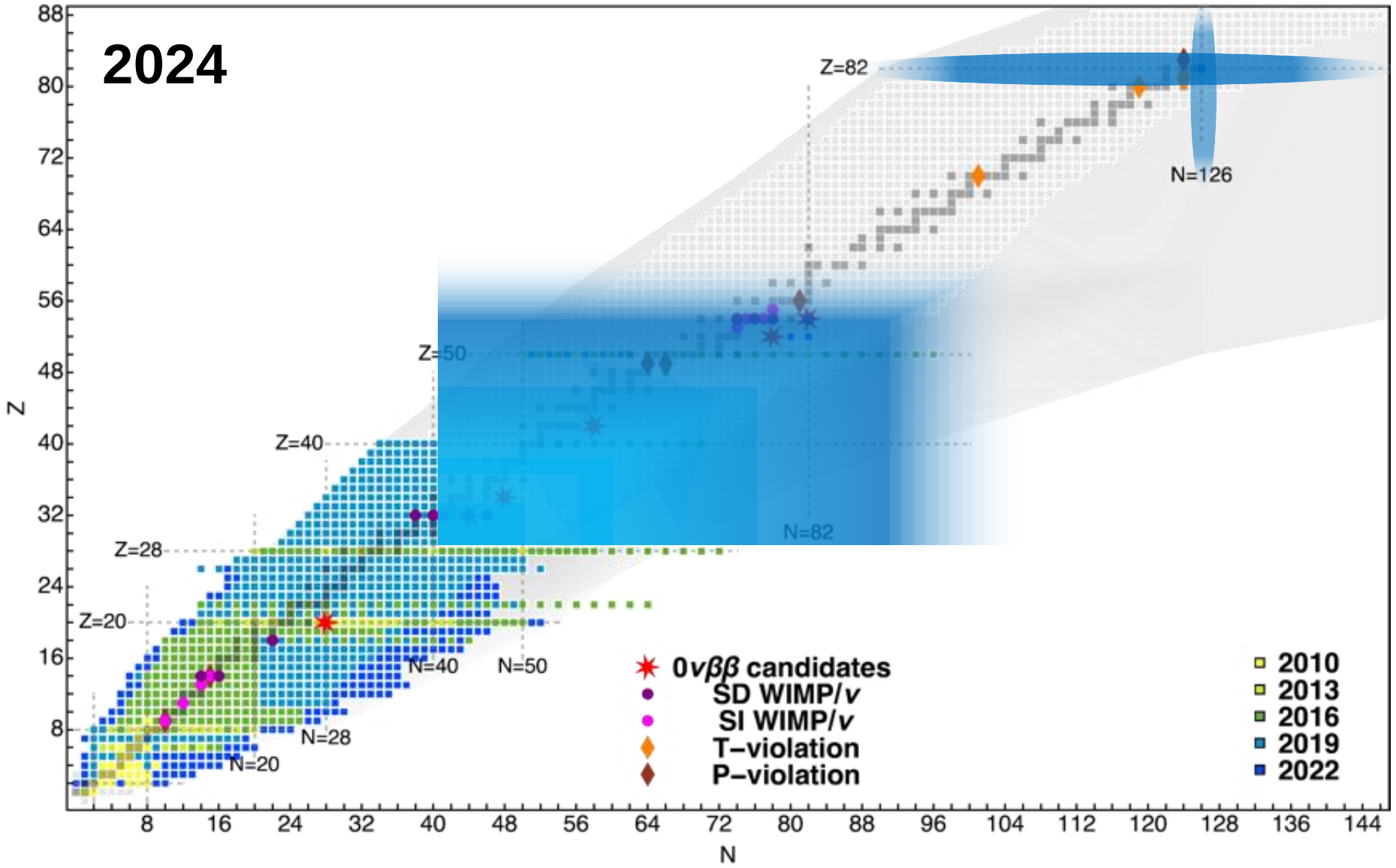


Antoine Belley

Jose Munoz

Act II Preview: Future of Ab Initio Theory

(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

Symmetry Violation
Schiff/anapole moments

CKM Unitarity (V_{ud})
Superallowed Fermi

Atomic/molecular/QC(?)

AI/Machine Learning
New emulators

TRIUMF

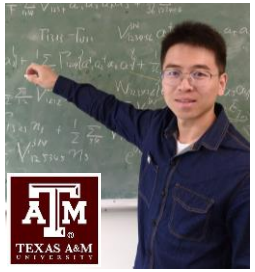
Future of Ab Initio Theory

(Former) Postdoctoral Fellows

Ragnar Stroberg

Takayuki Miyagi

Lotta Jokiniemi

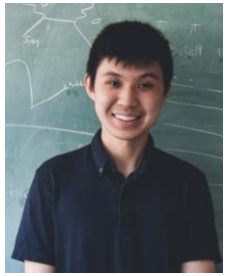

Baishan Hu

0νββ Decay

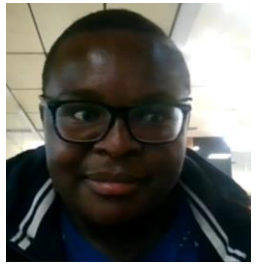
Antoine Belley Ginnette

Isabella

Alex Todd

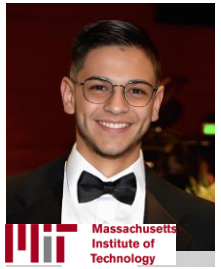

Michael Liudeng

Structure + Astrophysics


Kanting Motimele

Maude Larivière

Symmetry Violation


Jose Munoz

Jack Pitcher

CKM Unitarity

Emily Love

Matt Martin

AI/Machine Learning

Atomic Systems

Gaurav Tenkila

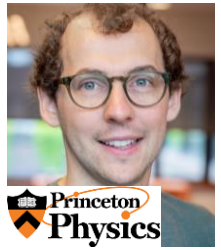
Hrishi Patel

Vijay Chand

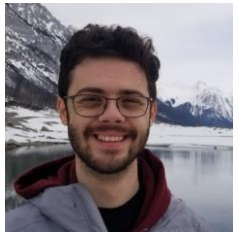
Just the beginning: join our revolution!

jholt@triumf.ca

Dark Matter/ν Scattering


Sam Leutheusser

Jose Padua


Mathieu Bruneault

Ab Initio Strategy IV: Rigorous Uncertainties

Construct predictive posterior distribution for NMEs – first case ^{76}Ge

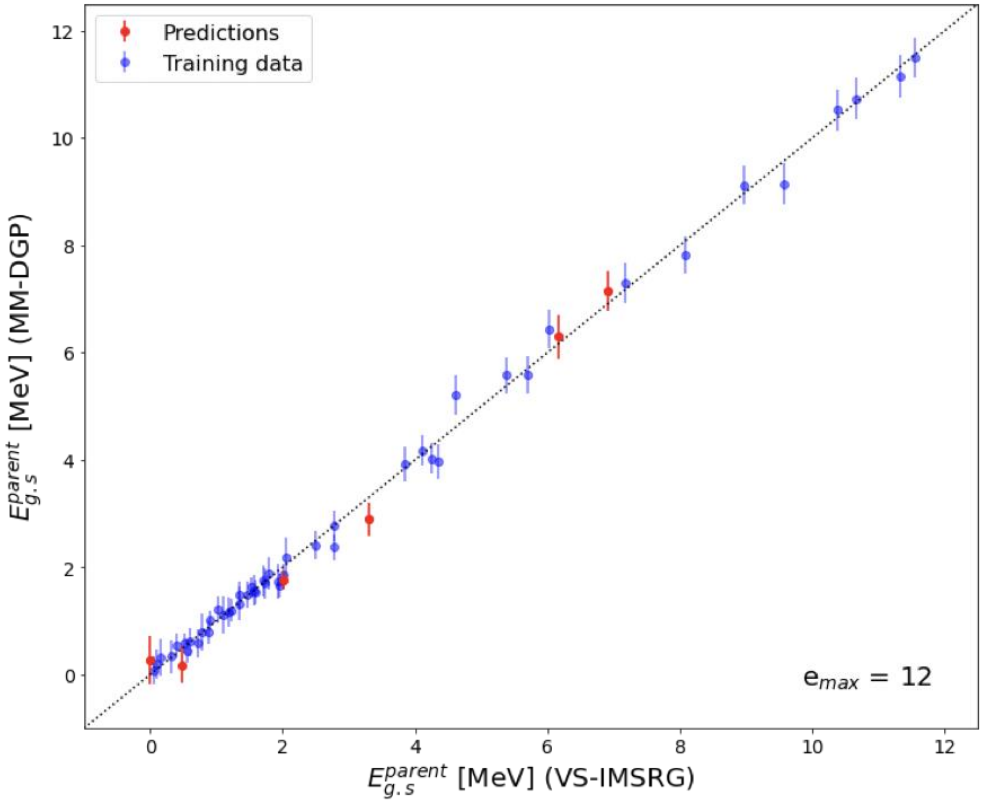
Consider all physics contributing to systematic error

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

Use 8100+ samplings of NN+3N forces - weighted by np $^1S_0$ phase shift

Solve many-body problem with MM-DGP

Emulator: from process itself



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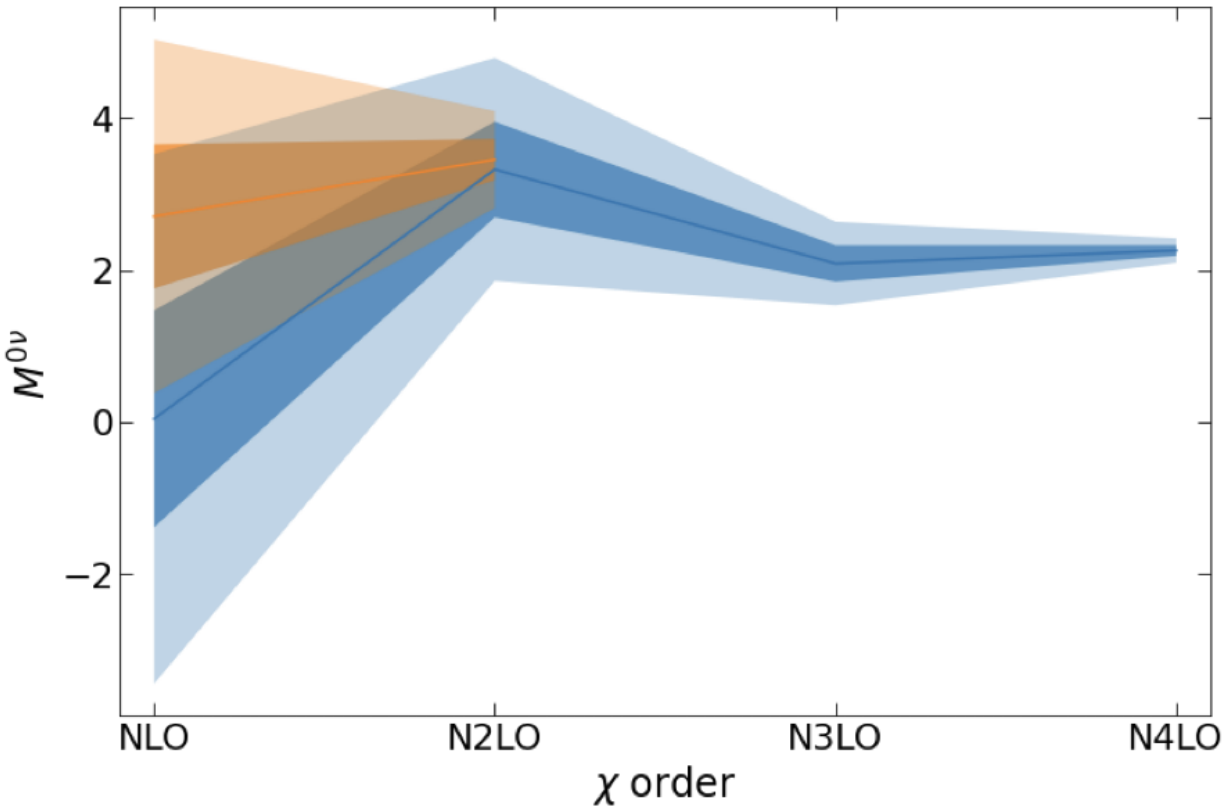
EFT: Truncation in nuclear forces

Belley et al, arXiv:2308.15634



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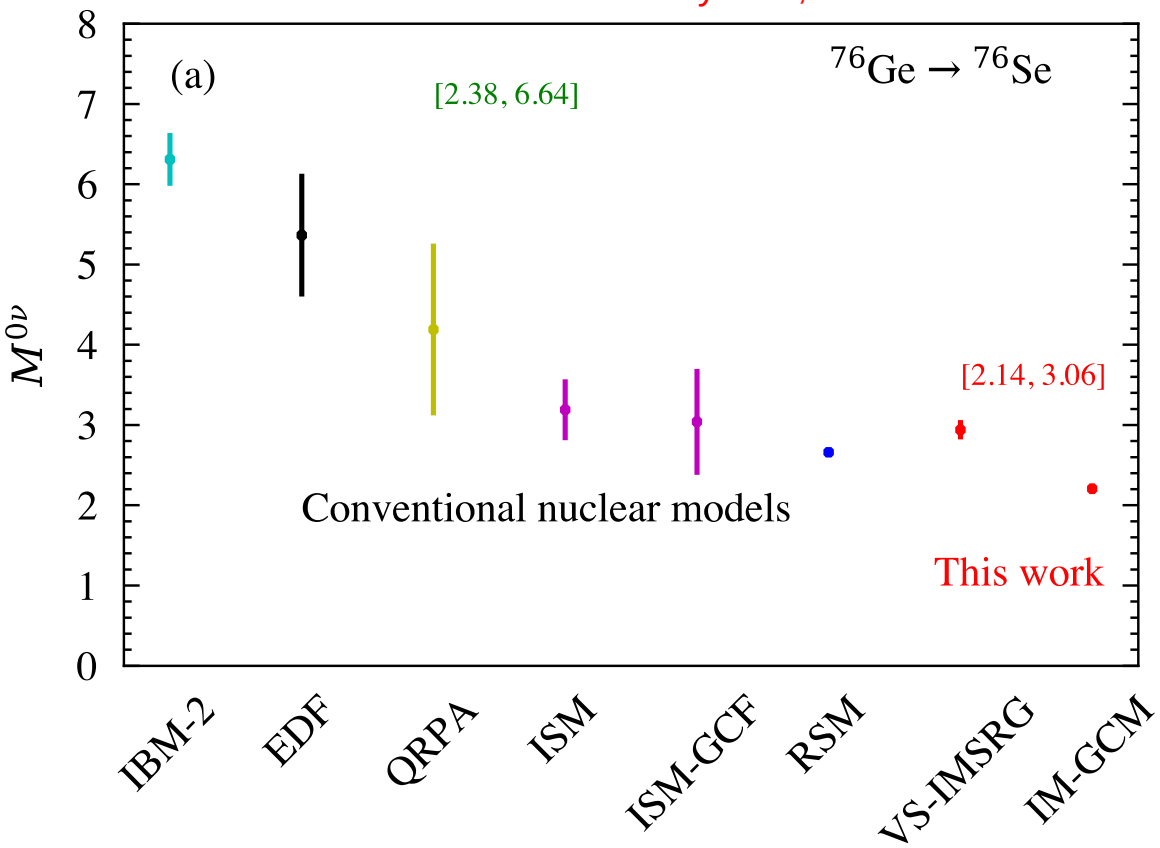

Ab Initio Strategy IV: Rigorous Uncertainties

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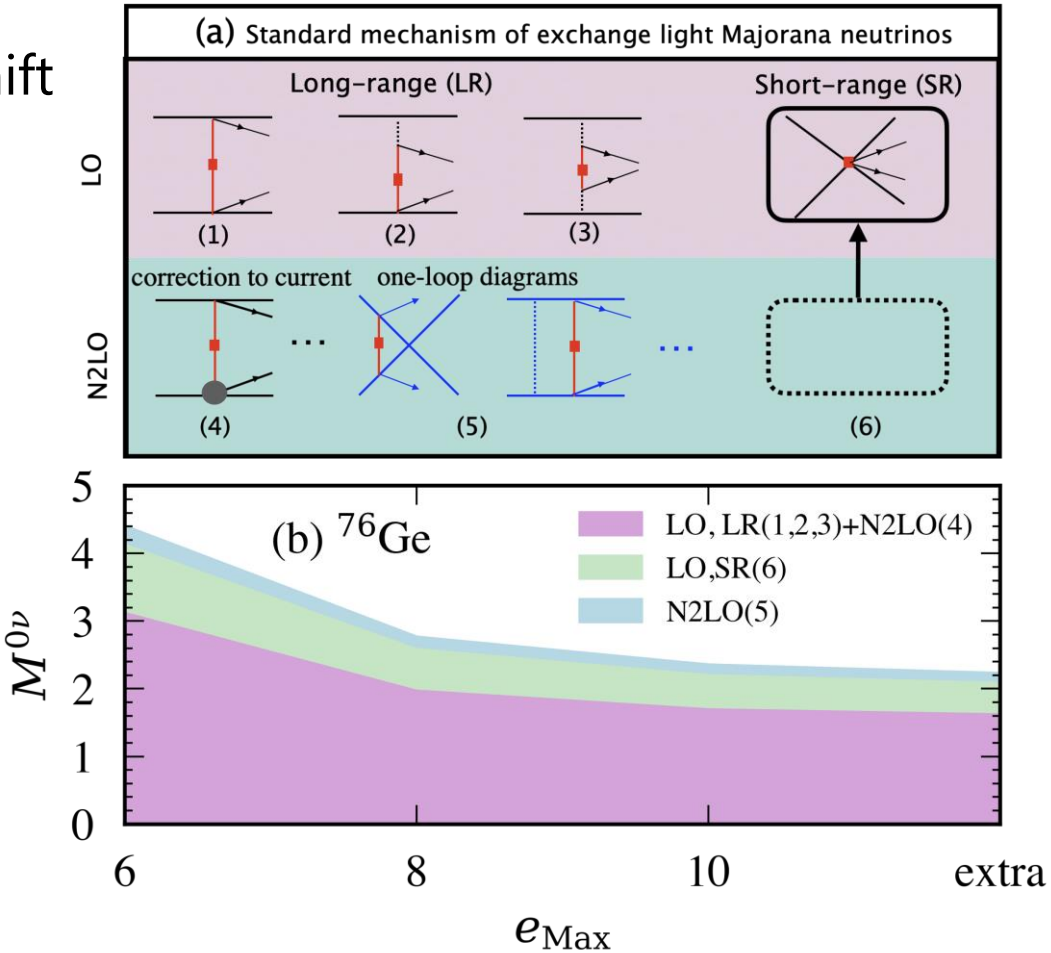
EFT: Truncation in nuclear forces

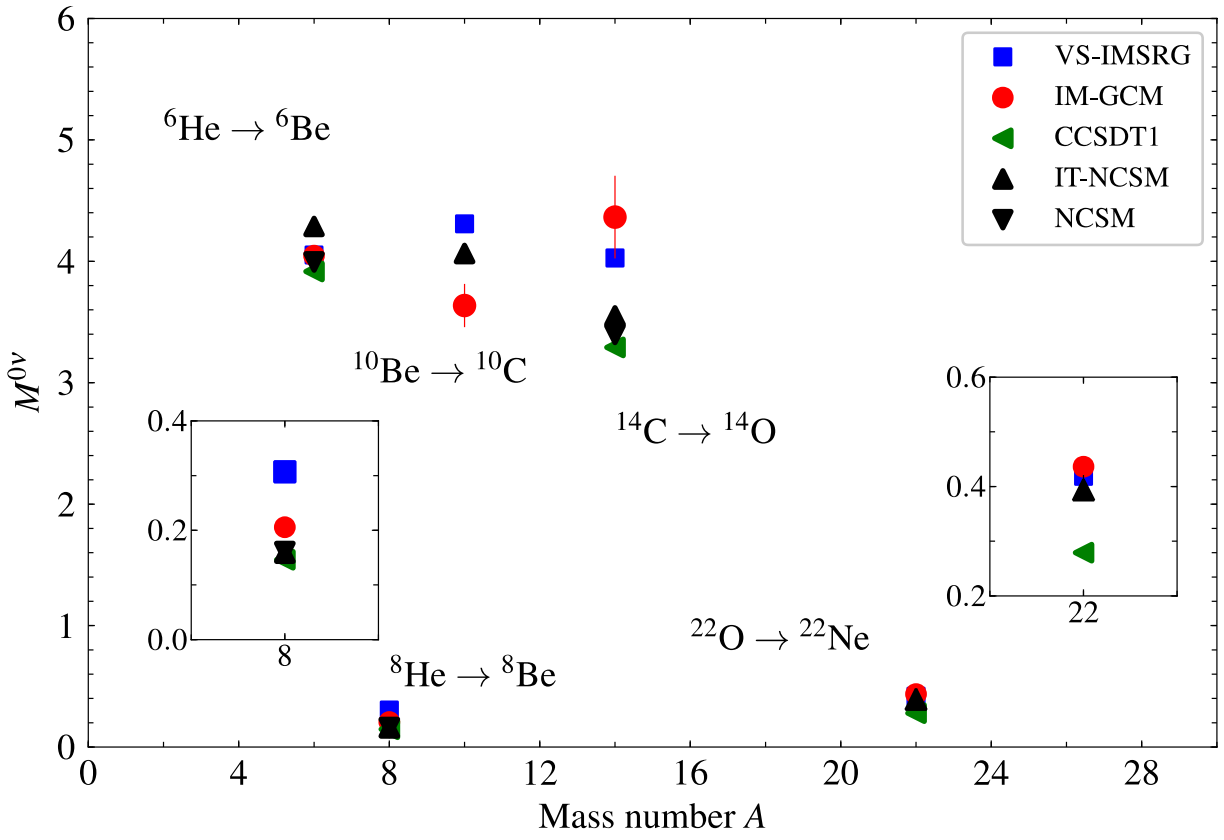
Many-body: Truncation in many-body physics

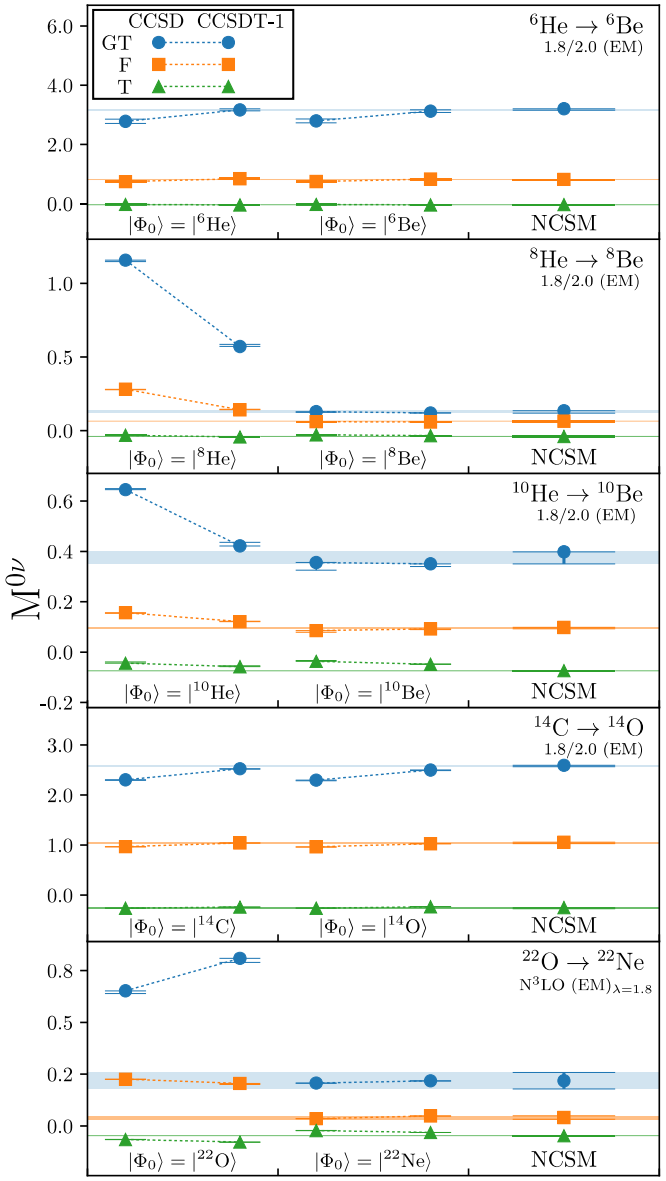
Operator: higher order contributions to operator



Ab Initio Strategy I: Benchmark in Light Nuclei

Benchmark with quasi-exact ab initio methods in light systems: A=6-22





Reasonable to good agreement in all cases

Pursue true double-beta decay candidates!

Yao, **Belley** et al., PRC (2020)

Valence-Space IMSRG

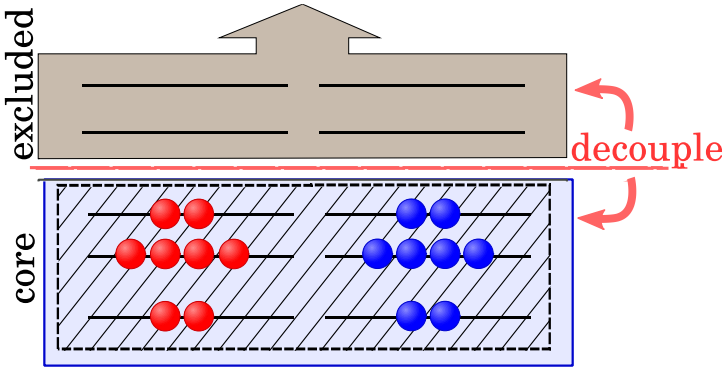
Explicitly construct unitary transformation from sequence of rotations

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

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

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

Step 1: Decouple core



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

Can we achieve accuracy of large-space methods?

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

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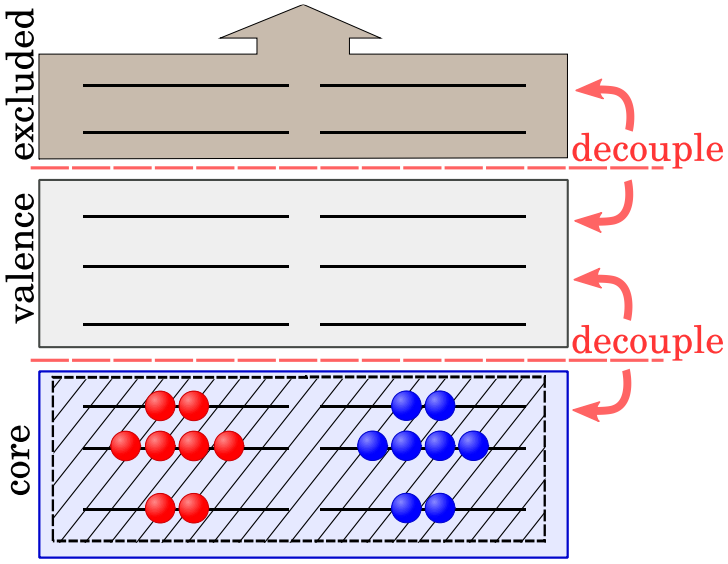
IMSRG(3) in progress

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



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Step 2: Decouple valence space

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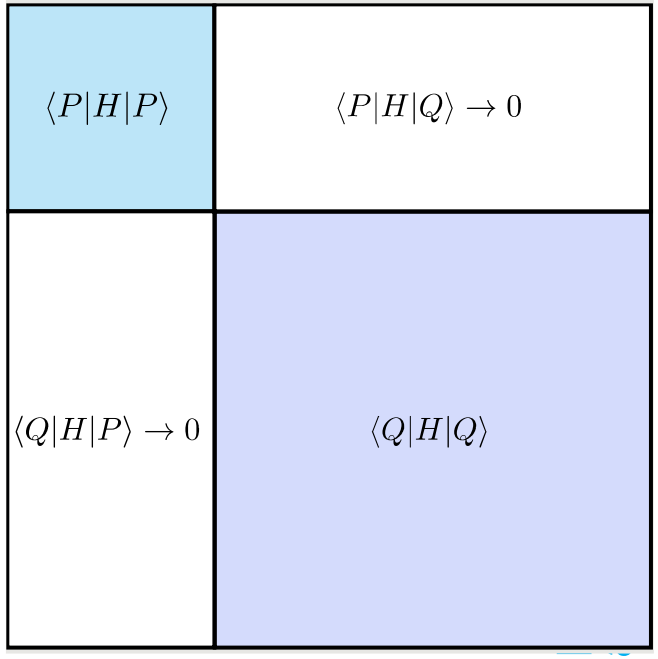

Valence-Space IMSRG

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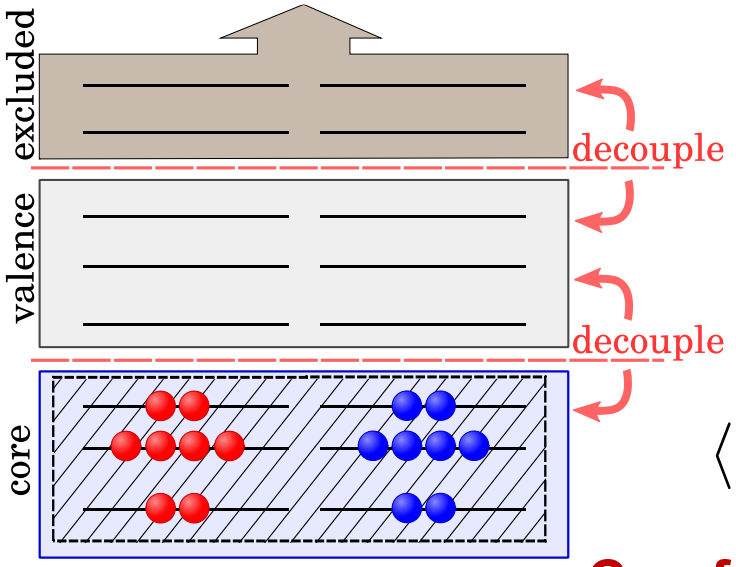
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

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



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

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

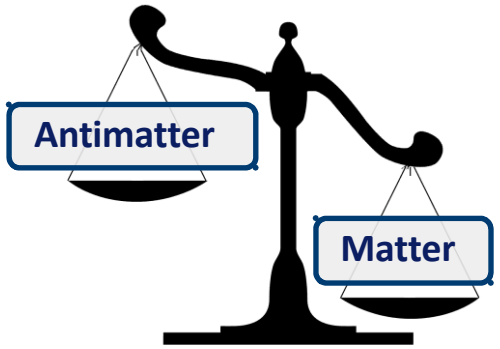
$\langle P\|H\|P\rangle$	$\langle P\|H\|Q\rangle \to 0$
$\langle Q\|H\|P\rangle \to 0$	$\langle Q\|H\|Q\rangle$

The Magic of Molecules: CP Violation

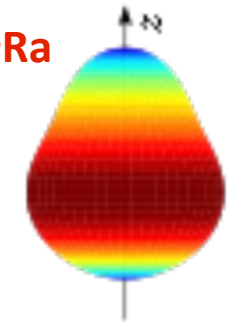
"One of the most compelling mysteries in all of science is how matter came to dominate over antimatter in the universe." – NSAC LRP

CP violation required beyond our current observations

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



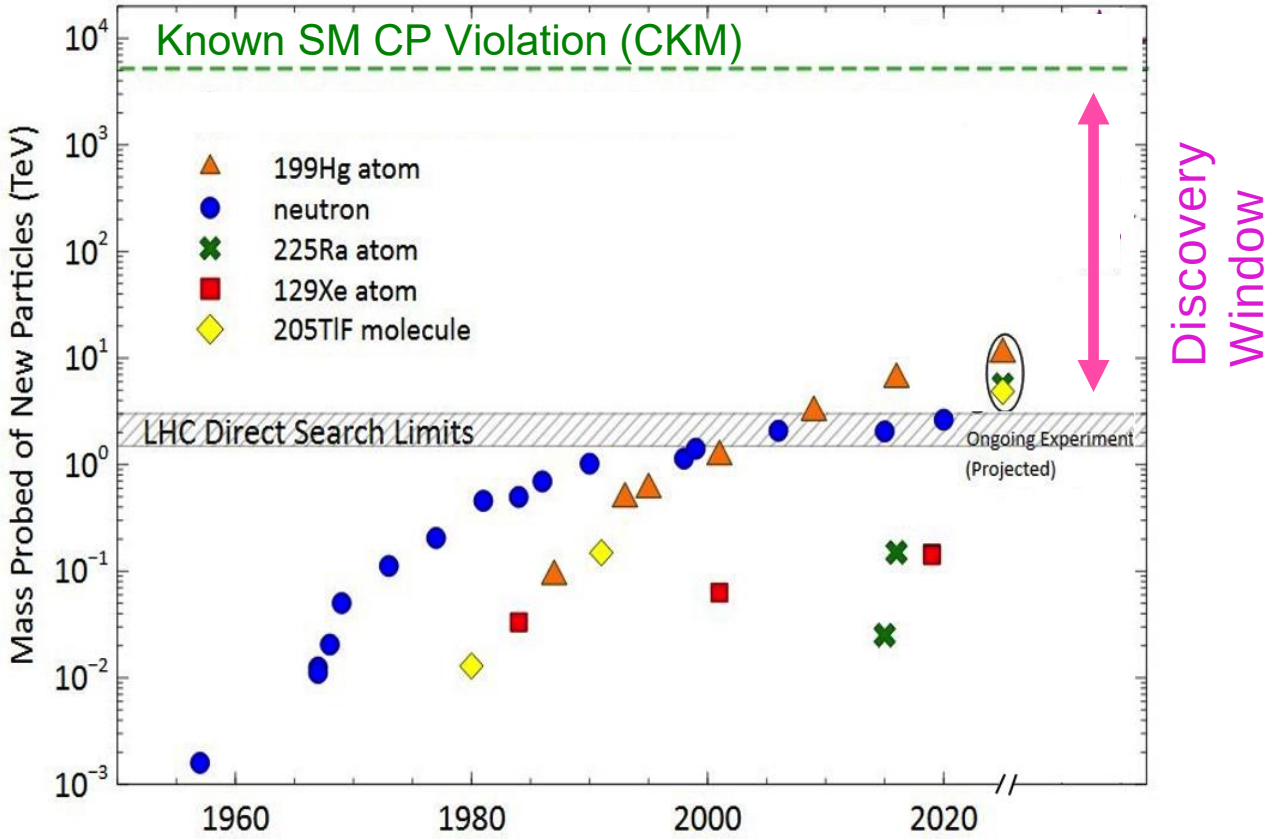
^{225}Ra



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

Effects enhanced in:

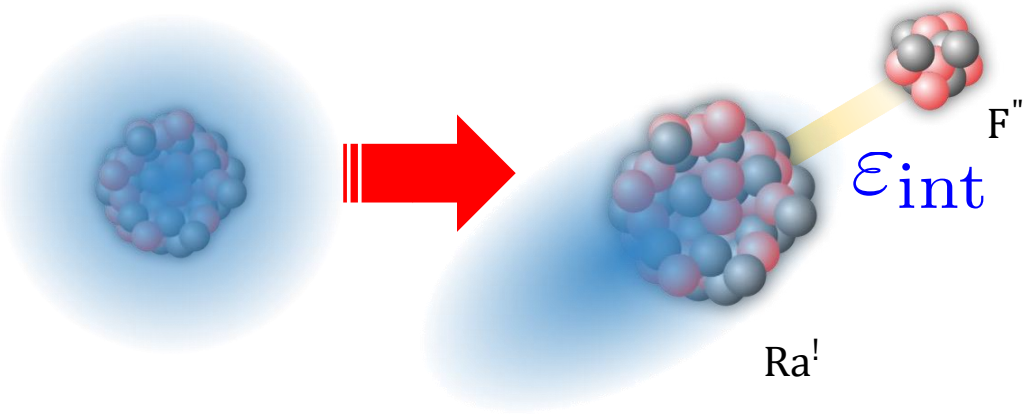
Heavy systems, Octupole deformed



The Magic of Molecules: CP Violation

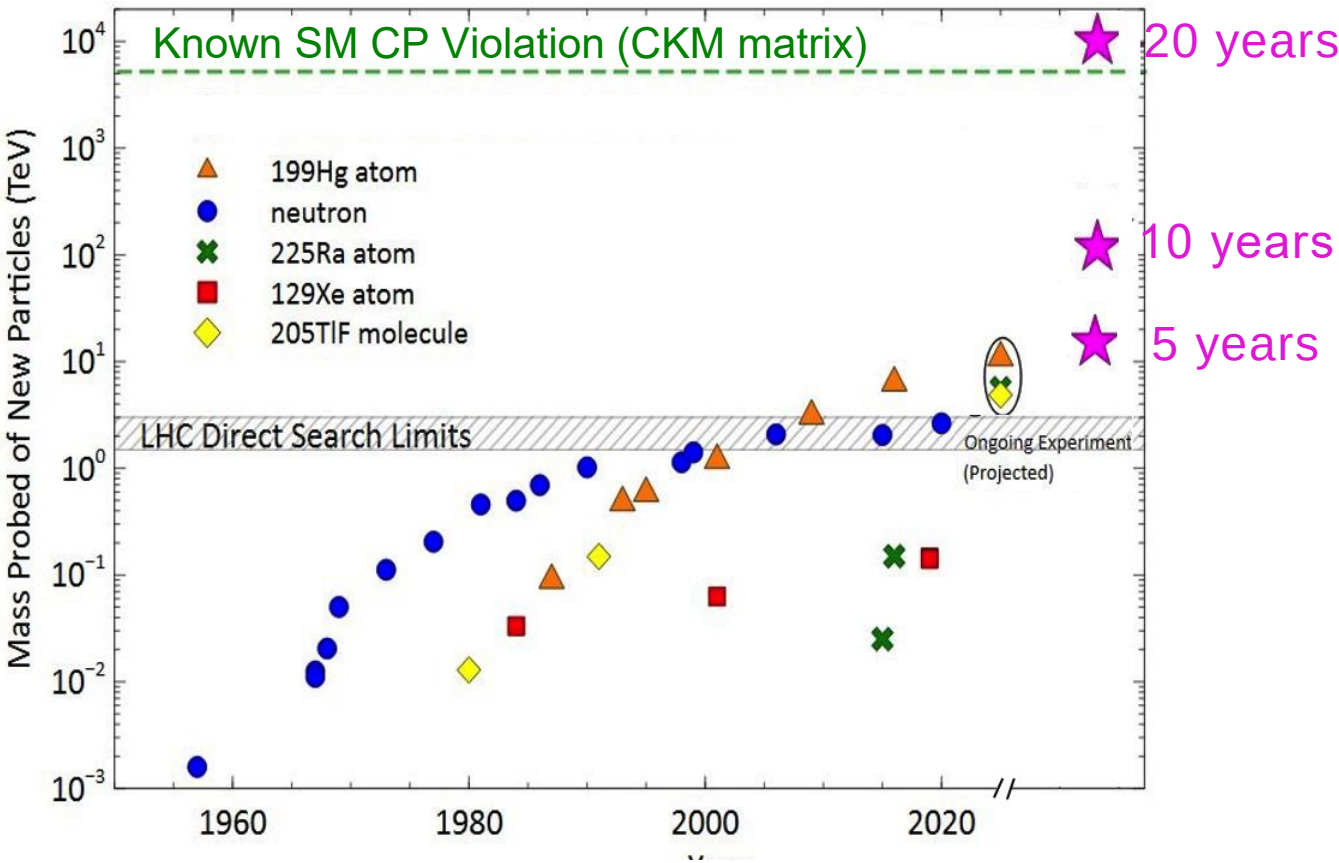
Worldwide race to exploit power of **Radioactive Molecules**

Generate internal fields orders of magnitude above lab possibilities



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

Probe **1000TeV** scale in our lifetimes



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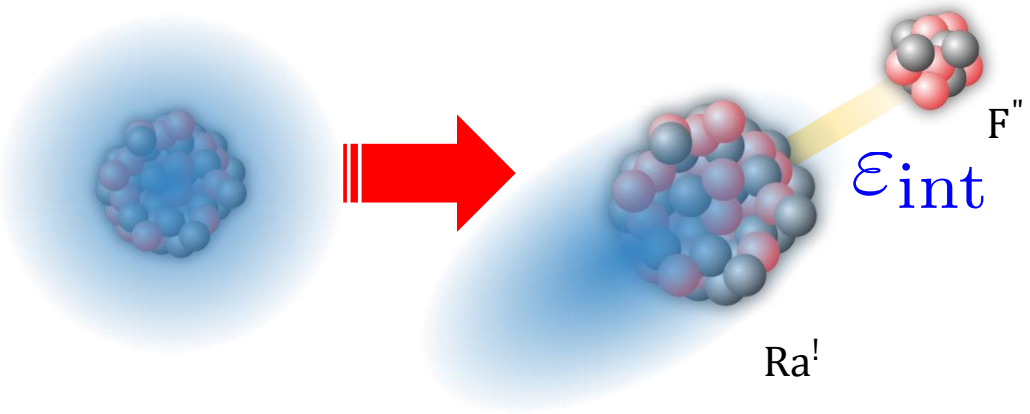

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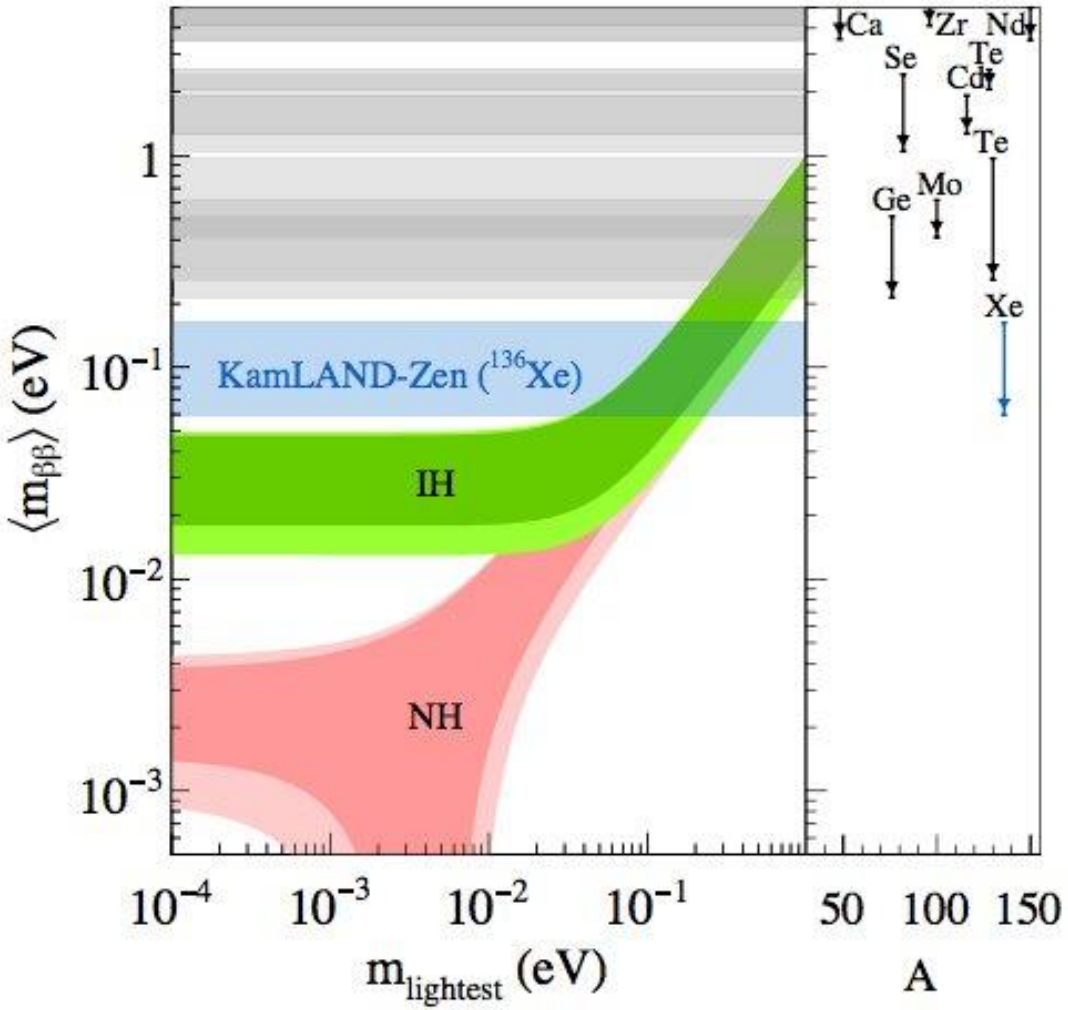

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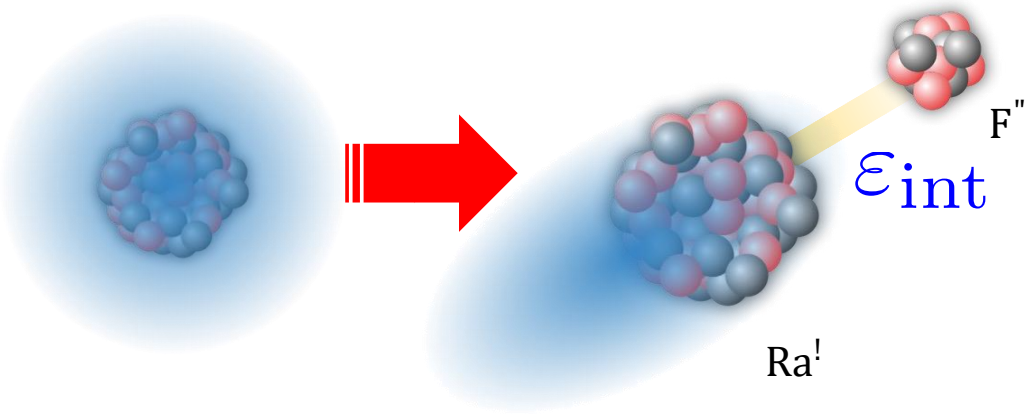

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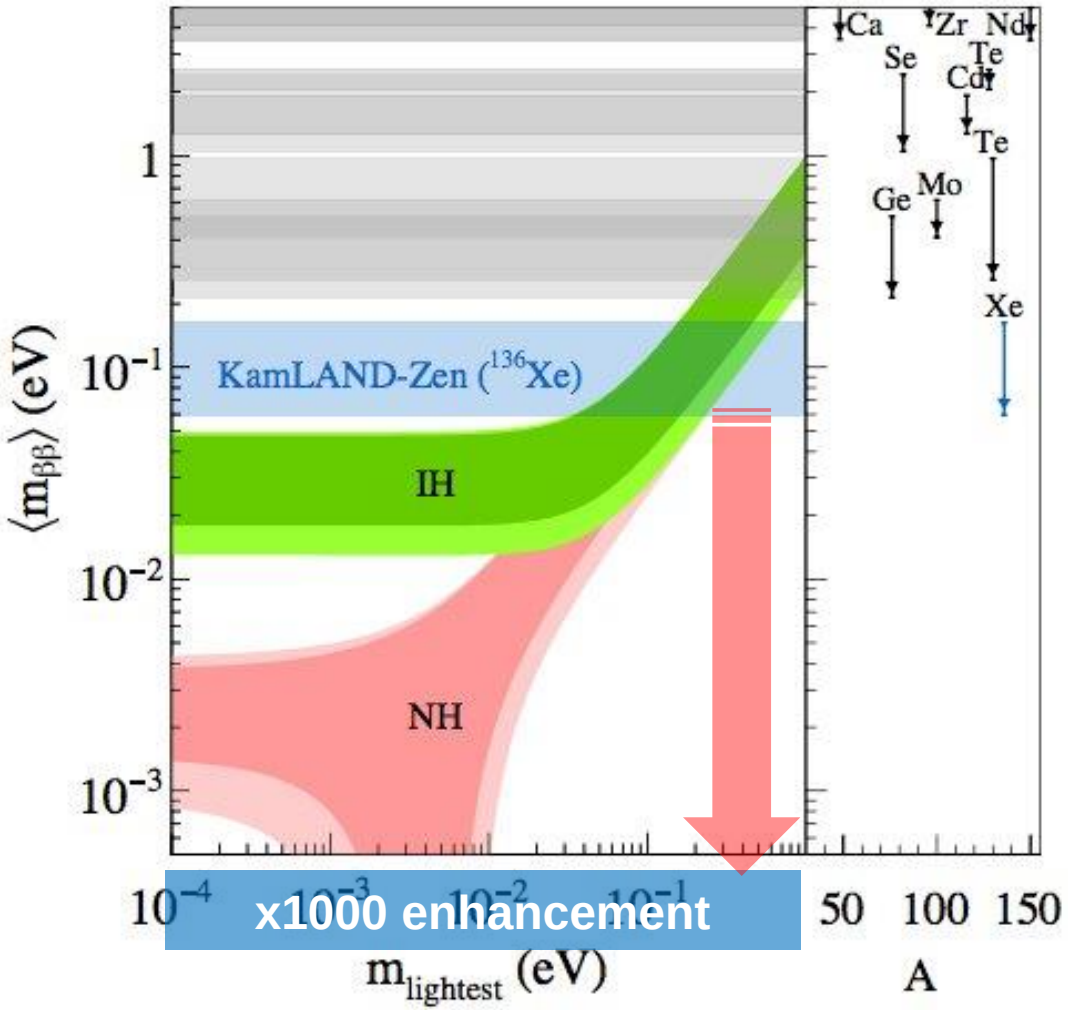

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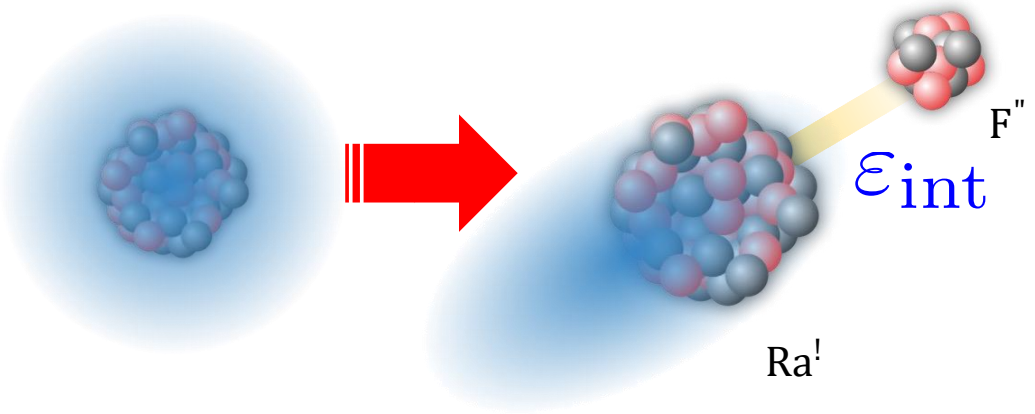
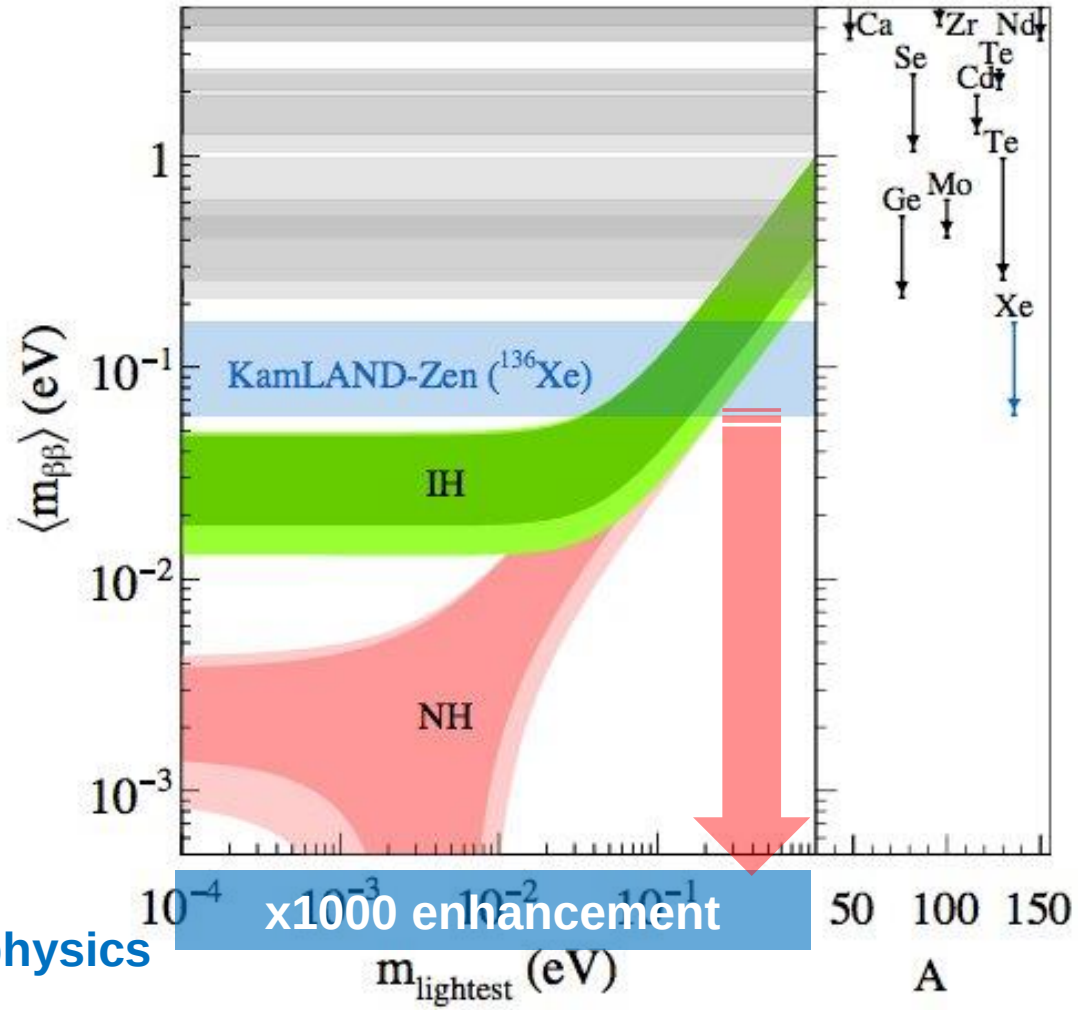




Enhancements in molecules vs atoms **>4000**

Probe 1000TeV scale in our lifetimes

To date, no rigorous nuclear theory

(motivation, interpretation)

Measurement — Nuclear structure — P,T odd NN int

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

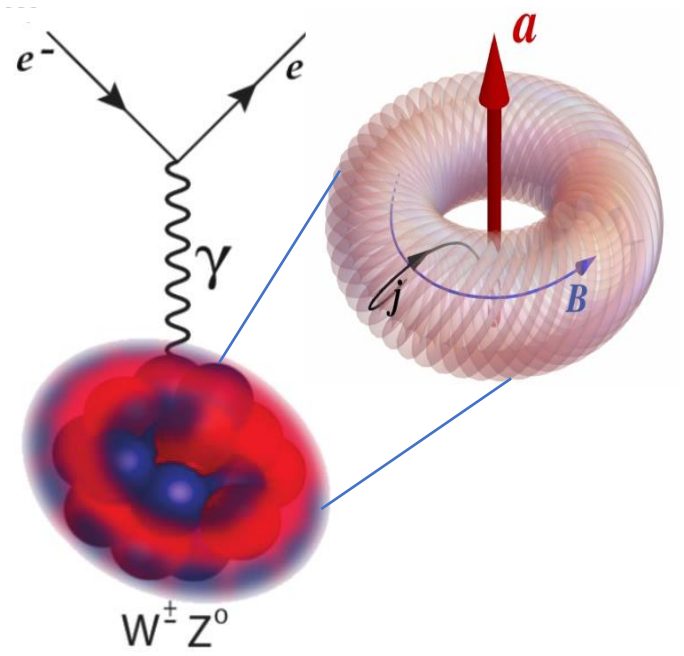
Experiment

New physics

The Magic of Molecules: Weak Structure of Nuclei

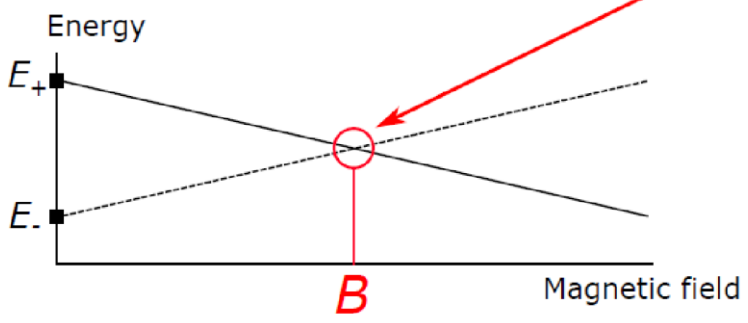
Hadronic P violation – probe the **weak structure** of the atomic nucleus!

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

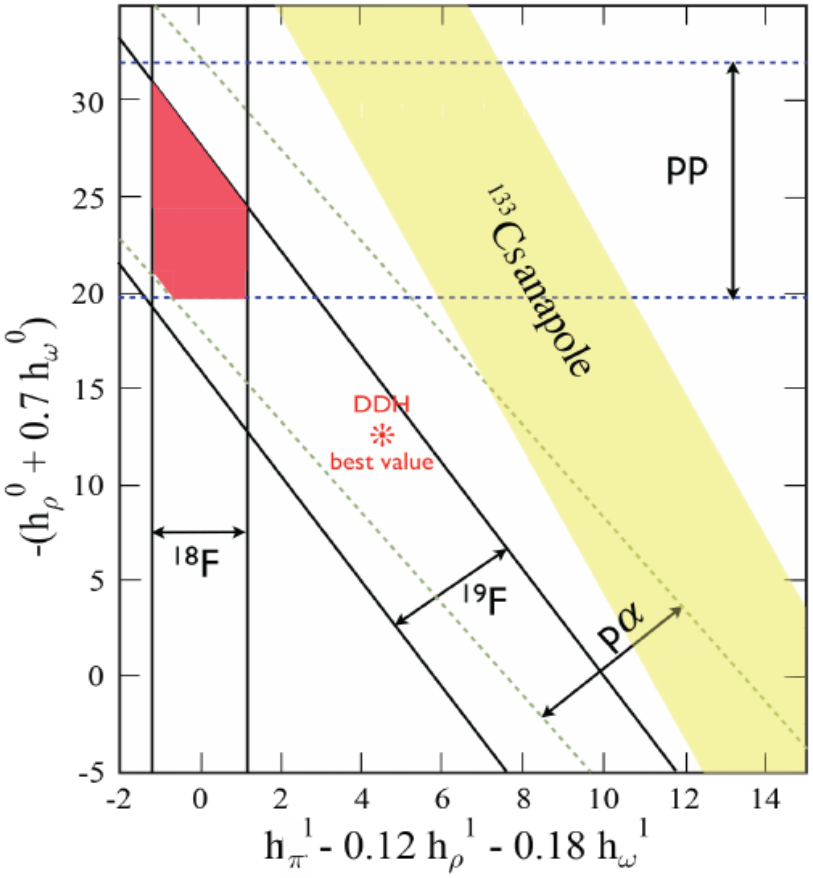


$$E_{PV} \sim \frac{\langle \psi_\uparrow^+ | H_\pm | \psi_\downarrow^- \rangle}{E_- - E_+}$$

$> 10^{11}$ molecular enhancement



Experimental tuning enhances $> 10^{11}$



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

To date, no rigorous nuclear theory

Nuclear structure — P-odd NN int

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

Experiment

New P-violating physics

RESEARCH ARTICLE

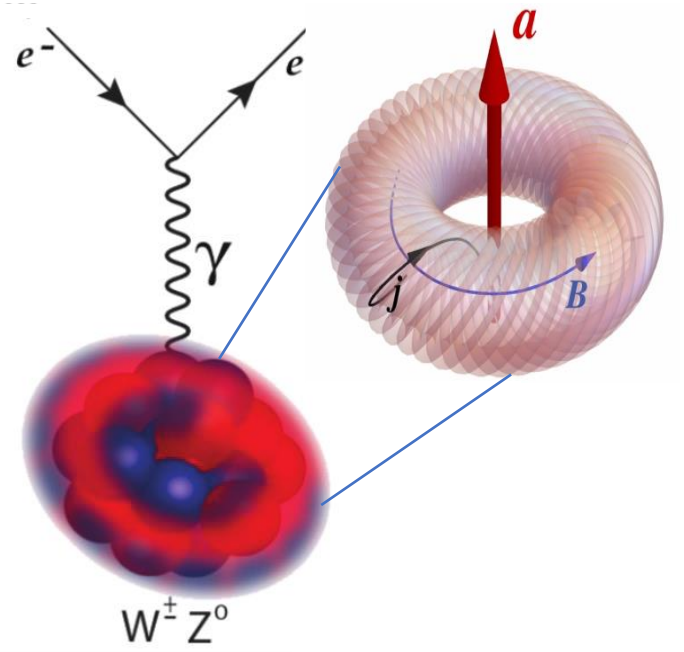
Measurement of Parity Nonconservation and an Anapole Moment in Cesium

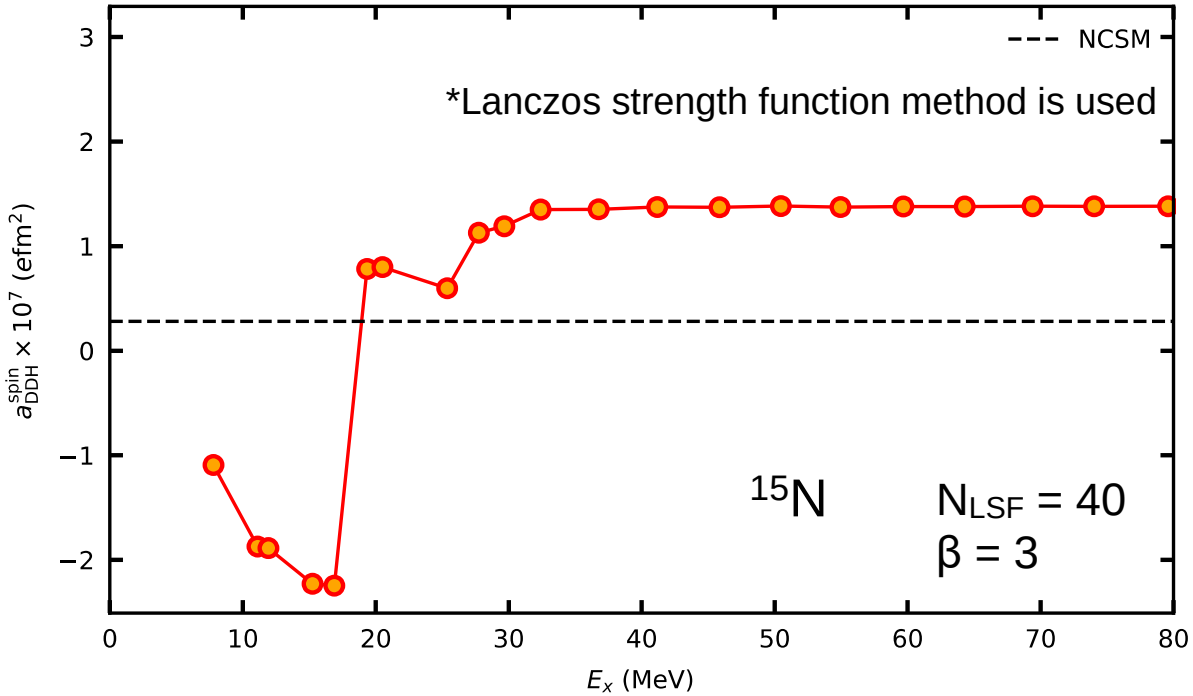
C. S. Wood, S. C. Bennett, D. Cho,* B. P. Masterson,† J. L. Roberts, C. E. Tanner,‡ C. E. Wieman§

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

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

Experiment

New P-violating physics