Overview on progress in theoretical nuclear physics

Jason D. Holt
Scientist, Theory Department
PANIC 2021, Lisbon (I wish…)
September 10, 2021

Discovery, accelerated

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McGill UNIVERSITY

Overview on progress in ab initio theoretical nuclear physics

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NSERC CRSNG

Arthur B. McDonald Canadian Astroparticle Physics Research Institute

NRC·CNRC

Discovery, accelerated

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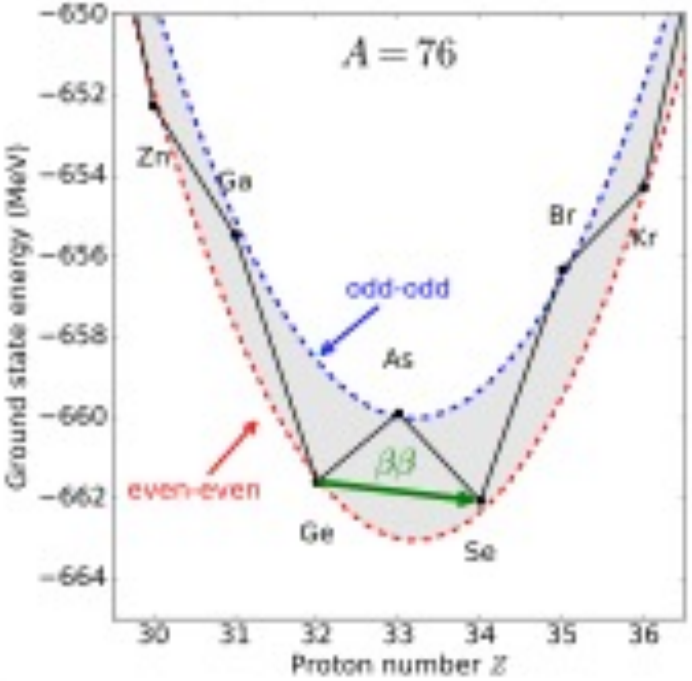
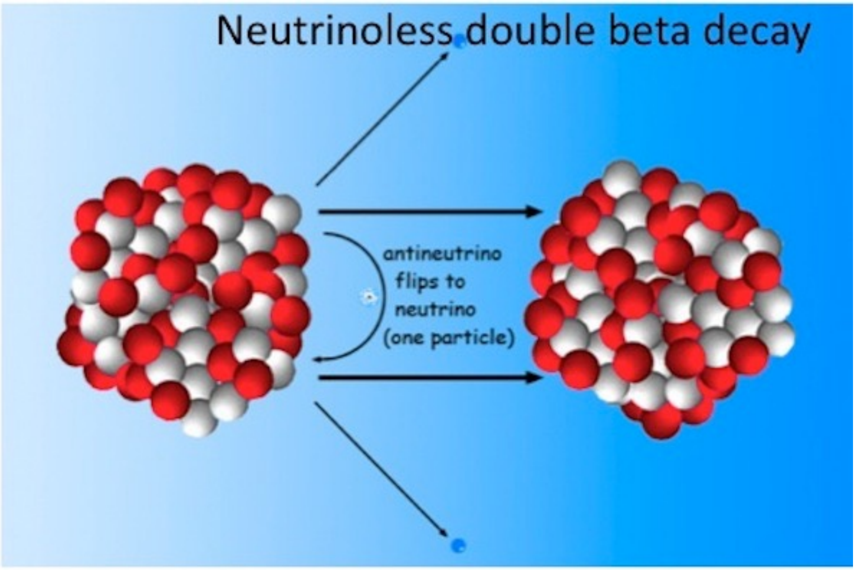
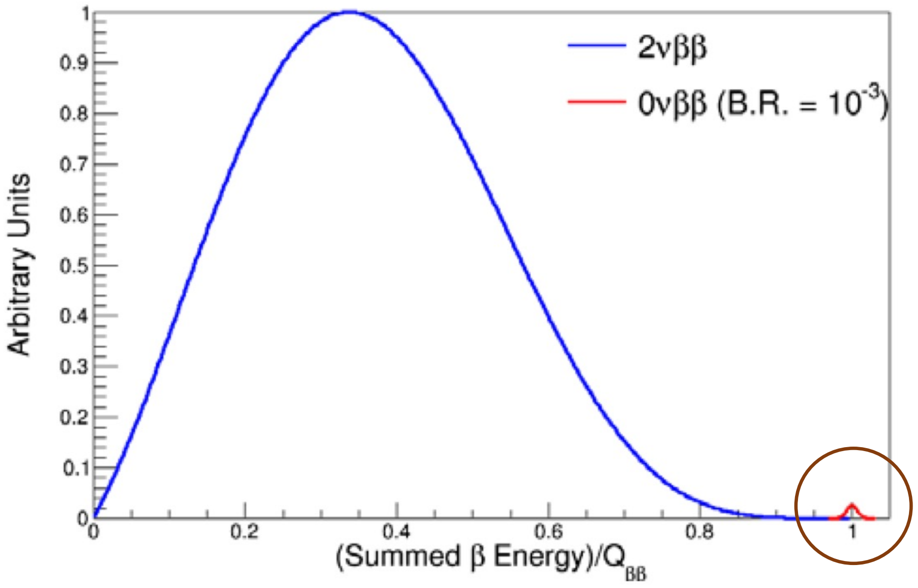
The Next Big Discovery? 0νββ-decay

Neutrino own antiparticle $\Longleftrightarrow$ 0νββ decay







Tremendous impact on BSM physics:

Lepton-number violating process

Majorana character of neutrino

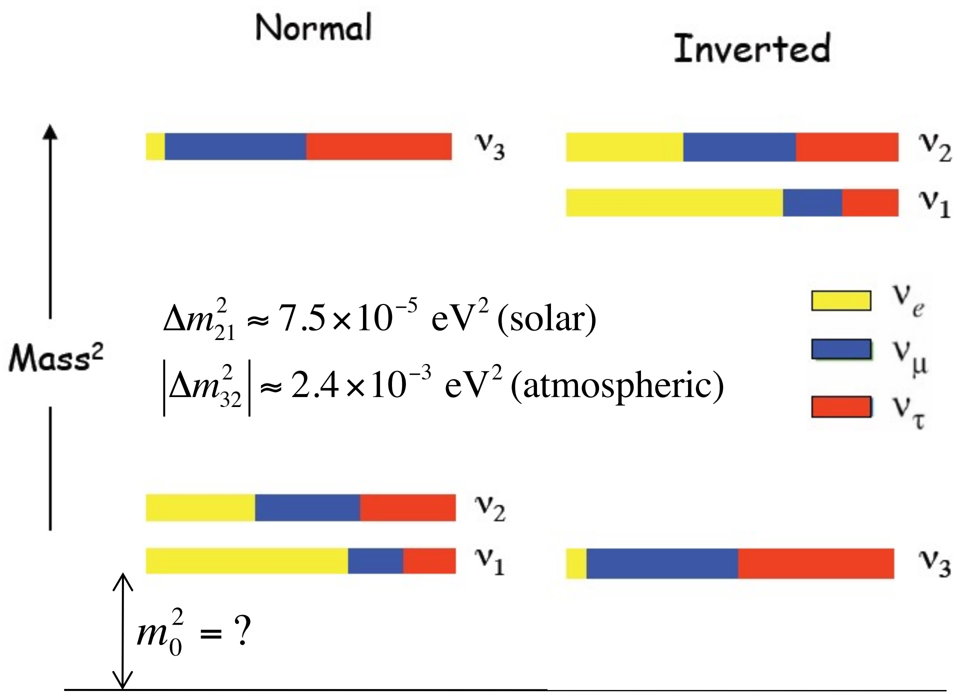
Absolute neutrino mass scale

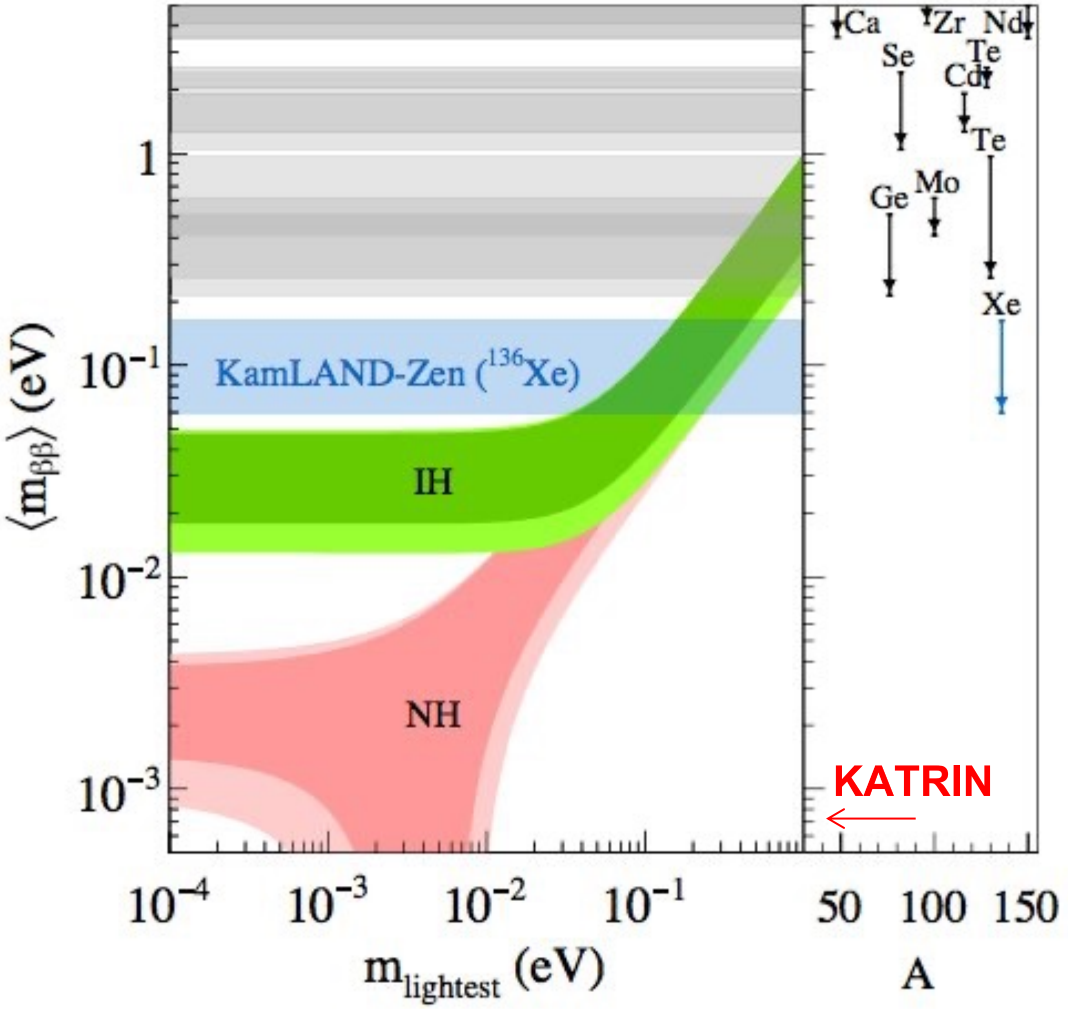
$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu}\left|M^{0\nu}\right|^2 \boxed{\langle m_{\beta\beta}\rangle^2} \qquad \langle m_{\beta\beta}\rangle = \left|\sum_{i=1}^{3} U_{ei} m_i\right|$$

NME not observable: must be calculated

Nature of Neutrino: 0νββ Decay

Next-generation searches push towards **IH**





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

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

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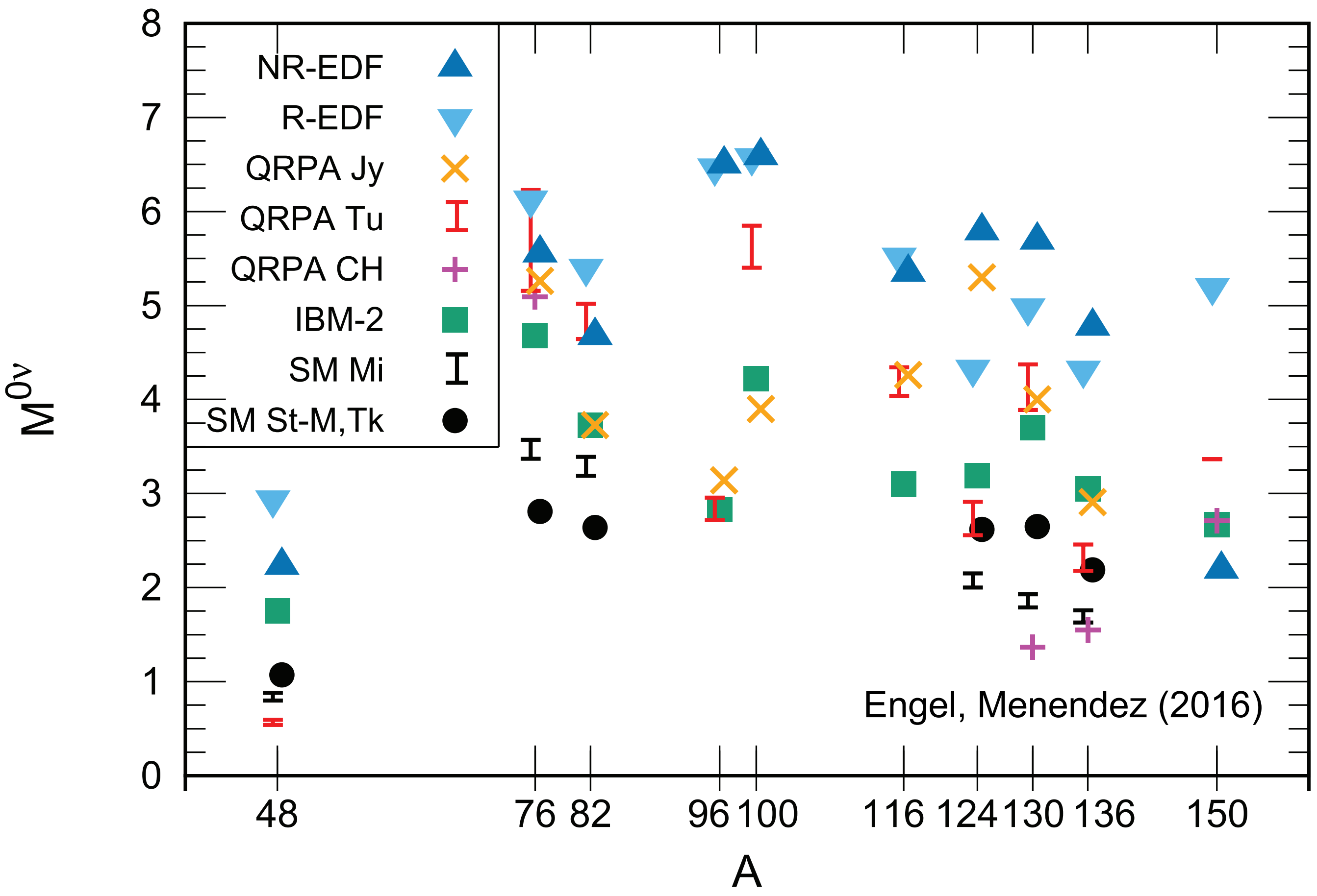
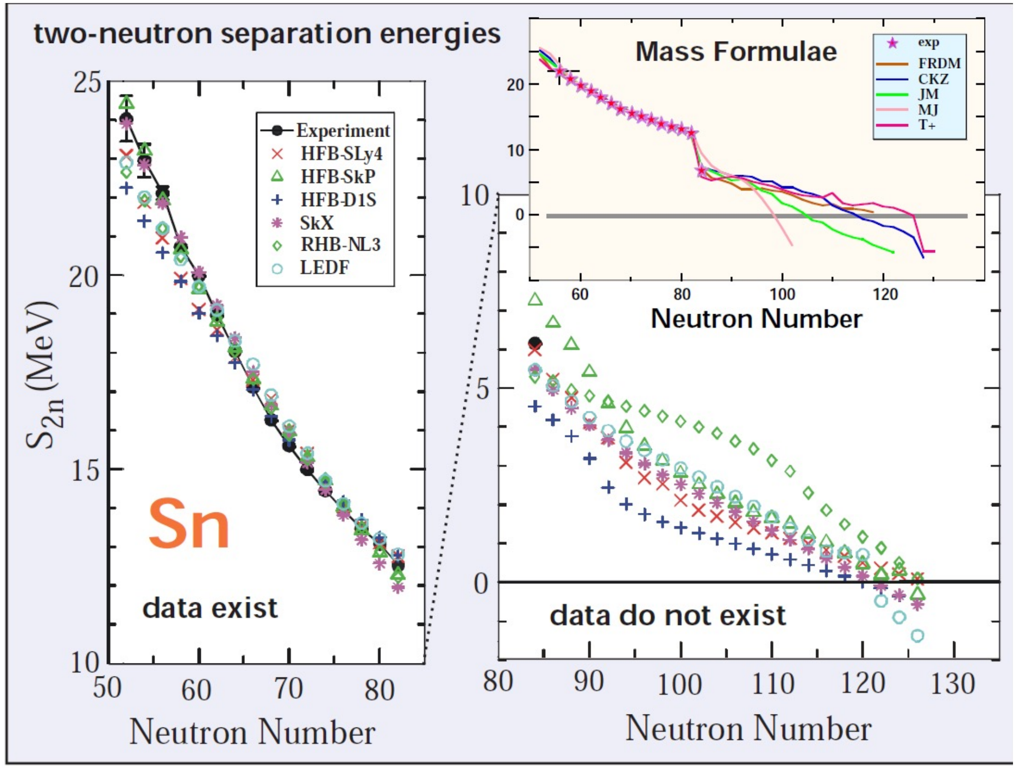
Status of $0\nu\beta\beta$-Decay Matrix Elements

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



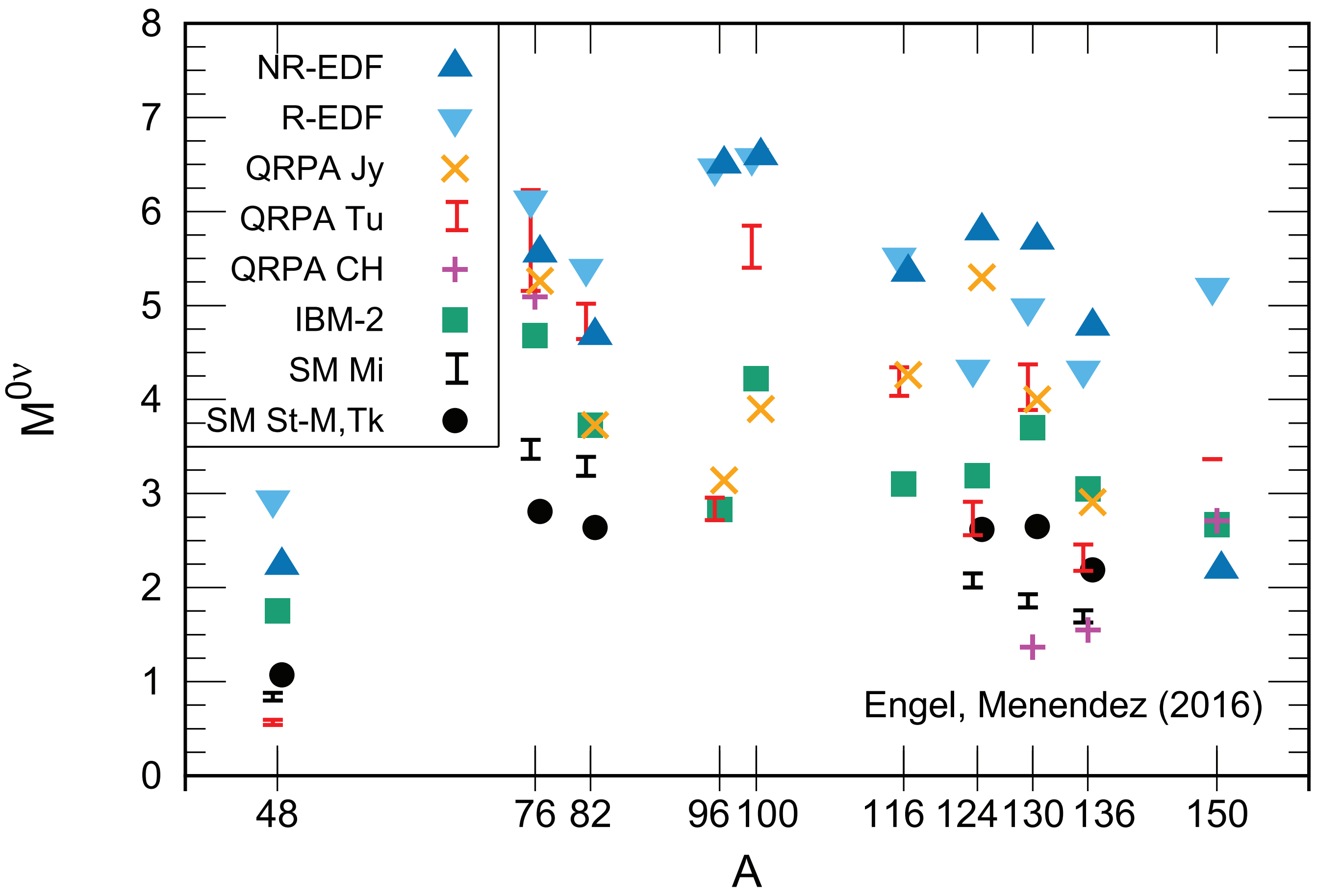


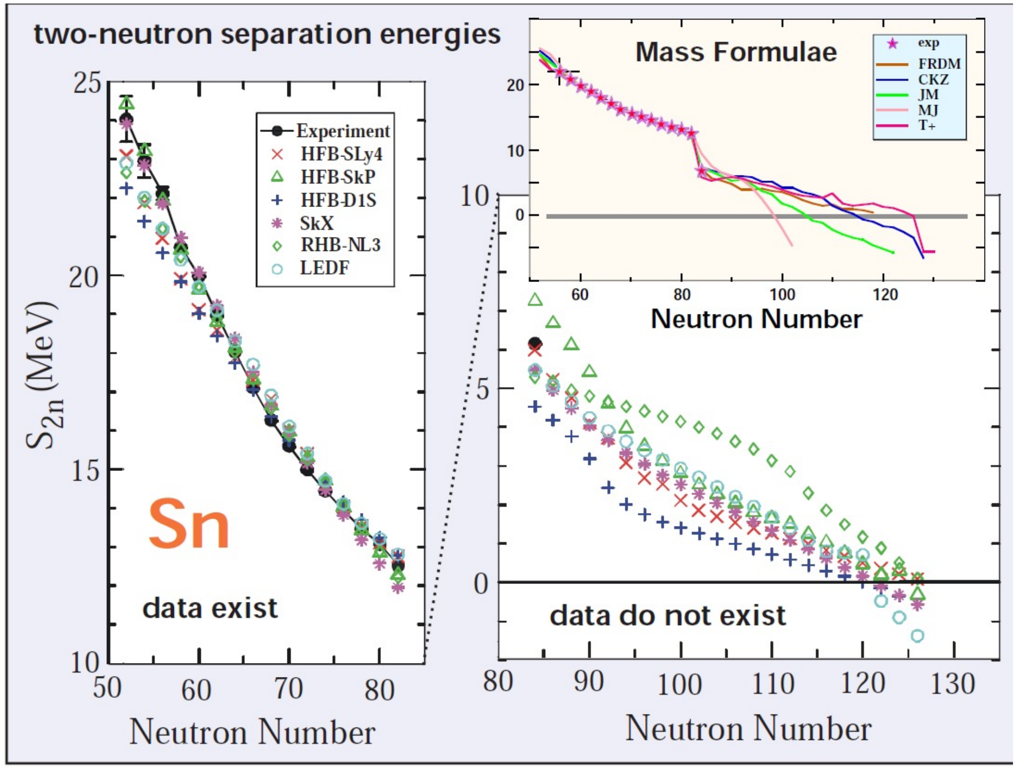
All models missing essential physics

Impossible to assign rigorous uncertainties

Status of 0νββ-Decay Matrix Elements

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



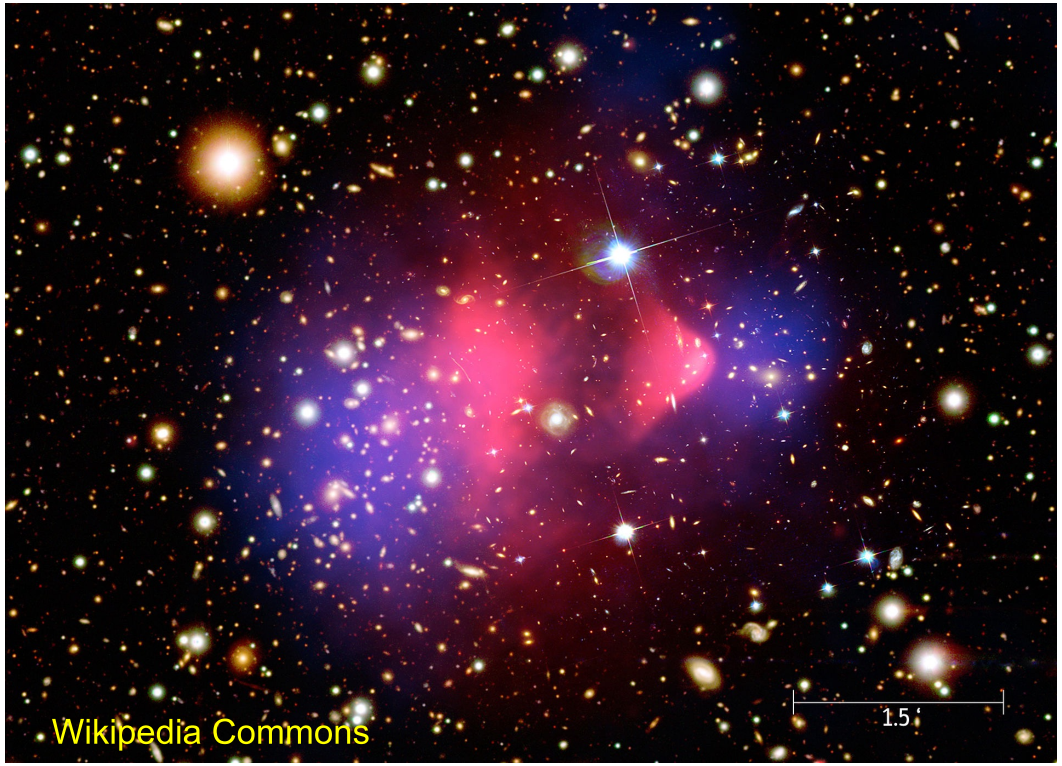


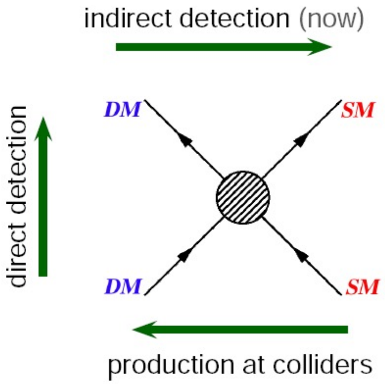
Rethink approach to NME calculations…

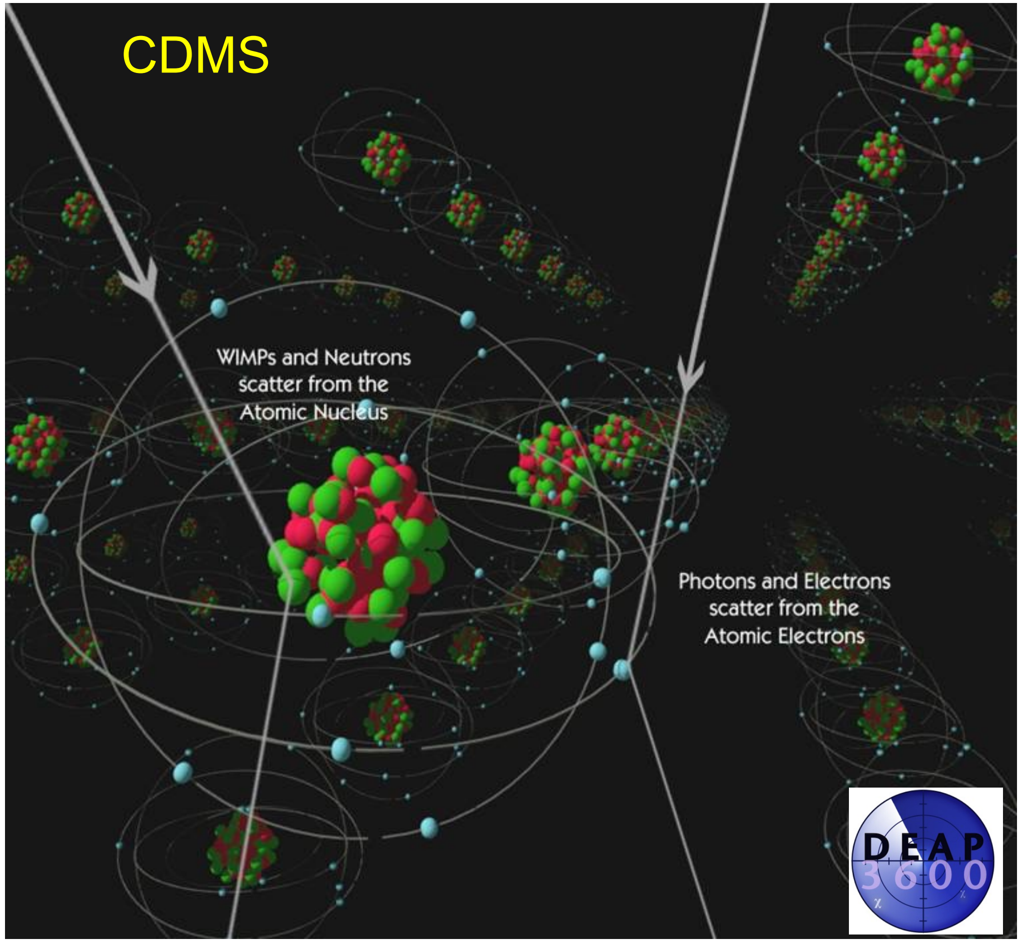
Next-generation NMEs needed for next-generation searches!

Dark Matter Direct Detection

Large-scale direct-detection searches underway worldwide







Observation of nuclear recoil

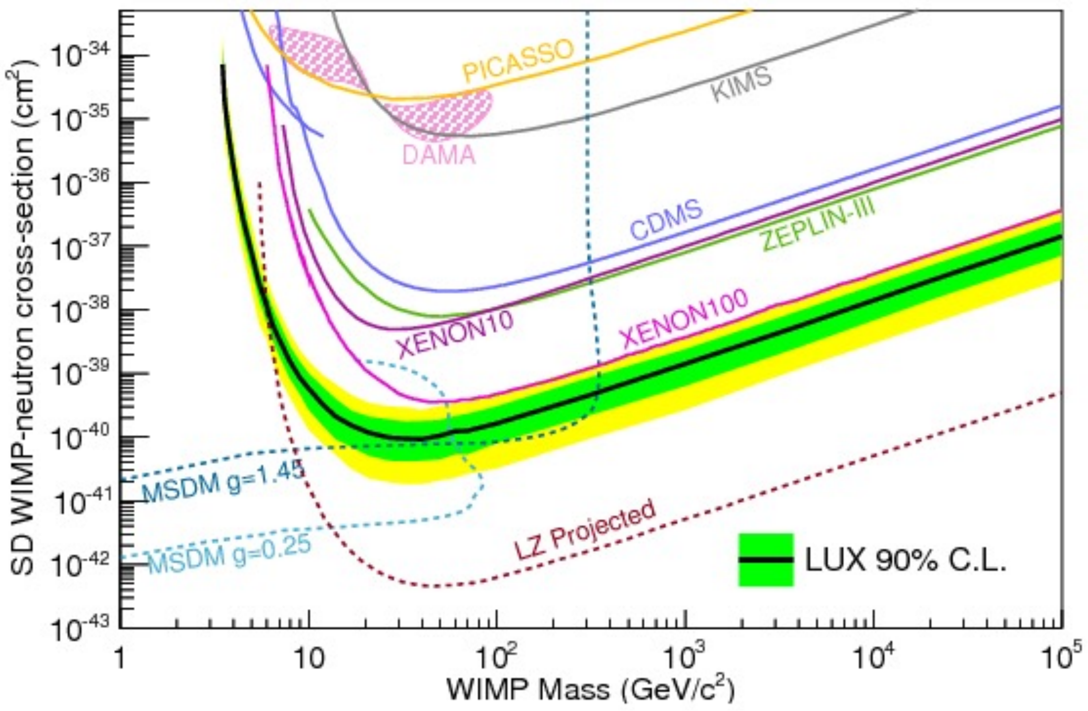
Direct detection: $X\,\mathrm{SM} \to X\,\mathrm{SM}$

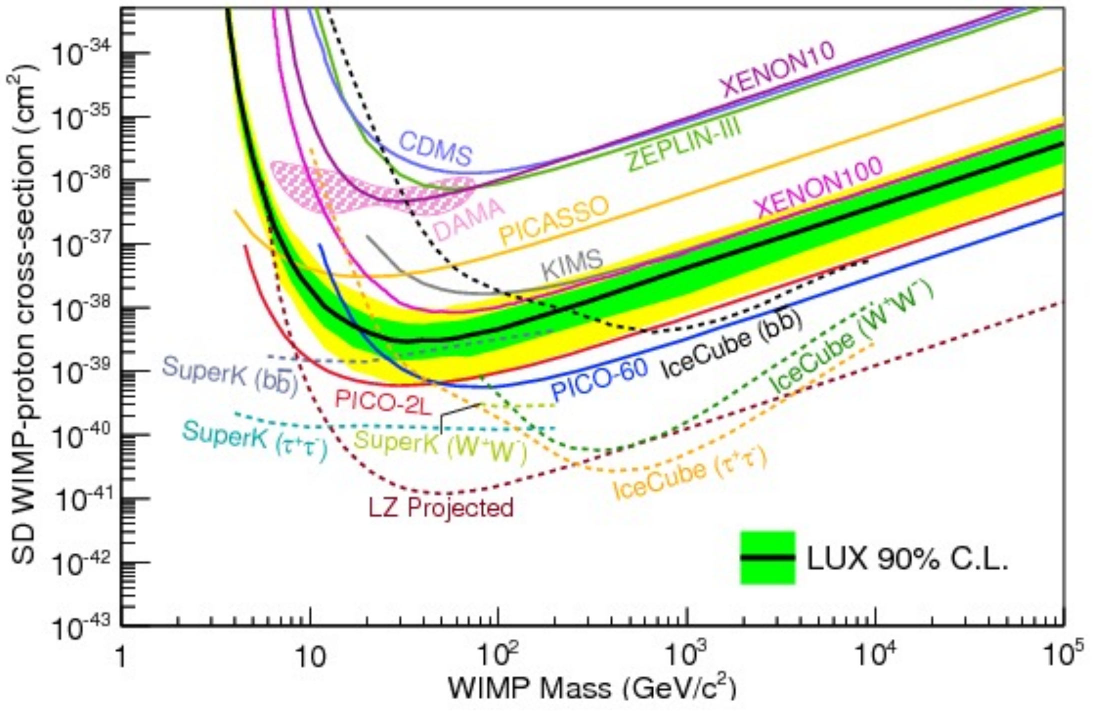
Leading candidates: neutralinos, ...?

Couple to scalar and axial-vector currents in atomic nuclei

Dark Matter Direct Detection

Exclusion plots for WIMP-nucleon total cross section require nuclear structure





Differential cross section: compare results from different target nuclei

$$\frac{\mathrm{d}\sigma}{\mathrm{d}p^2} = \frac{8G_F^2}{(2J_i+1)v^2} S_A(p)$$

Structure functions required from nuclear theory

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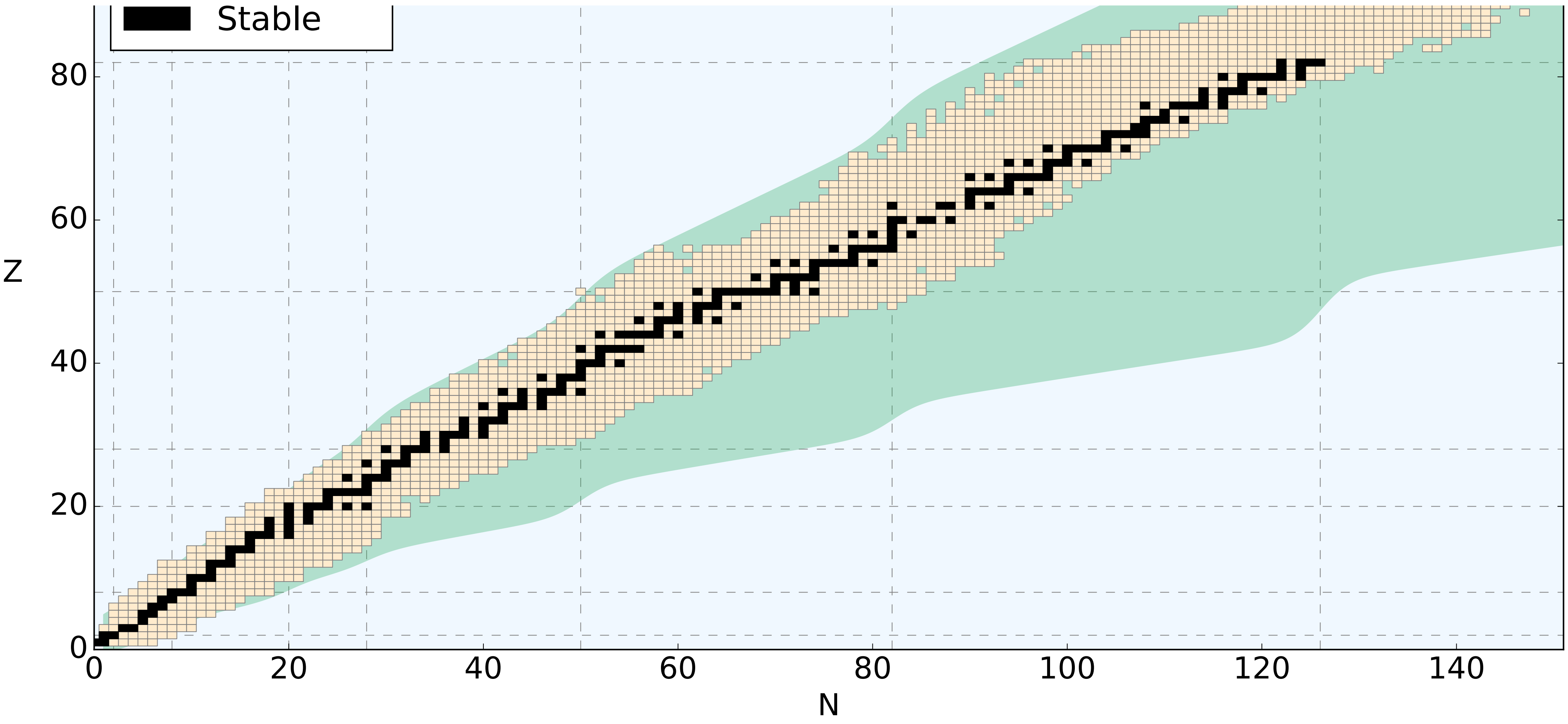
Obligatory Super Technical Theory Slide

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

$$H\psi_n = E_n\psi_n$$



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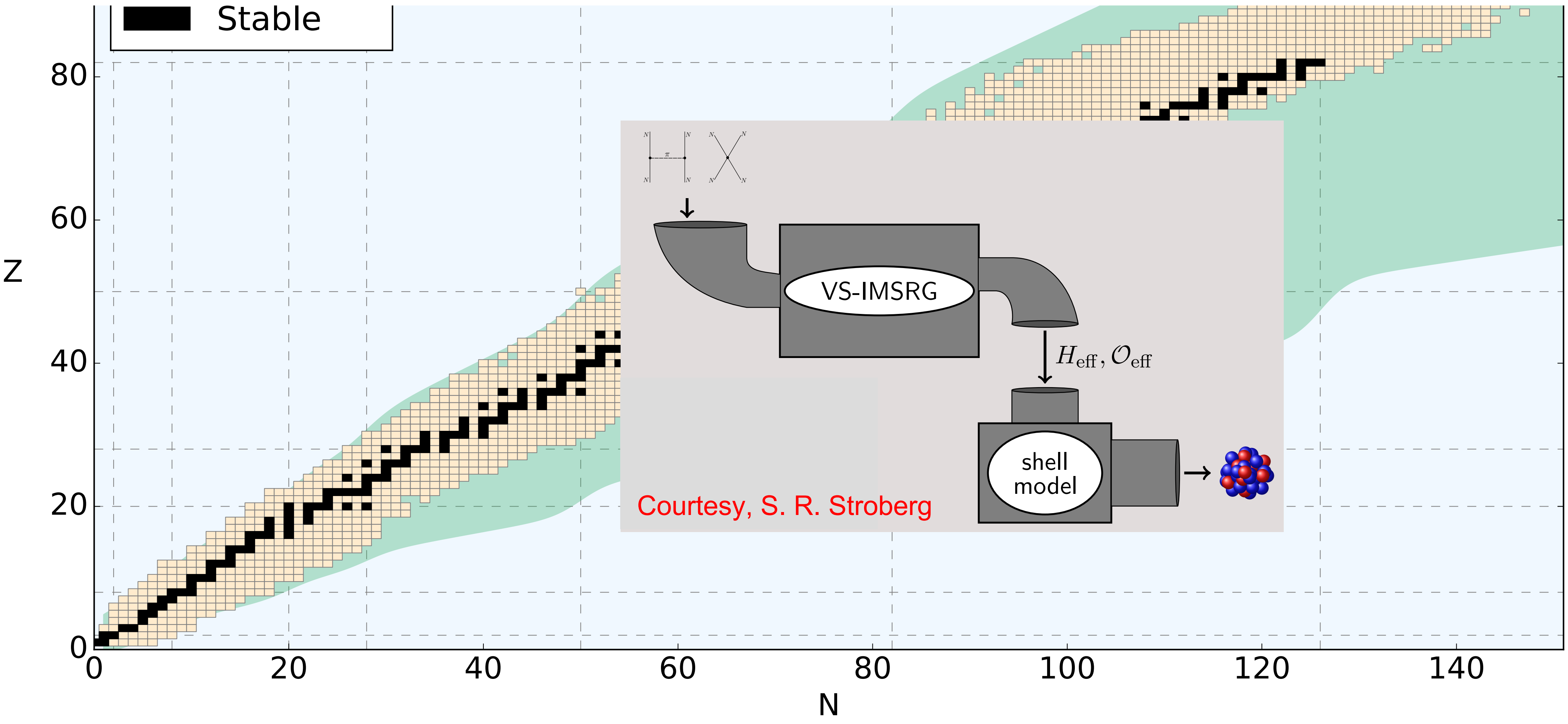

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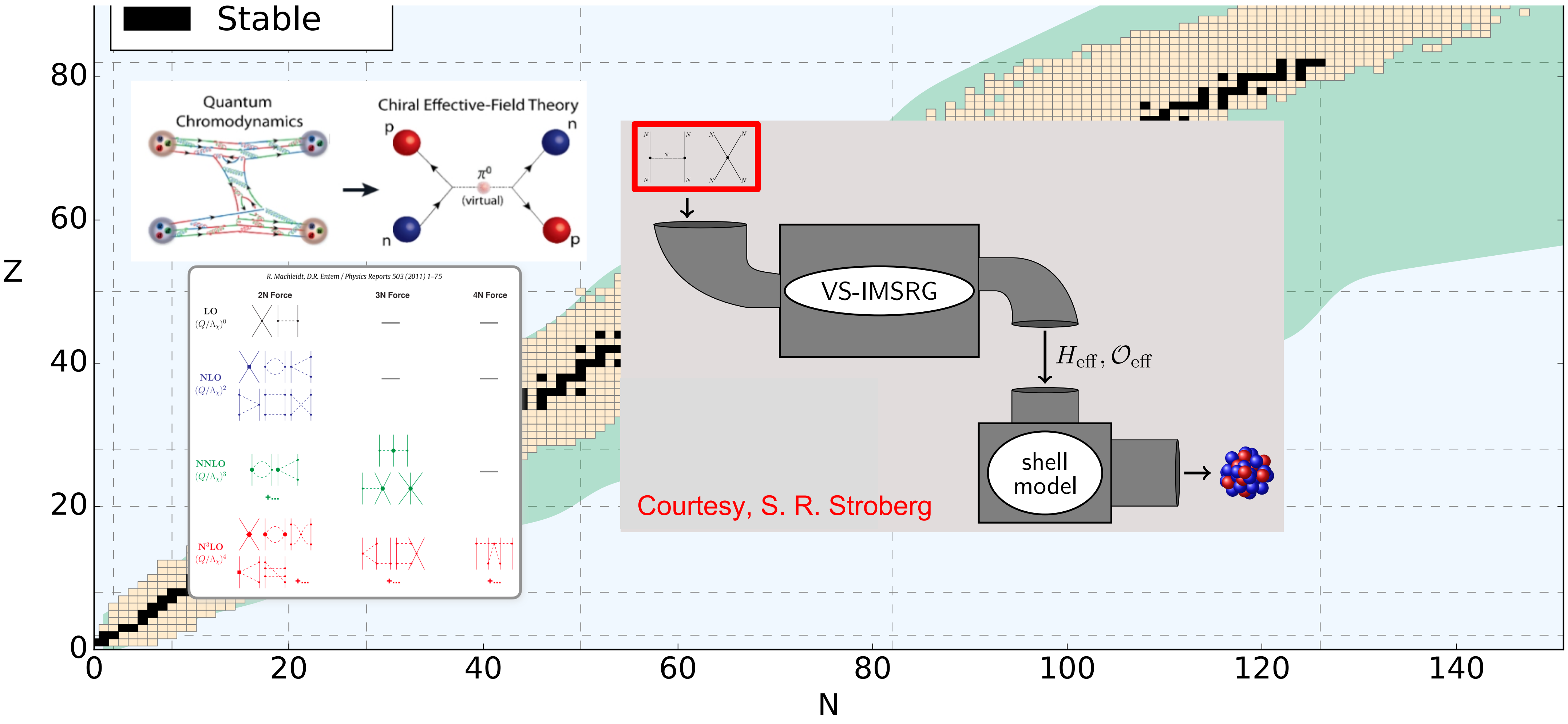

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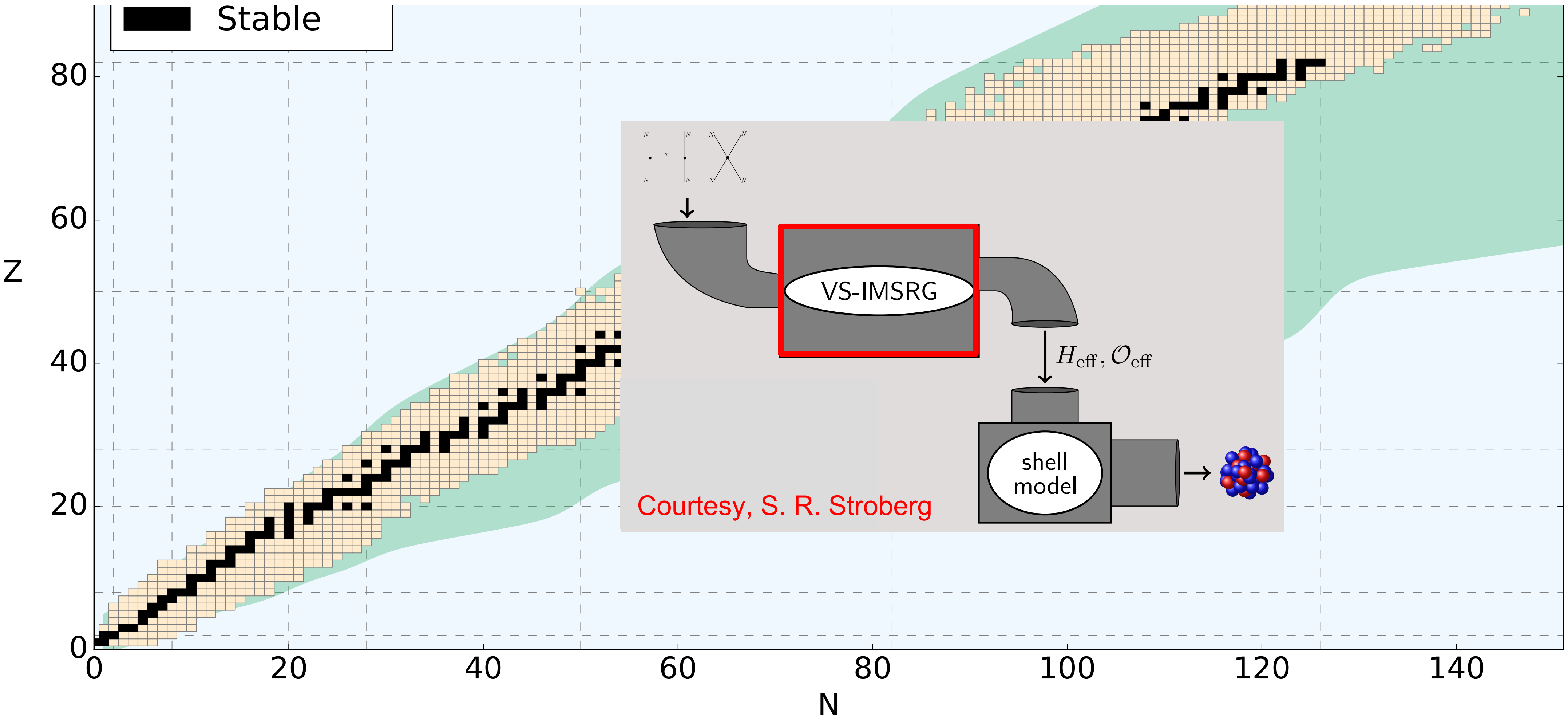

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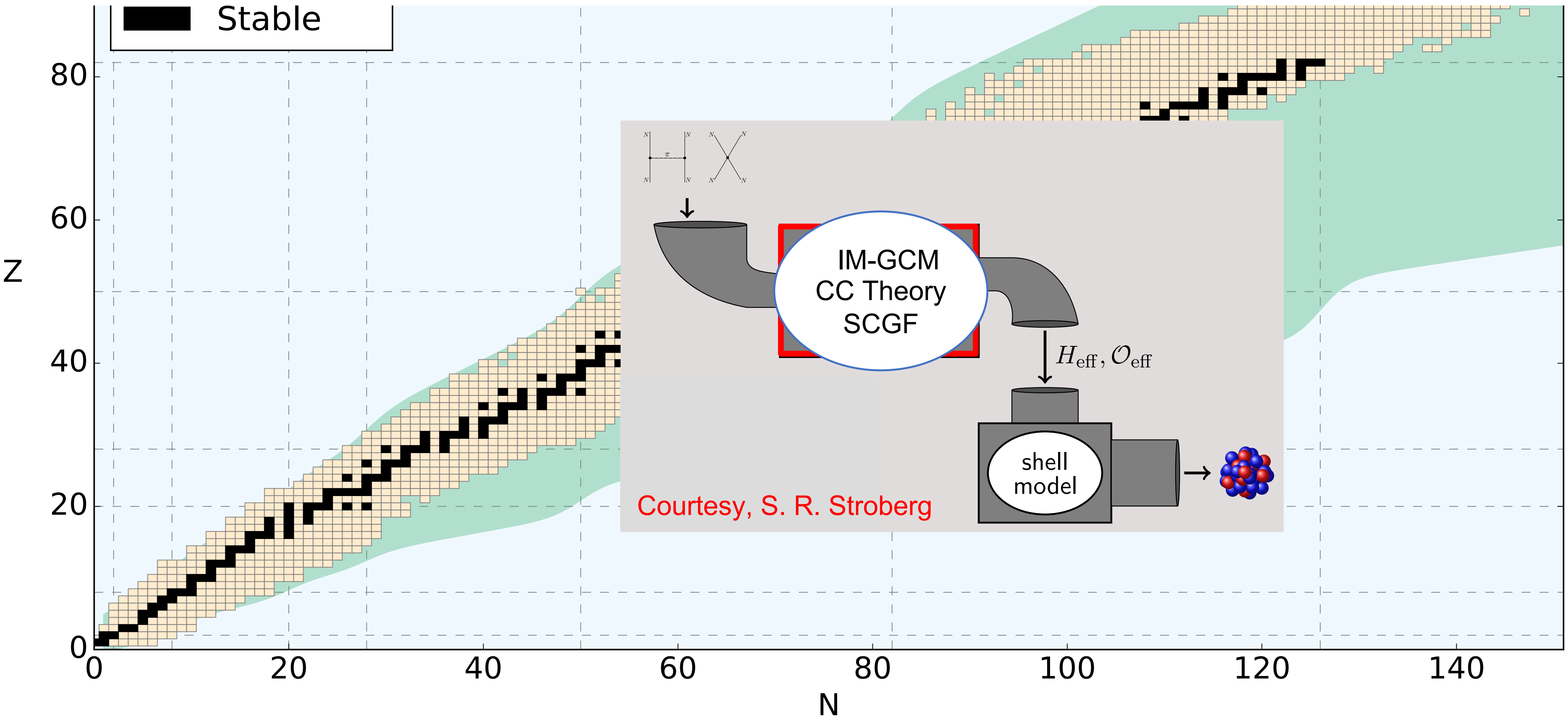
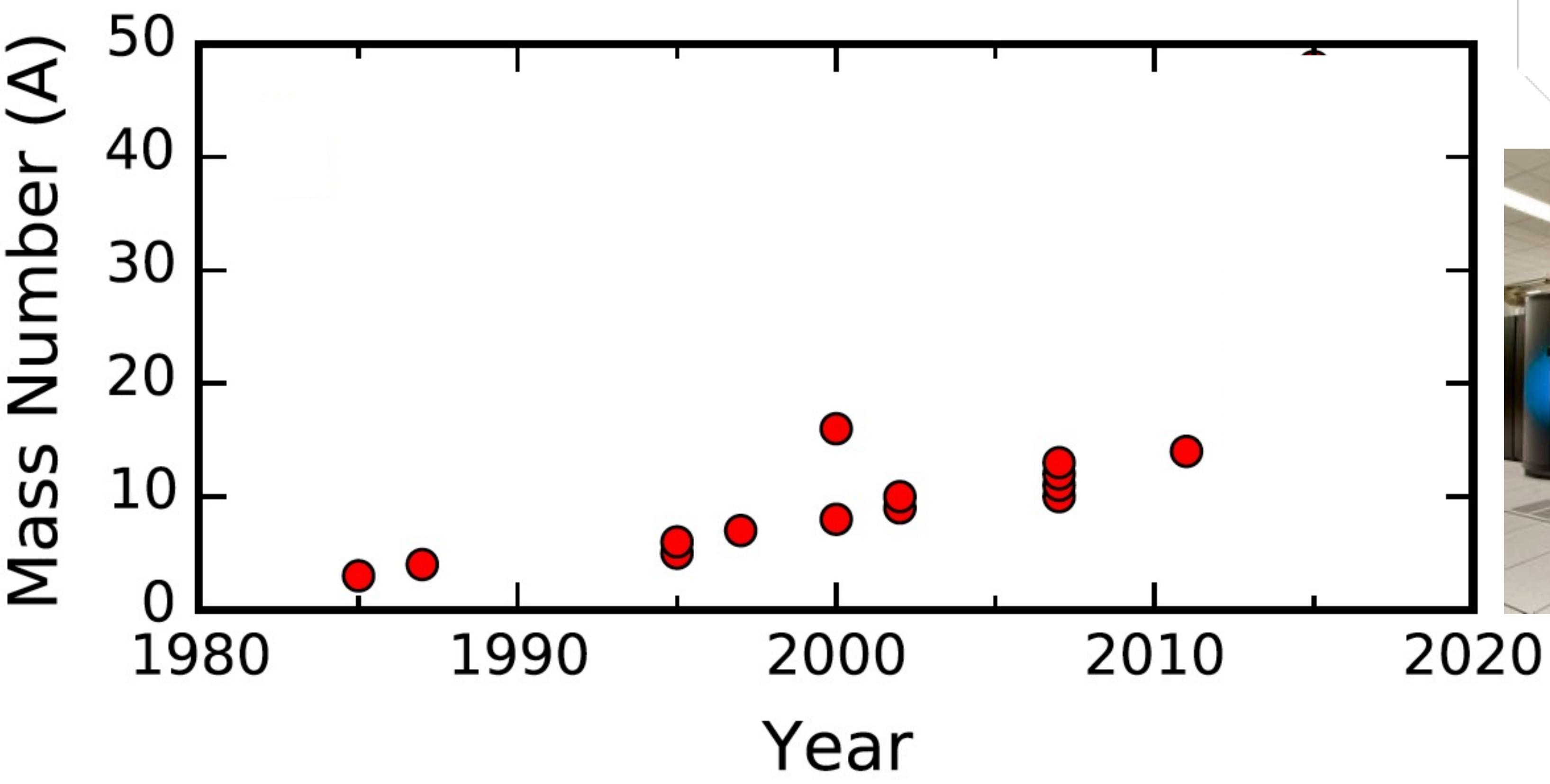
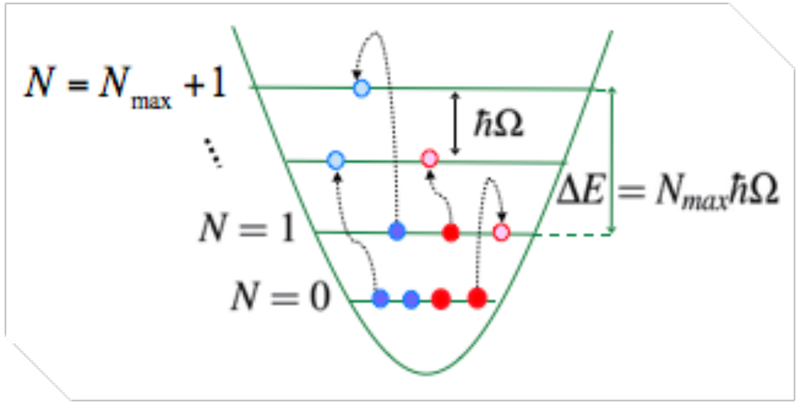


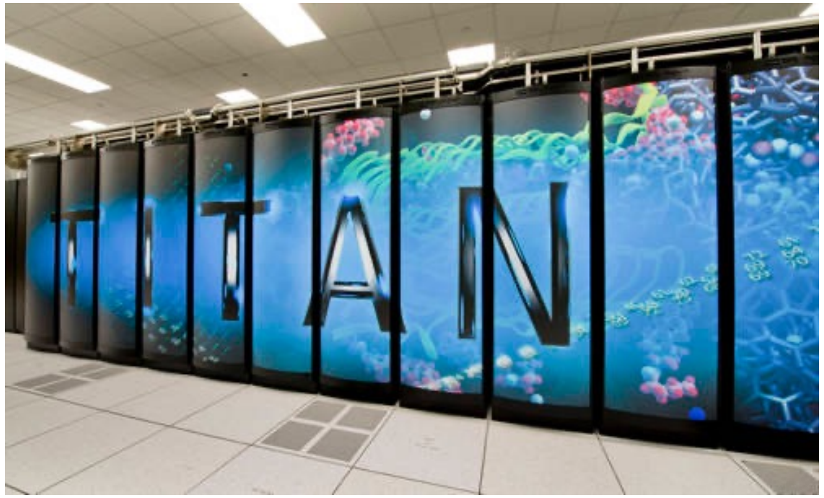
Chronological Reach of Ab Initio Theory

Moore's law: exponential growth in computing power

Methods for light nuclei (QMC, **NCSM**) scale exponentially with mass







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Methods for light nuclei (QMC, NCSM) scale exponentially with mass

Polynomial scaling methods developed (CC, **VS-IMSRG**, SCGF)

Explosion in limits of ab initio theory

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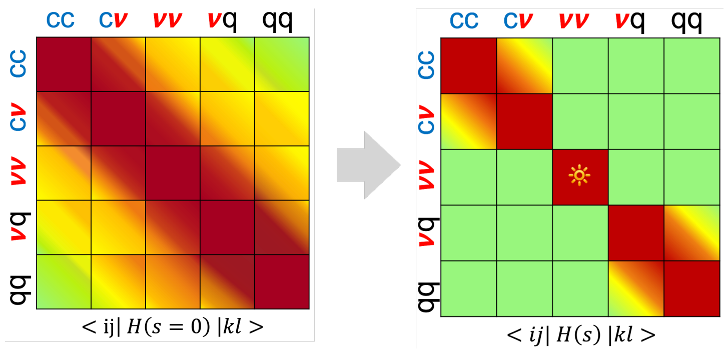

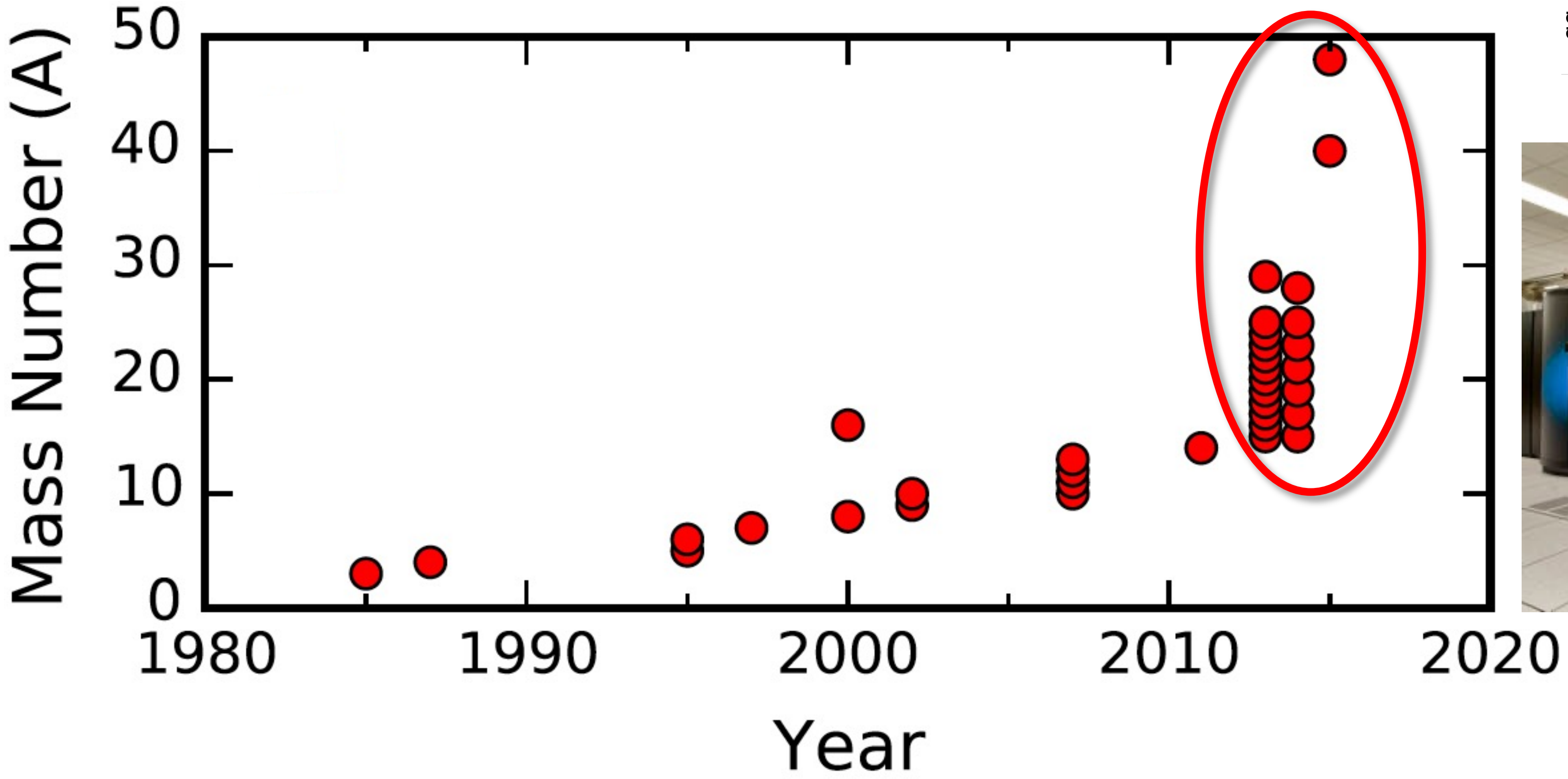

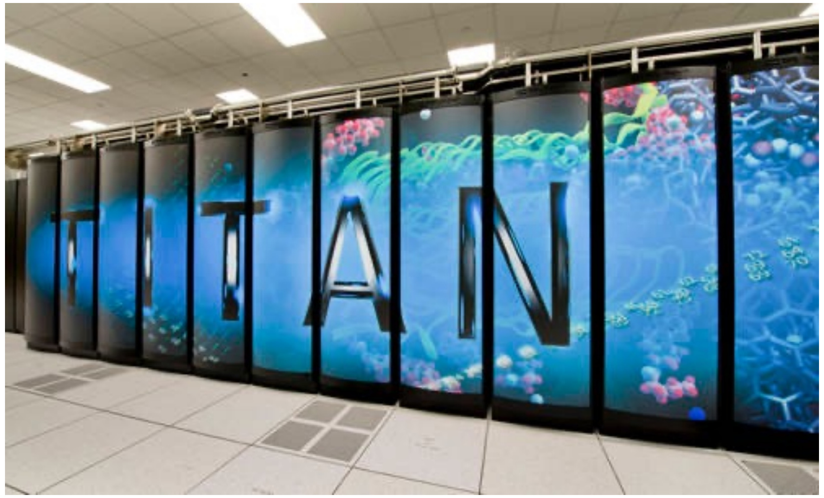

Chronological Reach of Ab Initio Theory

2021: A>(>)100

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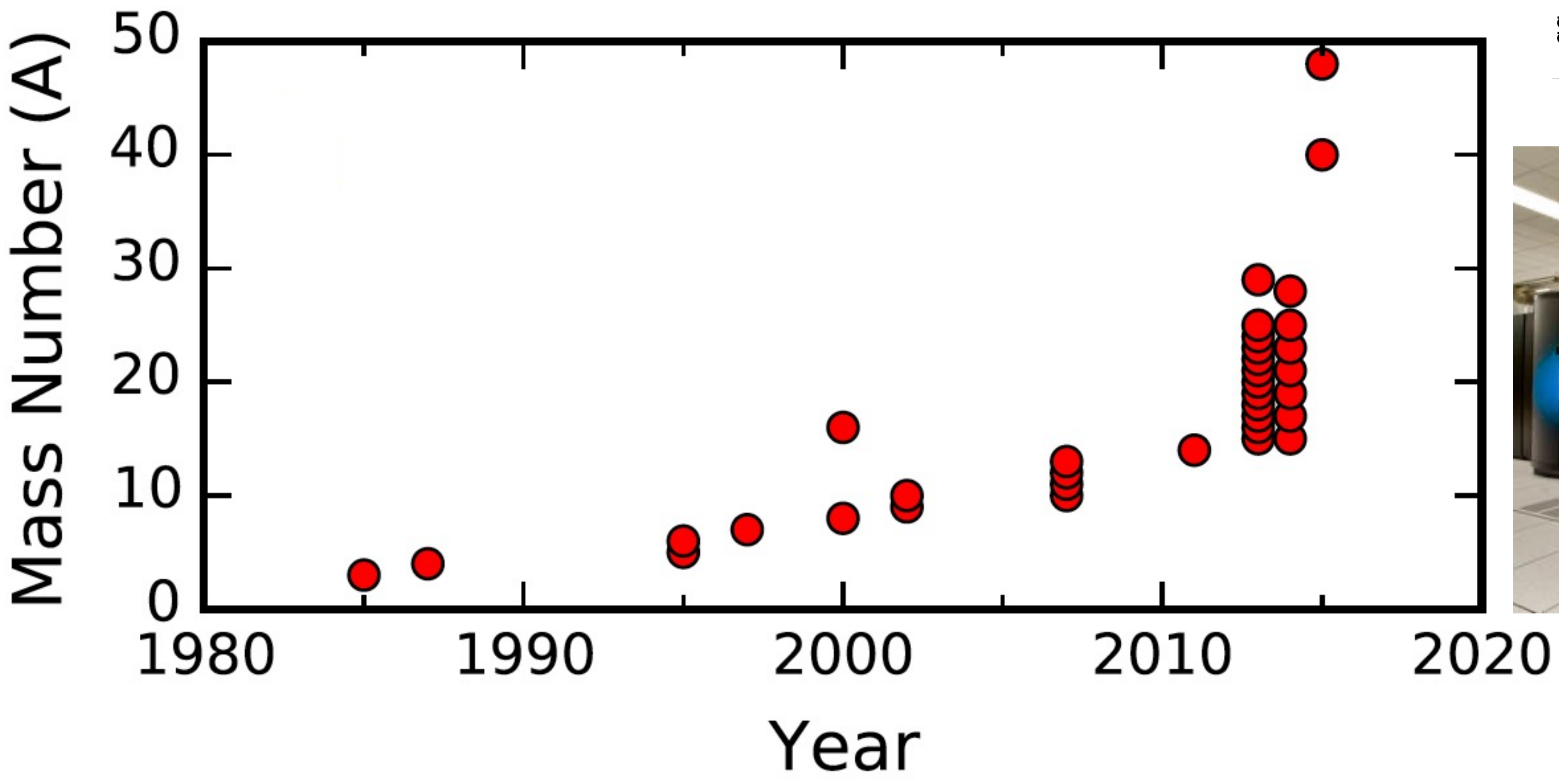
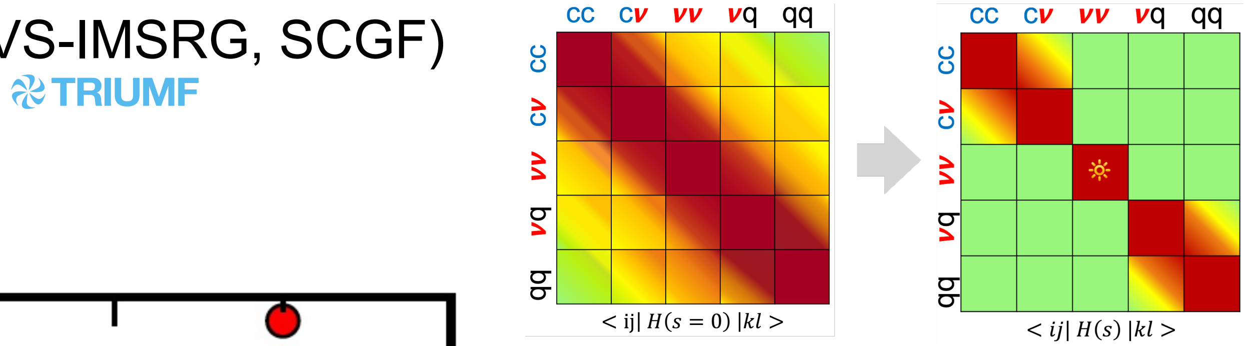
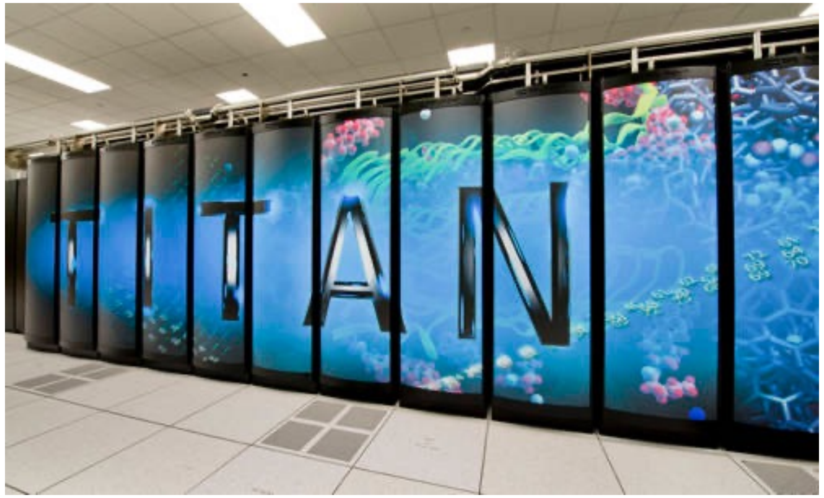




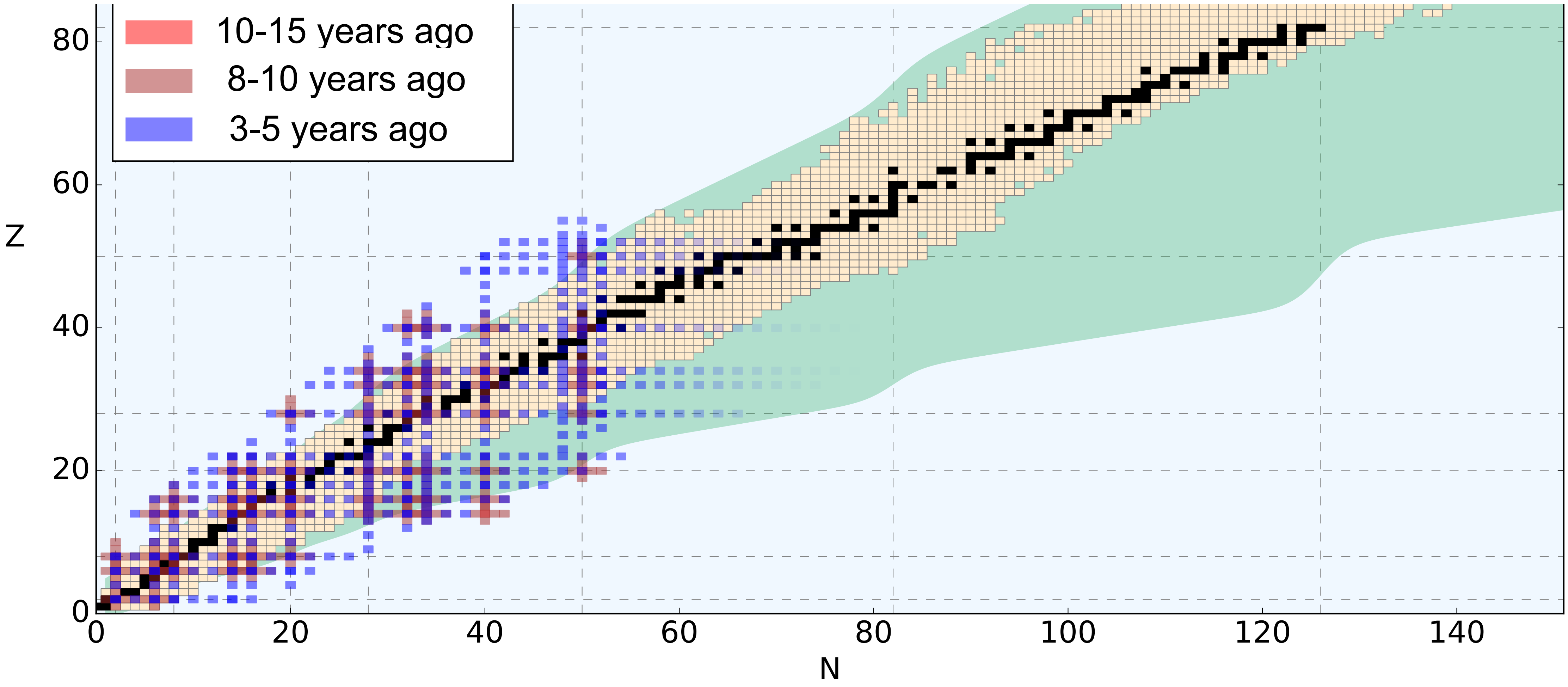


Recent Breadth of Ab Initio Theory

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

- Nuclear forces, electroweak physics
- Nuclear many-body problem

$$H\psi_n = E_n\psi_n$$



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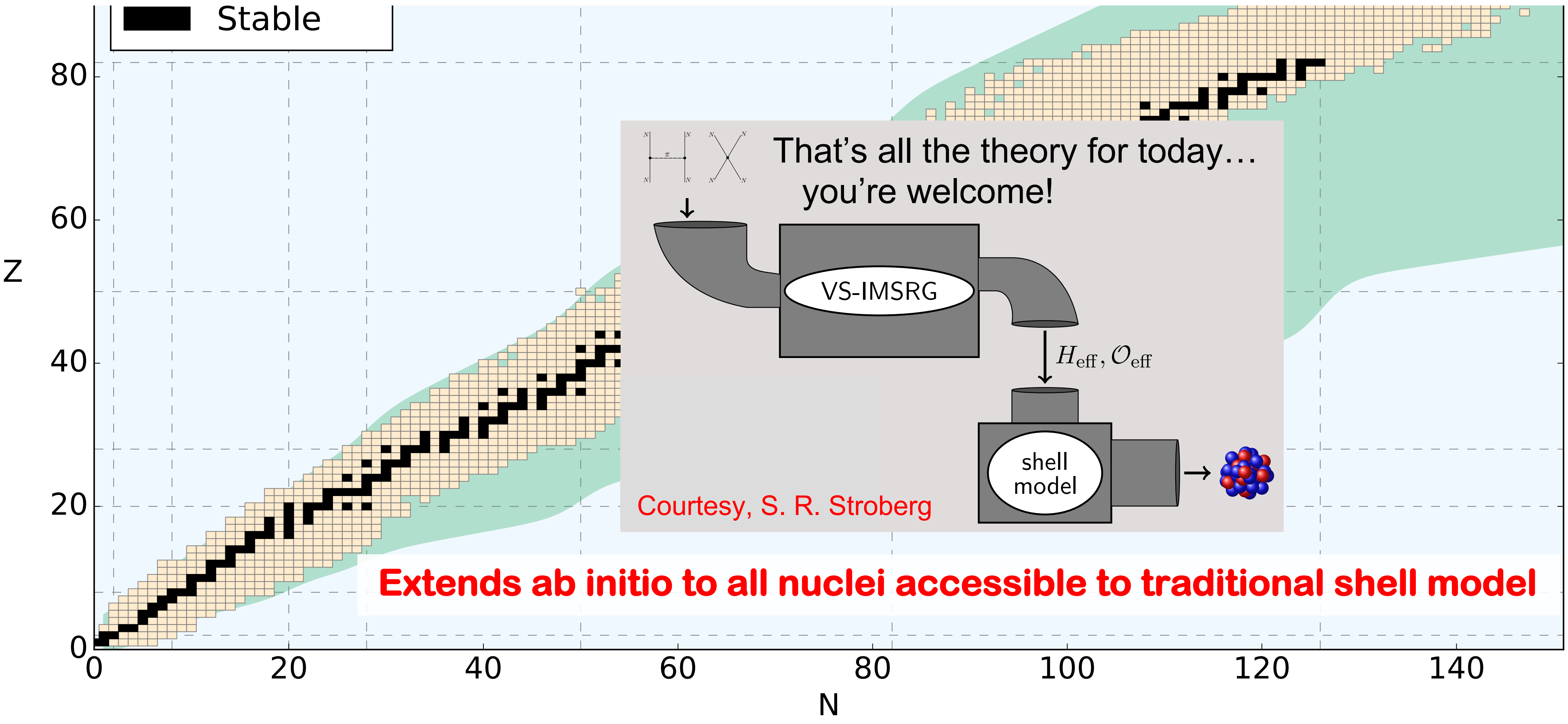

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Today: Global Ab Initio Calculations

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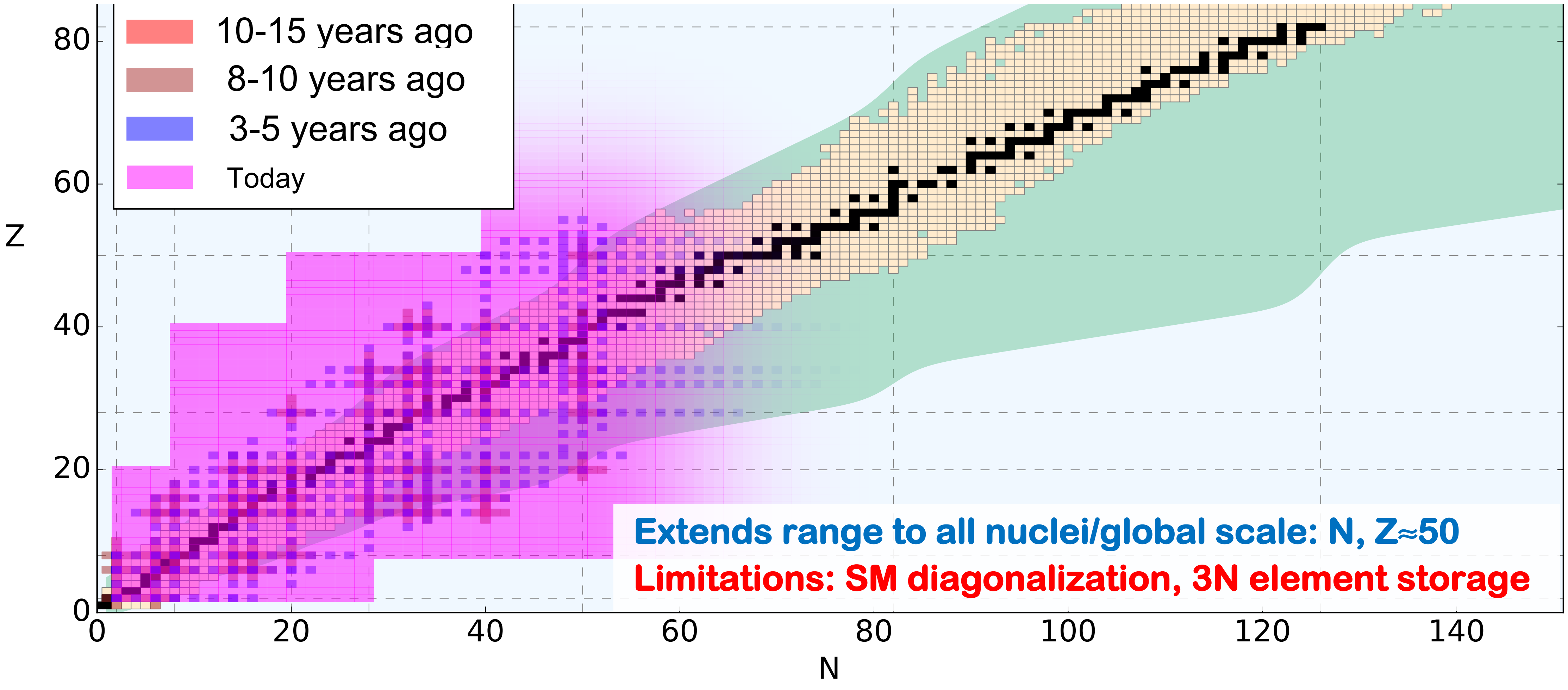
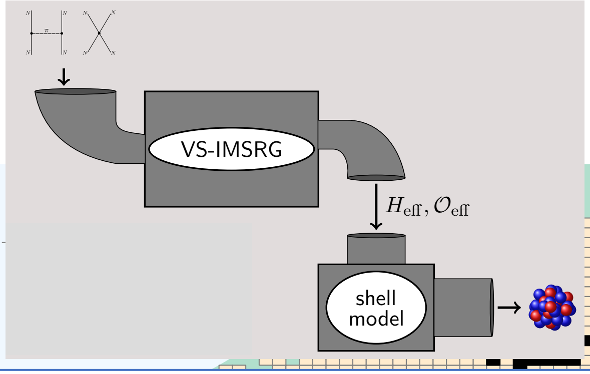
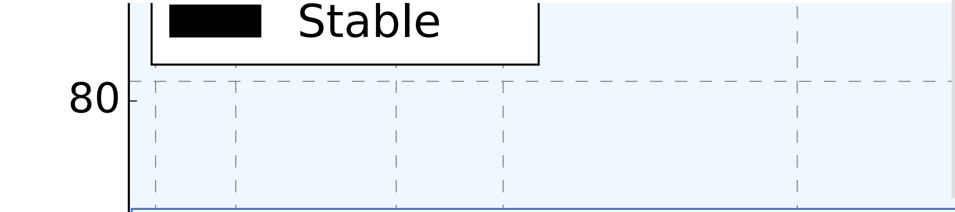


VS-IMSRG for Atomic Nuclei

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





Major Nuclear Structure Questions/Developments Underway

1) How do basic properties of nuclei emerge from fundamental interactions?

2) What are the limits of existence of matter?

3) How do magic numbers evolve?

4) Accessing the heaviest nuclei and r-process region

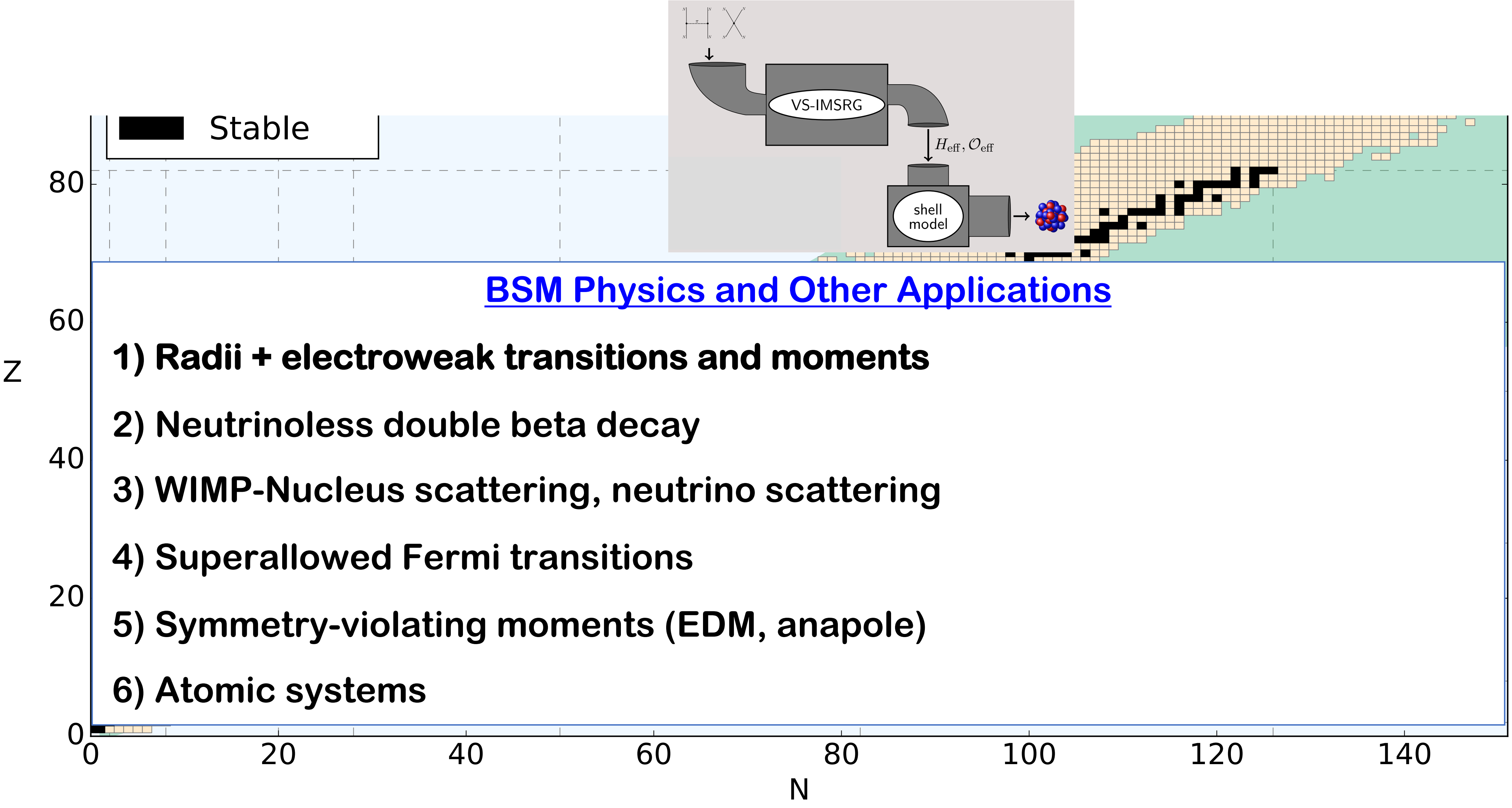
5) Incorporate coupling to continuum for unbound systems

6) Cross-shell physics for Islands of Inversion

7) Constraining properties relevant to neutron star physics

VS-IMSRG for Atomic Nuclei

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



BSM Physics and Other Applications

1) **Radii + electroweak transitions and moments**
2) **Neutrinoless double beta decay**
3) **WIMP-Nucleus scattering, neutrino scattering**
4) **Superallowed Fermi transitions**
5) **Symmetry-violating moments (EDM, anapole)**
6) **Atomic systems**

VS-IMSRG for Atomic Nuclei

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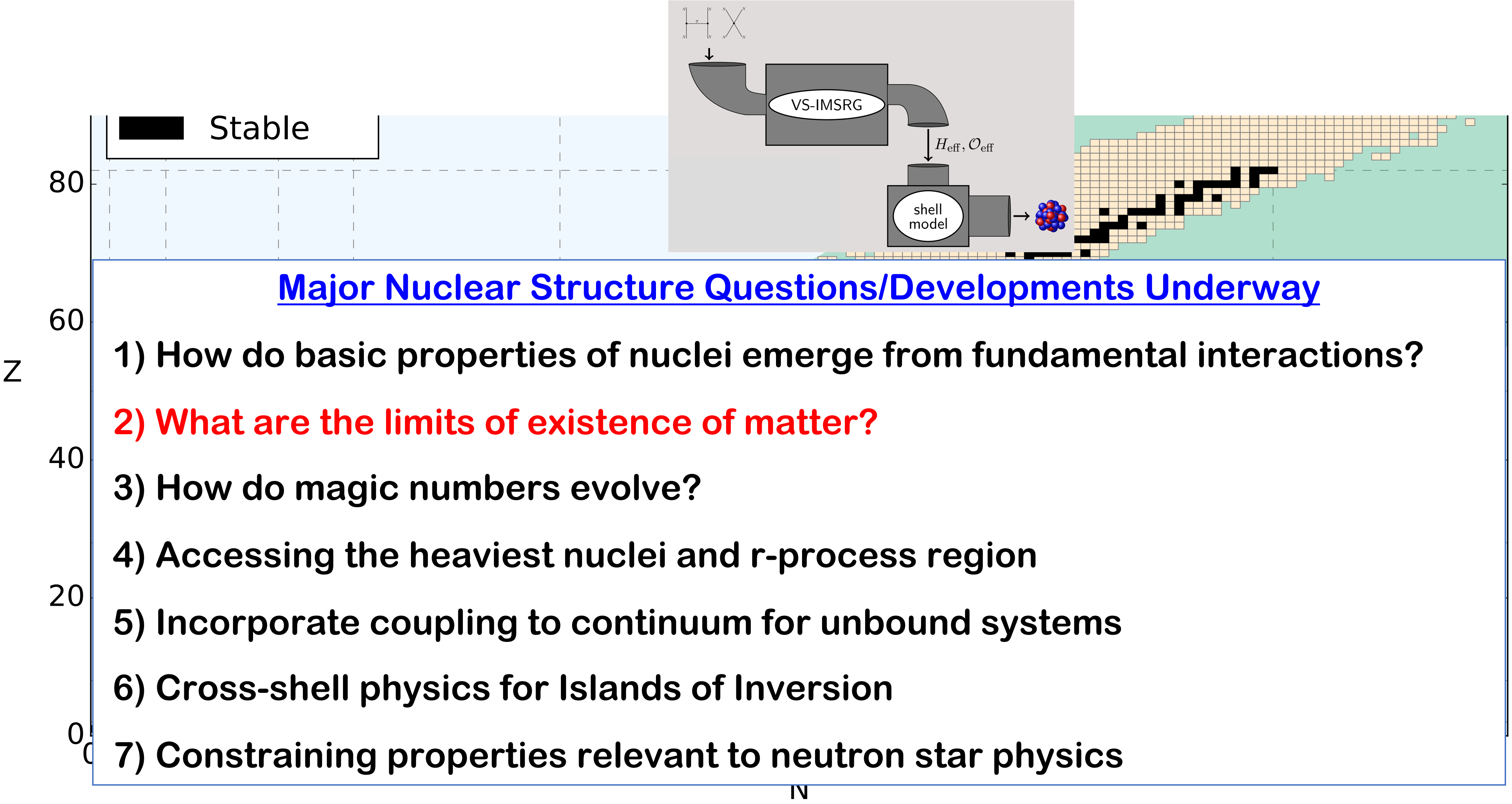

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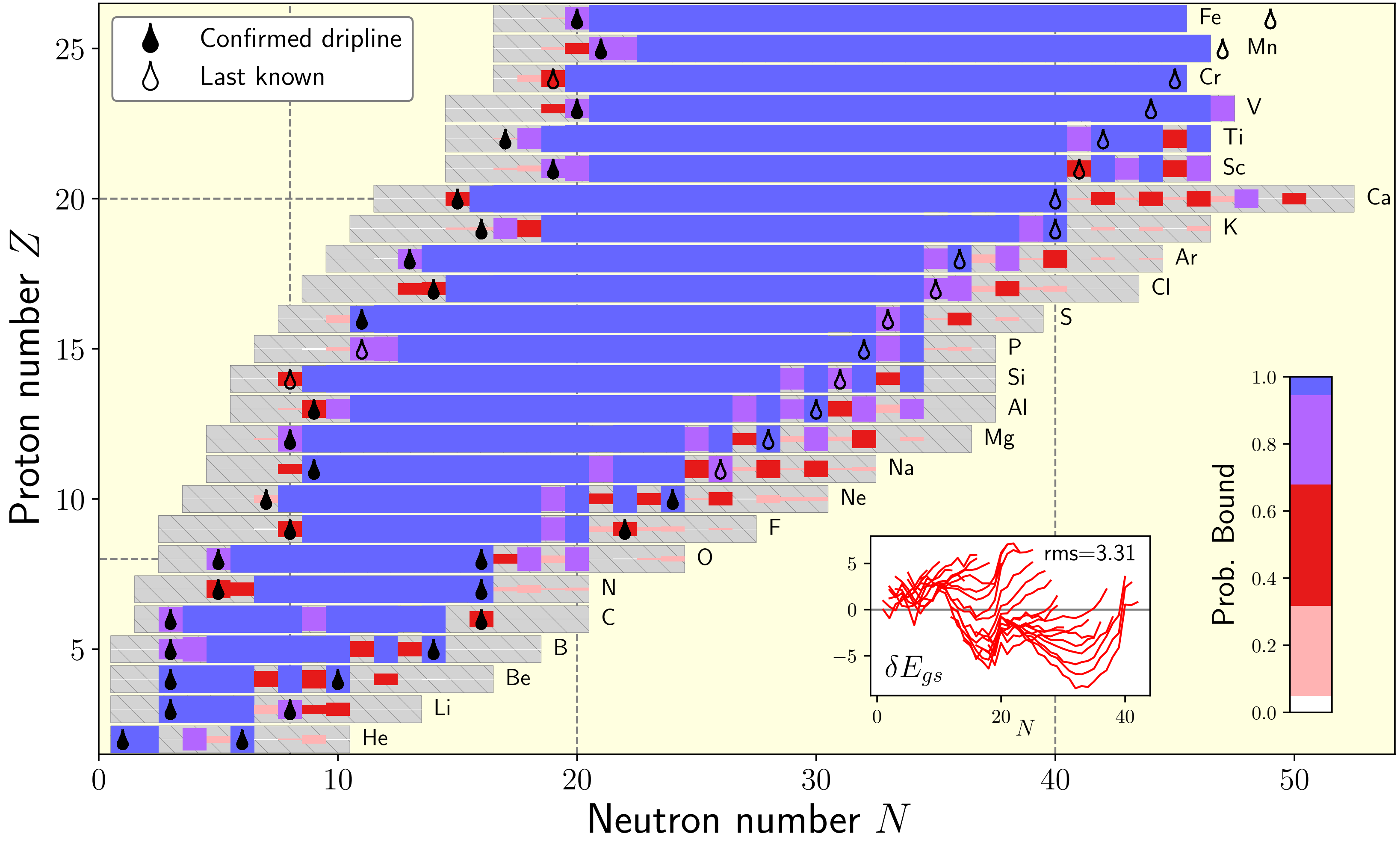
Dripline Predictions to Fe Isotopes

First predictions of proton and neutron driplines from first principles



From **few body** data only:

$$\mathcal{P}_{1n} = \frac{1}{\sqrt{2\pi}\sigma_{1n}} \int_0^\infty \exp \frac{(x - S_n^{th.corr})^2}{2\sigma_{1n}^2} dx$$

$$\mathcal{P}_{\text{bound}} = (\mathcal{P}_{1n}\mathcal{P}_{2n} + \xi_{1n,2n})(\mathcal{P}_{1p}\mathcal{P}_{2p} + \xi_{1p,2p})$$

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 largely predicted within uncertainties (artifacts at shell closures)

Provide ab initio predictions for neutron-rich region

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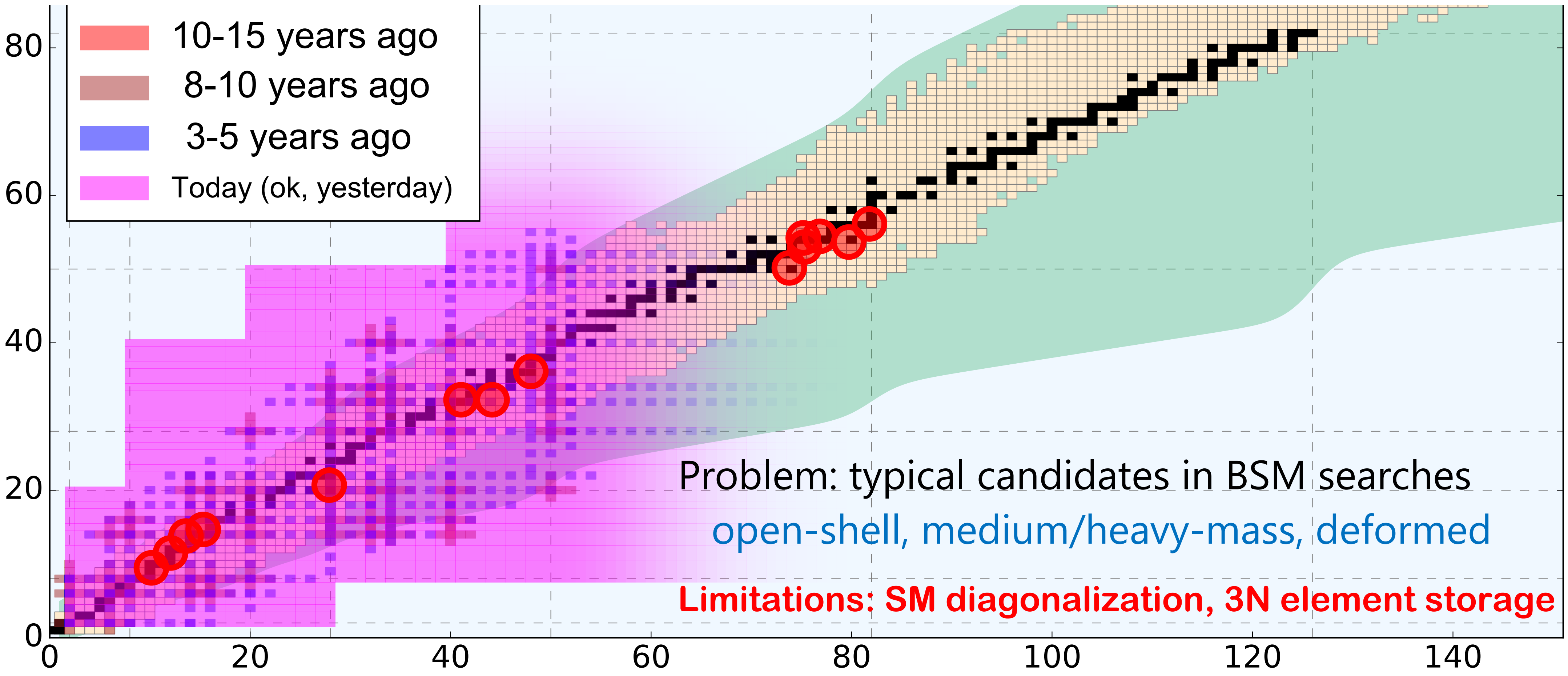
Nuclei in BSM Physics Searches

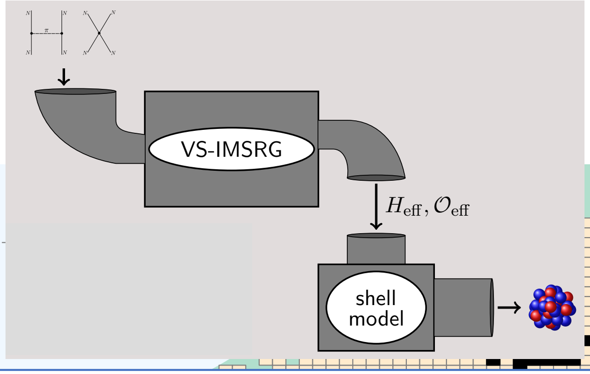
Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem



VS-IMSRG for Atomic Nuclei

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



Stable

Major Nuclear Structure Questions/Developments Underway

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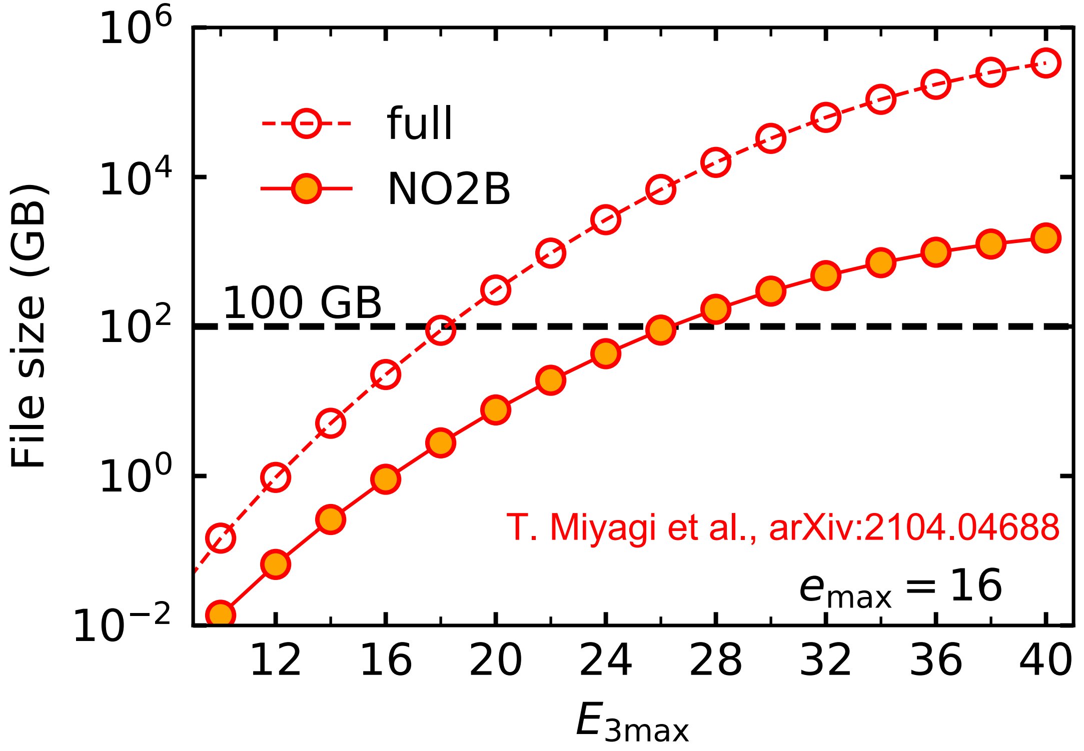
Ab Initio Calculations of Heavy Nuclei

Improvements in (clever) storage of 3N MEs *greatly* expands reach of ab initio theory

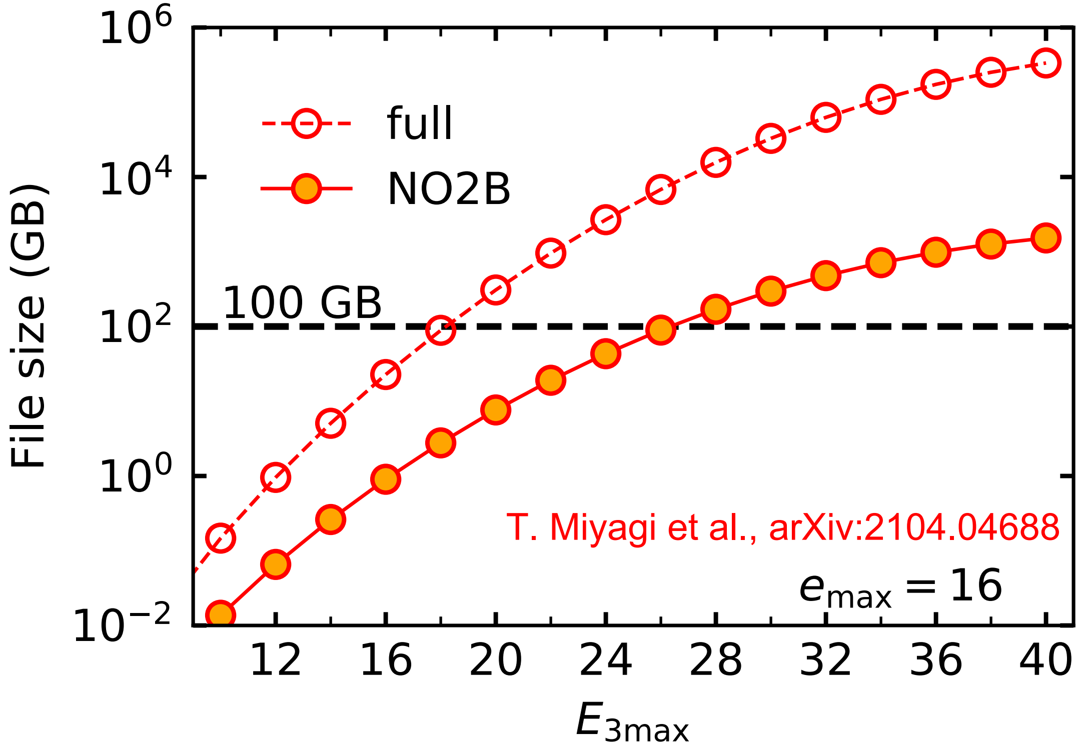
Previous limit: $e_1 + e_2 + e_3 \leq E_{3\text{max}} = 18$

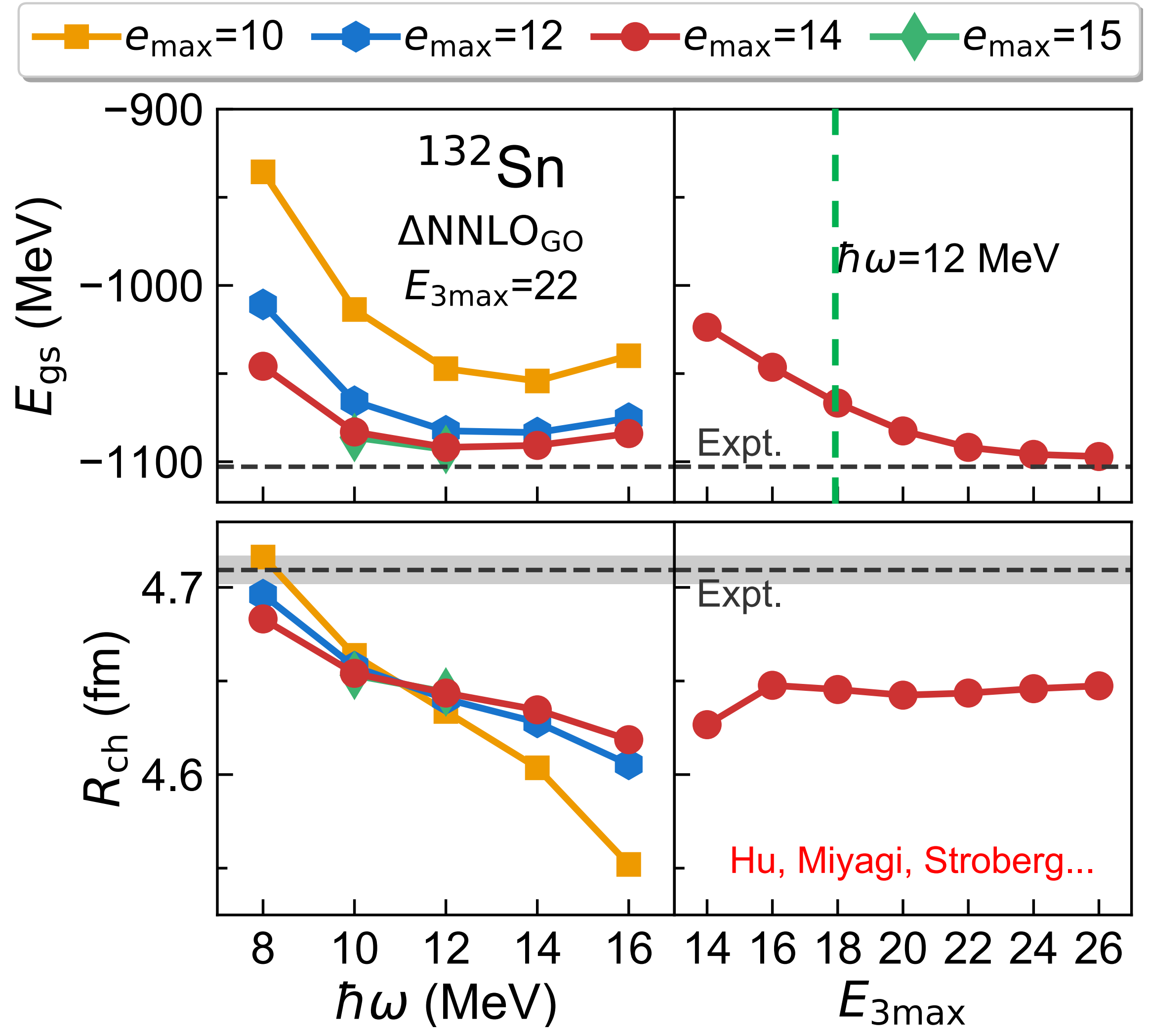


Convergence in Heavy Nuclei: ^{132}Sn

Improvements in (clever) storage of 3N MEs *greatly* expands reach of ab initio theory

Previous limit: E_{3max}=18 **not converged**





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

Opens path to heavy nuclei

Convergence in Heavy Nuclei: ^{208}Pb

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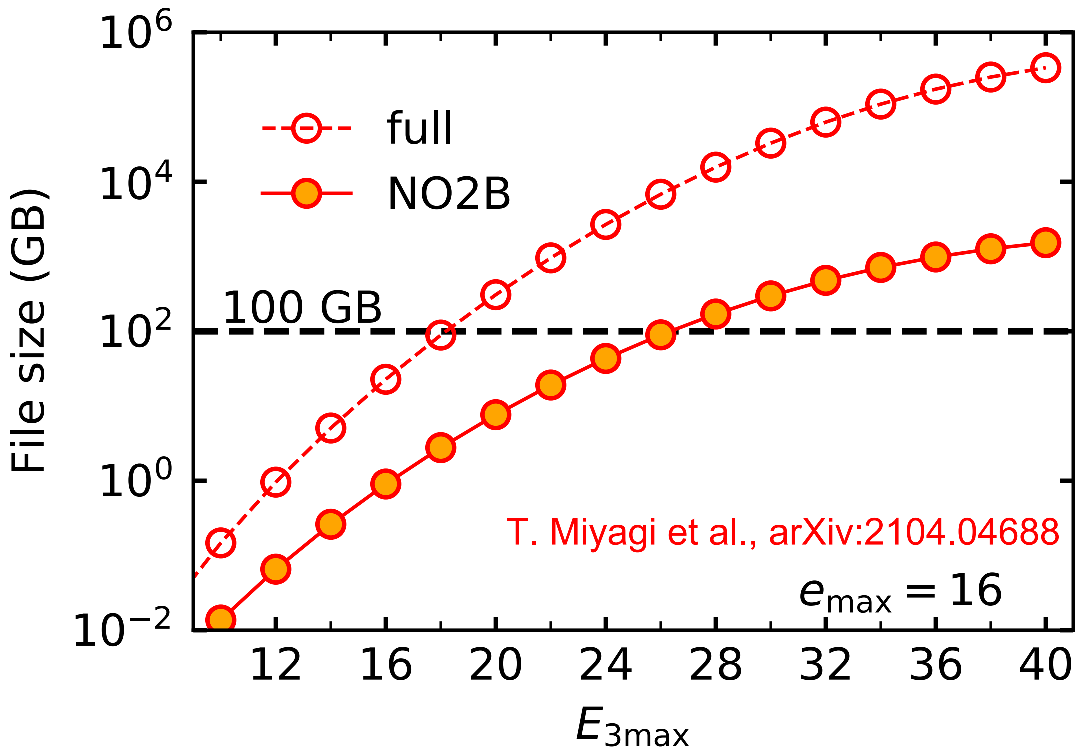

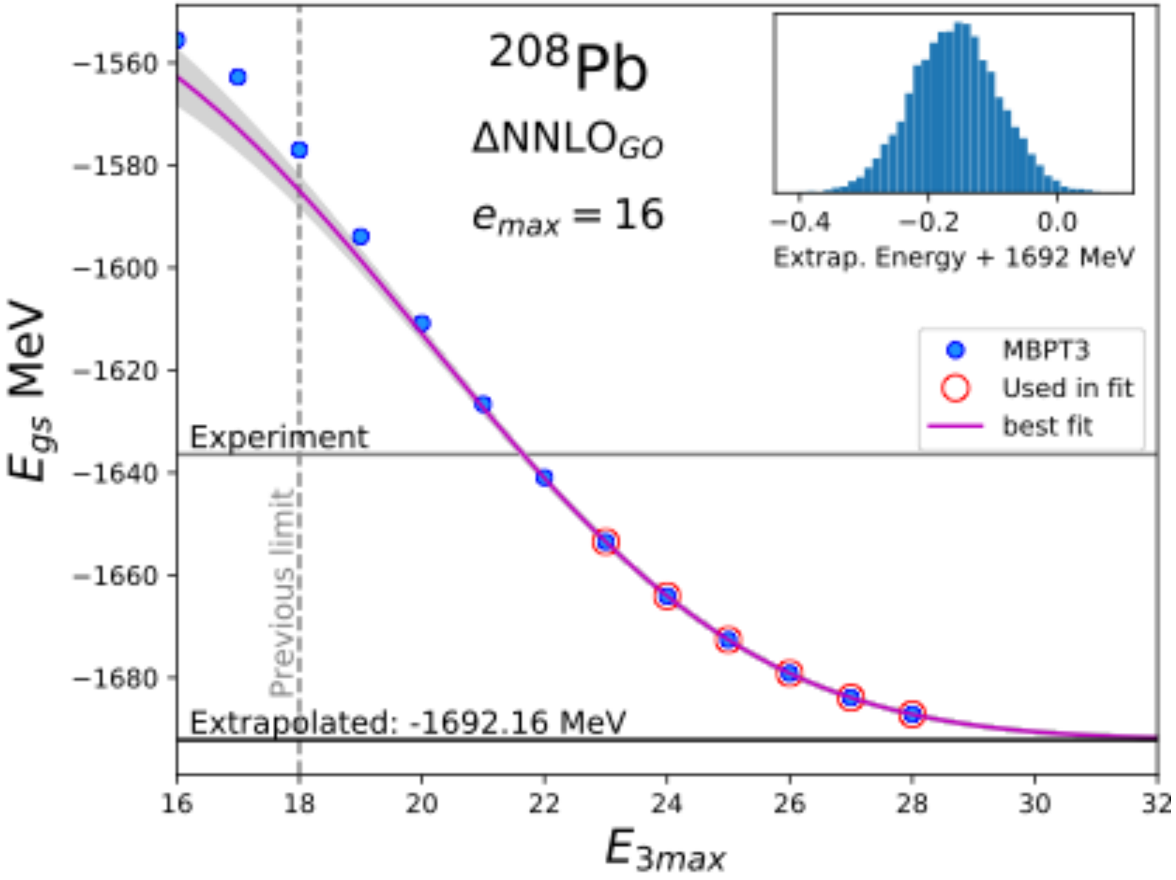

First converged ground-state properties of ^{132}Sn

Opens path to heavy nuclei!

Towards Neutrinoless Double Beta Decay

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

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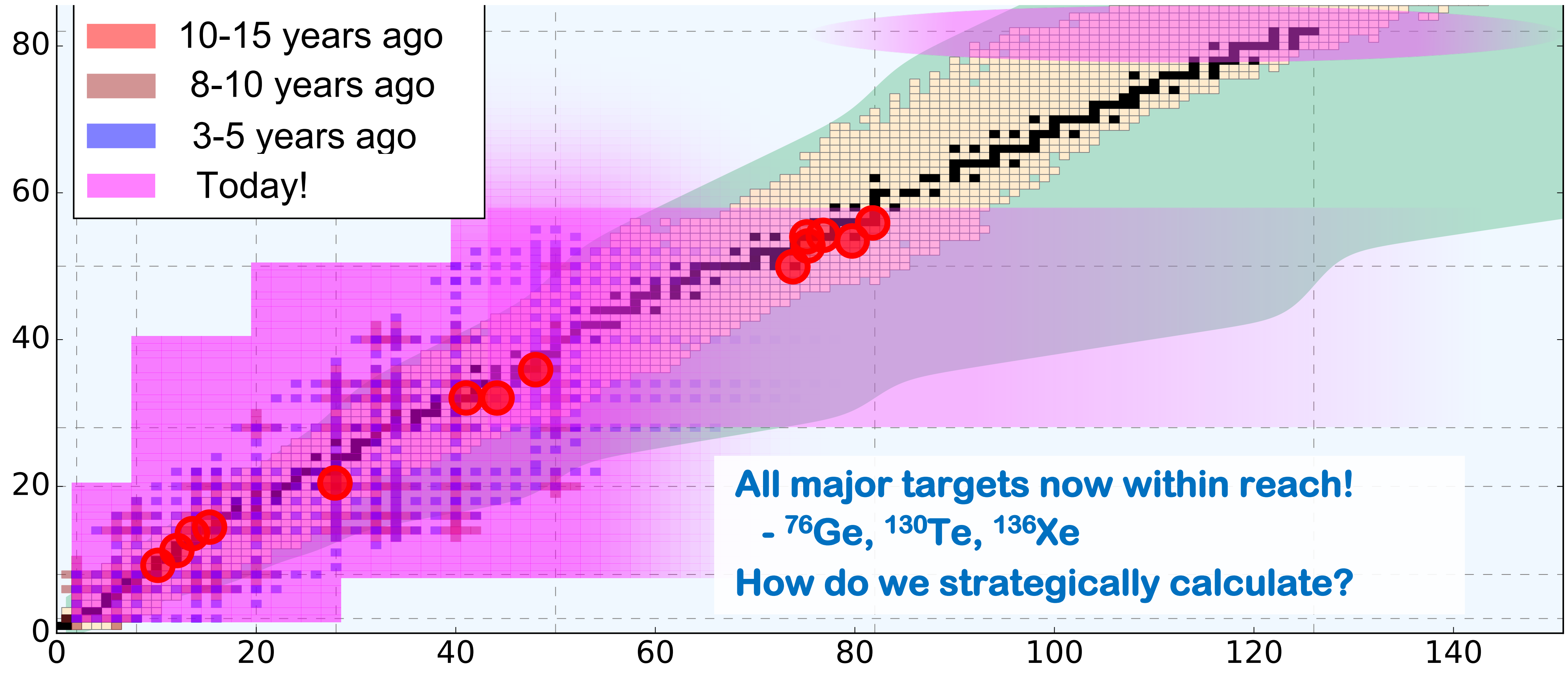


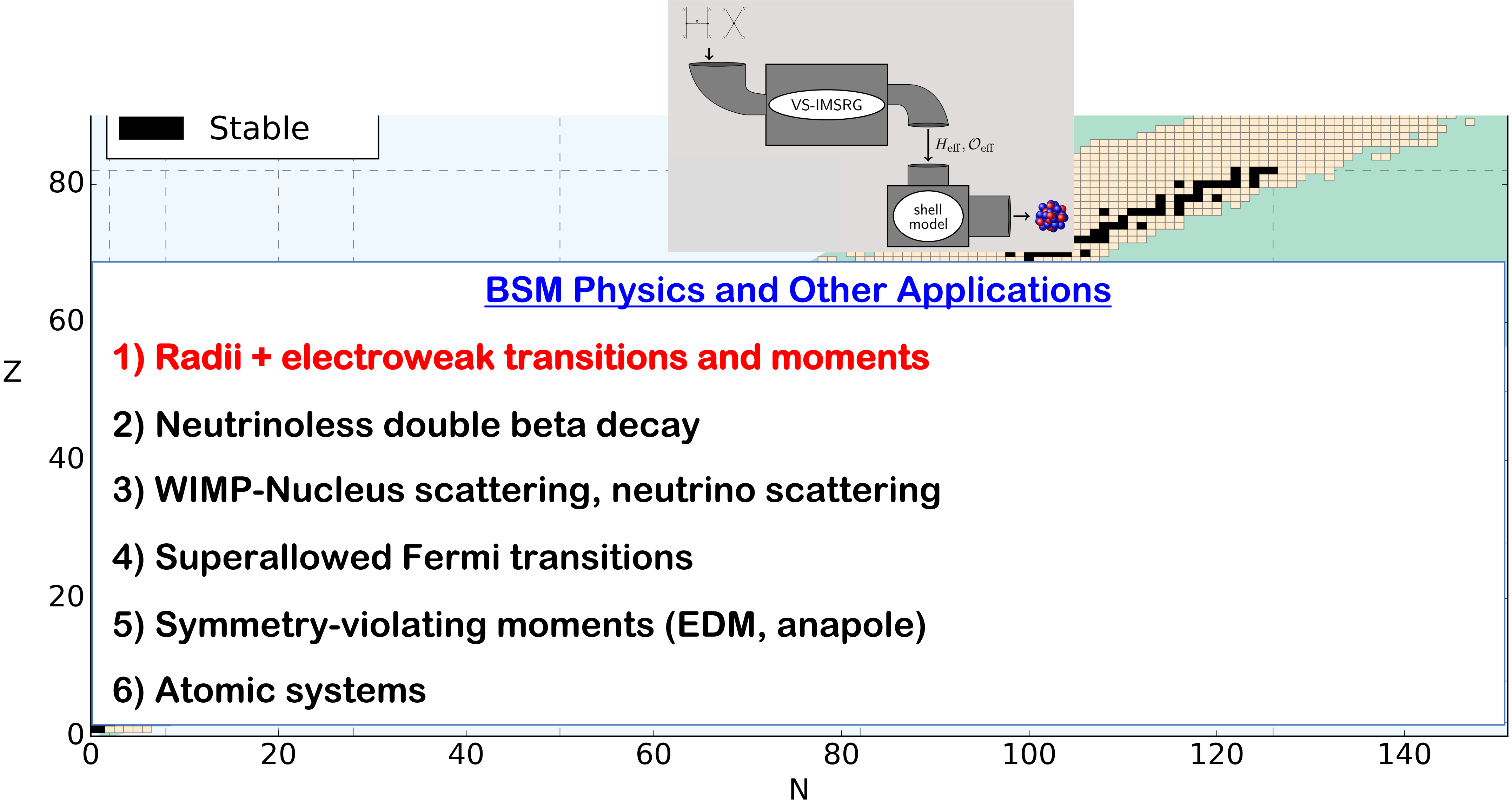
All major targets now within reach!

- ^{76}Ge, ^{130}Te, ^{136}Xe

How do we strategically calculate?

VS-IMSRG for Atomic Nuclei

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



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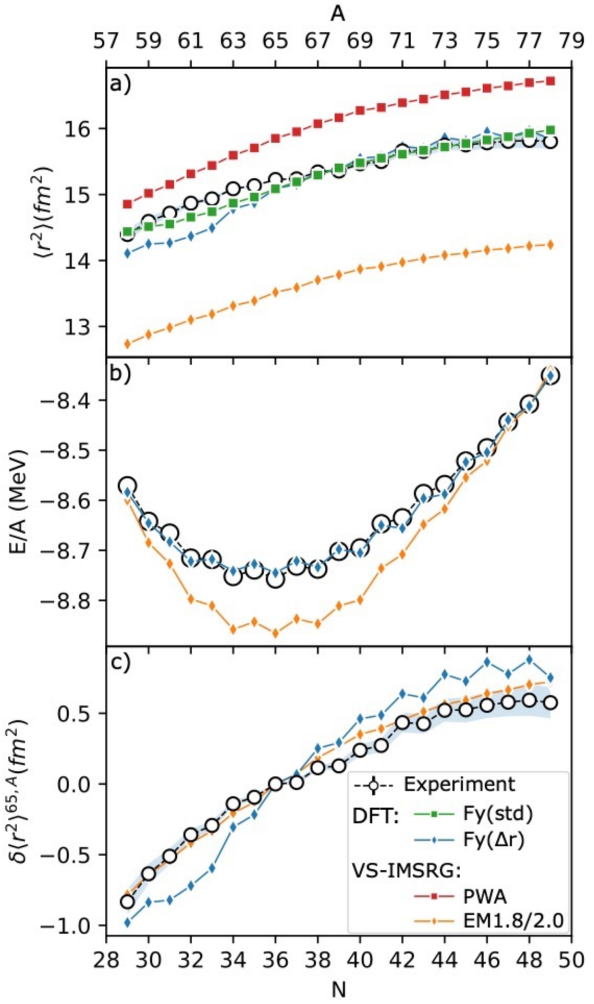
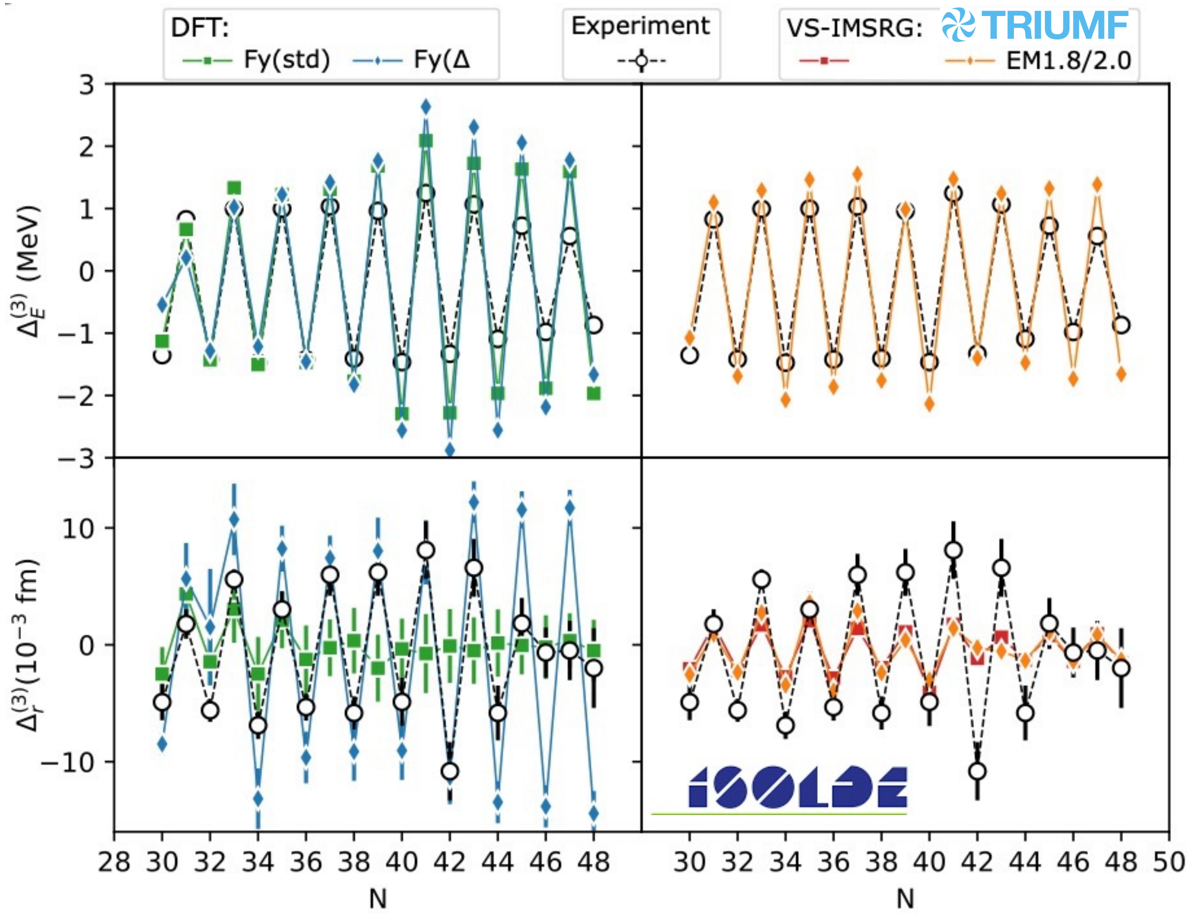
Laser Spectroscopy: Charge Radii Across Chains

Study odd-even staggering of charge radii across Cu isotopic chain





$$\langle R^2 \rangle = \left\langle \Phi_0 \mid \tilde{R}^2 \mid \Phi_0 \right\rangle + \left\langle \Phi_{\rm SM} \mid \tilde{R}^2 \mid \Phi_{\rm SM} \right\rangle$$

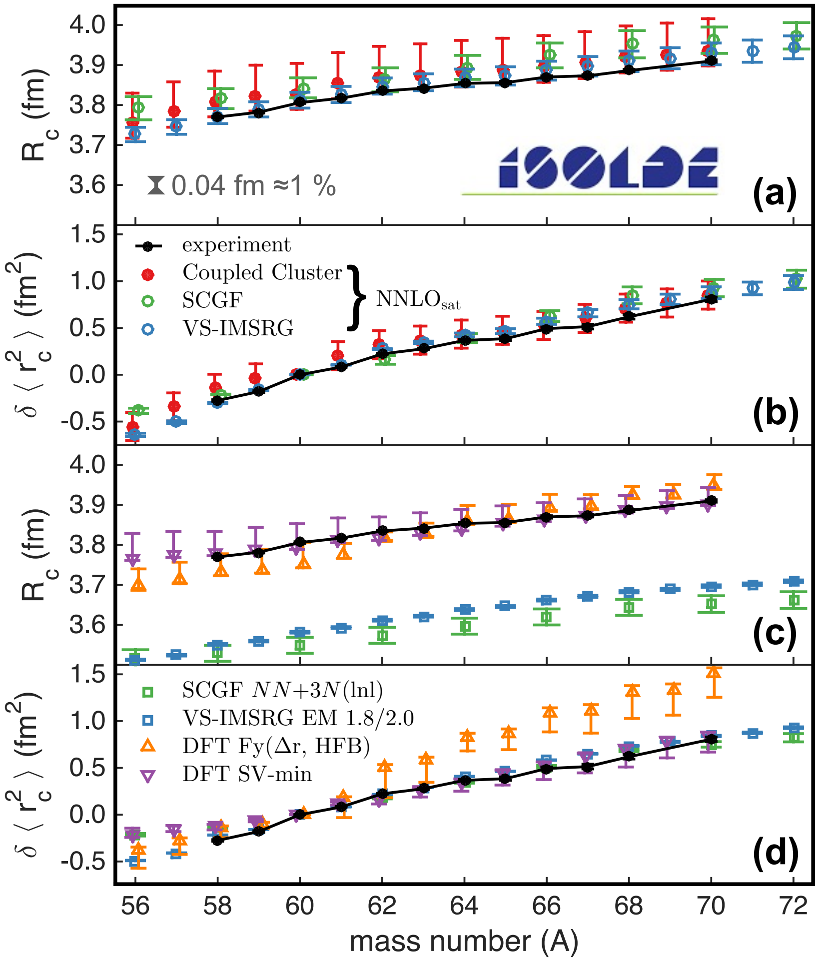
de Groote et al., Nature Phys. (2020)

Cu isotopes, odd-even staggering well reproduced

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

Laser Spectroscopy: Charge Radii Across Chains

Study charge radii systematics across Ni isotopic chain



$$\langle R^2 \rangle = \left\langle \Phi_0 \mid \tilde{R}^2 \mid \Phi_0 \right\rangle + \left\langle \Phi_{SM} \mid \tilde{R}^2 \mid \Phi_{SM} \right\rangle$$

Malbrunot-Ettenauer et al., submitted

Multiple ab-initio methods generally agree within uncertainties

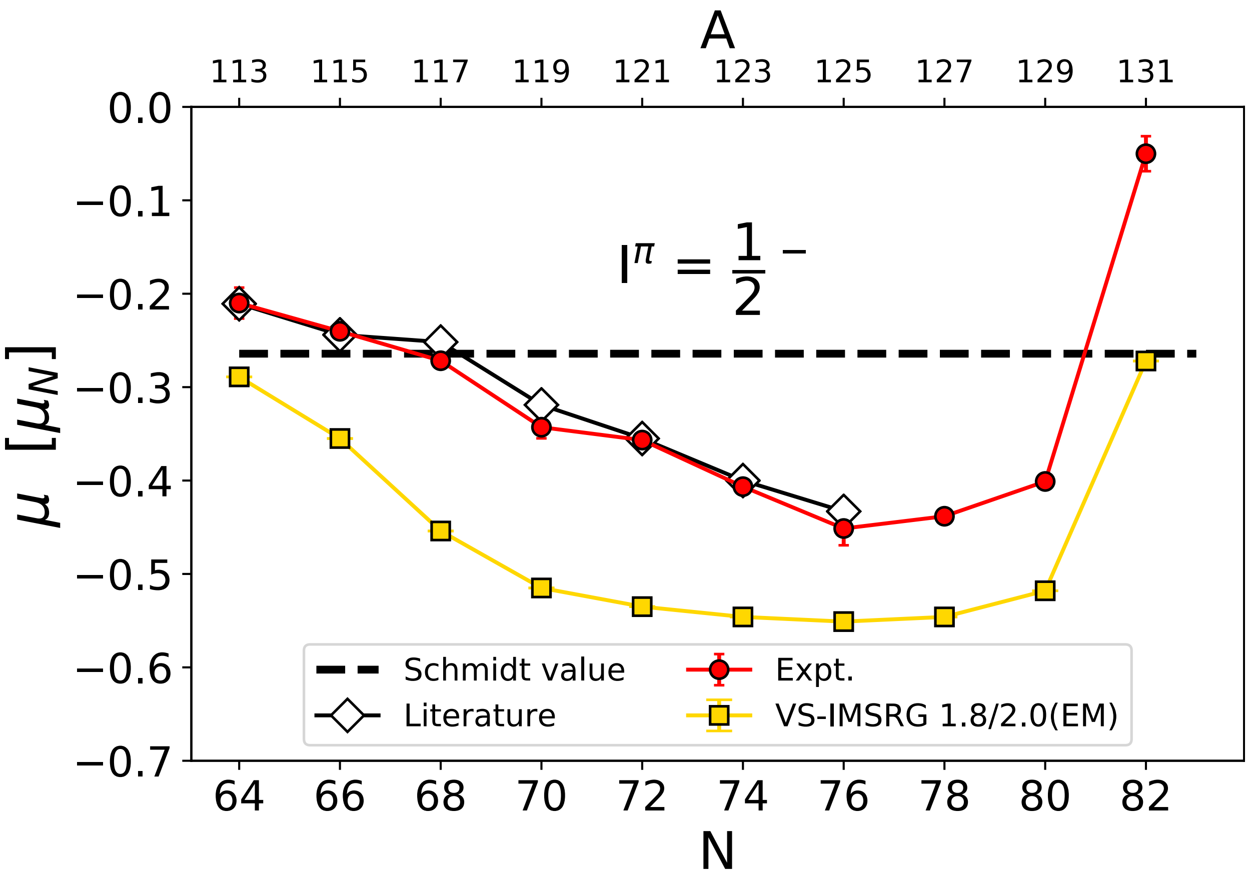
Ab initio (again) competitive with DFT

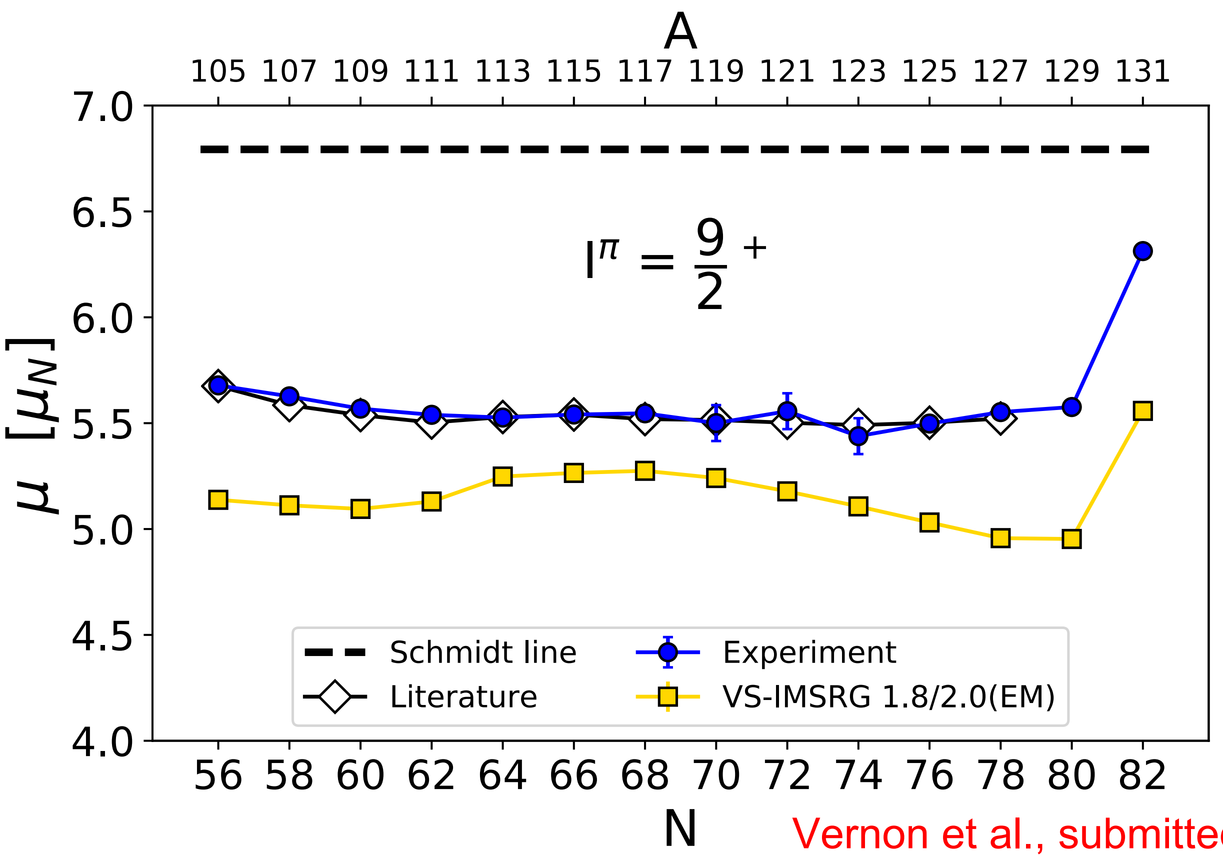
EM Moments in Heavy Nuclei: In

Improvements in storage of 3N matrix elements greatly expands reach of ab initio theory!

Calculate radii, moments of entire In chain – focus on odd-even

Reproduces trends of new measurements



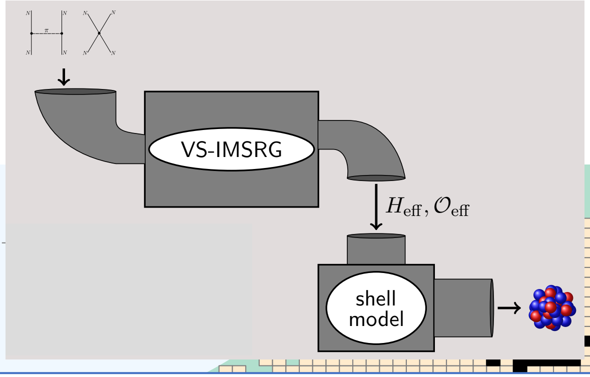


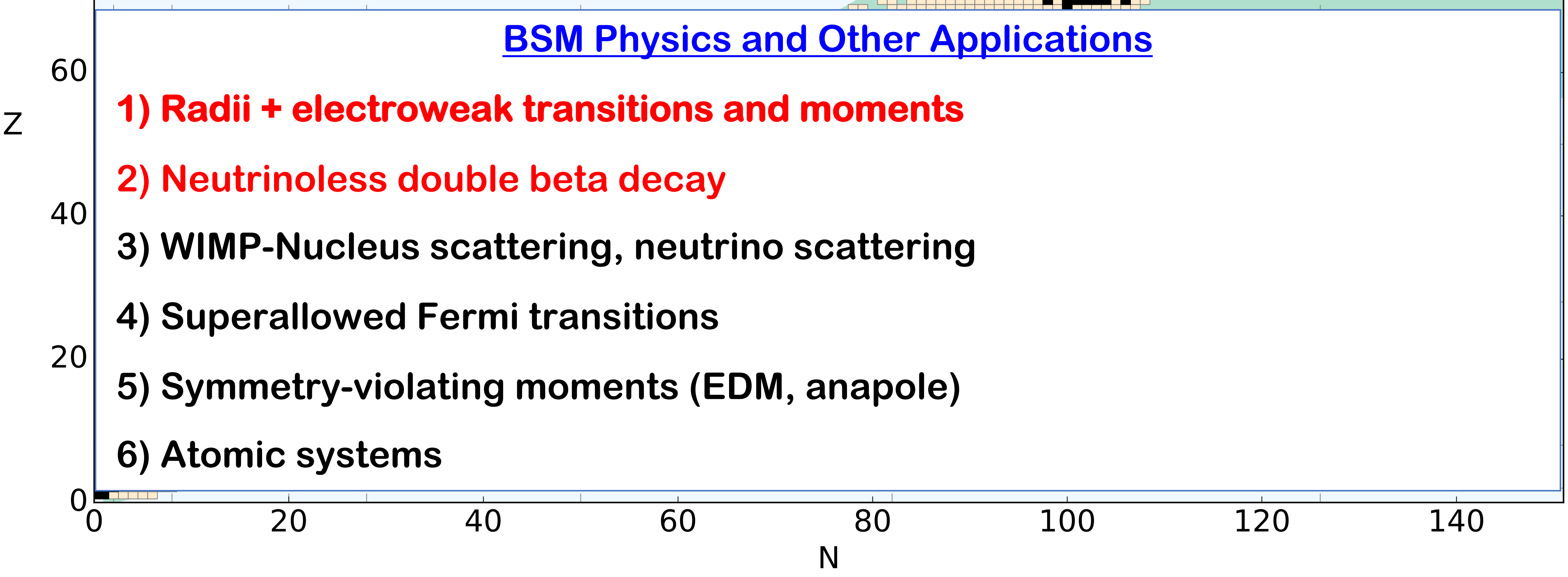
Vernon et al., submitted

Neglected physics: two-body meson-exchange currents

VS-IMSRG for Atomic Nuclei

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





BSM Physics and Other Applications

1) Radii + electroweak transitions and moments

2) Neutrinoless double beta decay

3) WIMP-Nucleus scattering, neutrino scattering

4) Superallowed Fermi transitions

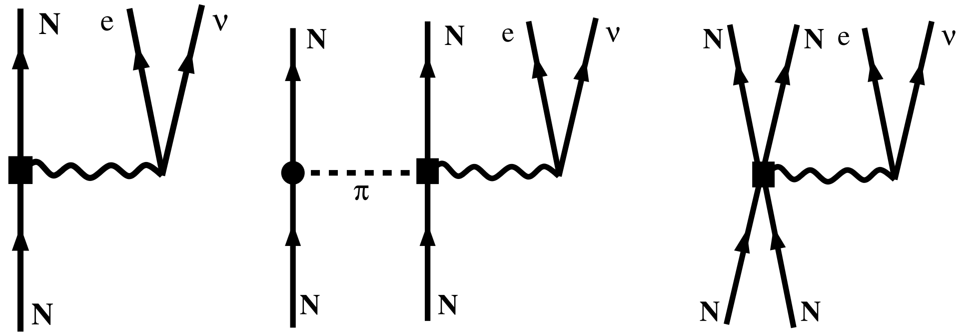
5) Symmetry-violating moments (EDM, anapole)

6) Atomic systems

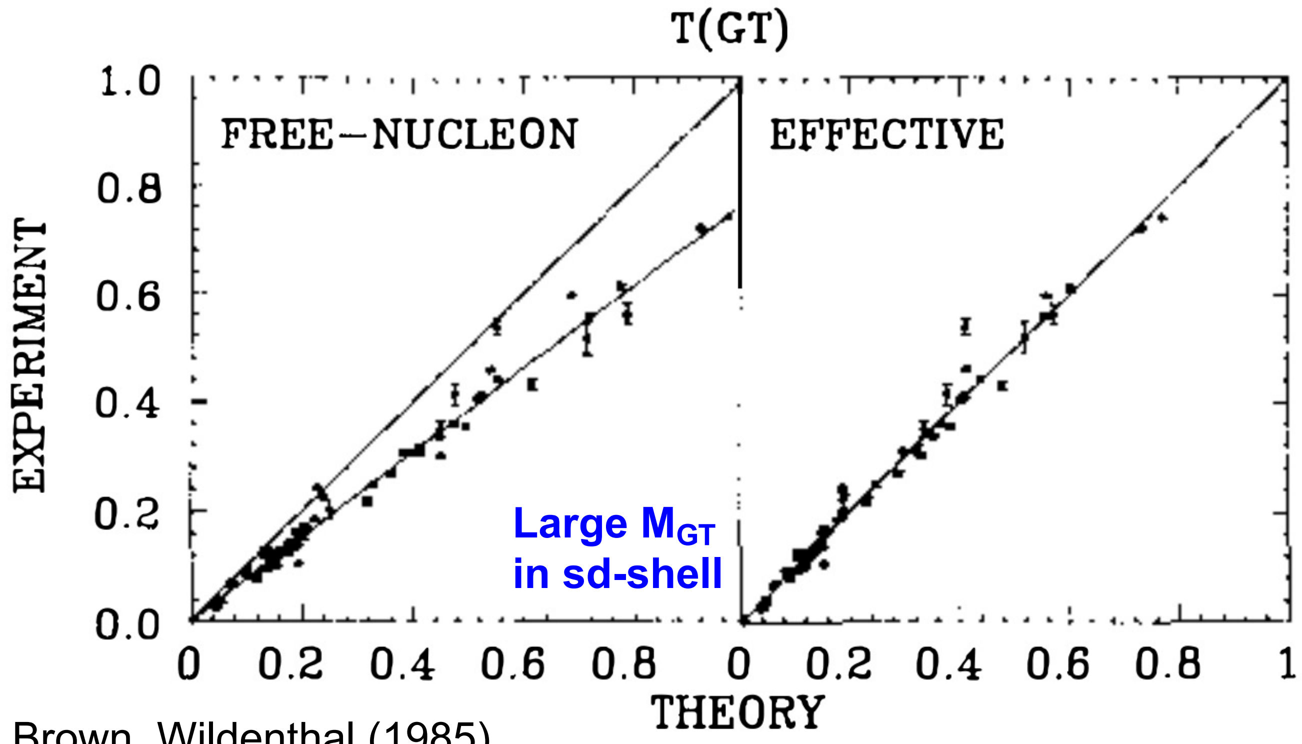
Strategy I: Study Simpler, Relevant Cases

Long-standing puzzle[1] 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)

- Should g_A be quenched in medium?
- Missing wavefunction correlations
- Renormalized VS operator?
- Neglected two-body currents?
- Model-space truncations?

Explore in ab initio framework

[1] papers from the 1970's

Large-Scale Efforts for Ab Initio GT Transitions

Calculate **large GT matrix elements**

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

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

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

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

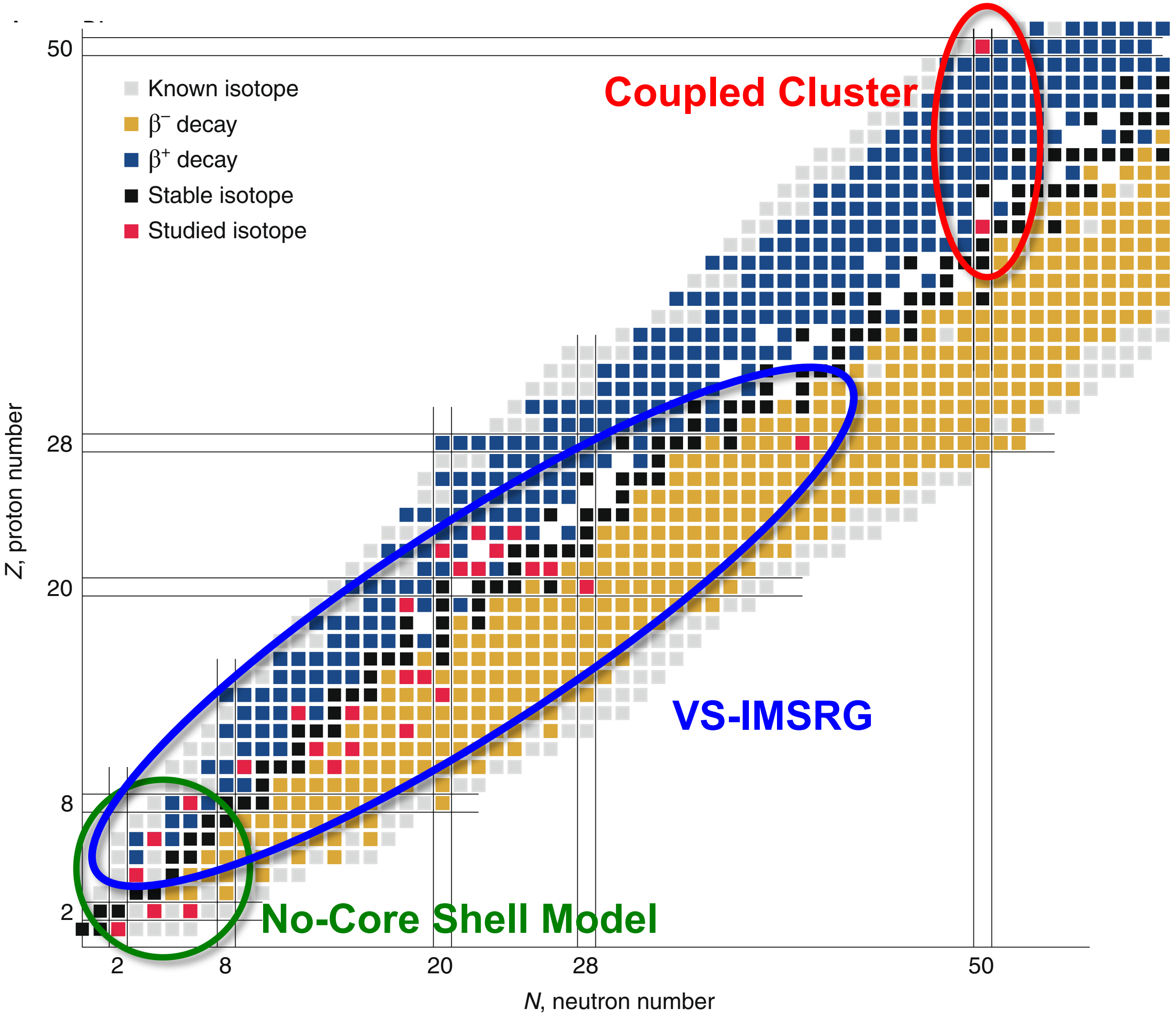
Discrepancy between experimental and theoretical β-decay rates resolved from first principles

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]

NUCLEAR PHYSICS

Beta decay gets the ab initio treatment

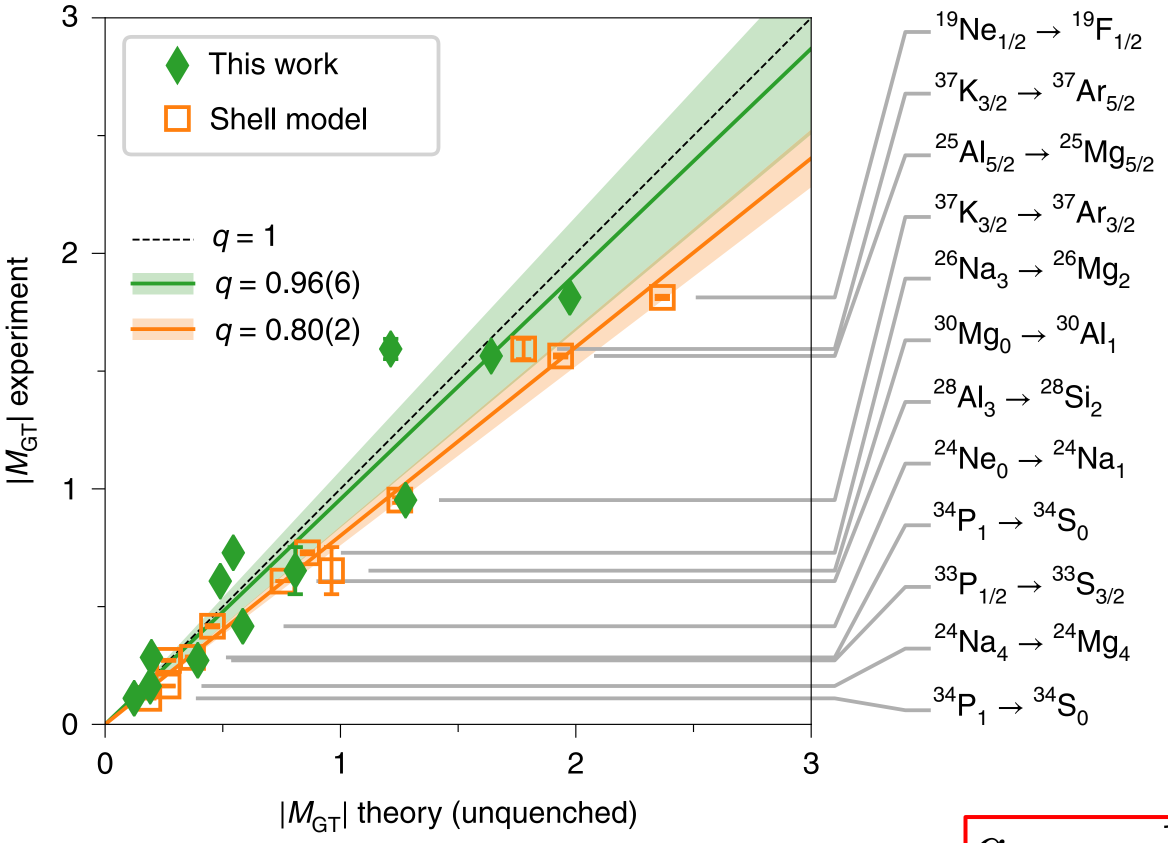
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.

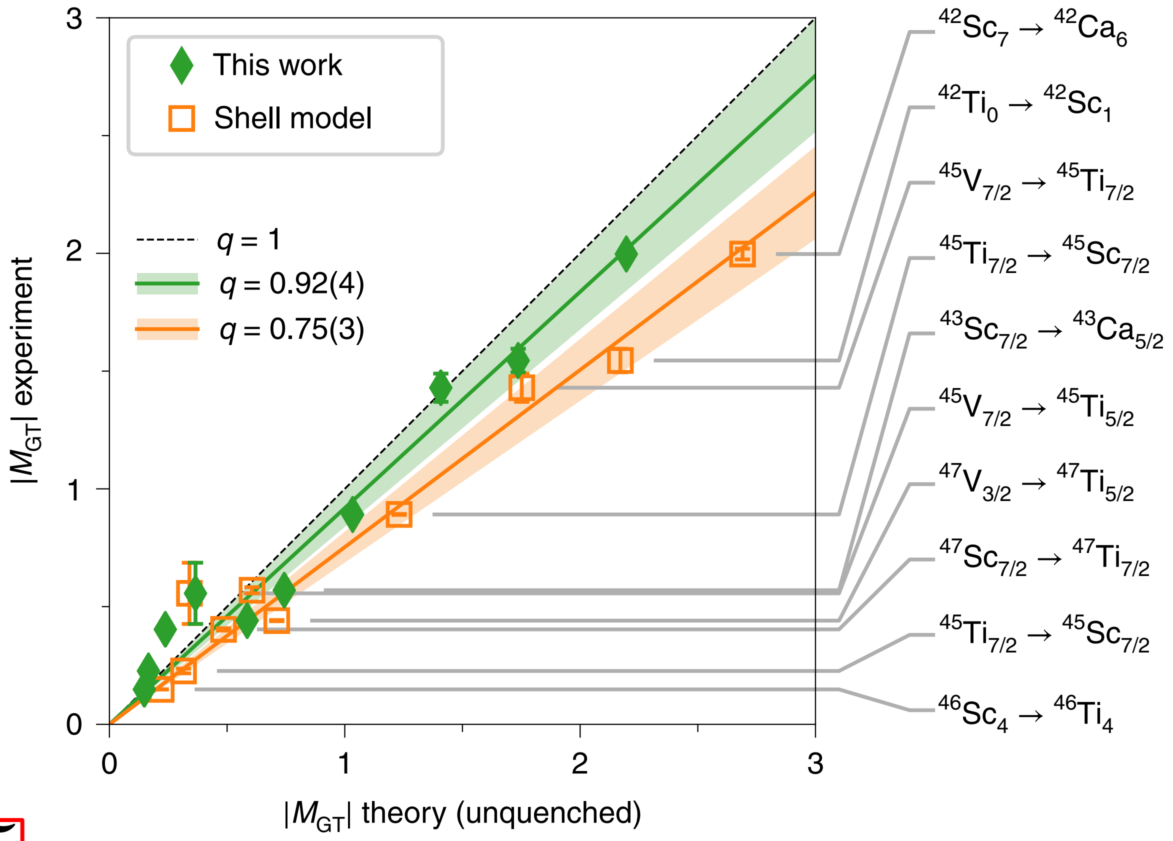


Solution to g_A-Quenching Problem

Comparison to standard phenomenological shell model

Ab initio calculations across the chart explain data with unquenched g_A





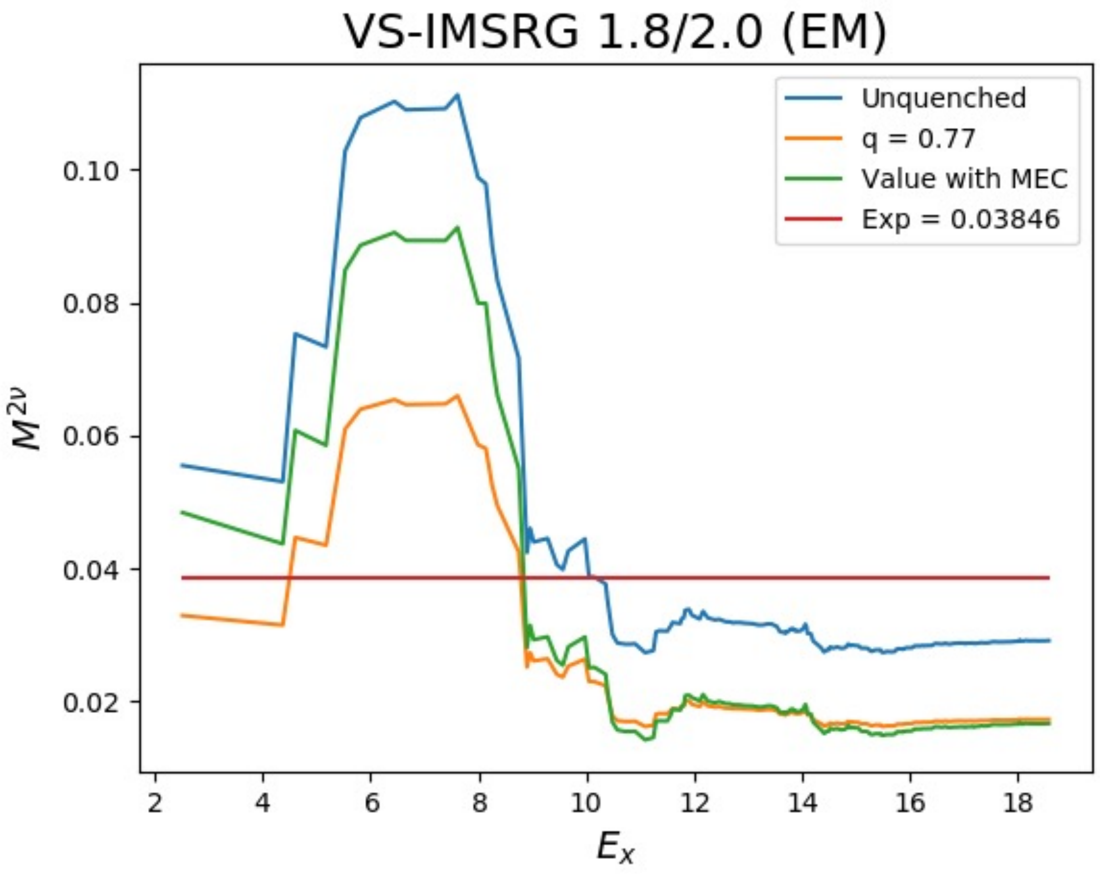
$$\boxed{g_A = 1.25}$$

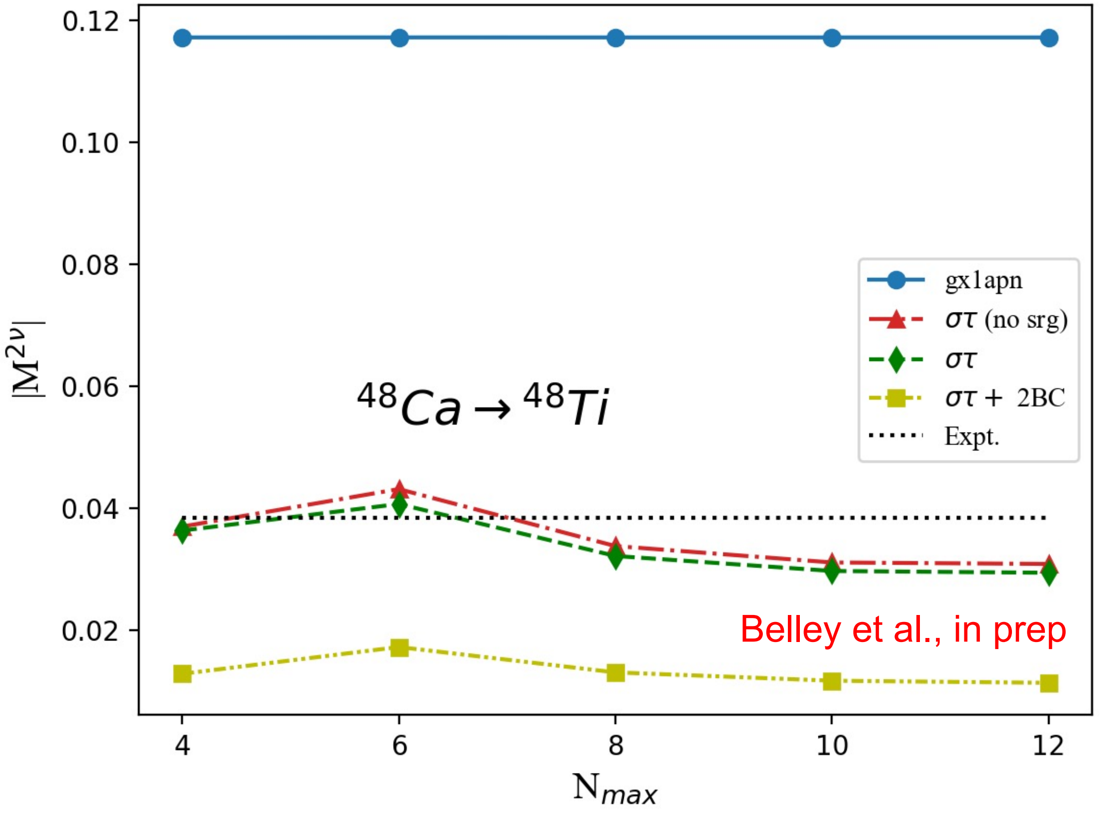
Gysbers et al., Nature Phys. (2019)

Refine results with improvements in forces and many-body methods

Ab Initio $2\nu\beta\beta$ Decay: ^{48}Ca

Consistent many-body wfs/operators from chiral NN+3N forces (**with 2b currents**)



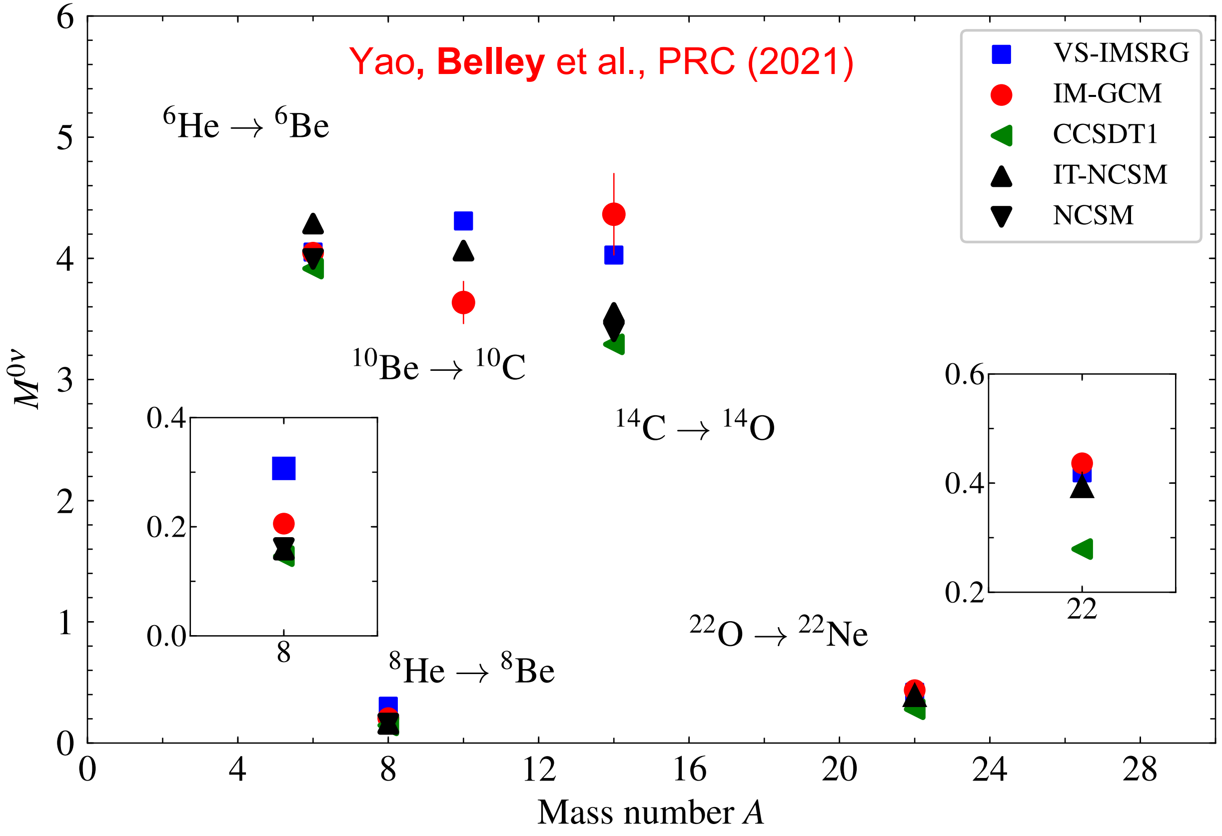


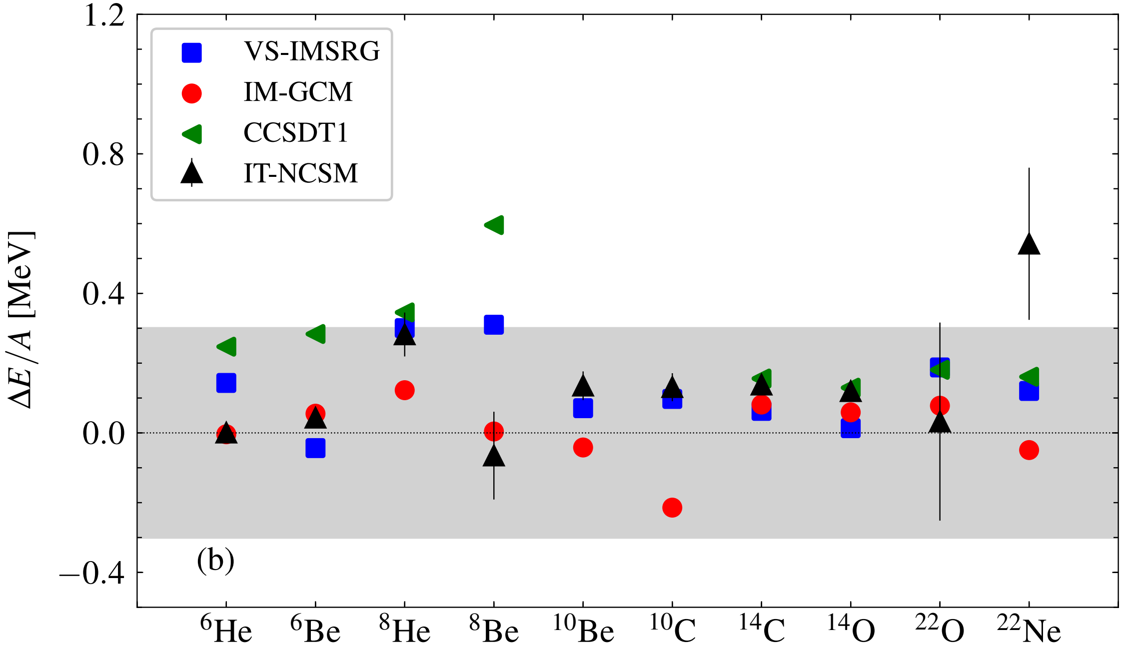
VS-IMSRG: decrease in final matrix element

Potential issues: limited 1^+ states, missing IMSRG(3)... Benchmarks with CC underway

Strategy II: Benchmark NMEs in Light Nuclei

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





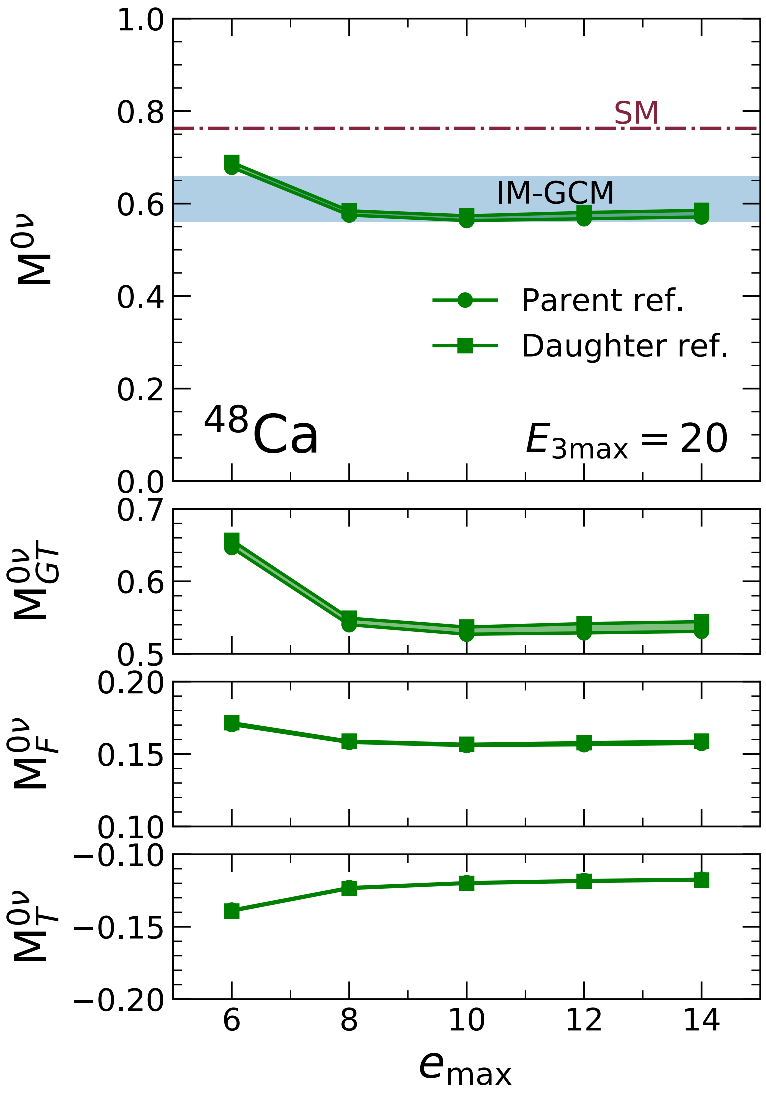
Reasonable to good agreement in all cases!

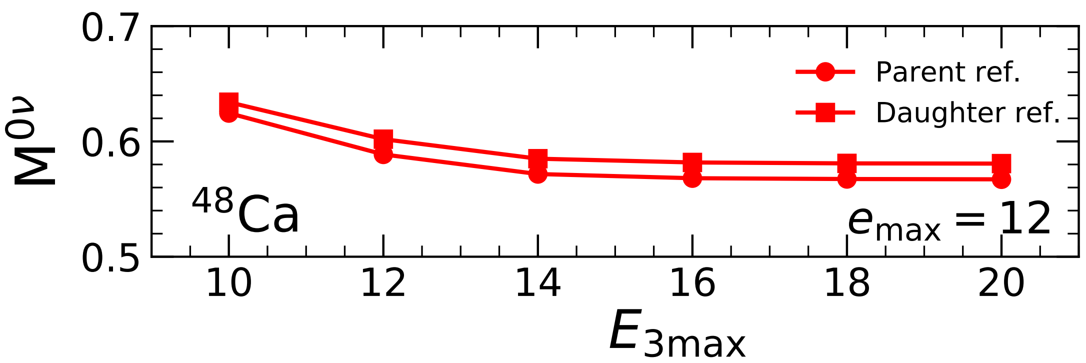
Pursue true double-beta decay nuclei

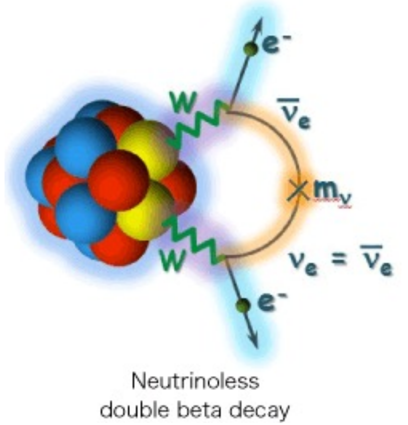
Strategy III: Final Predictions ^{48}Ca

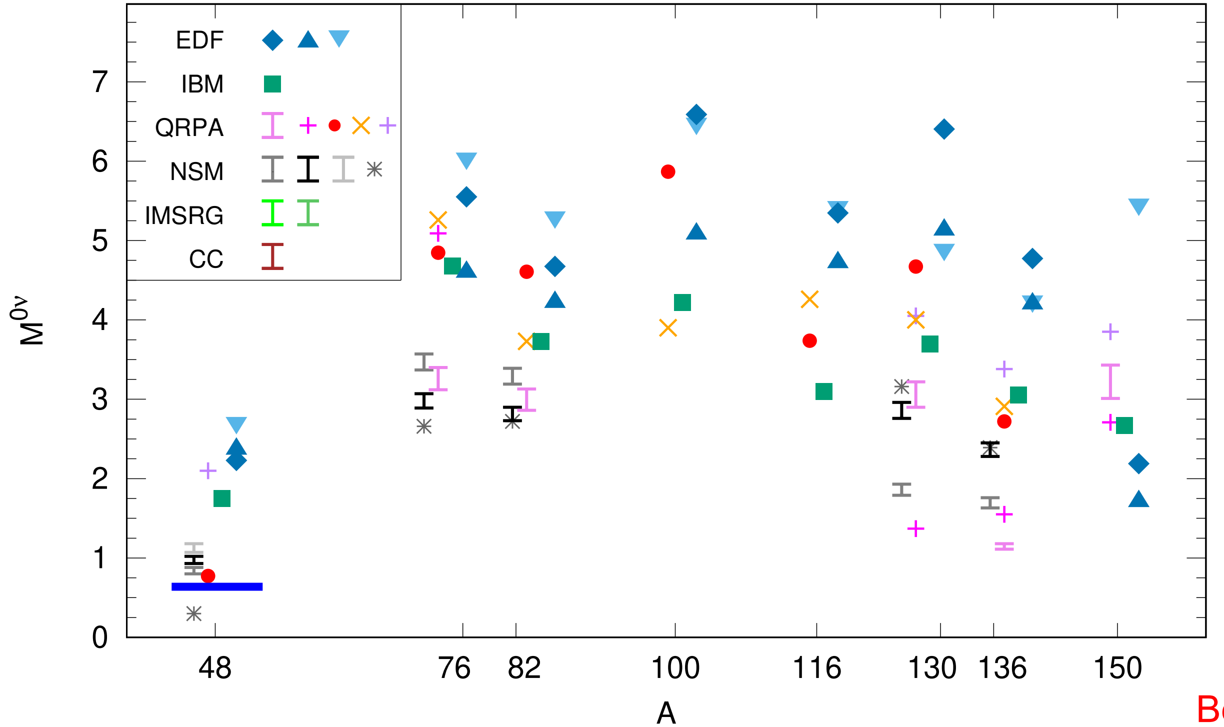
Ab initio: consistent many-body wfs/operators from chiral NN+3N forces (**no 2b currents**)

Small uncertainty from NO reference indicated; well converged in e_{max}, E_{3max}







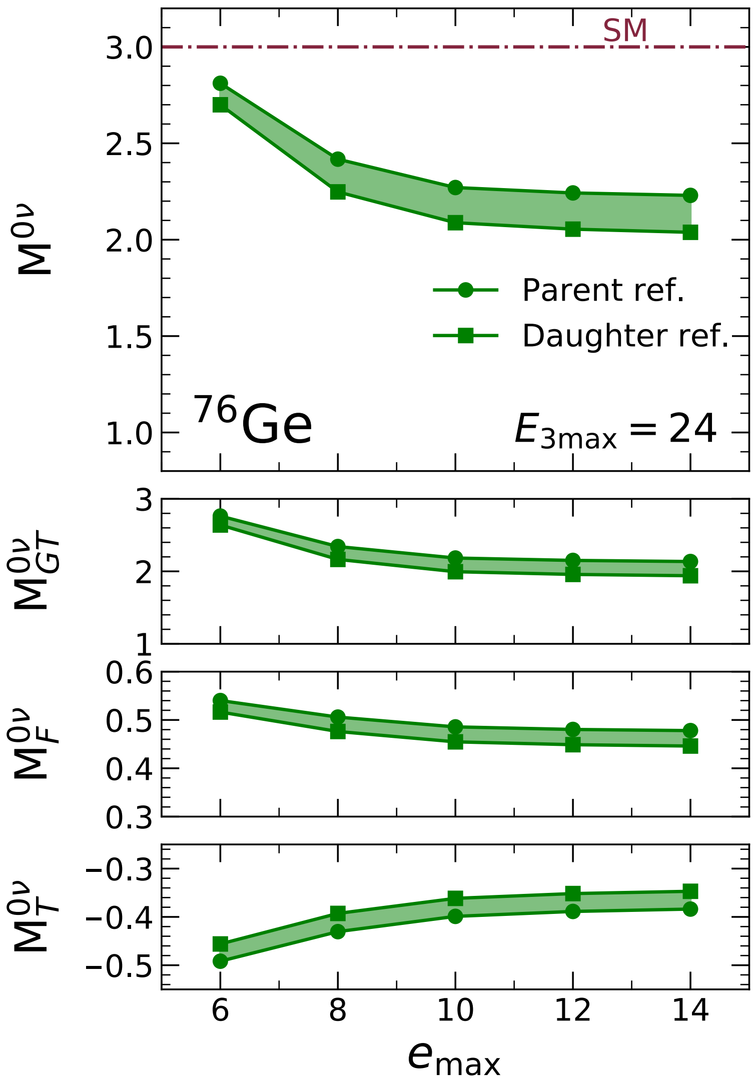


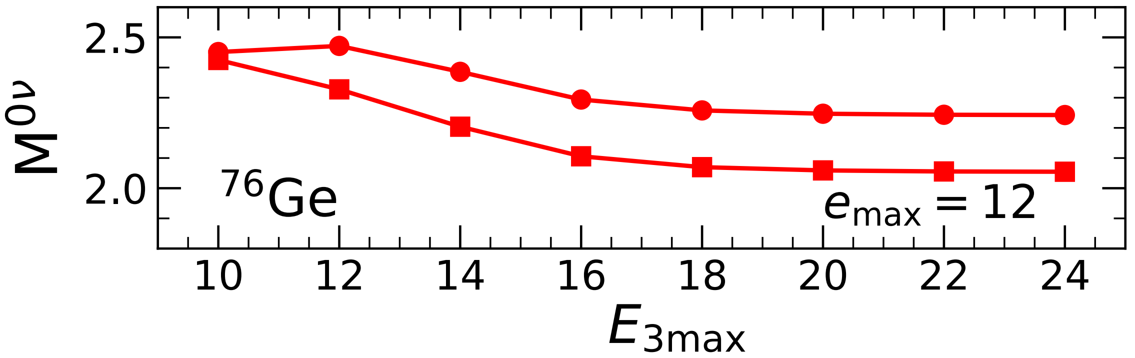
Belley et al., PRL (2021)

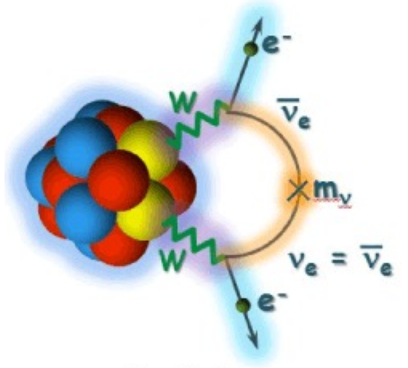
Strategy III: Final Predictions ^{76}Ge

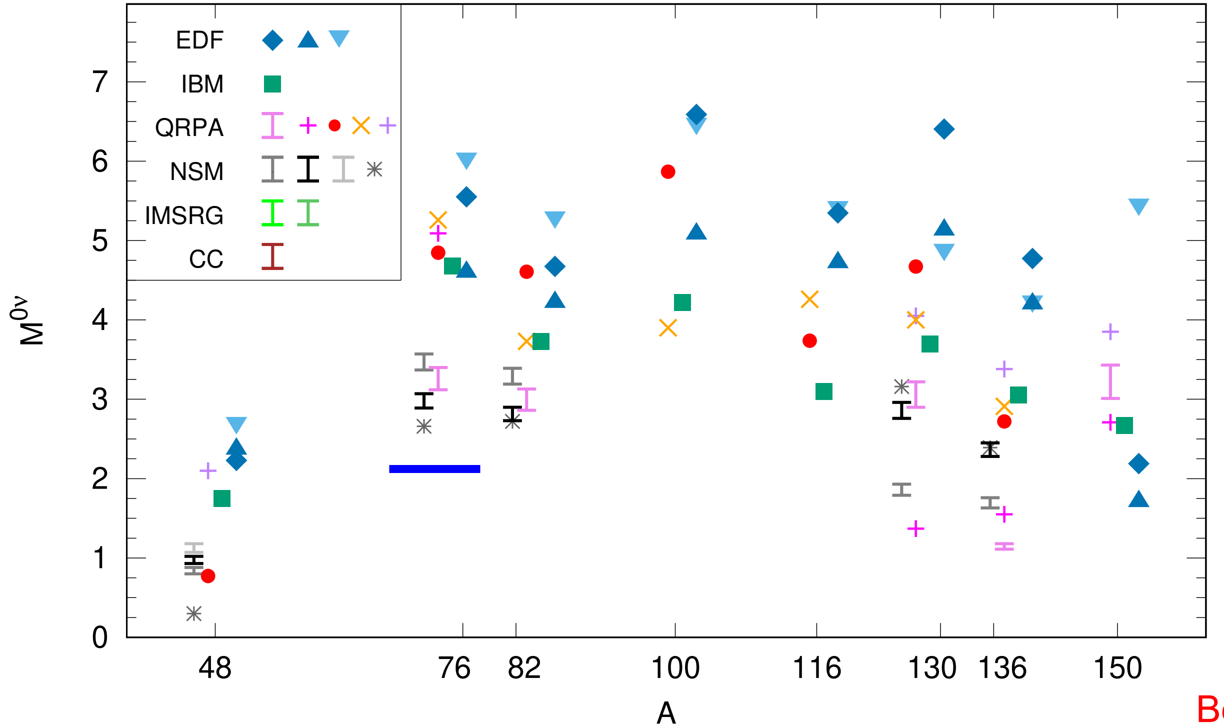
Key nucleus in worldwide searches

NME smaller than all previous calculations...







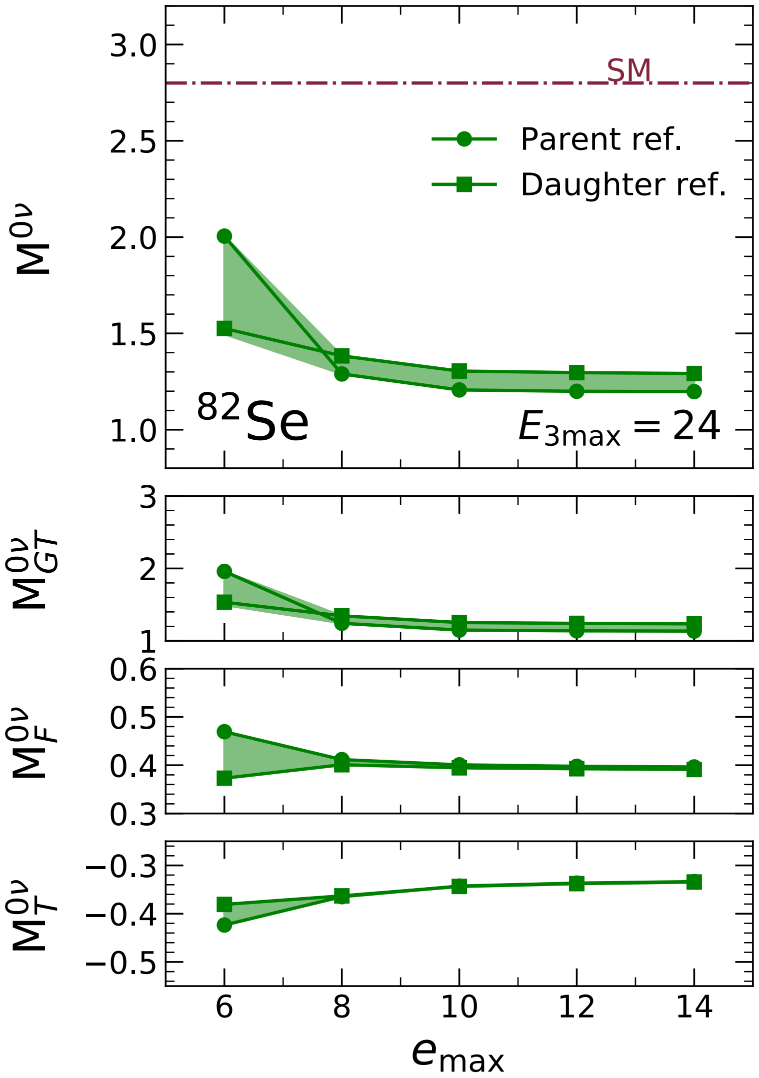


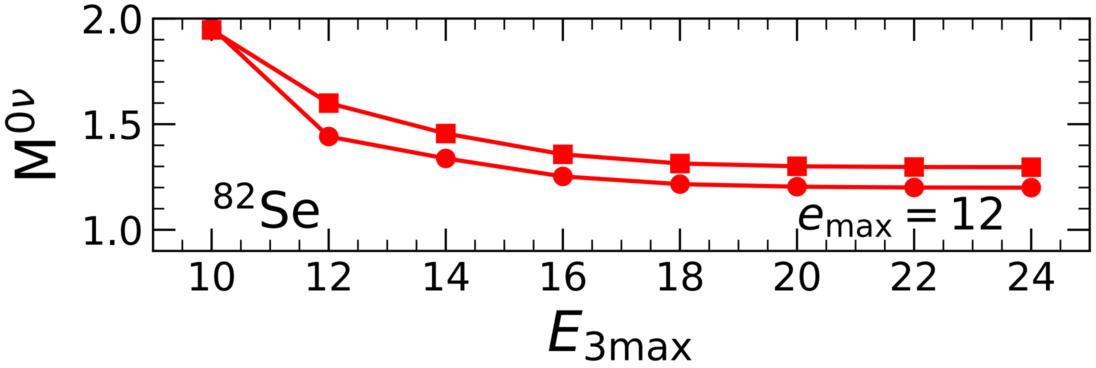
Belley et al., PRL (2021)

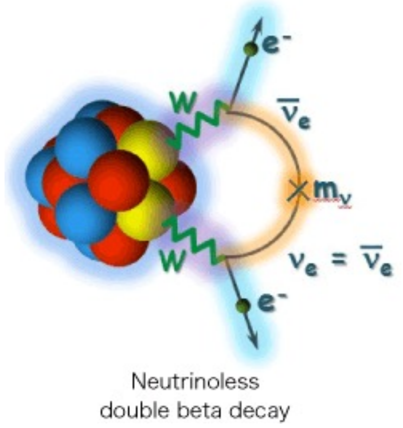
Strategy III: Final Predictions ^{82}Se

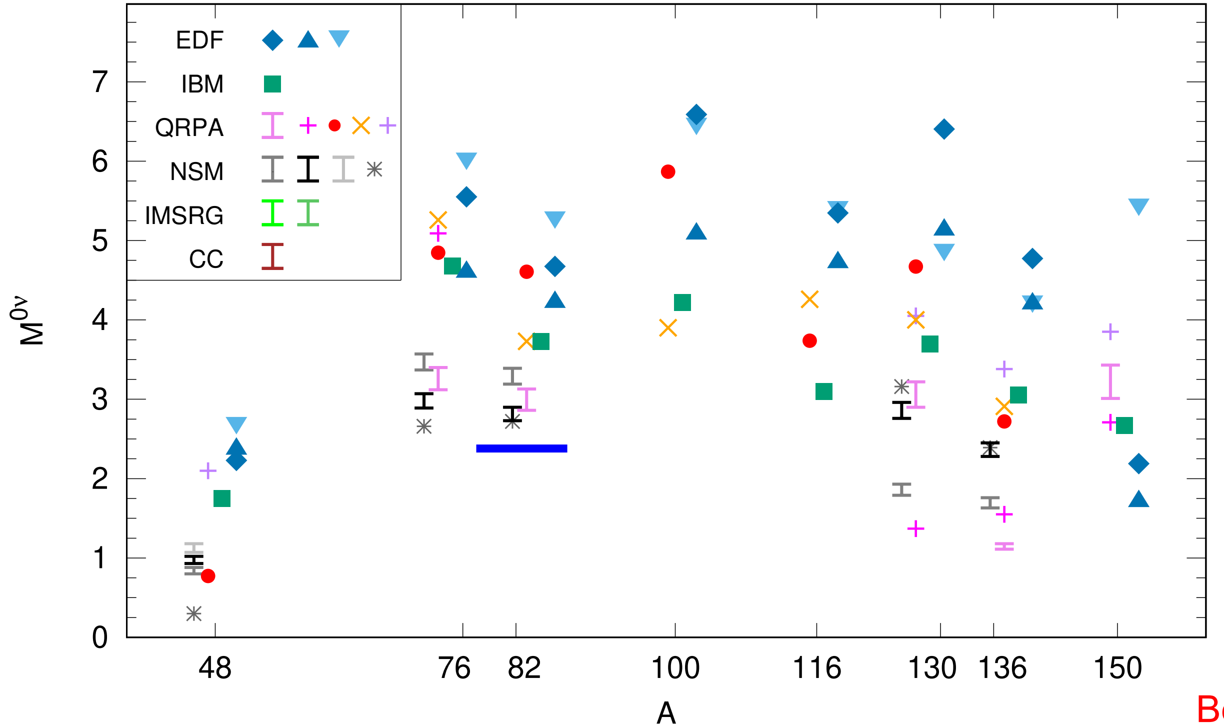
Ab initio: consistent many-body wfs/operators from chiral NN+3N forces (**no 2b currents**)

Small uncertainty from NO reference indicated; well converged in e_{max}, E_{3max}









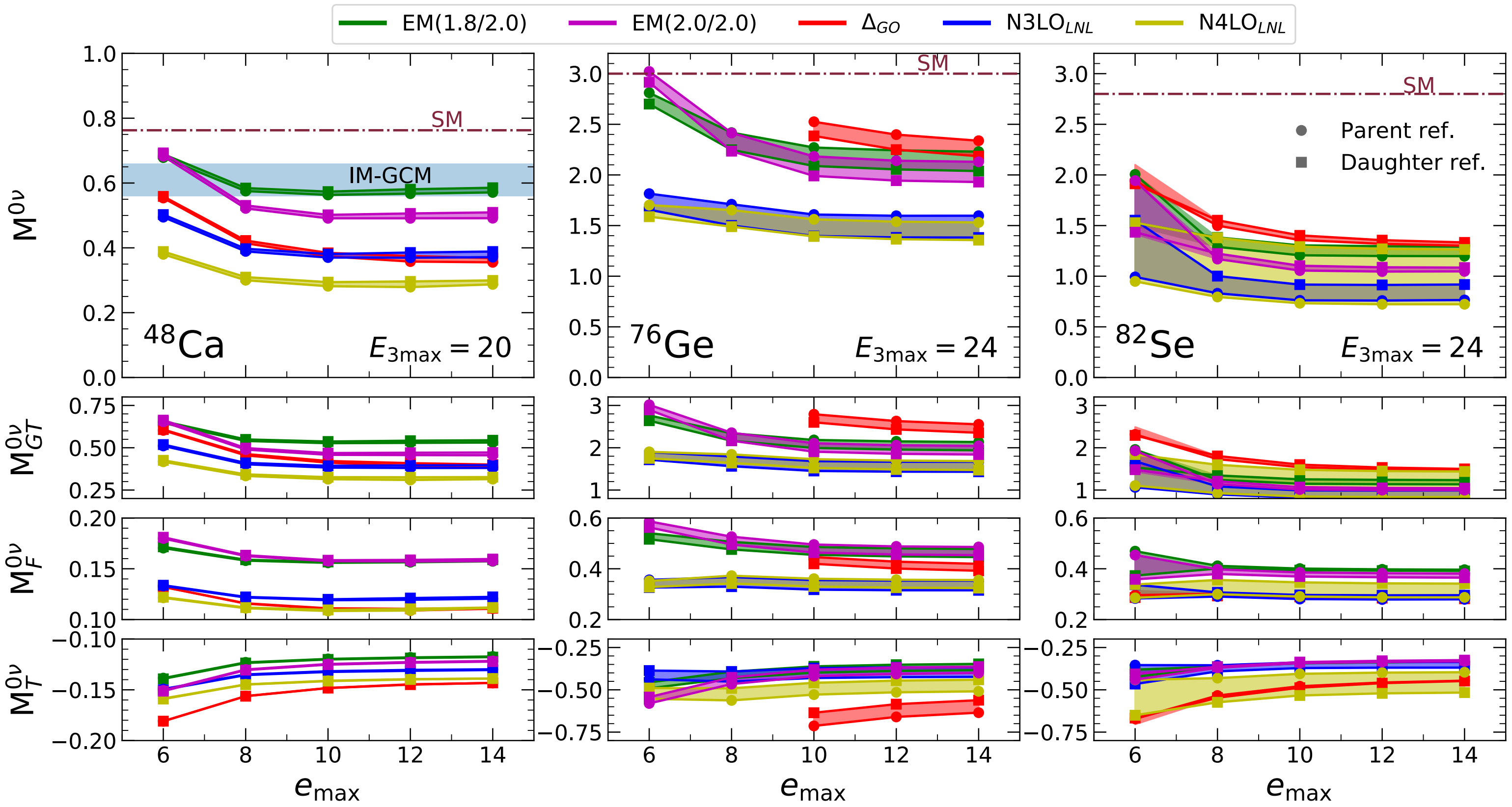
Belley et al., PRL (2021)

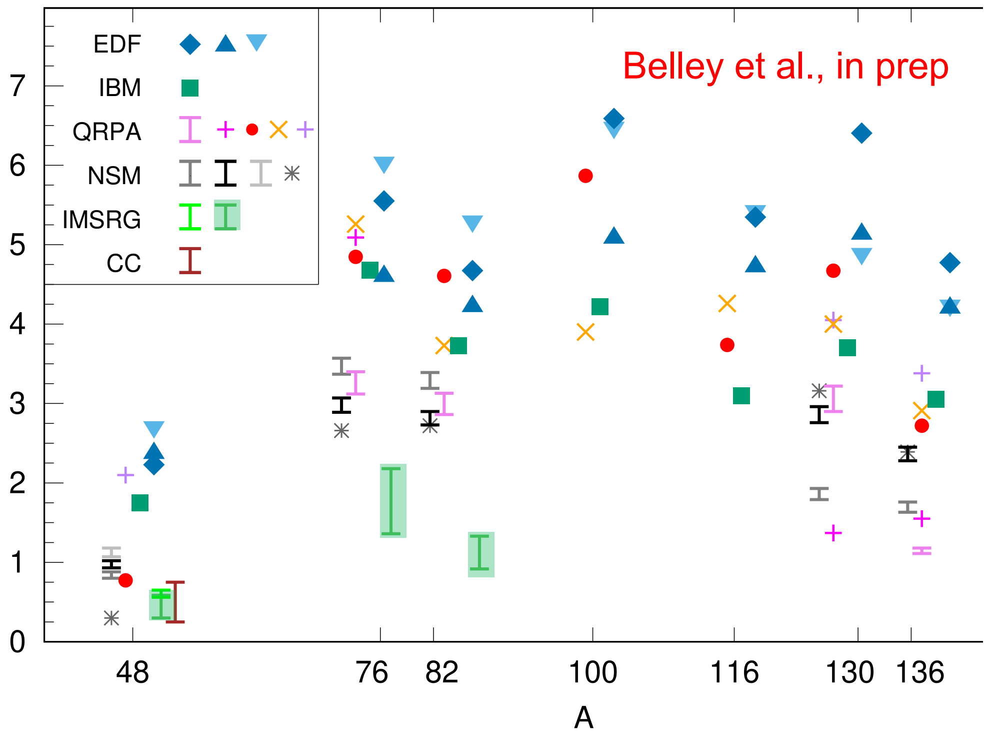
TRIUMF

Ab Initio 0νββ Decay: Multiple Interactions

Study uncertainty from input NN+3N forces with **5 chiral Hamiltonians**

Convergence in virtually all cases: globally smaller than phenomenology, much less spread





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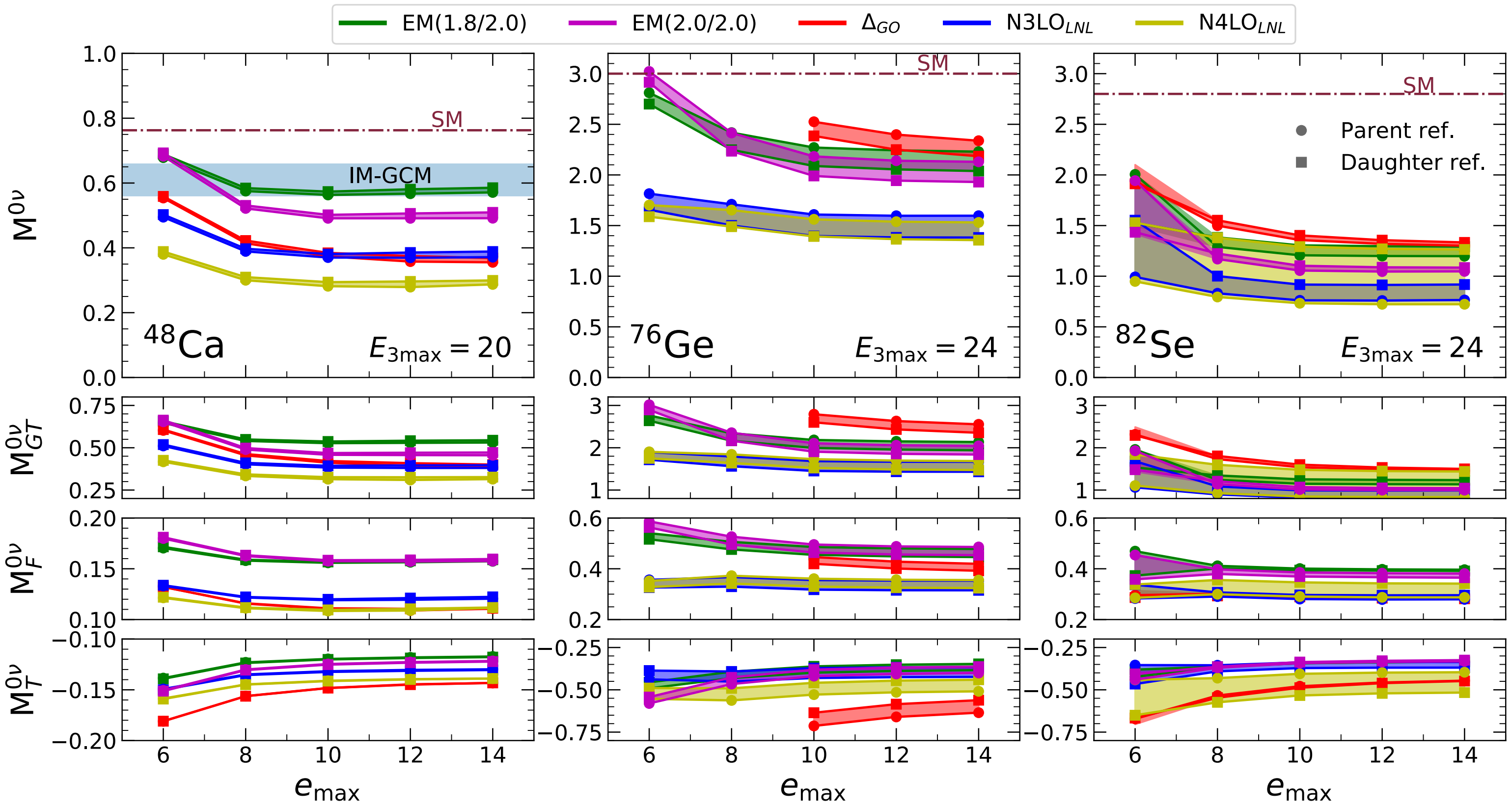
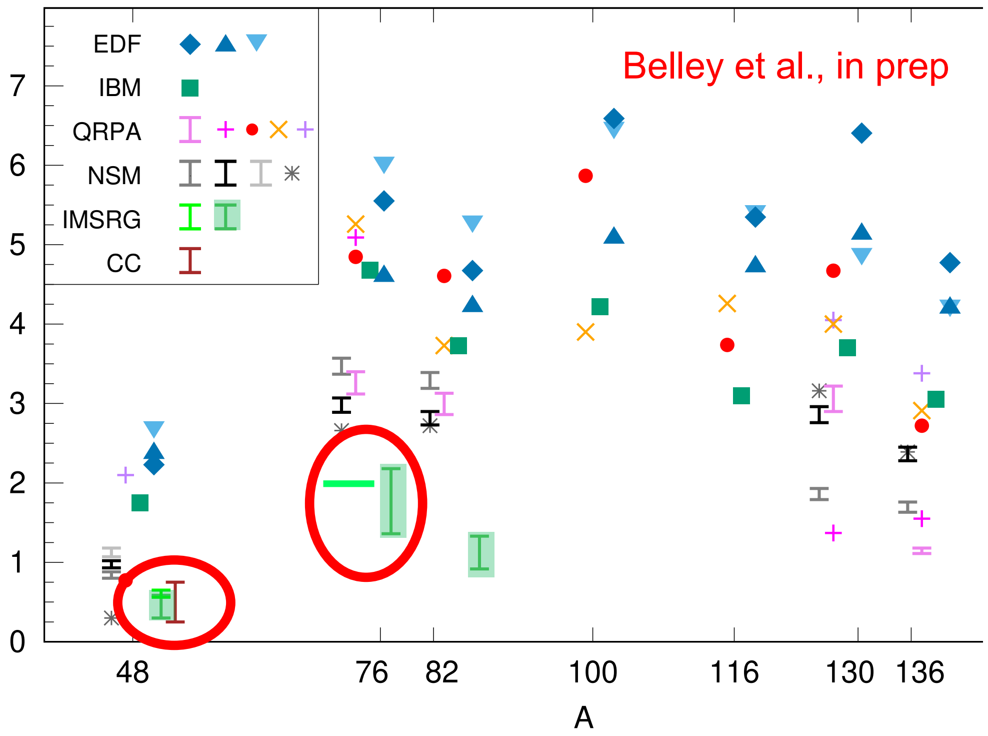
In agreement with other ab initio approaches in ^{48}Ca, ^{76}Ge (preliminary)



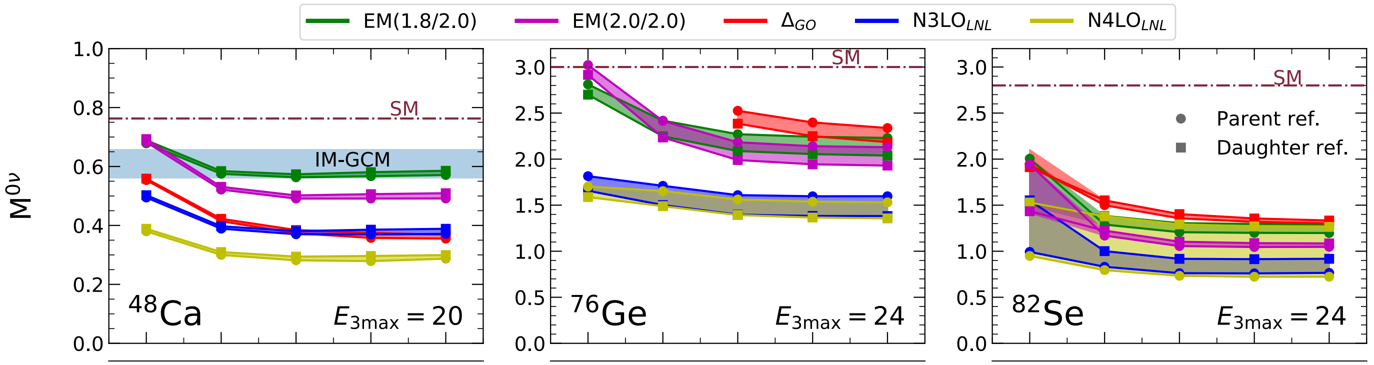


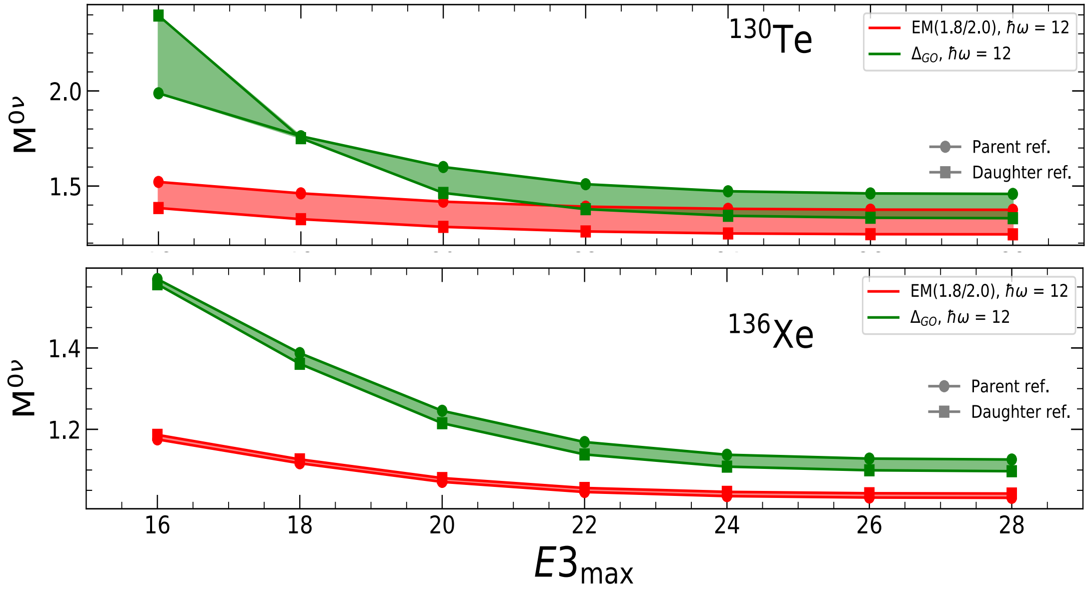
All ab initio calculations agree within uncertainties!

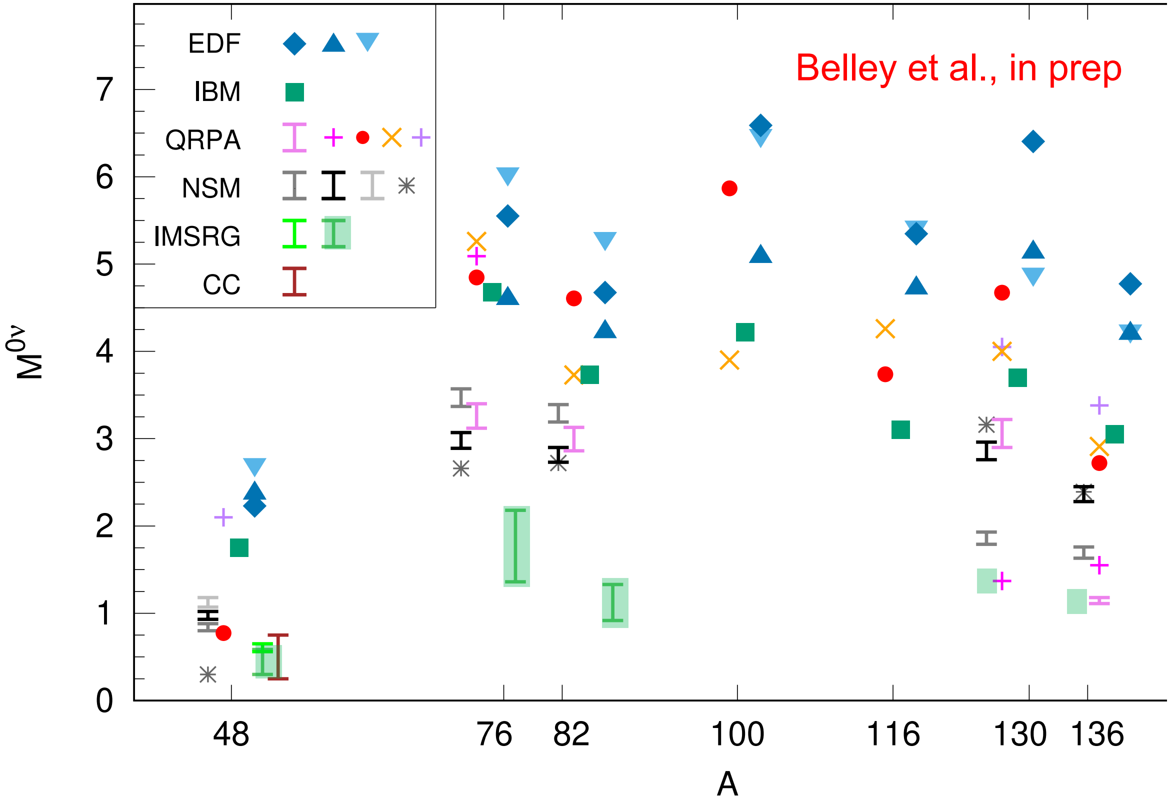
Strategy III: Final Predictions (with uncertainties!)

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

Significant differences from nuclear model/phenomenological calculations







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

TRIUMF

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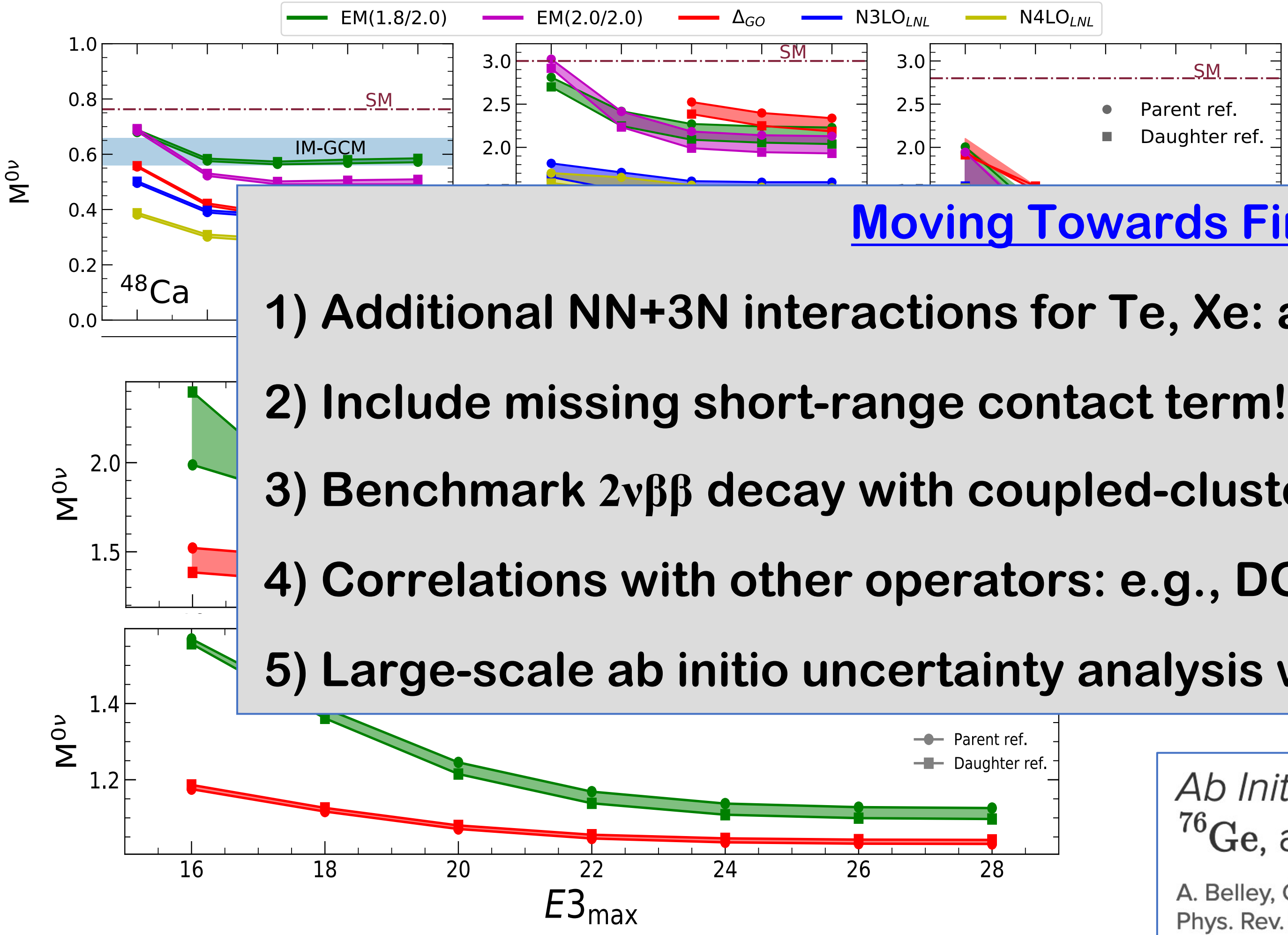

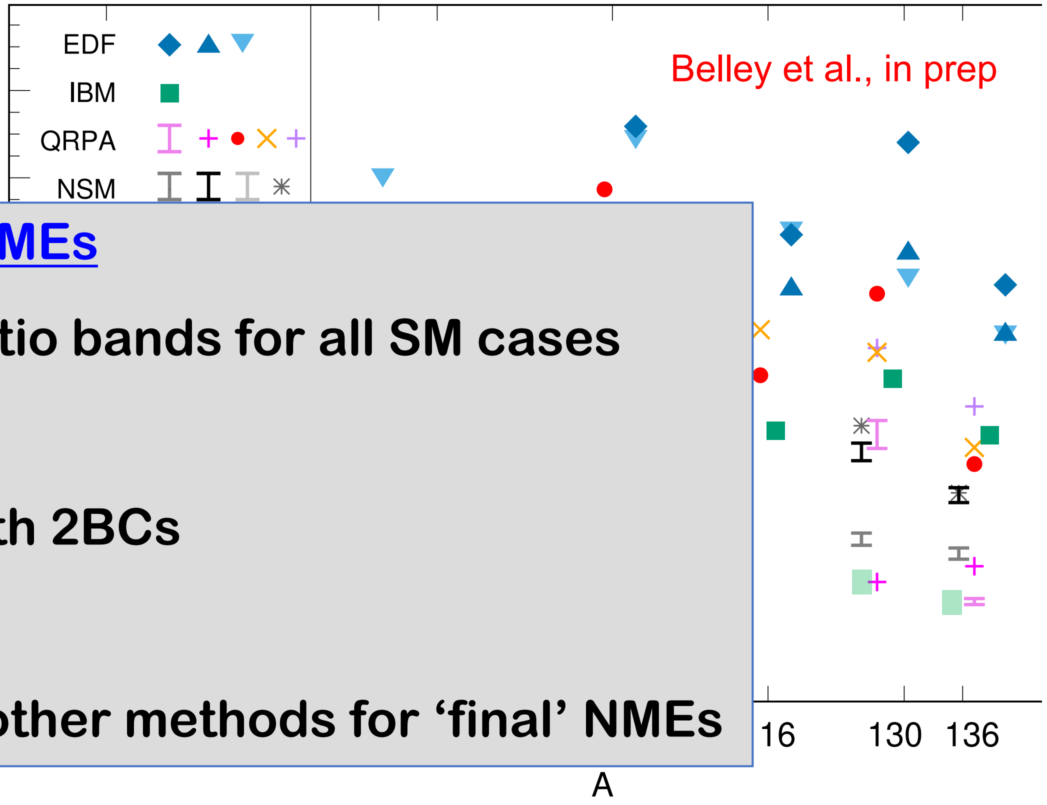

Moving Towards Final NMEs

1) Additional NN+3N interactions for Te, Xe: ab initio bands for all SM cases
2) Include missing short-range contact term!
3) Benchmark $2\nu\beta\beta$ decay with coupled-cluster with 2BCs
4) Correlations with other operators: e.g., DGT
5) Large-scale ab initio uncertainty analysis with other methods for 'final' NMEs

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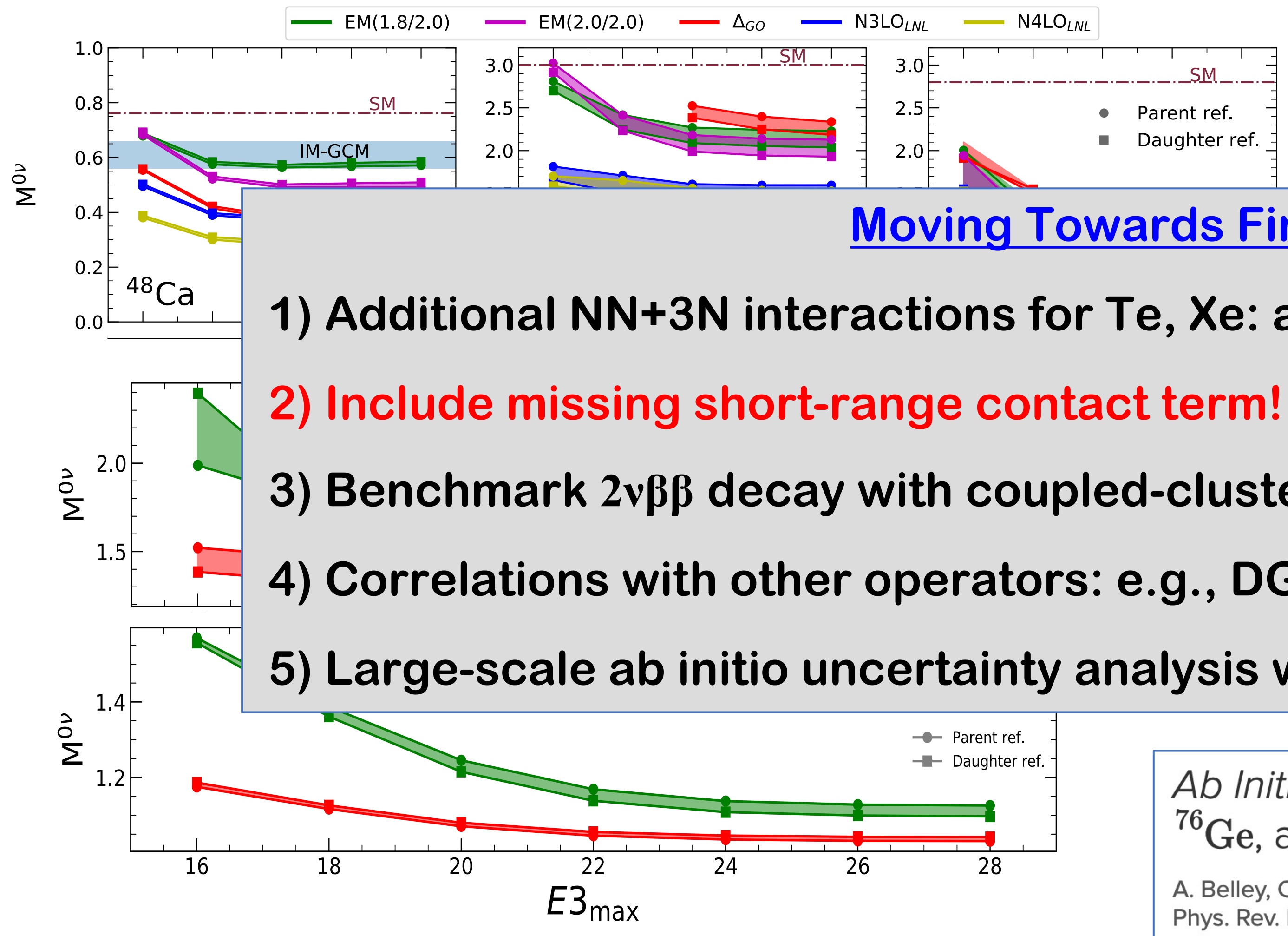

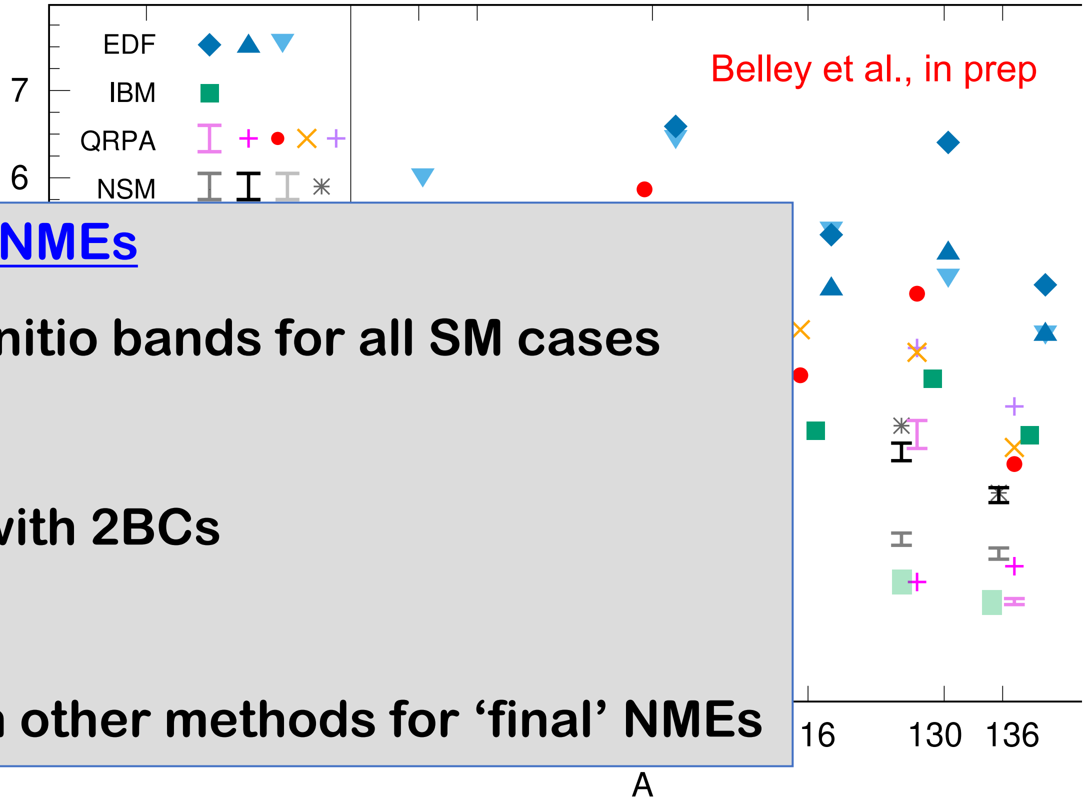

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TRIUMF

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

Proper renormalization requires short-range contact term at leading order

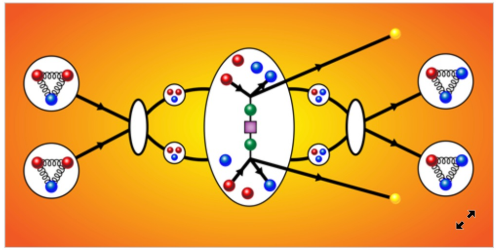
Physics Cirigliano et al. PRL (2018)

SYNOPSIS

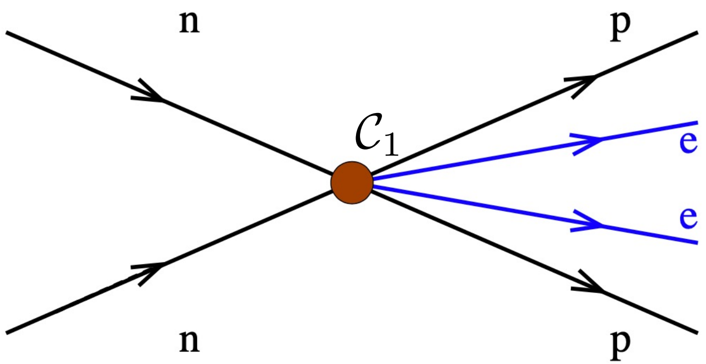
A Missing Piece in the Neutrinoless Beta-Decay Puzzle

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

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

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

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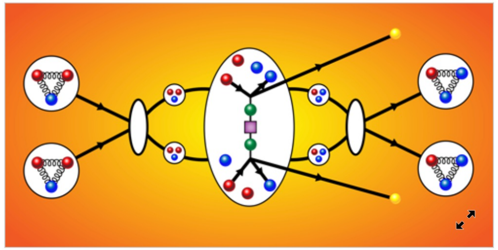

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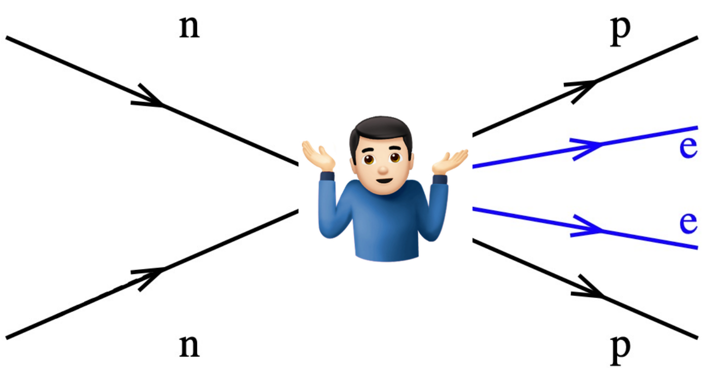

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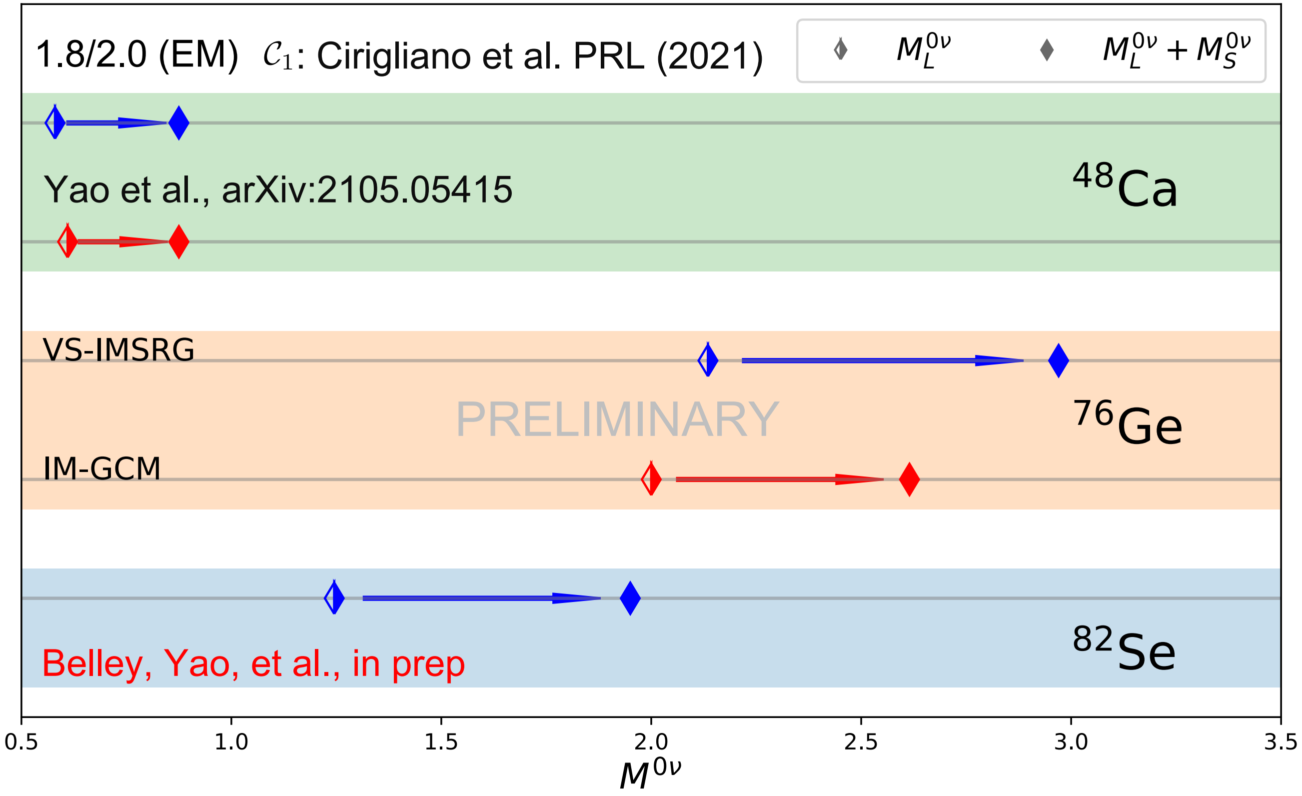
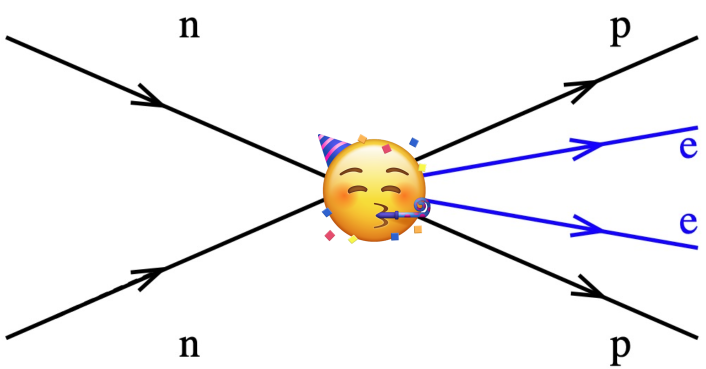
Huge problem: unclear how to fix undetermined coupling constant $\mathcal{C}_1$

The Year We Regained Hope: Coupling Constant Fit

Cirigliano et al. propose new method to estimate the size of the contact term

First ab initio calculations with short-range term from IM-GCM, VS-IMSRG





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Overall increase of 40% in ^{76}Ge to 60% in ^{82}Se!

^{130}Te, ^{136}Xe waiting in computing queue… results in days

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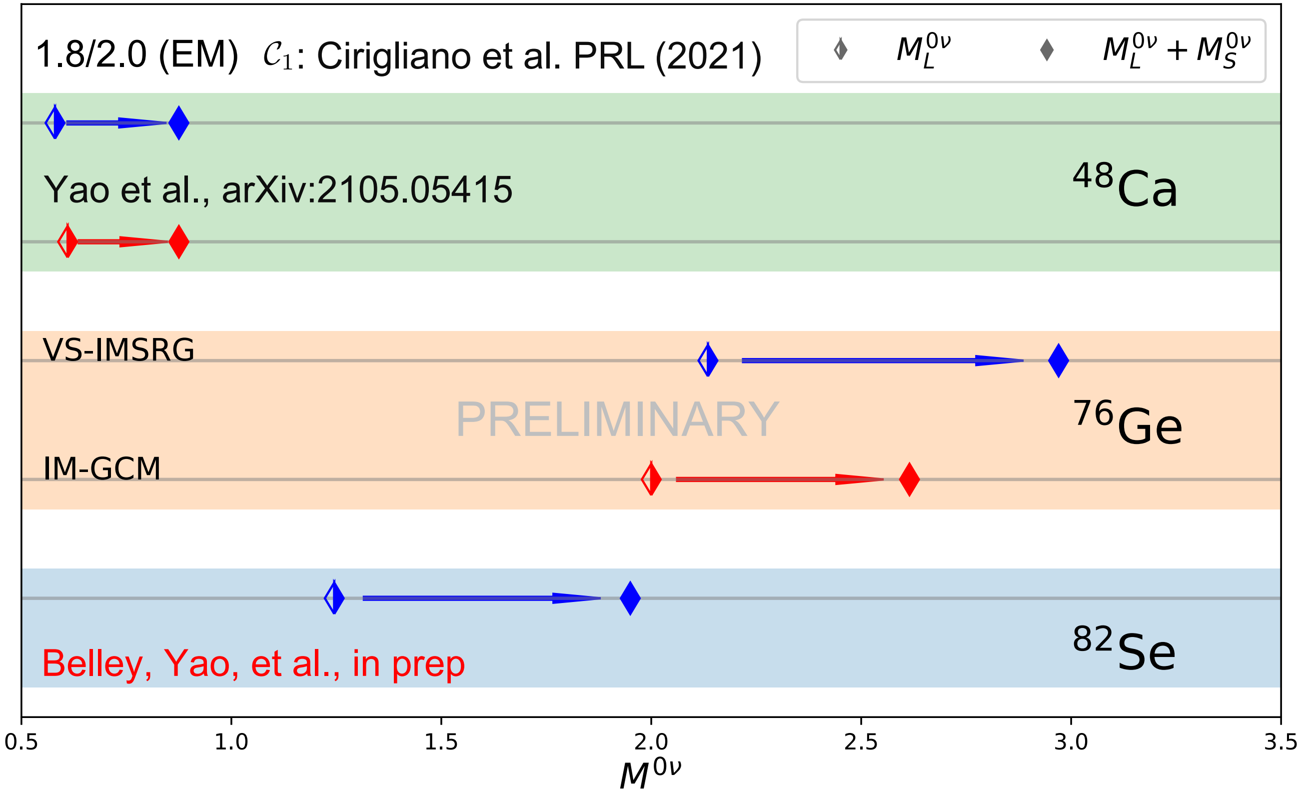

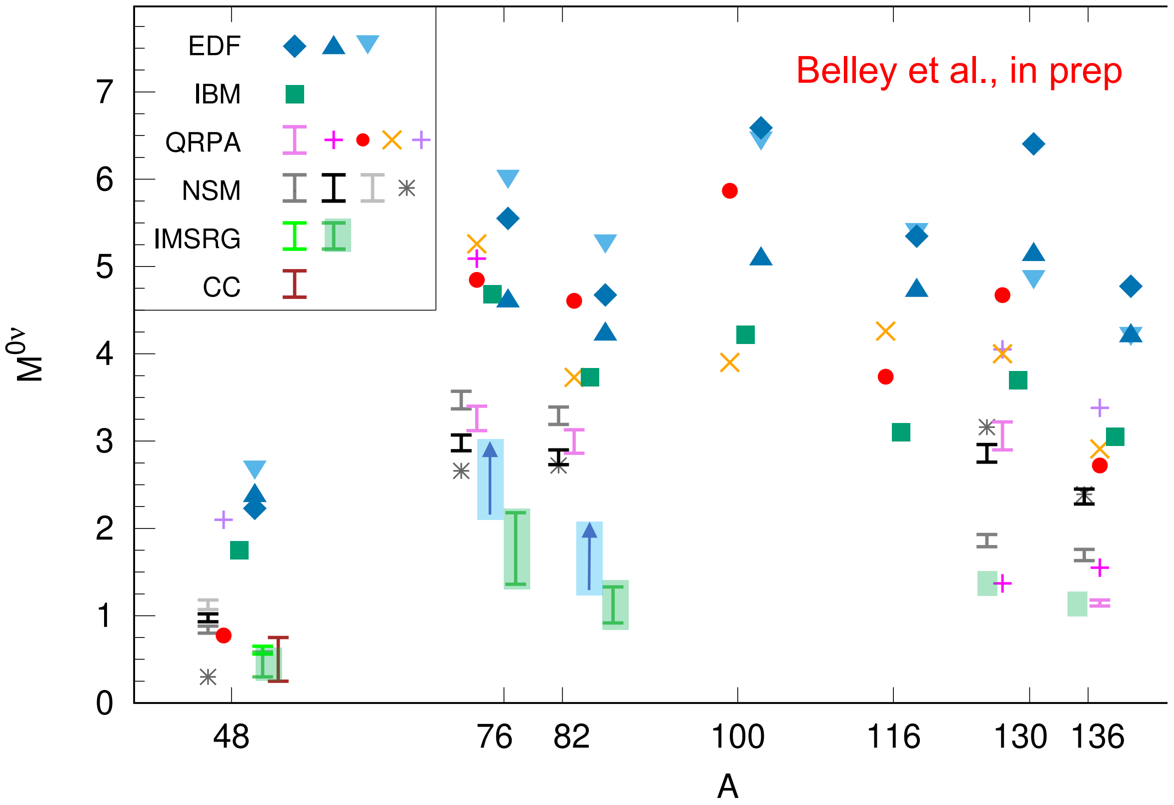

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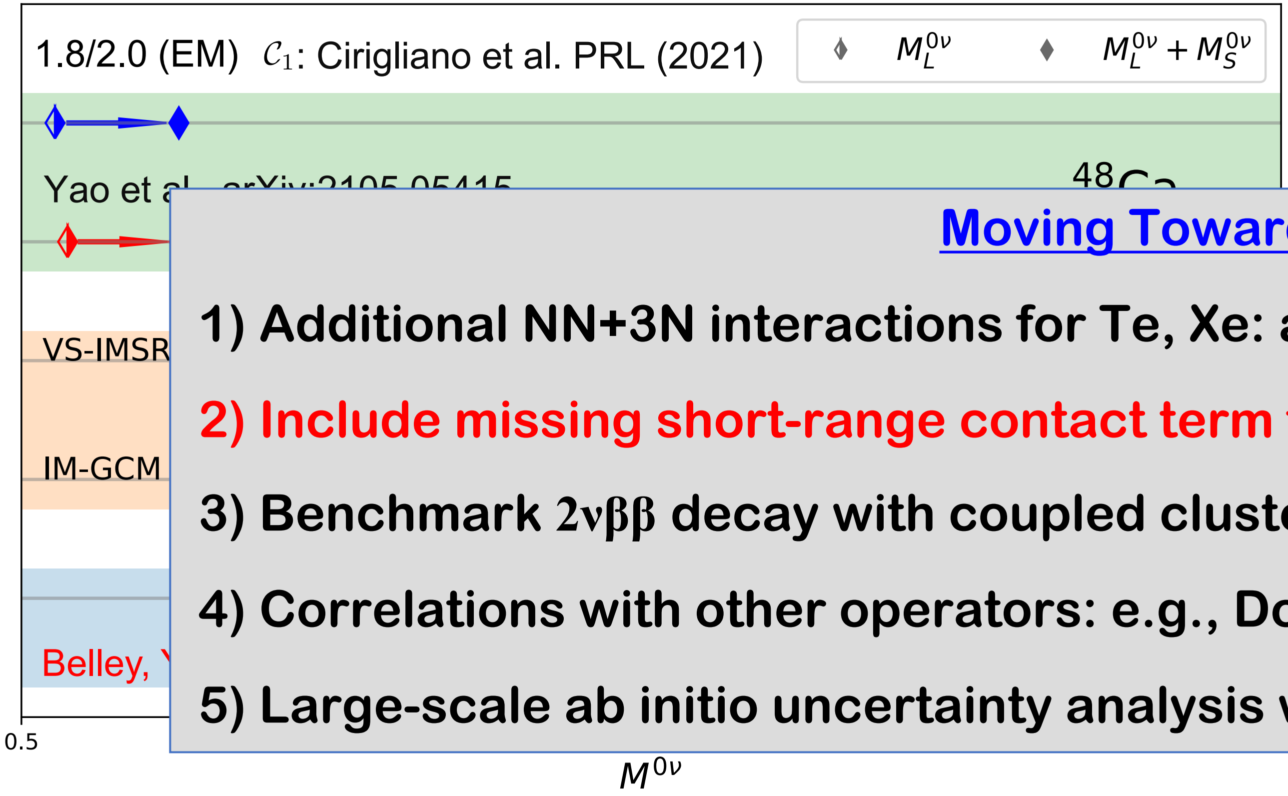

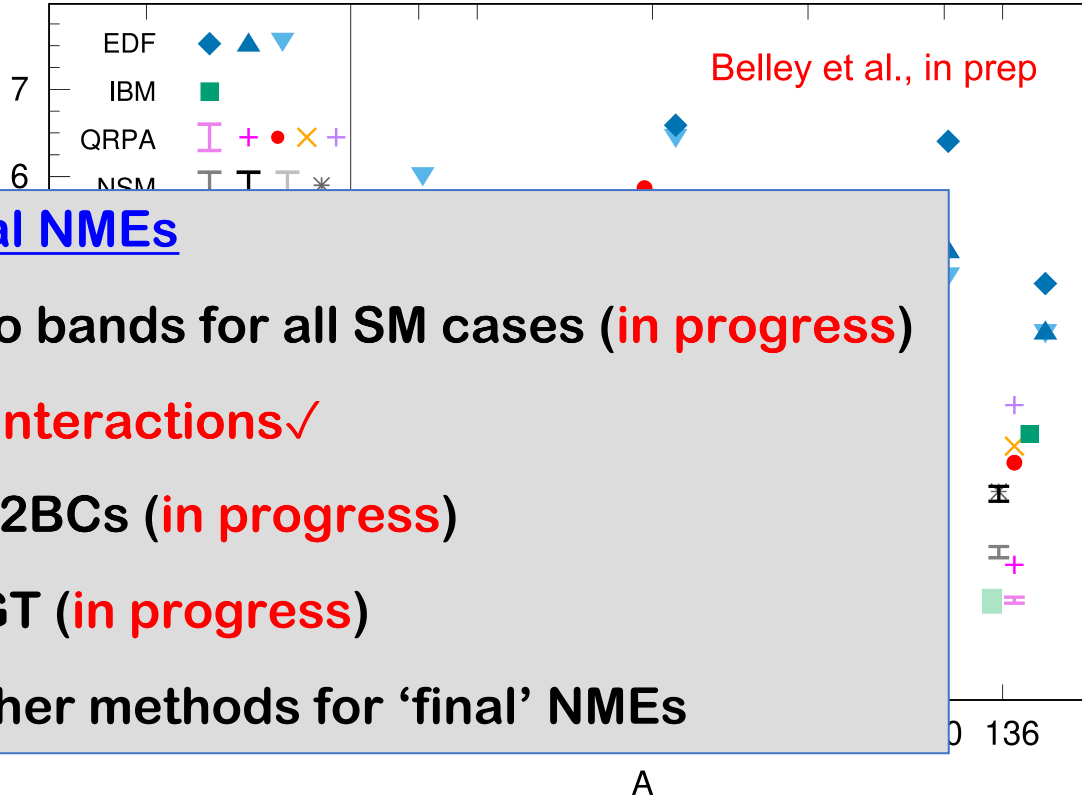

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2) Include missing short-range contact term for all interactions✓

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Overall increase of 40% in ^{76}Ge to 60% in ^{82}Se!

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Structure Functions from Large-Scale Shell Model

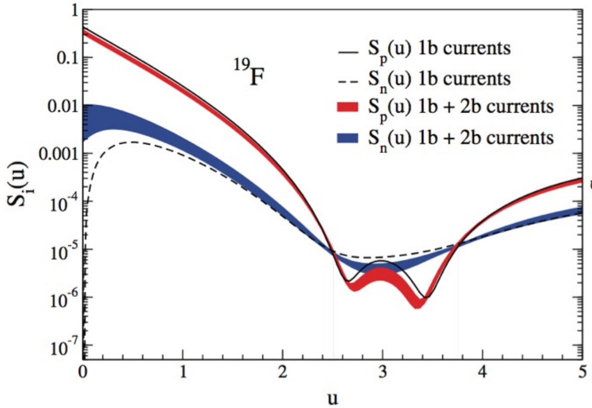
Best to date: phenomenological wfs + bare operator (**axial currents**)

$$S_A(p) = \langle f|\mathcal{L}^A|i\rangle = a_0^2 S_{00}(p) + a_0 a_1 S_{01}(p) + a_1^2 S_{11}(p)$$

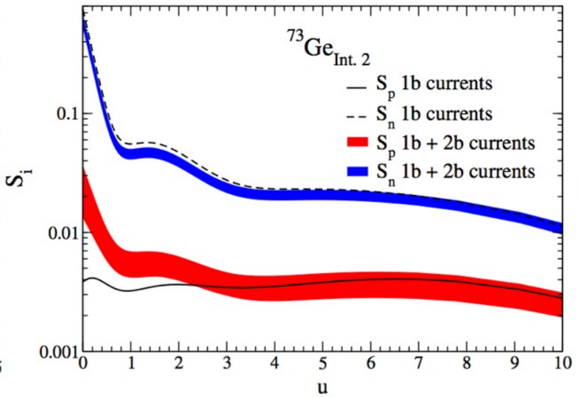
Isoscalar Coupling   Isovector Coupling

$$S_p(q) = S_{00}(q) + S_{01}(q) + S_{11}(q)$$

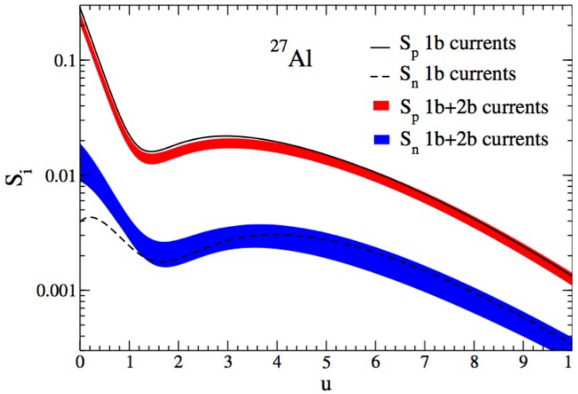
$$S_n(q) = S_{00}(q) - S_{01}(q) + S_{11}(q)$$



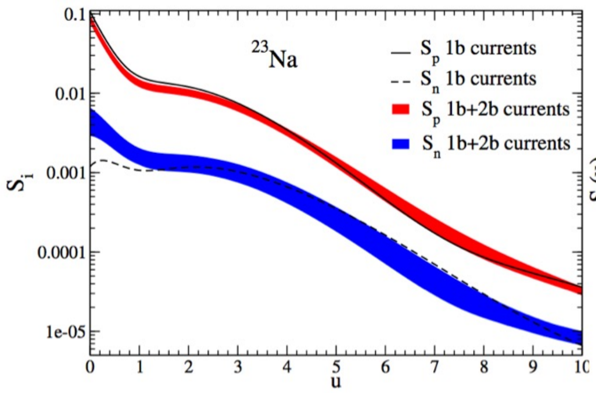
PICASSO, COUPP, SIMPLE



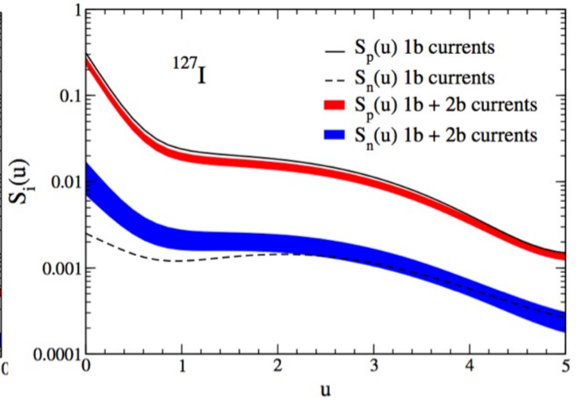
CDMS, EDELWEISS, EURECA



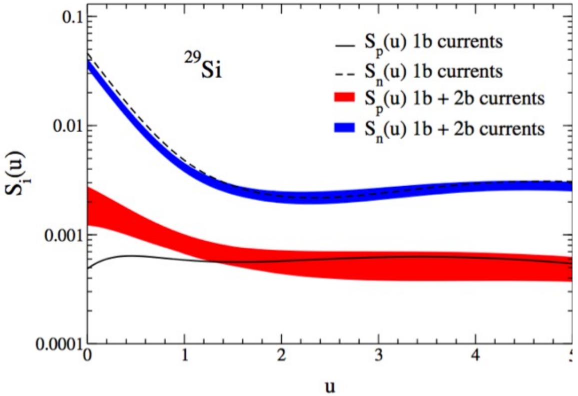
CRESST



DAMA, ANAIS, DM-Ice



DAMA, ANAIS, DM-Ice, KIMS



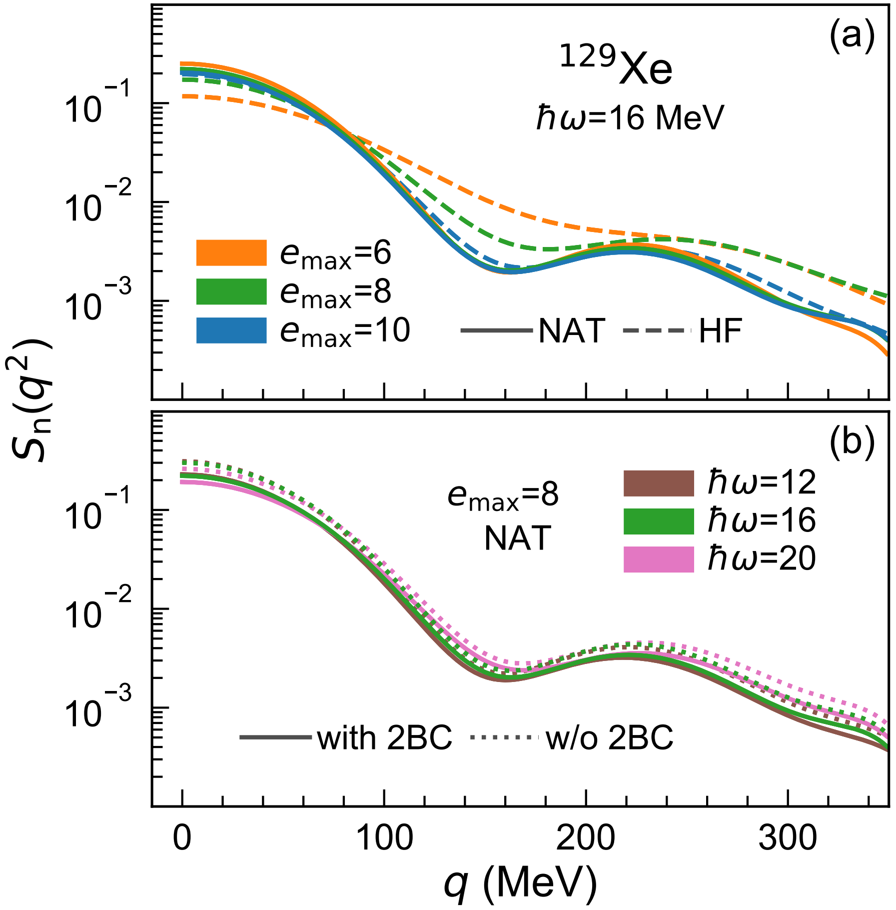
CDMS-II

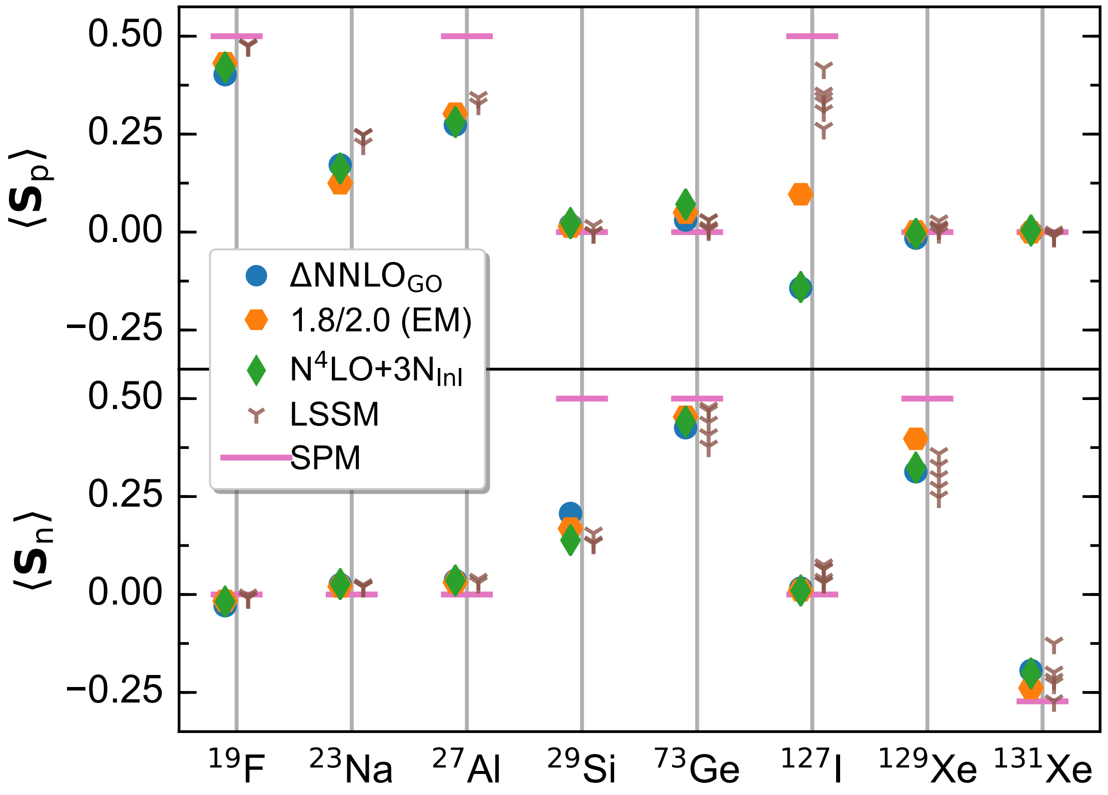
Klos et al, PRD (2013)

Ab Initio Convergence and Spin Expectations

Use consistent NN+3N forces and 2-body currents

Natural orbitals basis (NAT) displays much more rapid convergence in ^{129}Xe



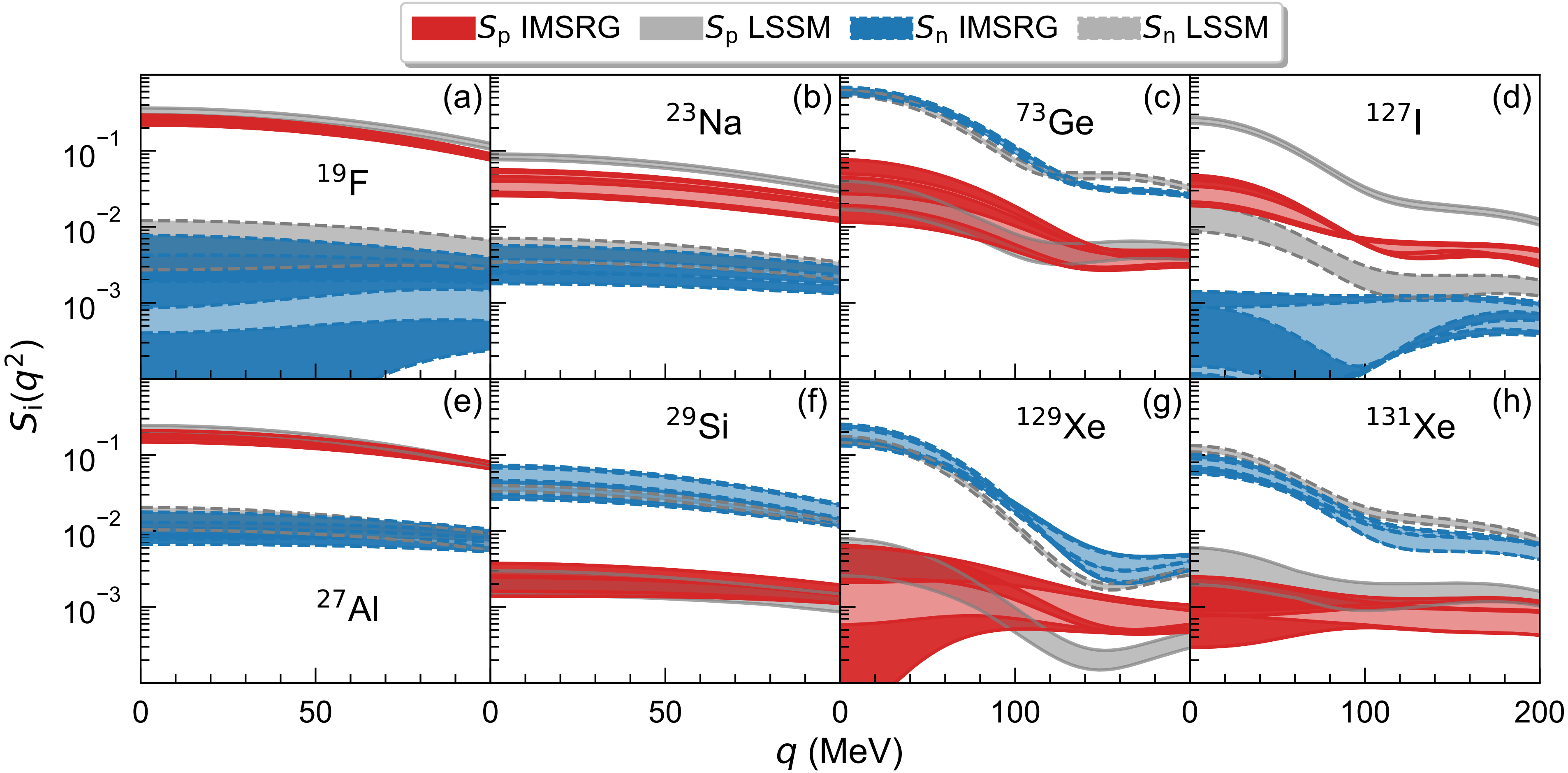


Hu et al. arXiv: 2109.00193

Ab Initio SD WIMP-Nucleus Response Overview

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

Overall similar to phenomenology at low q, discrepancies in 127I



Hu et al. arXiv: 2109.00193

Provide new structure functions for all SD direct-detection candidates

Present and Future for Theory

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

Nuclear Structure

Development of forces and currents

Dripline predictions up to Fe

Evolution of magic numbers:

  masses, radii, spectra, EM transitions

Multi-shell theory:

  Islands of inversion

  Forbidden decays

Atomic systems

Fundamental Symmetries/BSM Physics

EW operators: GT quenching, muon capture

$0\nu\beta\beta$ decay matrix elements

WIMP-Nucleus/neutrino scattering

Superallowed Fermi transitions

Symmetry-violating moments [molecules]

Work in progress

Higher-order many-body effects: IMSRG(3)

Monte Carlo shell model diagonalization

Extension to superheavy nuclei

Precision data on GT transitions

TRIUMF / The University of British Columbia / McGill University: S. R. Stroberg, T. Miyagi, B. Hu, A. Belley, I. Ginnett, E. Love, M. Bruneault, J. Padua, G. Tenkila, H. Patel

Technische Universität Darmstadt: A. Schwenk

The University of Tennessee Knoxville: G. Hagen, T. Papenbrock

Massachusetts Institute of Technology: R. F. Garcia-Ruiz

Michigan State University: J.M. Yao, H. Hergert

Colorado School of Mines: M. Martin, K. G. Leach

Universitat de Barcelona: L. Jokiniemi, J. Menéndez

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

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

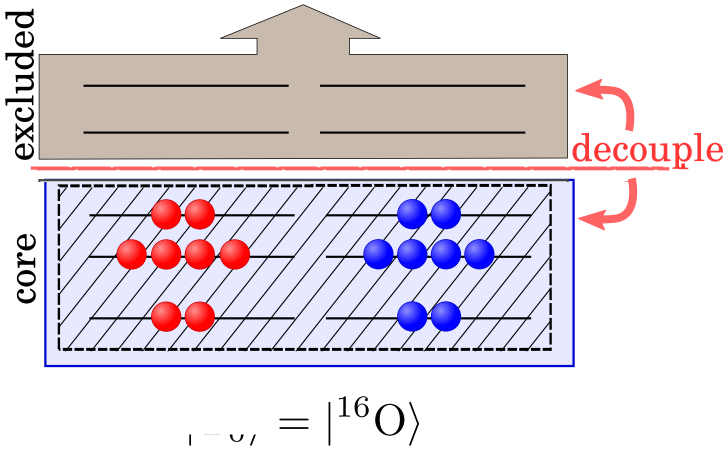
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

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

IMSRG(3) in progress

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

Step 1: Decouple core



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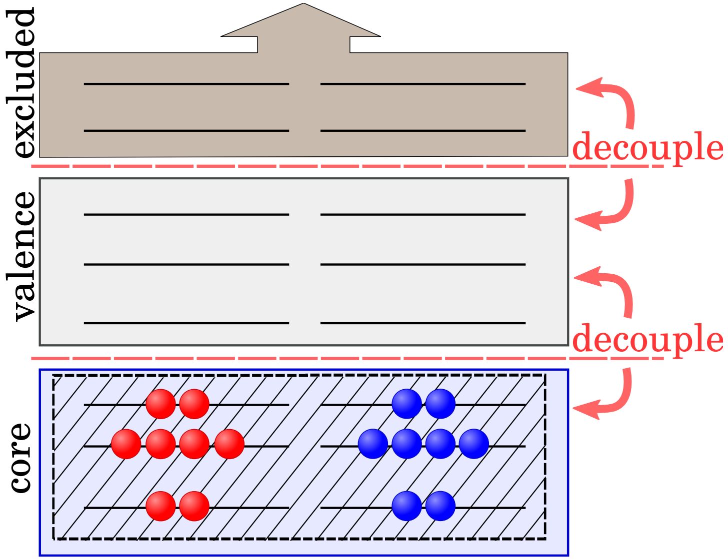

$= |^{16}\mathrm{O}\rangle$

Step 1: Decouple core
Step 2: Decouple valence space

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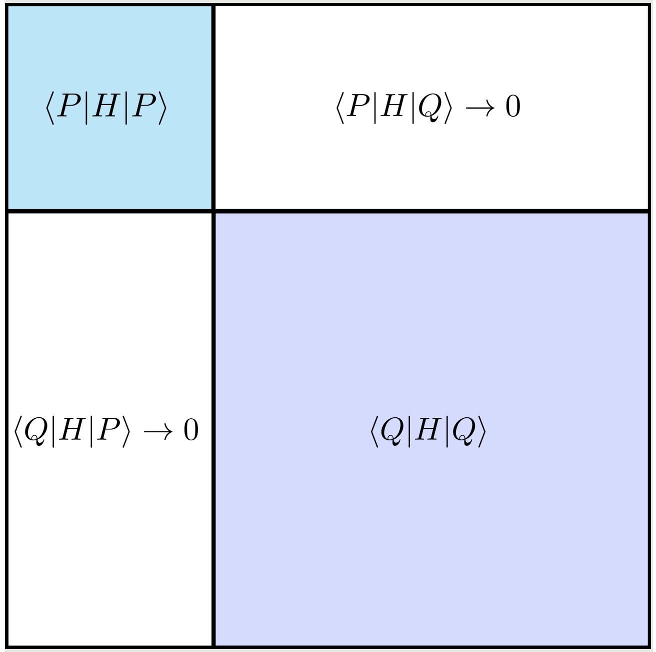

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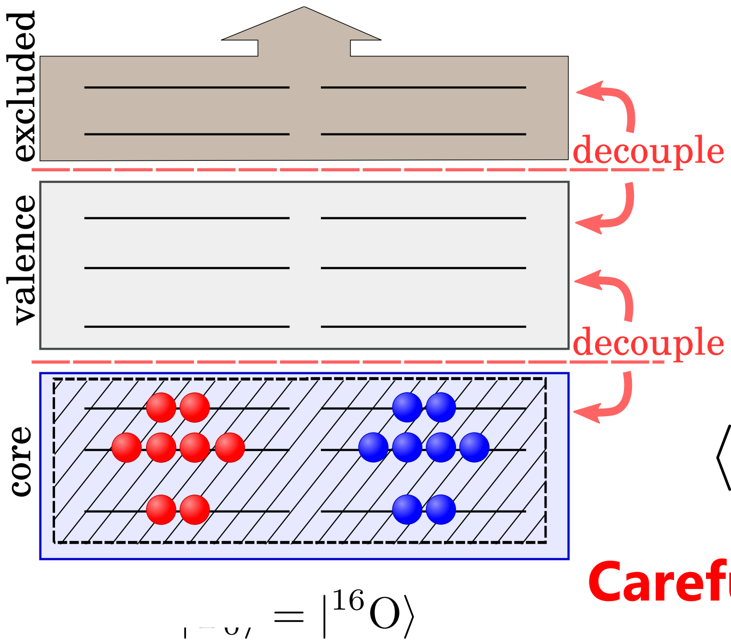

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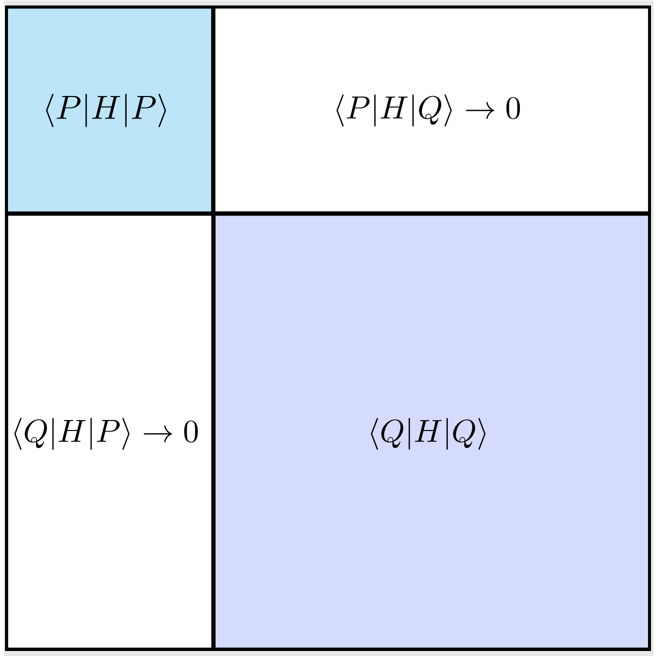
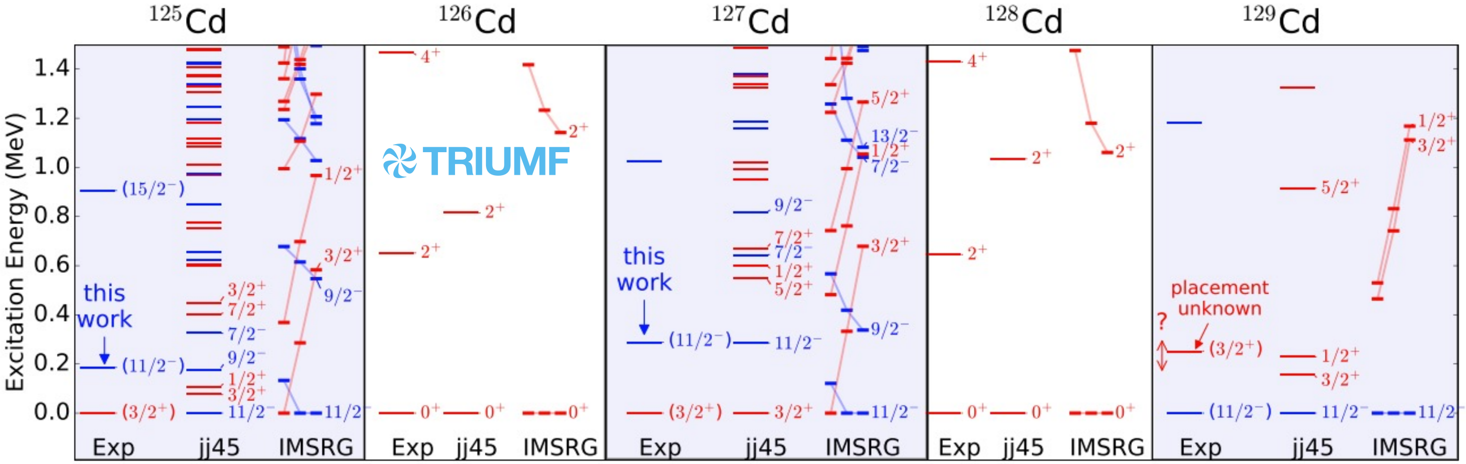
Careful benchmarking essential



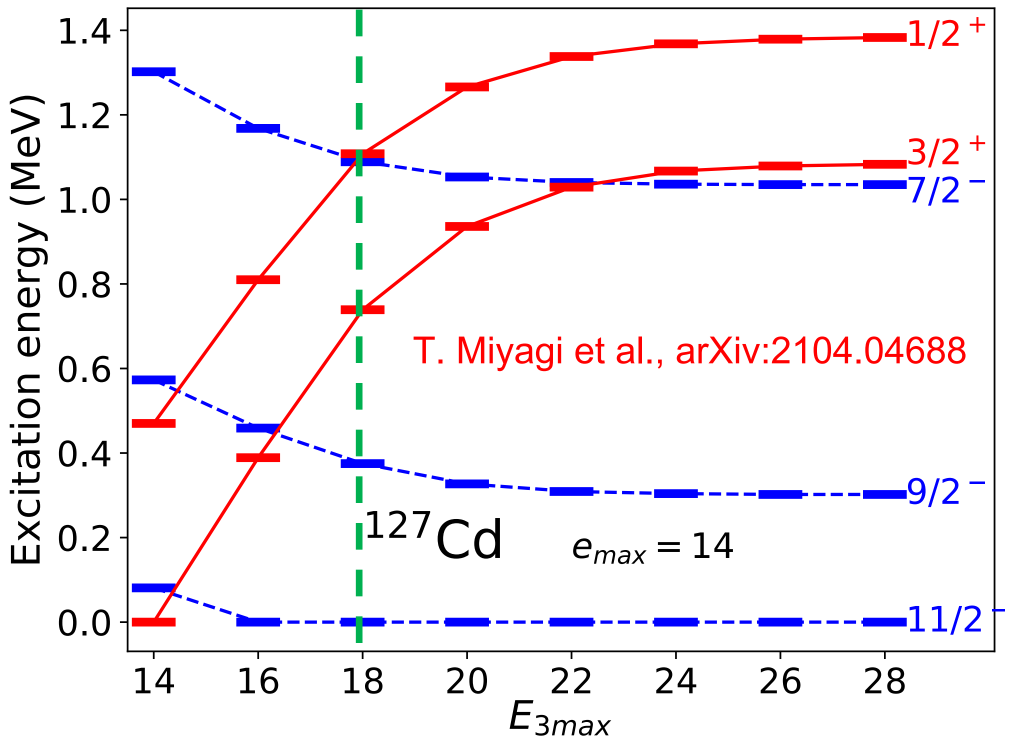
TRIUMF

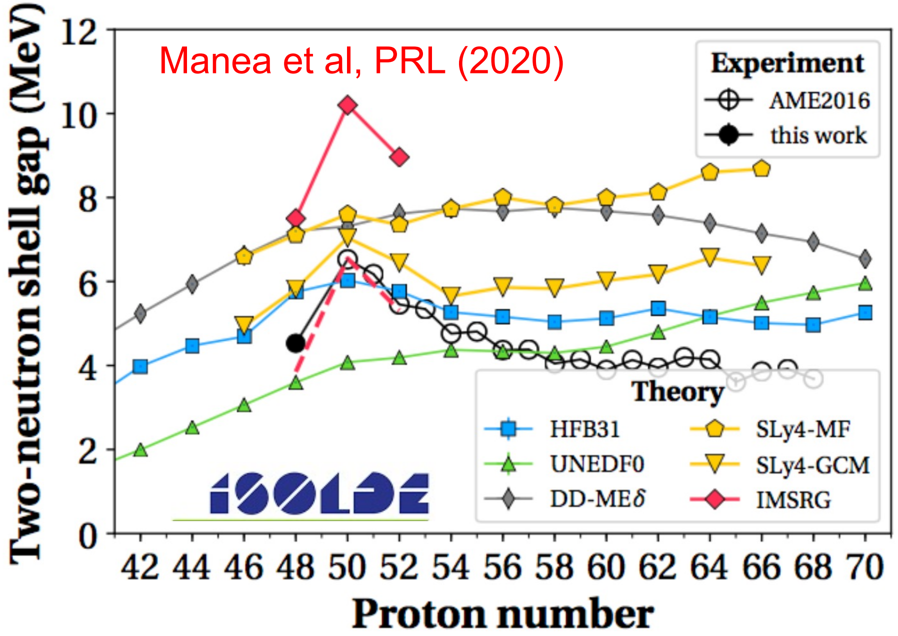
Convergence of N=82 Gap

Size of N=70 gap not converged at E_{3max}=18: for neutron-rich Sn, In, Cd…



Lascar et al PRC (2017)





Resorted to unreliable extrapolations…

New capabilities: converged spectra in N=82 region

TRIUMF

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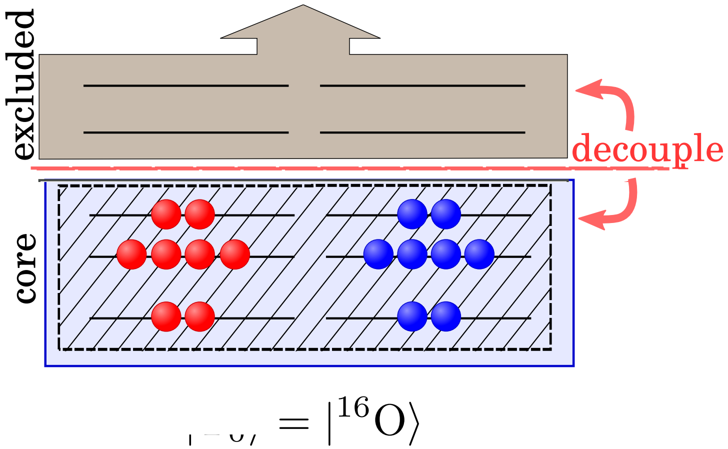

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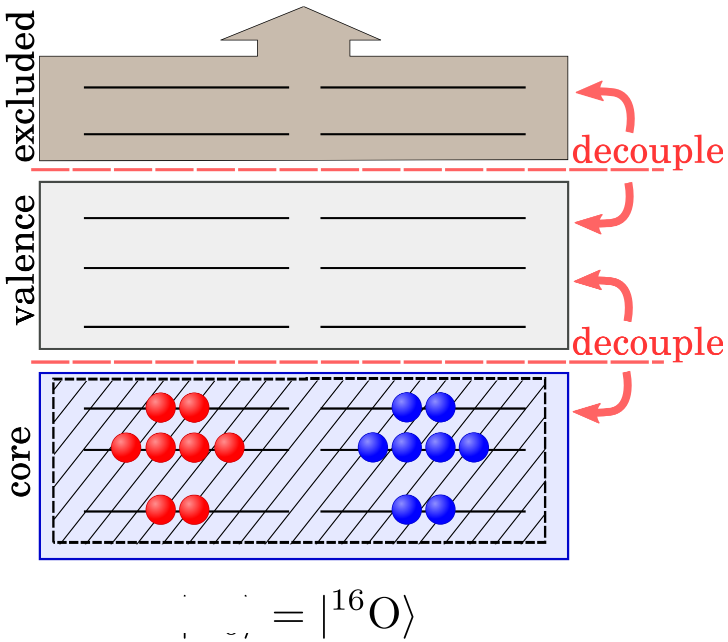

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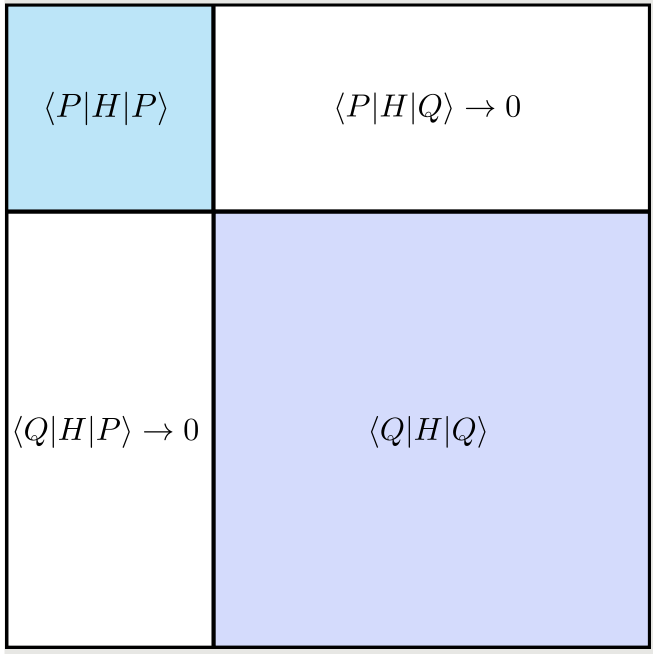

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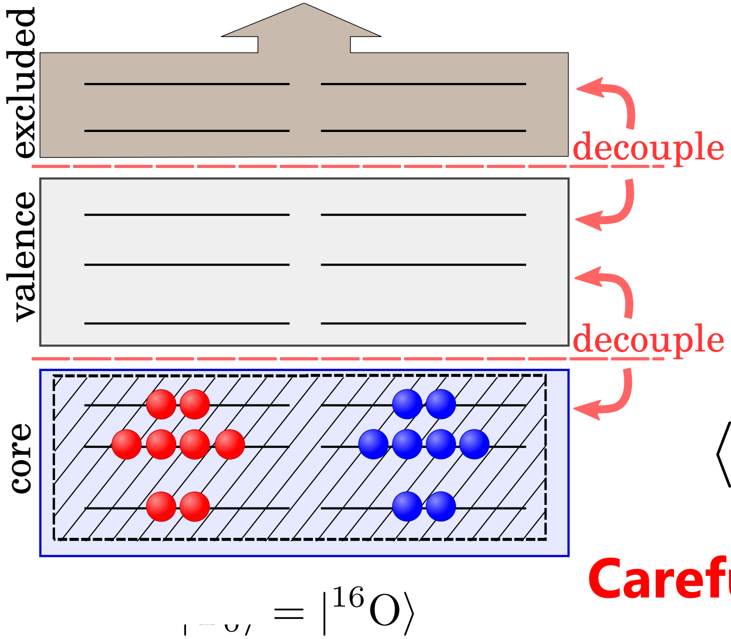

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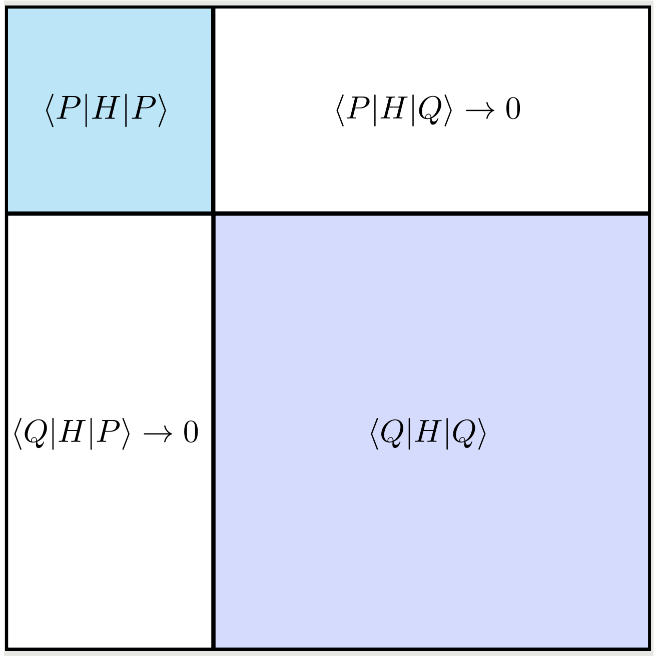
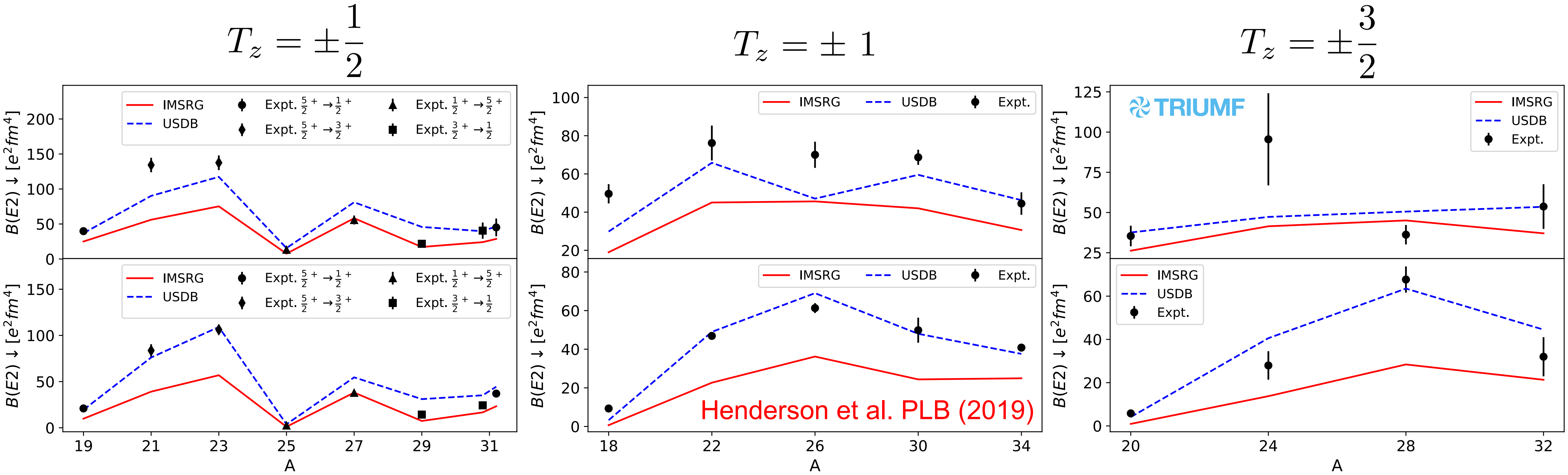


Global Trends in Absolute B(E2): sd Shell

Study charge E2 transitions across sd-shell



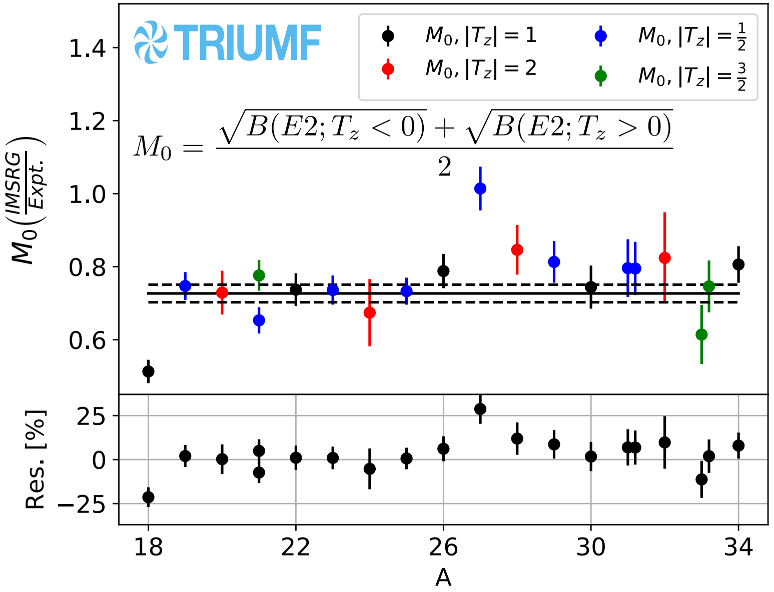
USDB with effective charges typically reproduces absolute values well

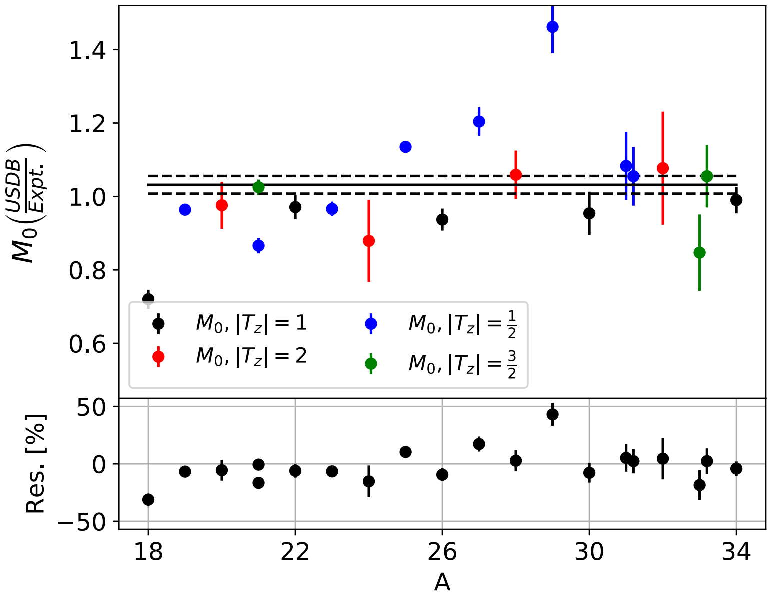
VS-IMSRG (**no effective charges**) typically underpredicts experiment

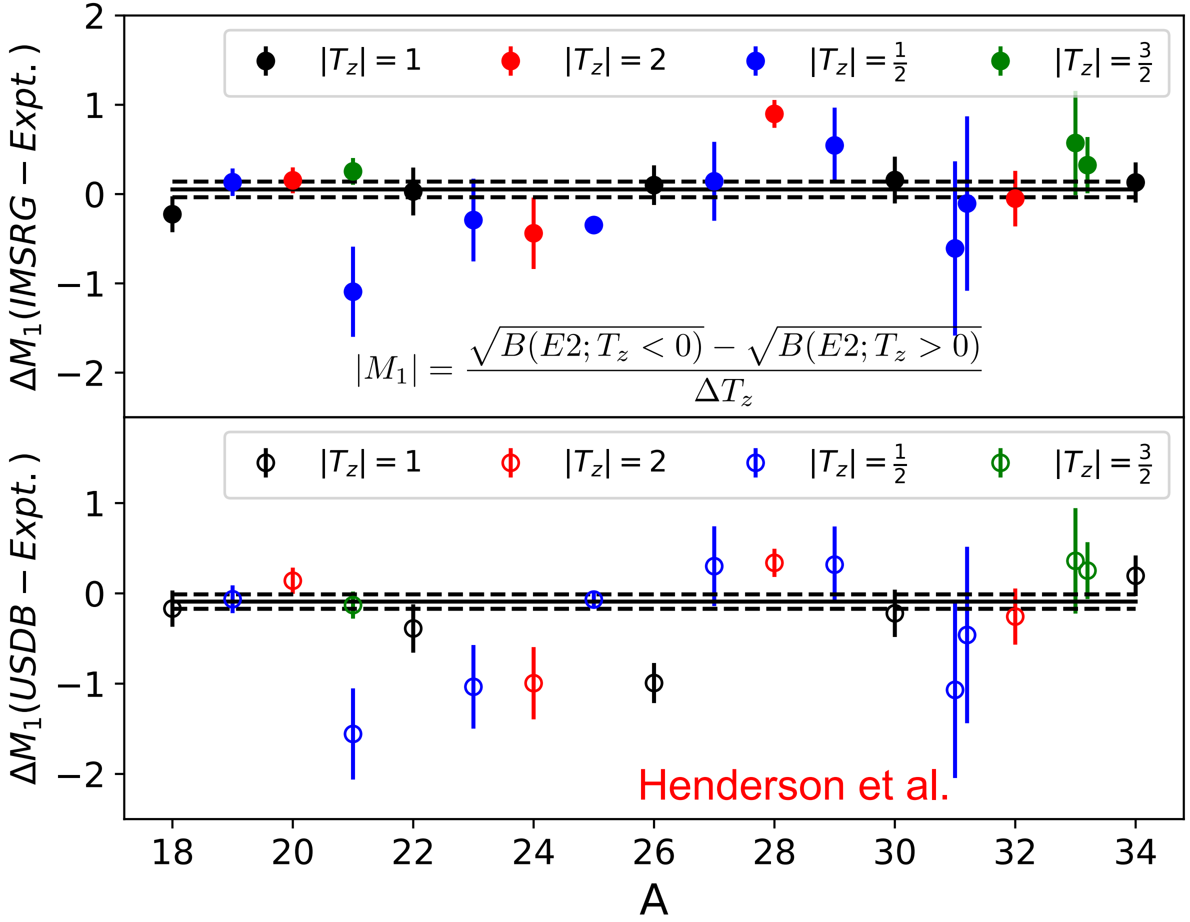
Trends well reproduced in both…

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

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







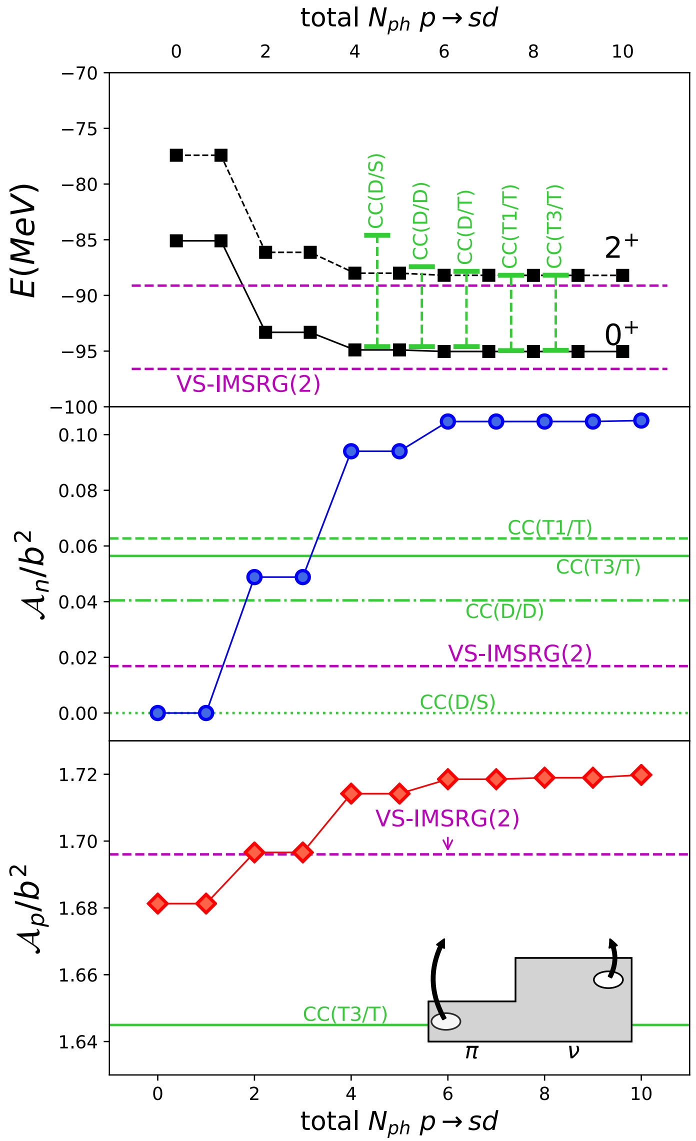
IS: USDB good agreement, VS-IMSRG systematically small

IV: Both agree well

Deficiencies in IS only

Origin of E2 Puzzle ^{14}C in psd Shell

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



Energies well converged all around

p/n amplitudes increase with p/h ex.

Only converged at ~6 Nph

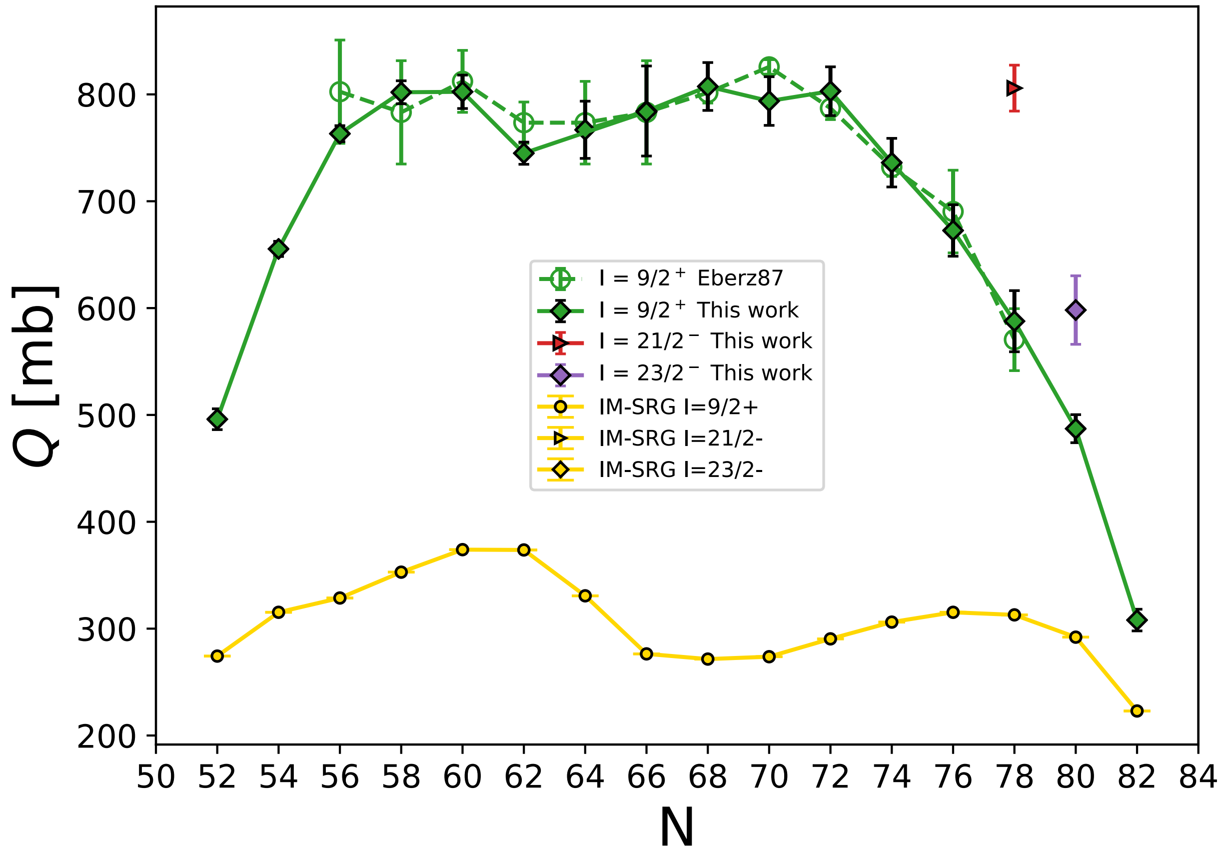
Not possible to capture fully in CC or IMSRG

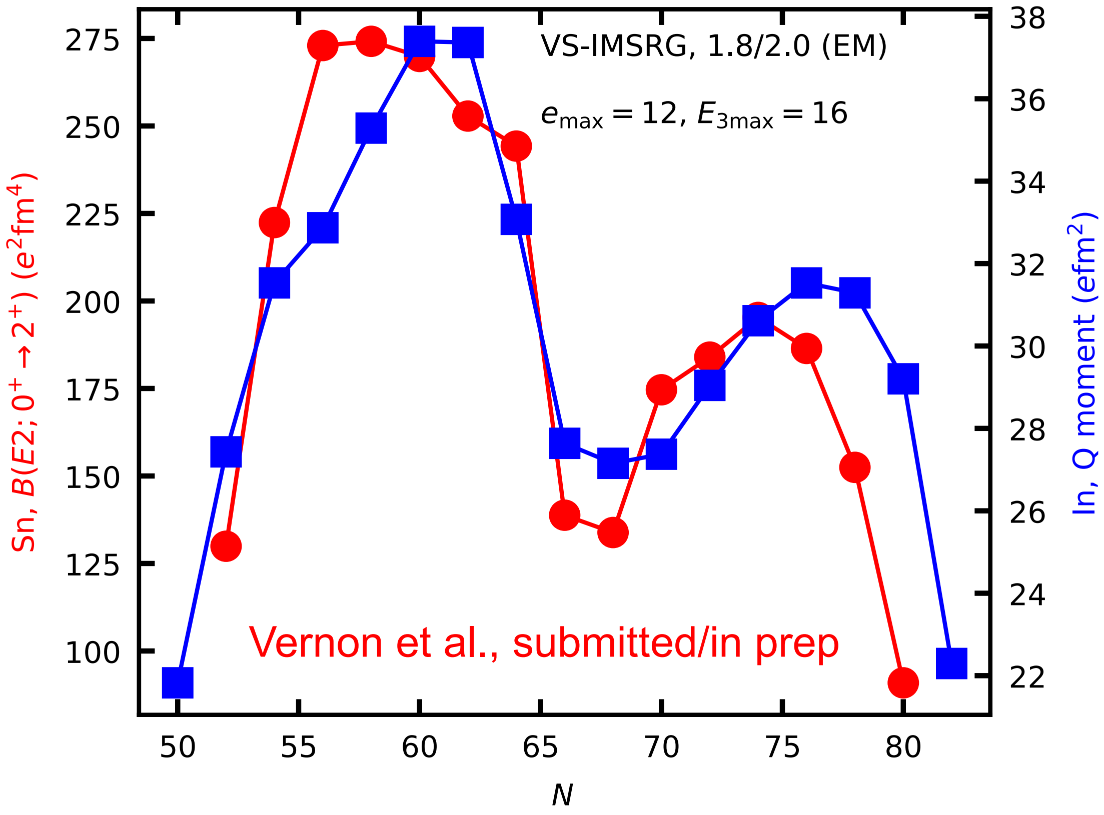
Systematic Studies in Heavy Region: In/Sn

Improvements in storage of 3N matrix elements greatly expands reach of ab initio theory!

Calculate radii, EM moments of entire In chain!

Reproduces trends of new measurements – correlates with B(E2) in Sn chain

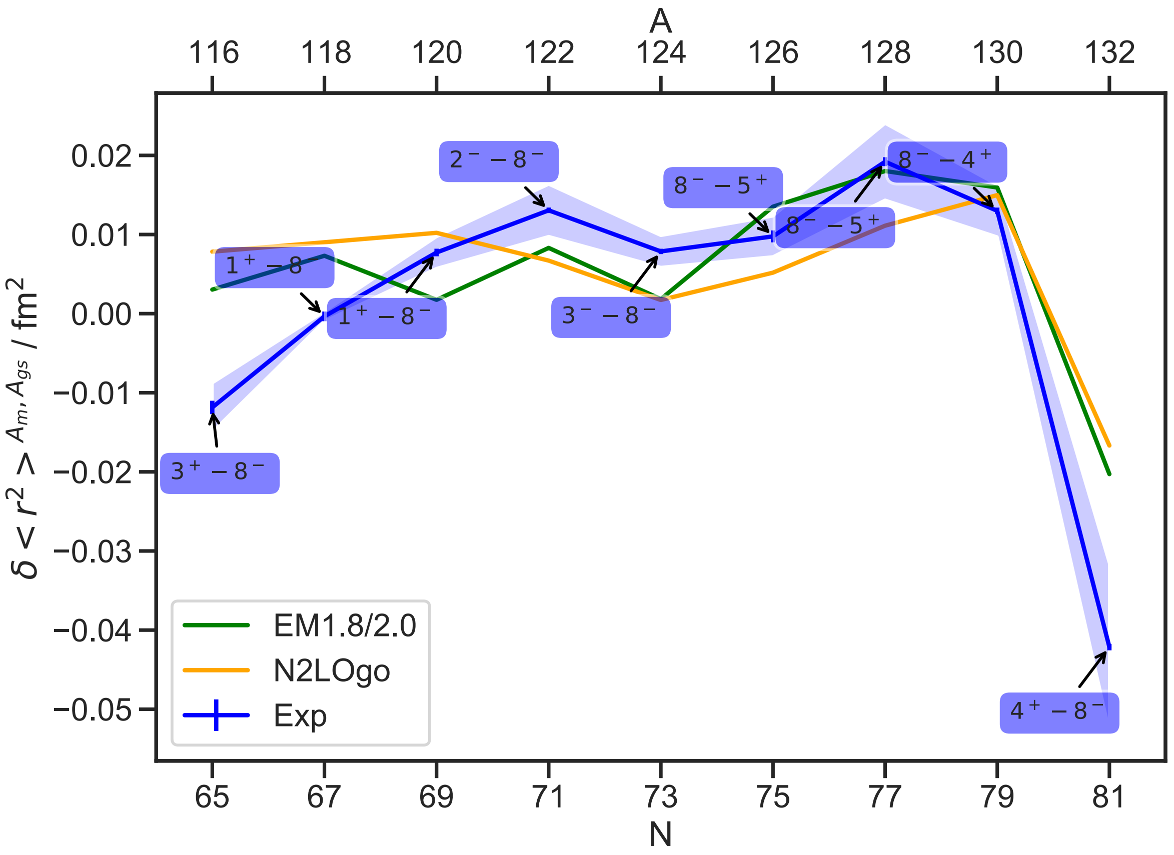


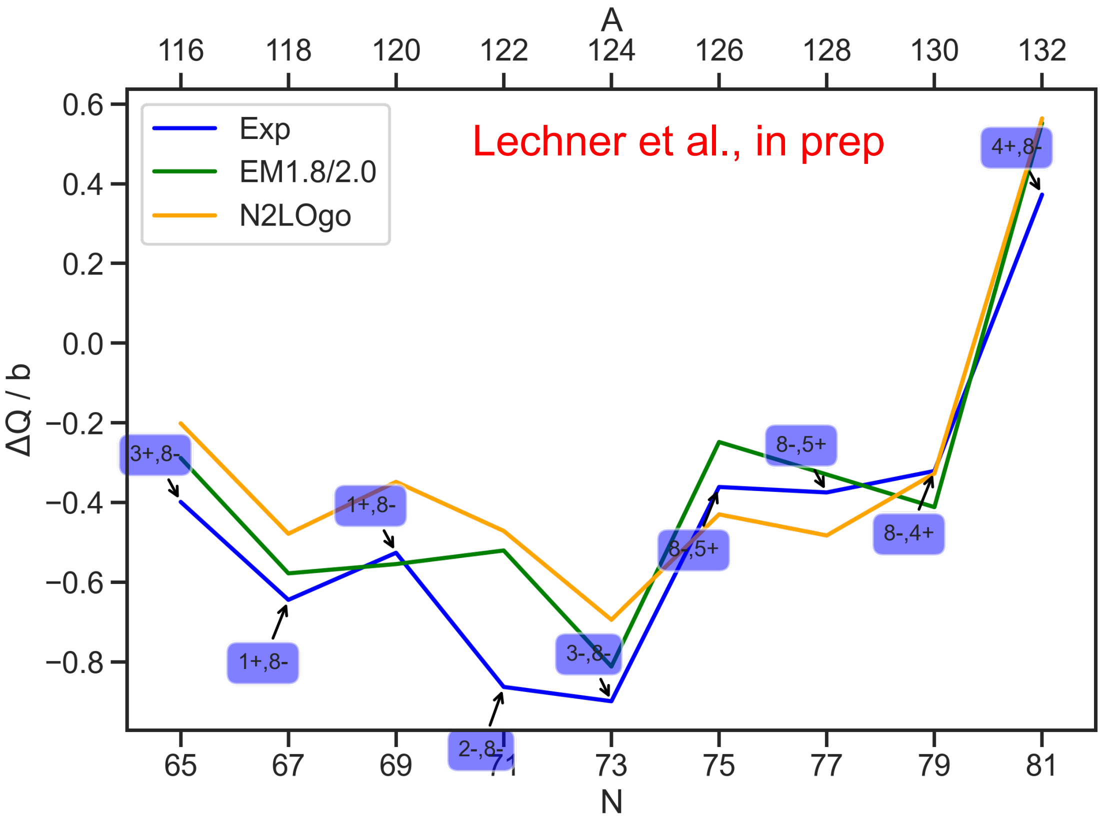


Systematic studies in Sn region: Sb

Improvements in storage of 3N matrix elements greatly expands reach of ab initio theory!

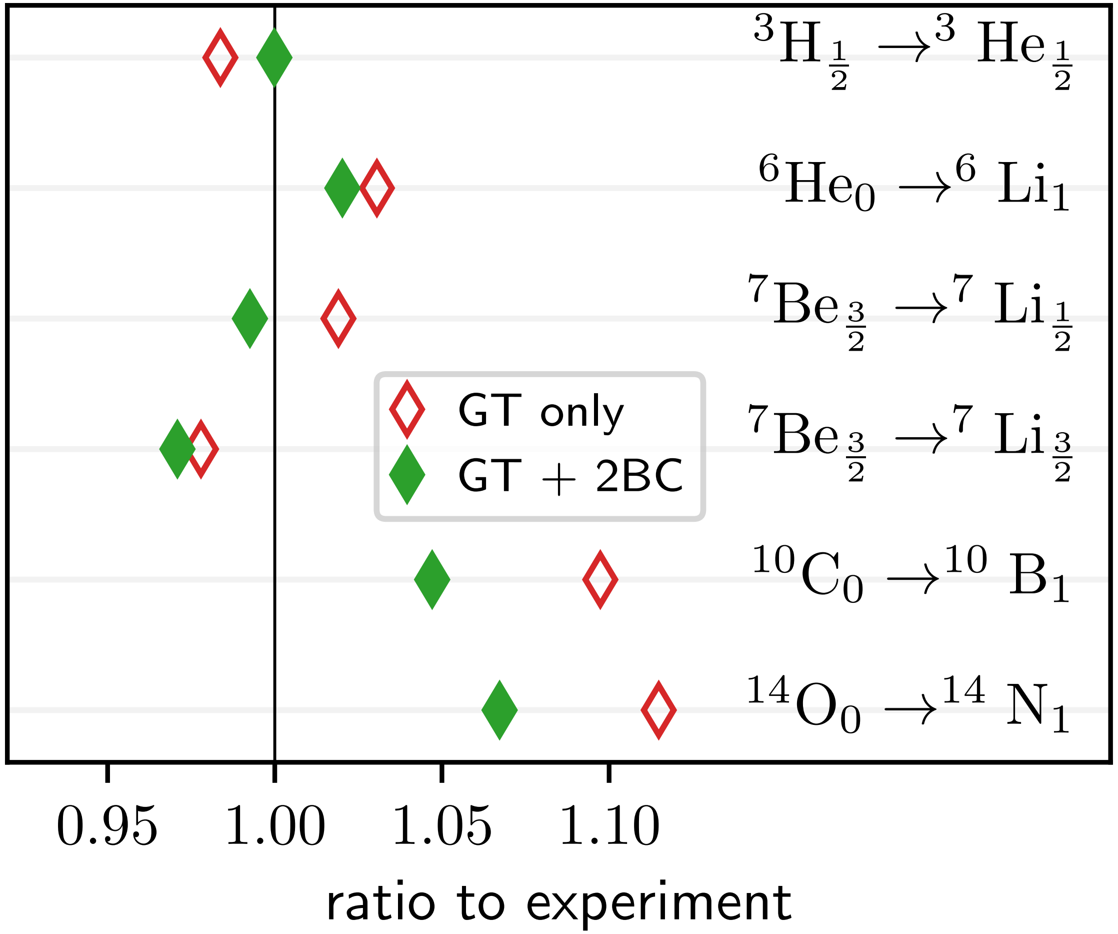
Calculate radii, moments of entire Sb chain… explore new physics

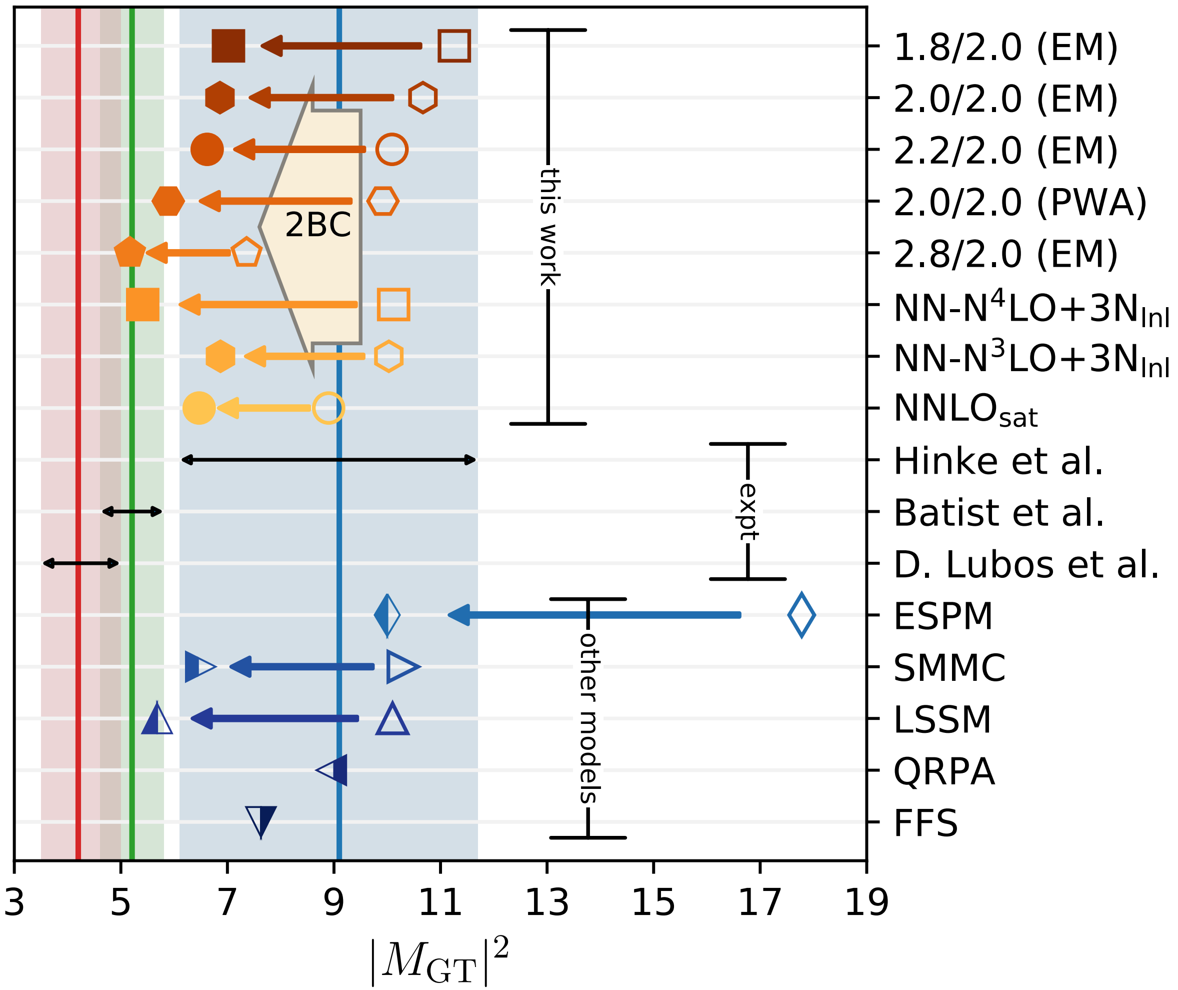




GT Transitions in Light nuclei and ^{100}Sn

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





Large quenching effect from correlations

Gysbers et al., Nature Phys. (2019)

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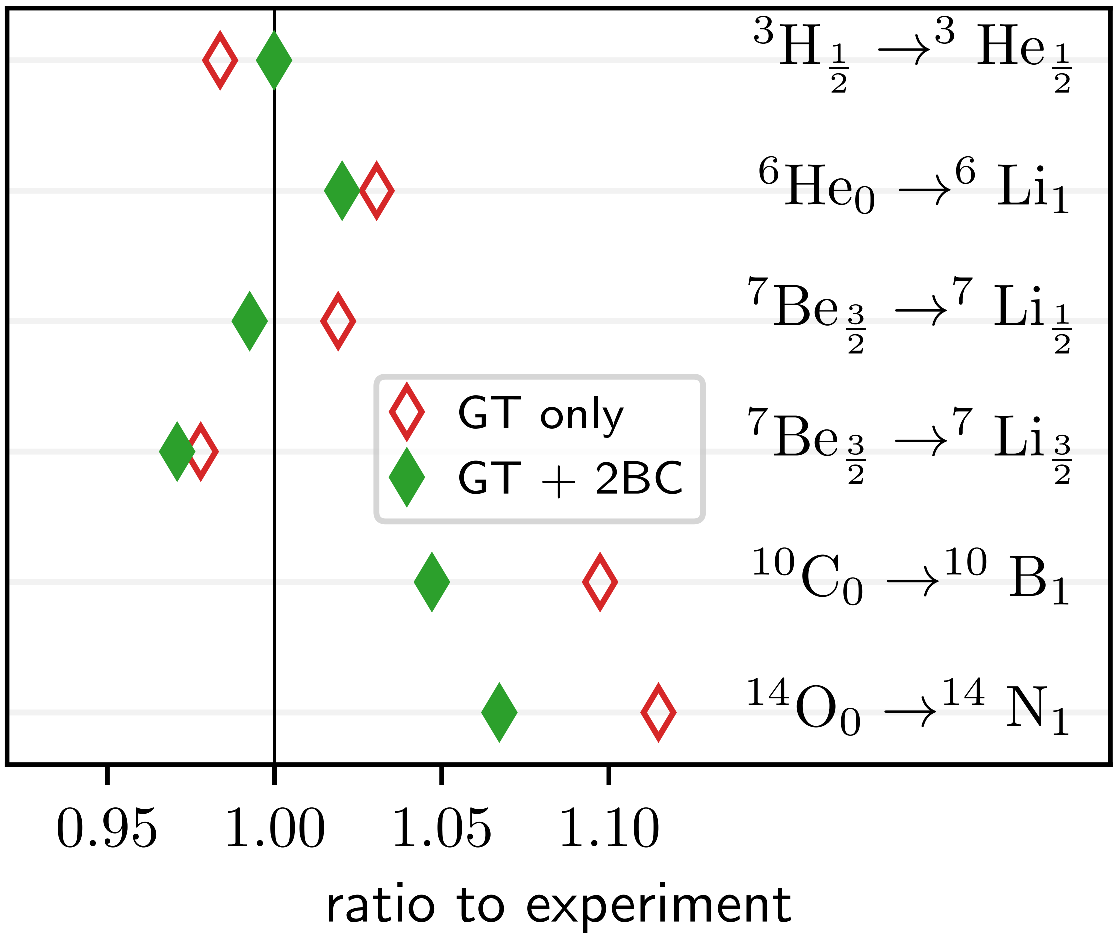

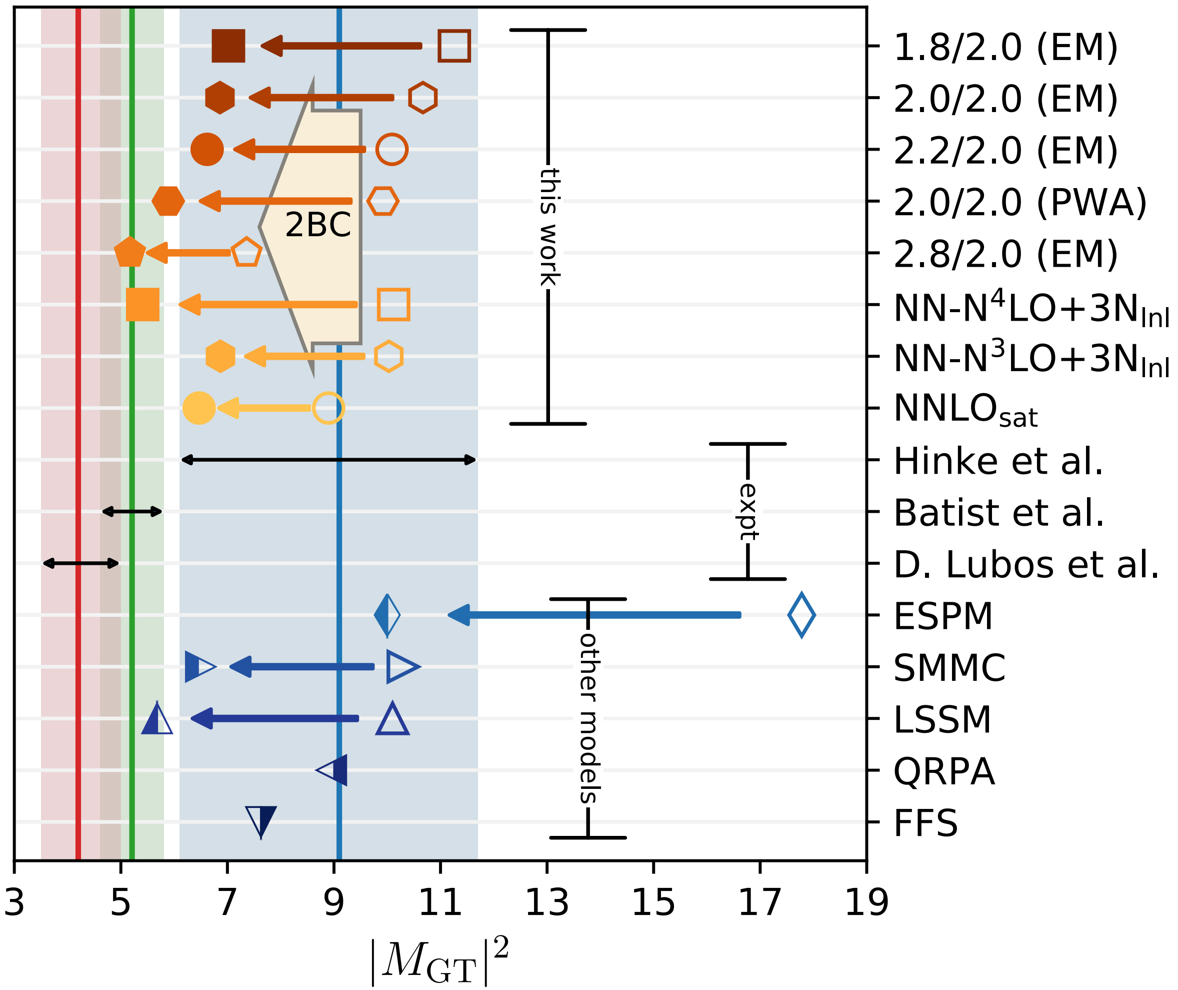

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Addition of 2BC further quenches and reduces spread in results

Discovery, accelerated

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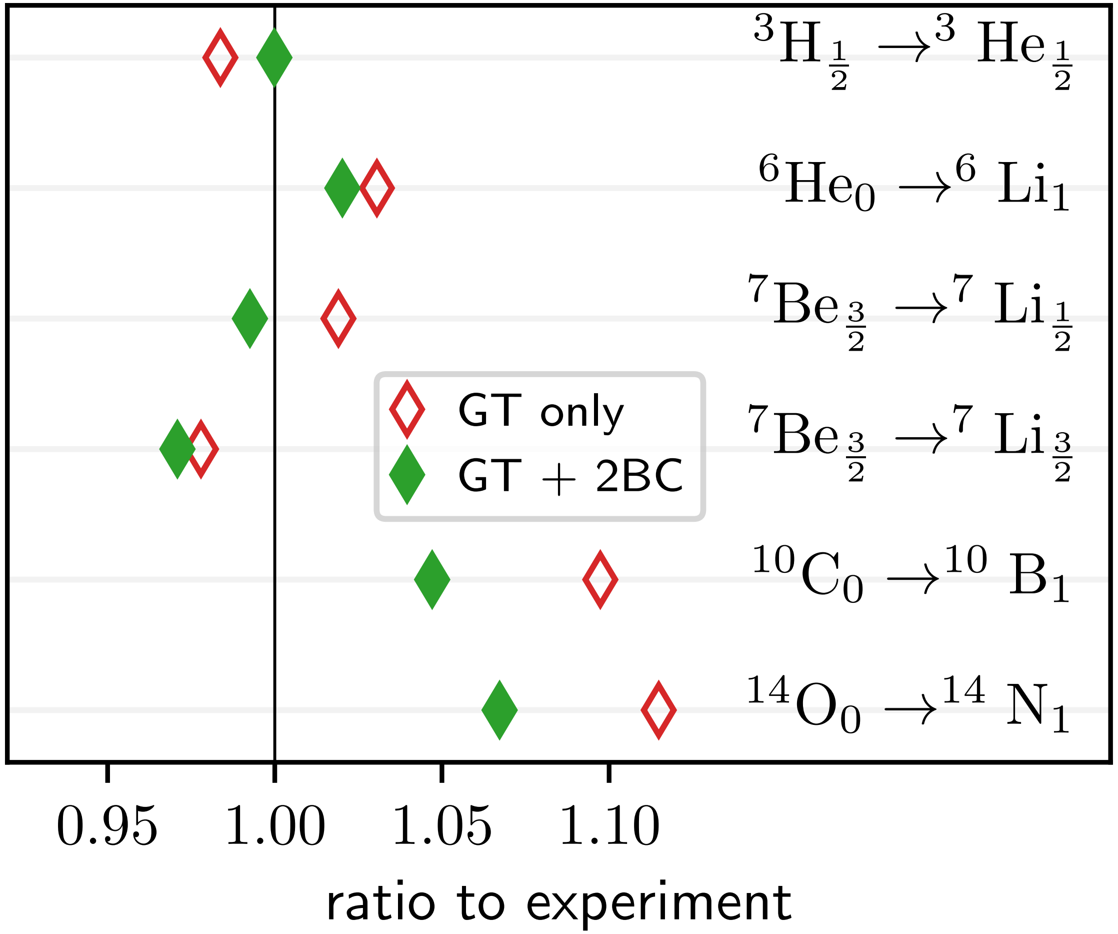

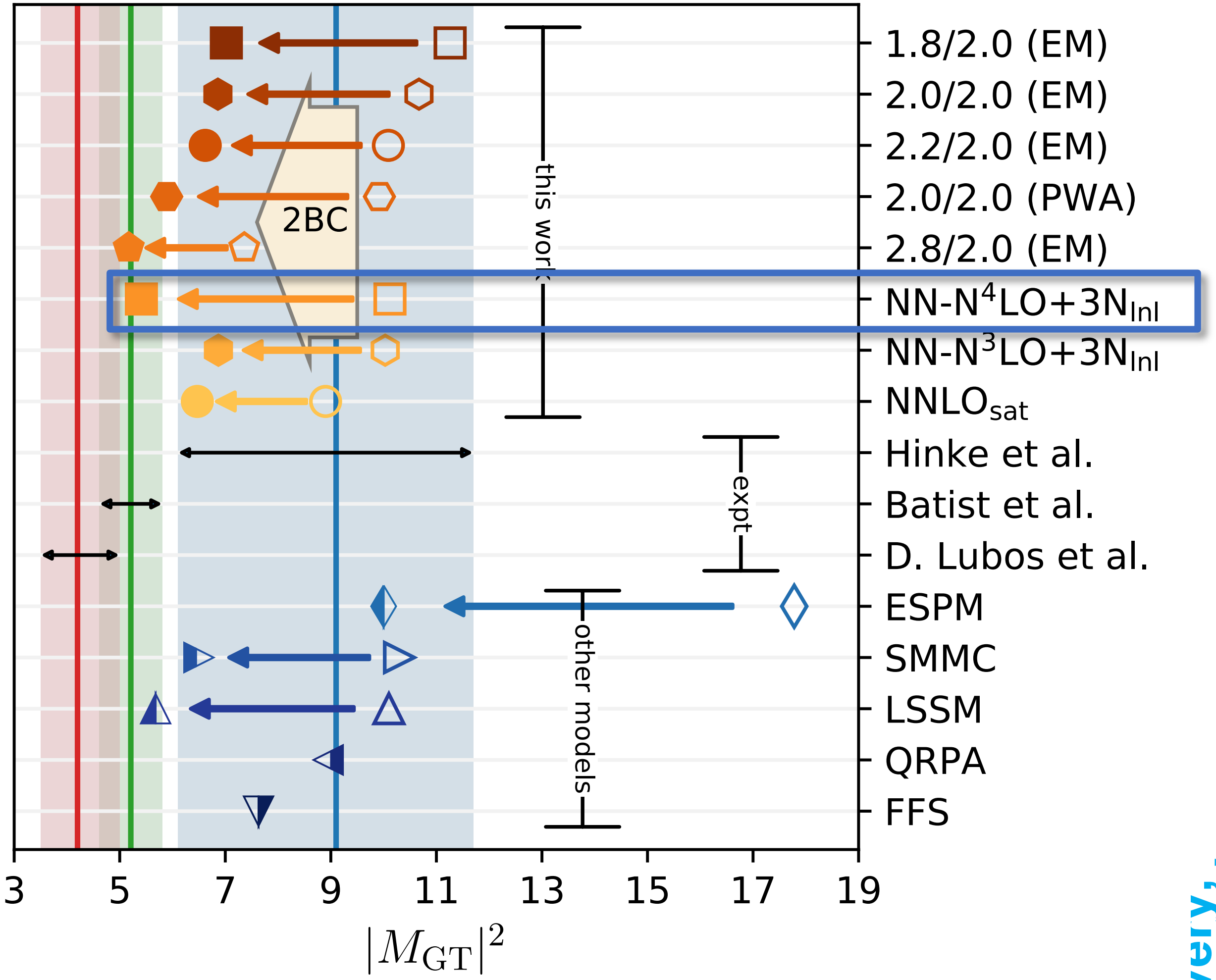

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Gysbers et al., Nature Phys. (2019)

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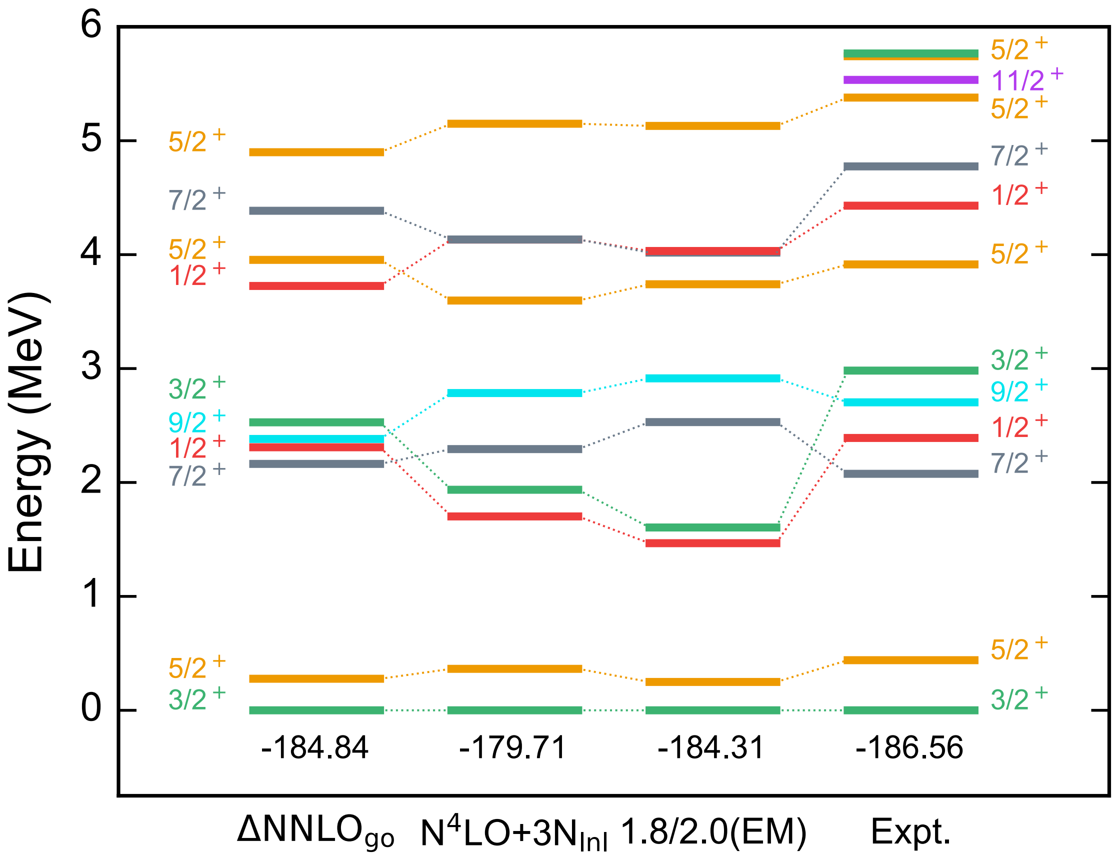
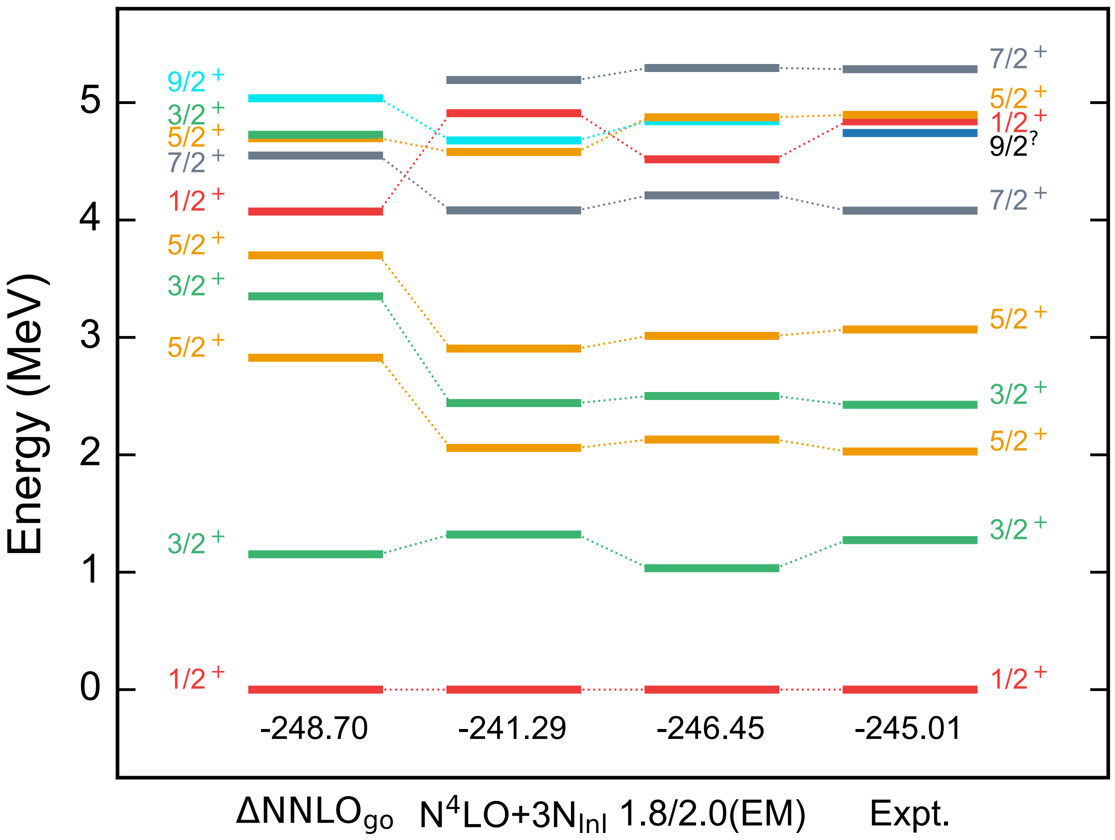
Spectroscopy

Ab initio: Consistent many-body wfs/operators from chiral NN+3N forces + 2b currents

Calculated spectroscopy (generally) well reproduces experiment





Hu, Padua, in prep.

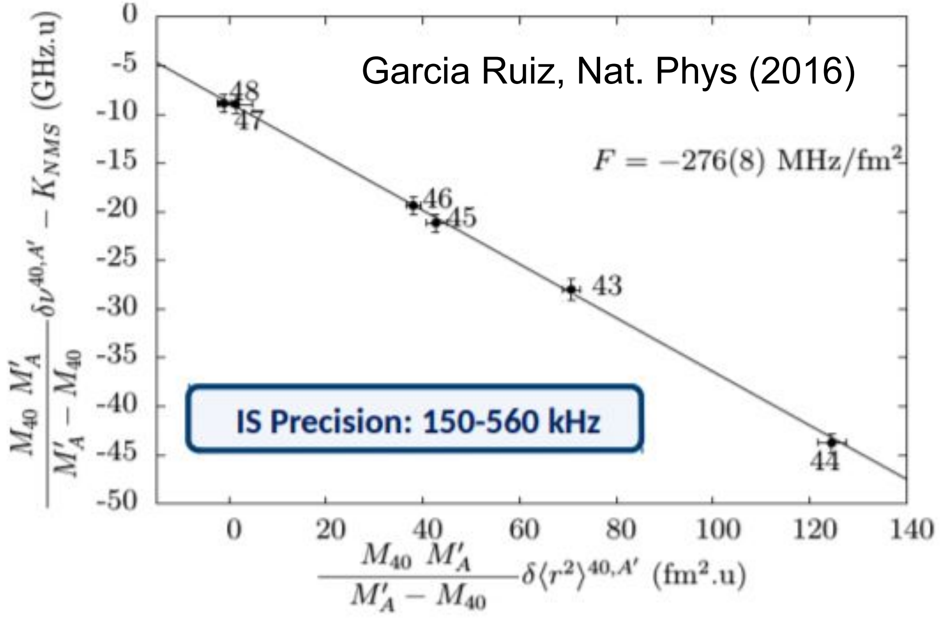
Extent to Ab Initio Atomic Systems

Motivation: isotope shifts in atoms needed for laser spec. experiments

Mass Shift: $$\delta E_{i,\mathrm{MS}}^{A,A'} = \left(\frac{M'-M}{MM'}\right)(K_{i,\mathrm{NMS}} + K_{i,\mathrm{SMS}}) = \left(\frac{M'-M}{MM'}\right) K_{i,\mathrm{MS}}$$

Field Shift: $$\delta E_{i,\mathrm{FS}}^{(1)A,A'} = -\int_{\mathbf{R}^3} \left[V^A(\mathbf{r}) - V^{A'}(\mathbf{r})\right] \rho_i^e(\mathbf{r}) d^3\mathbf{r} \approx \sum_n F_{i,n}\delta\langle r^{n+2}\rangle^{A,A'}$$

$$\delta\nu^{A,A'} = K_{MS}\frac{M_{A'}-M_A}{M_{A'}M_A} + F\delta\langle r^2\rangle^{A,A'}$$



➔ Non-linearities in "**King plots**" point to new electron-nucleon interactions.

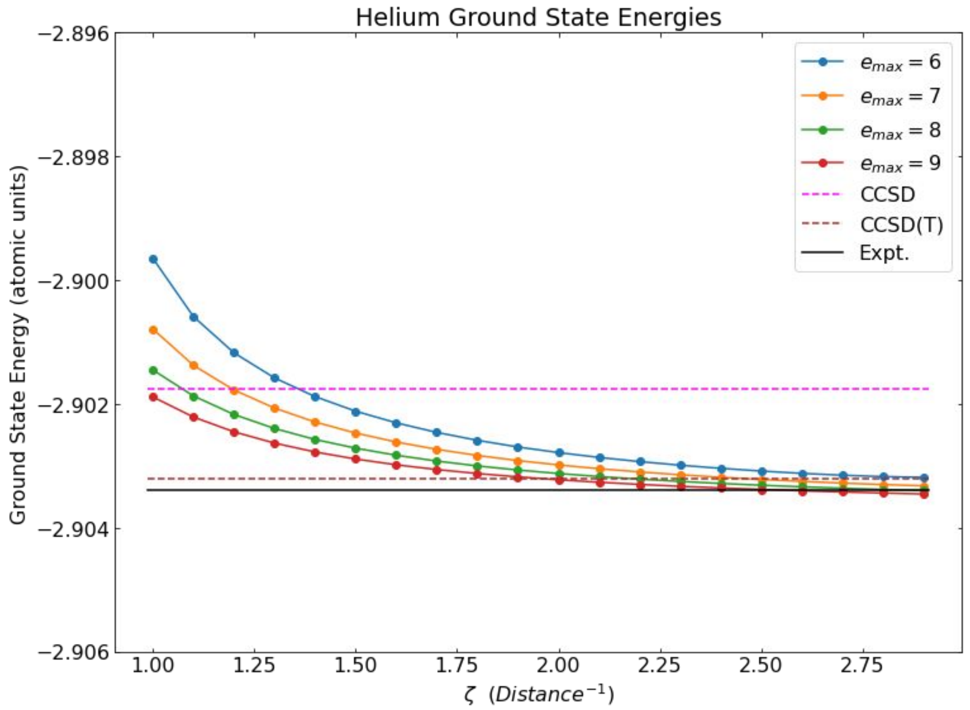
Flambaum et al. Phys Rev A 97, 032510 (2018)

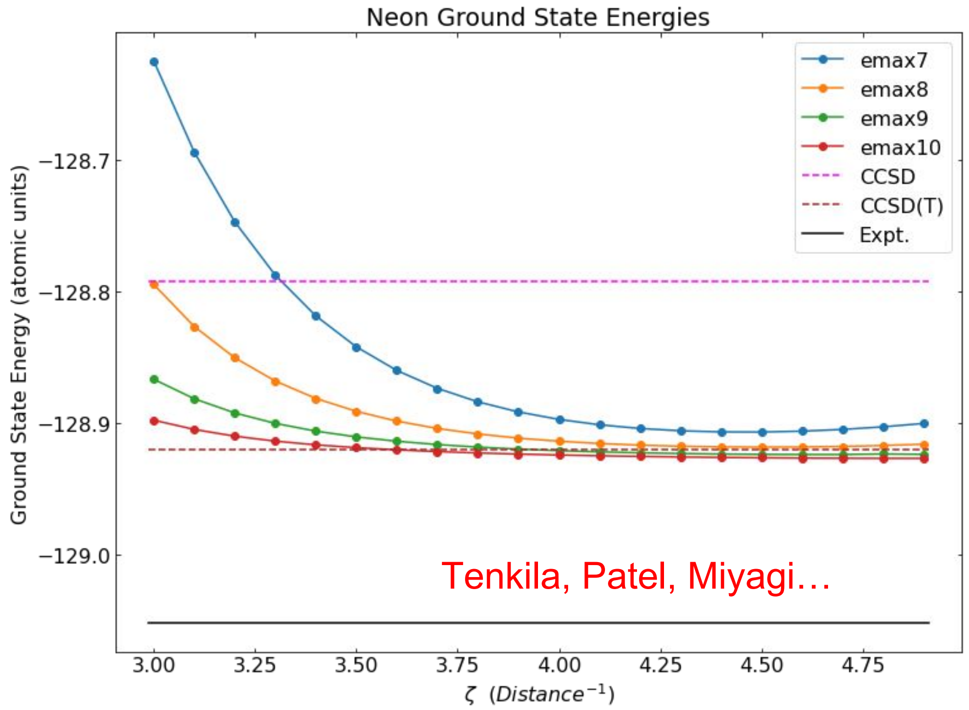
➔ Laser spectroscopy can be used to probe BSM physics

Stadnik et al. Phys Rev Lett 120, 223202 (2018) - Long range neutrino mediated forces

IMSRG for Closed-Shell Atoms

Apply single-reference IMSRG for closed-shell systems





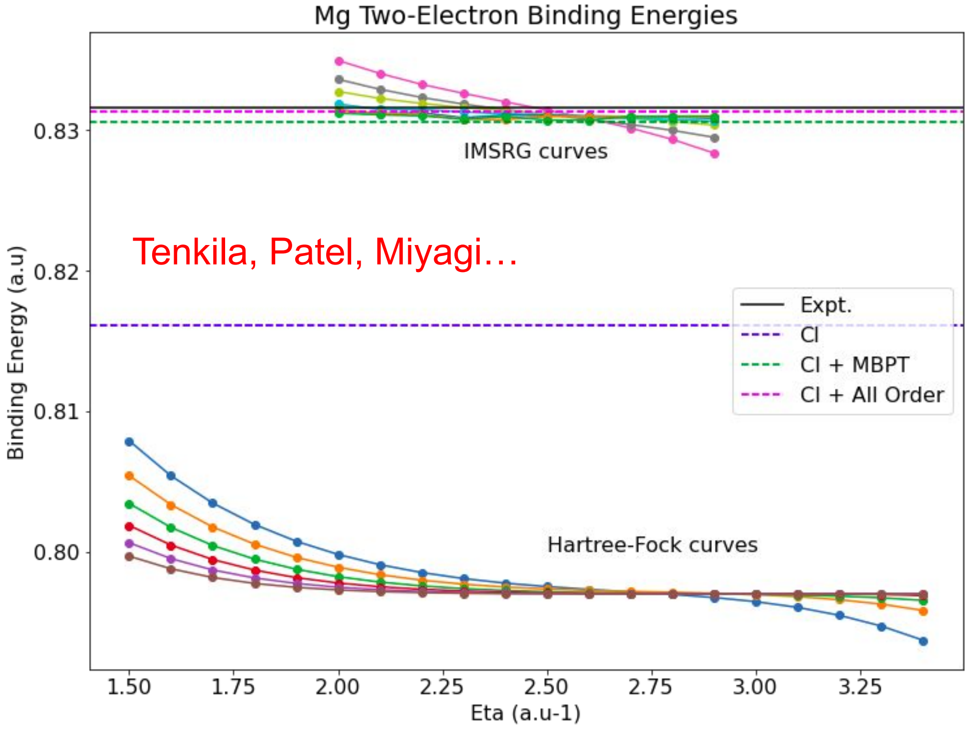
Converges to “best” coupled-cluster results

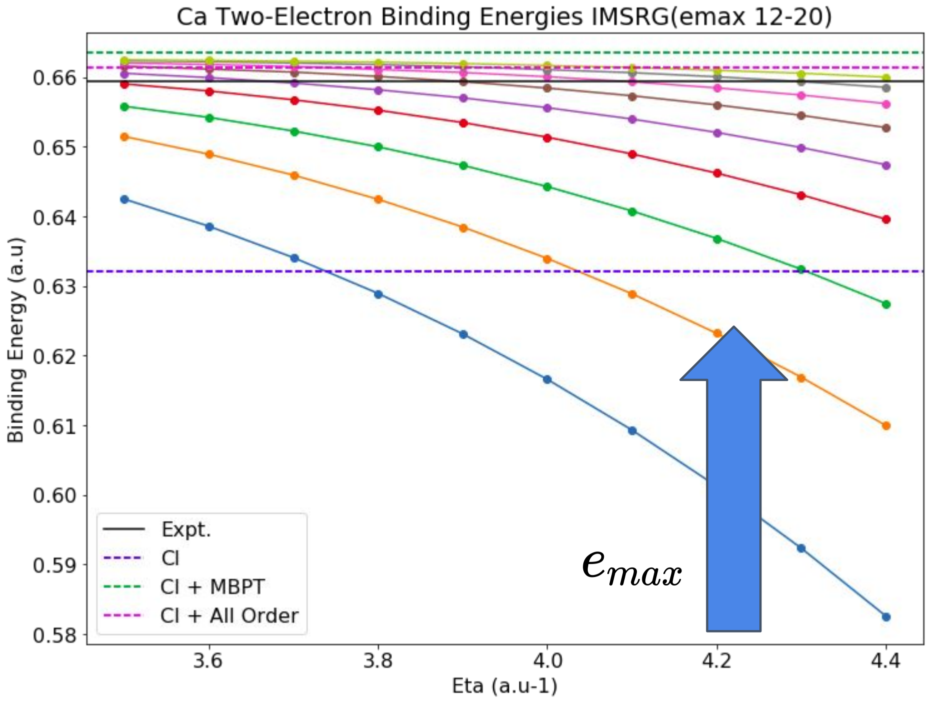
Good experimental agreement for light atoms…

Discrepancies point to neglected relativistic effects

VS-IMSRG for Open-Shell Atoms

Apply VS-IMSRG for binding energies of systems: Mg, Ca



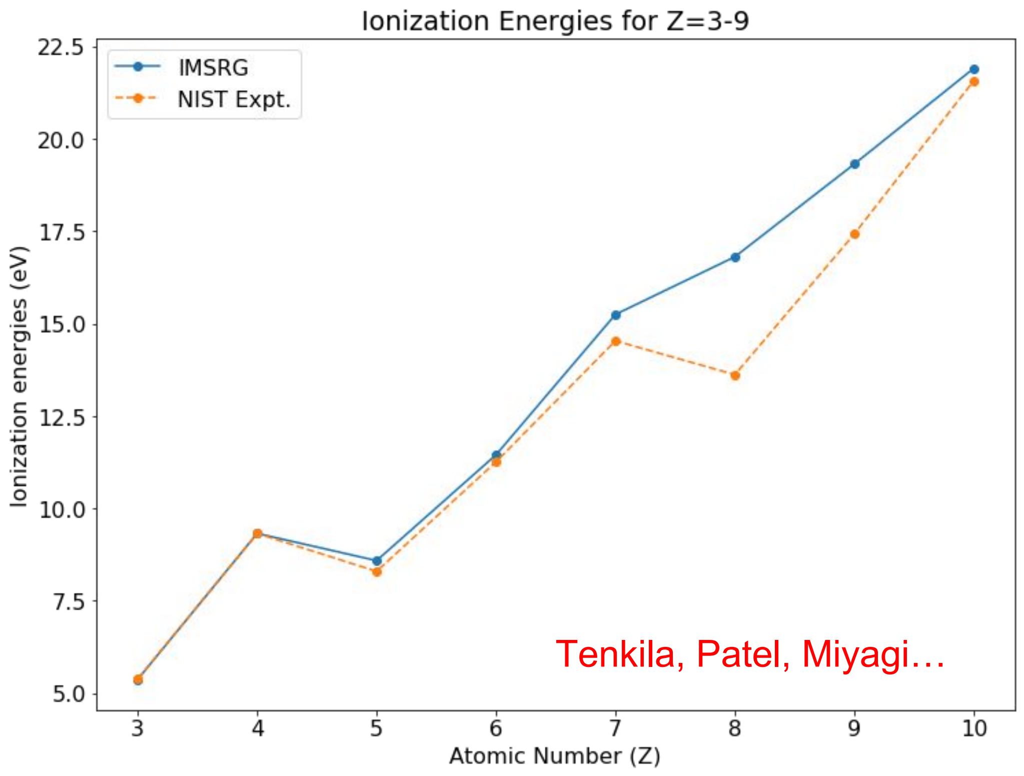


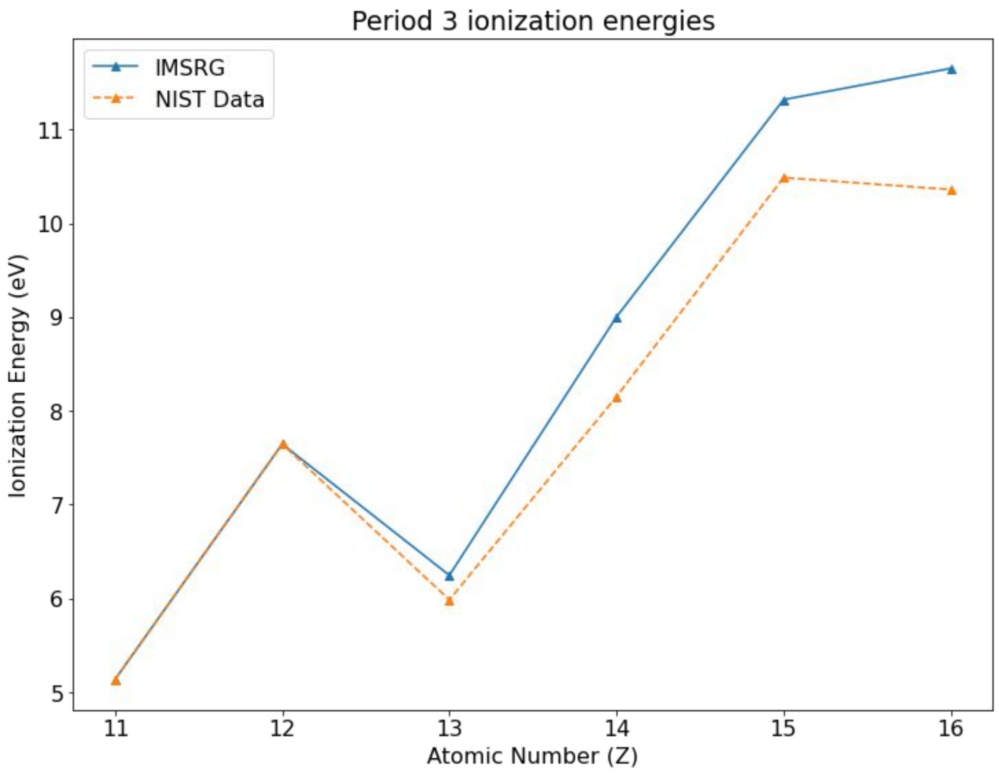
Converges to best available many-body results

Good(?) experimental agreement in both cases

VS-IMSRG for Open-Shell Atoms

Apply VS-IMSRG for ionization energies of systems



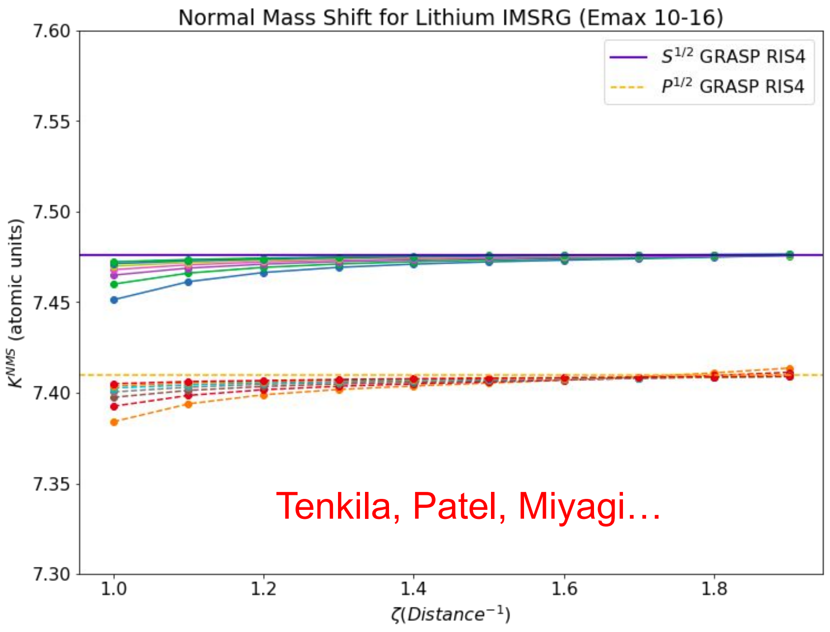


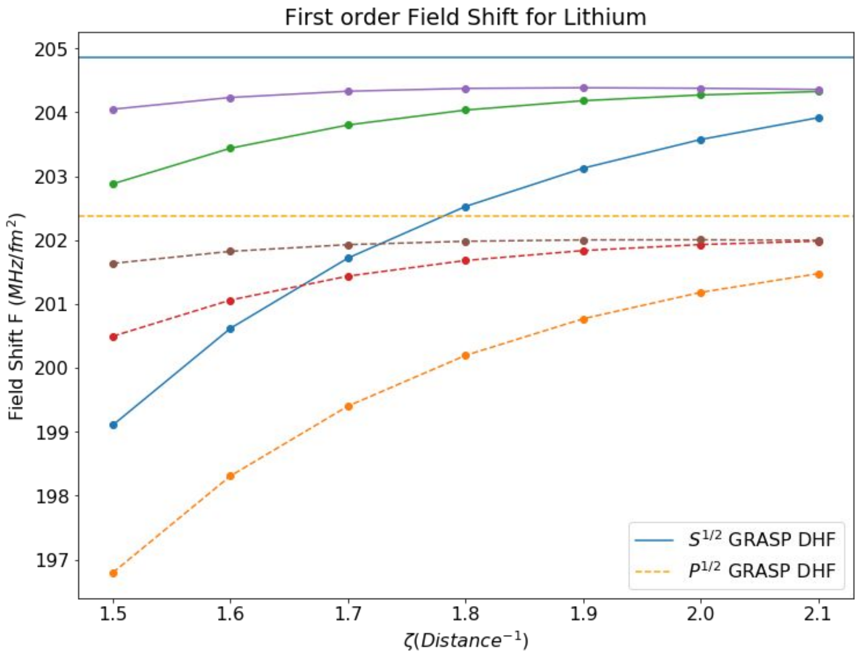
No ab initio calculations available

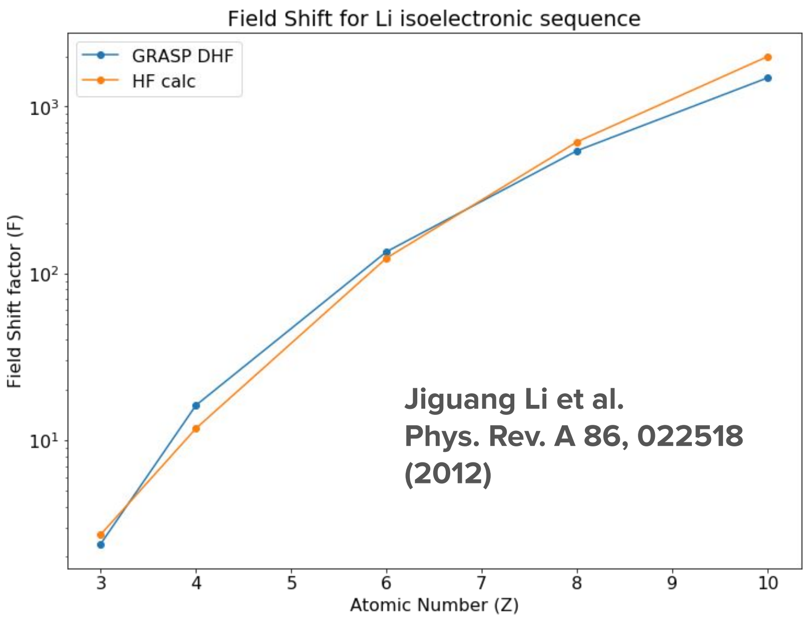
Good(at times) experimental agreement in both cases

VS-IMSRG for Isotope Shifts

VS-IMSRG calculations of isotope shifts in light atoms







Results comparable to currently used code

Extension to Dirac-Hartree-Fock in progress to access heavy atomic systems!