Exploring major nuclear structure issues with rare isotopes

Jason D. Holt
Scientist, Theory Department
Science Week
August 19, 2020

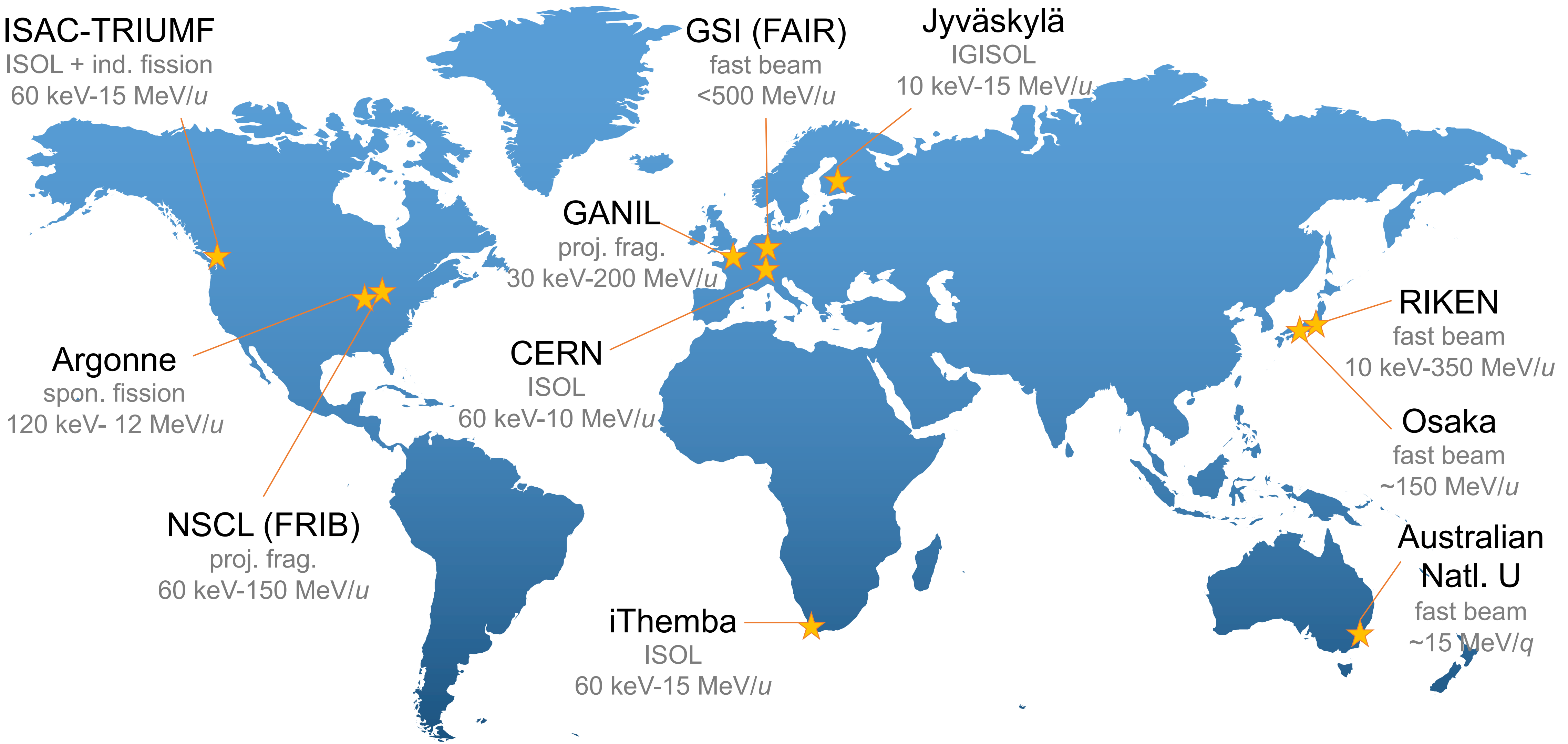
Discovery, accelerated

Next-generation RIB facilities: unprecedented era of nuclear science

Major RIB Facilities

Thousands of new isotopes to be produced – need intense beams to probe essential properties

Q: How do we avoid “stamp collecting”?

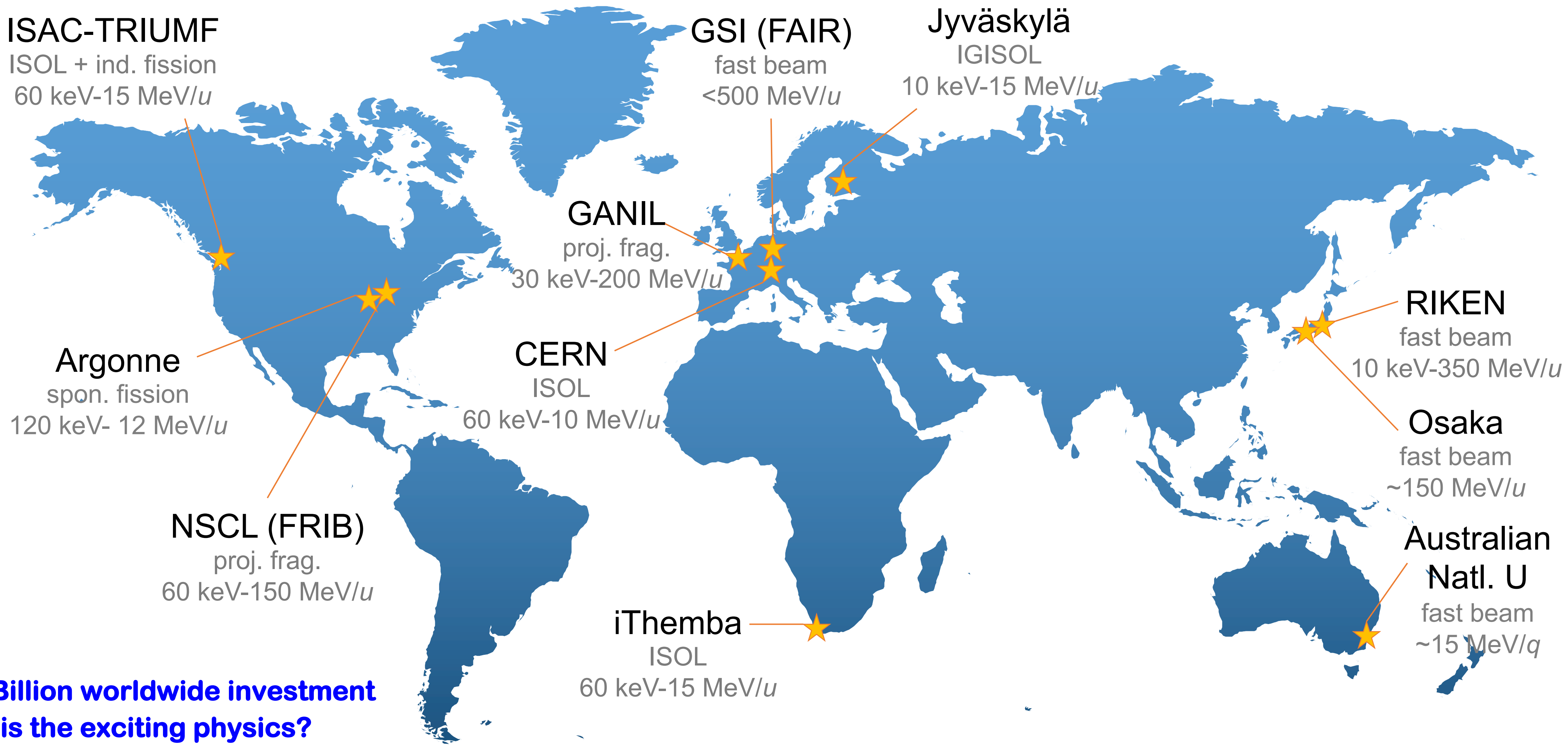


Next-generation RIB facilities: unprecedented era of nuclear science

Major RIB Facilities

Thousands of new isotopes to be produced – need intense beams to probe essential properties

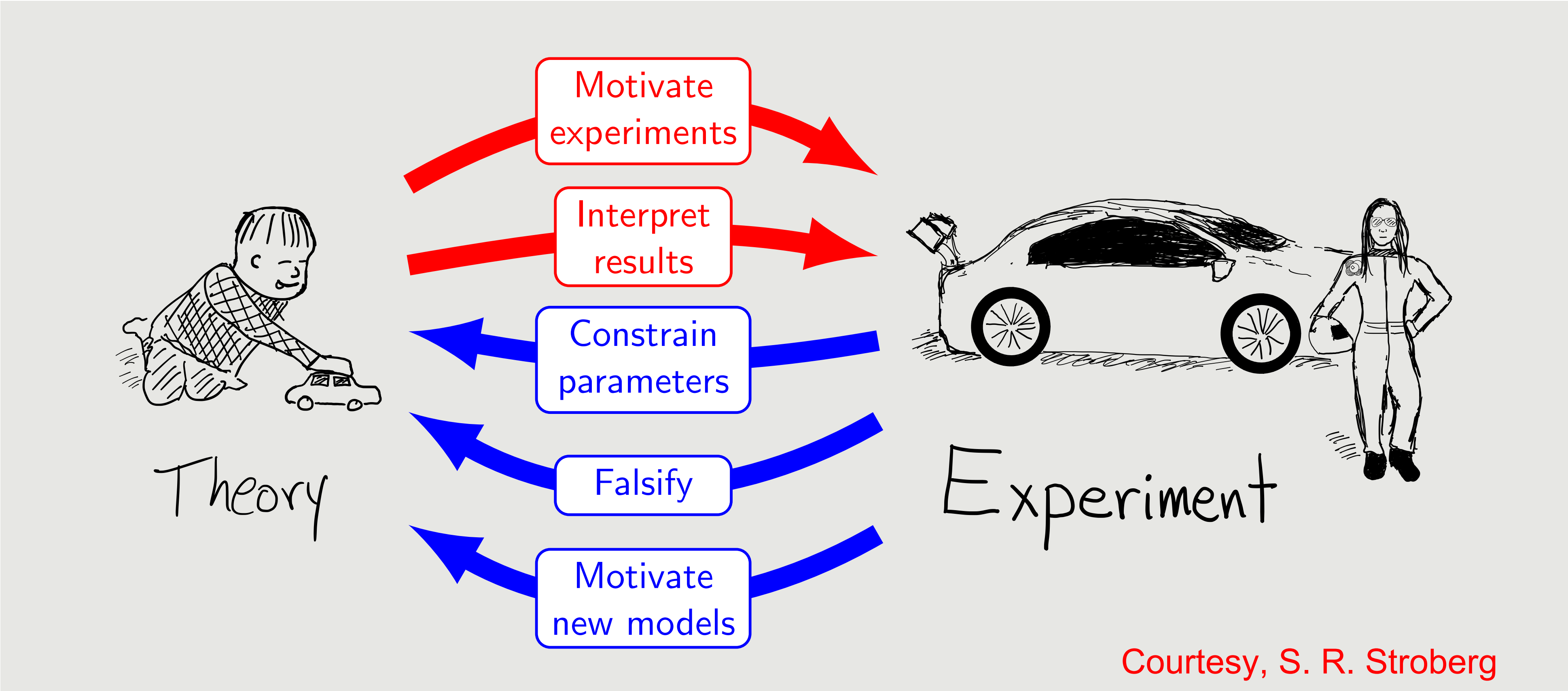
Q: How do we avoid “stamp collecting”? A: **Meaningful interplay with theory**



$4-5 Billion worldwide investment
What is the exciting physics?

How Science Works

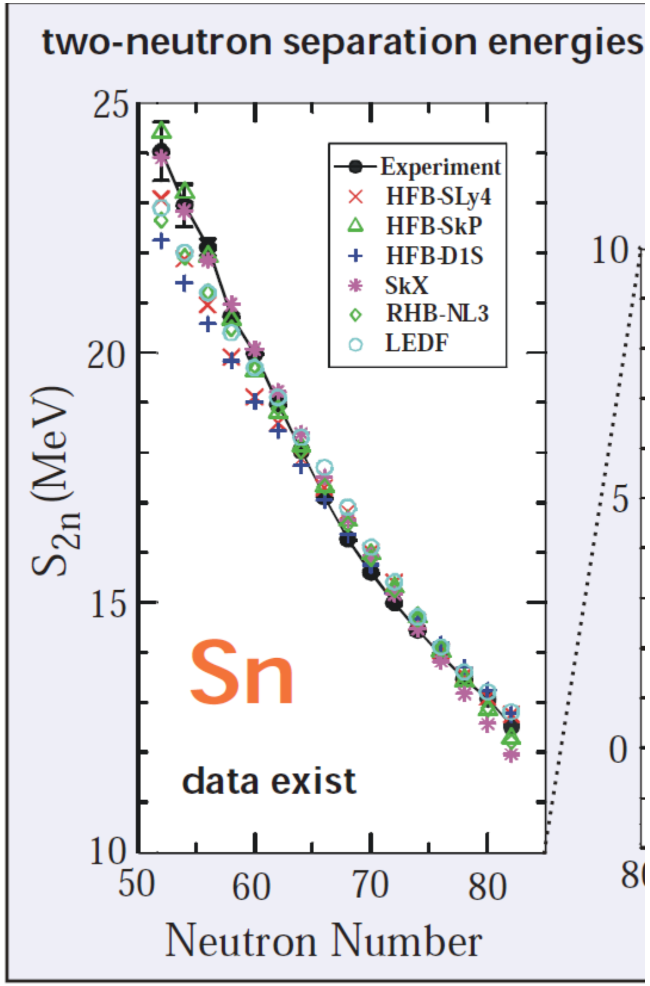
Big questions largely driven by theory; similar needs for all RIB facilities – is theory ready??



How do we currently approach nuclear theory?

Predictions with Nuclear Models

How well can models motivate experiments?



Agreement good where data exists

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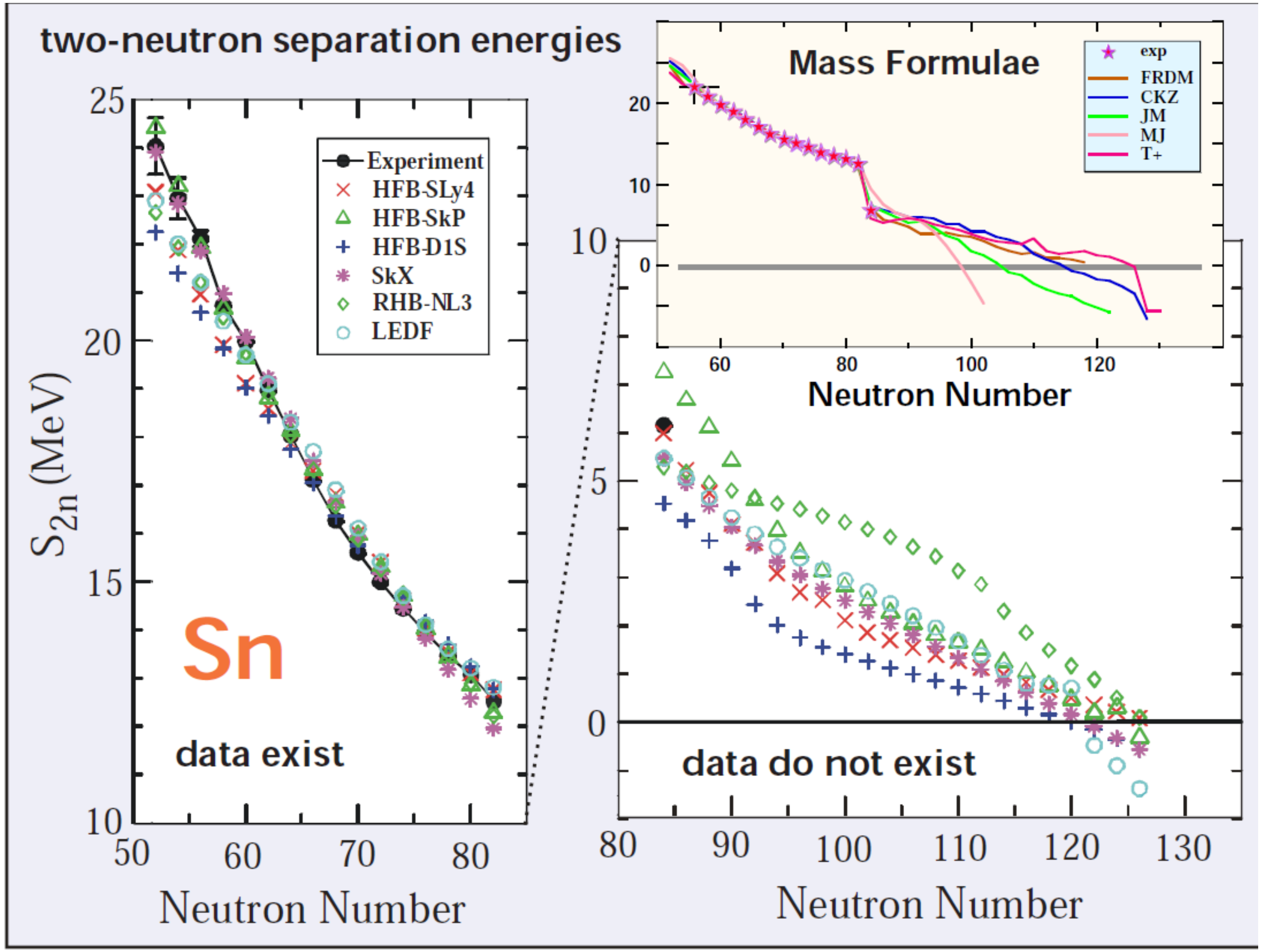
How well can models motivate experiments?



Often extrapolates unreliably

Spread in results = meaningful uncertainty?

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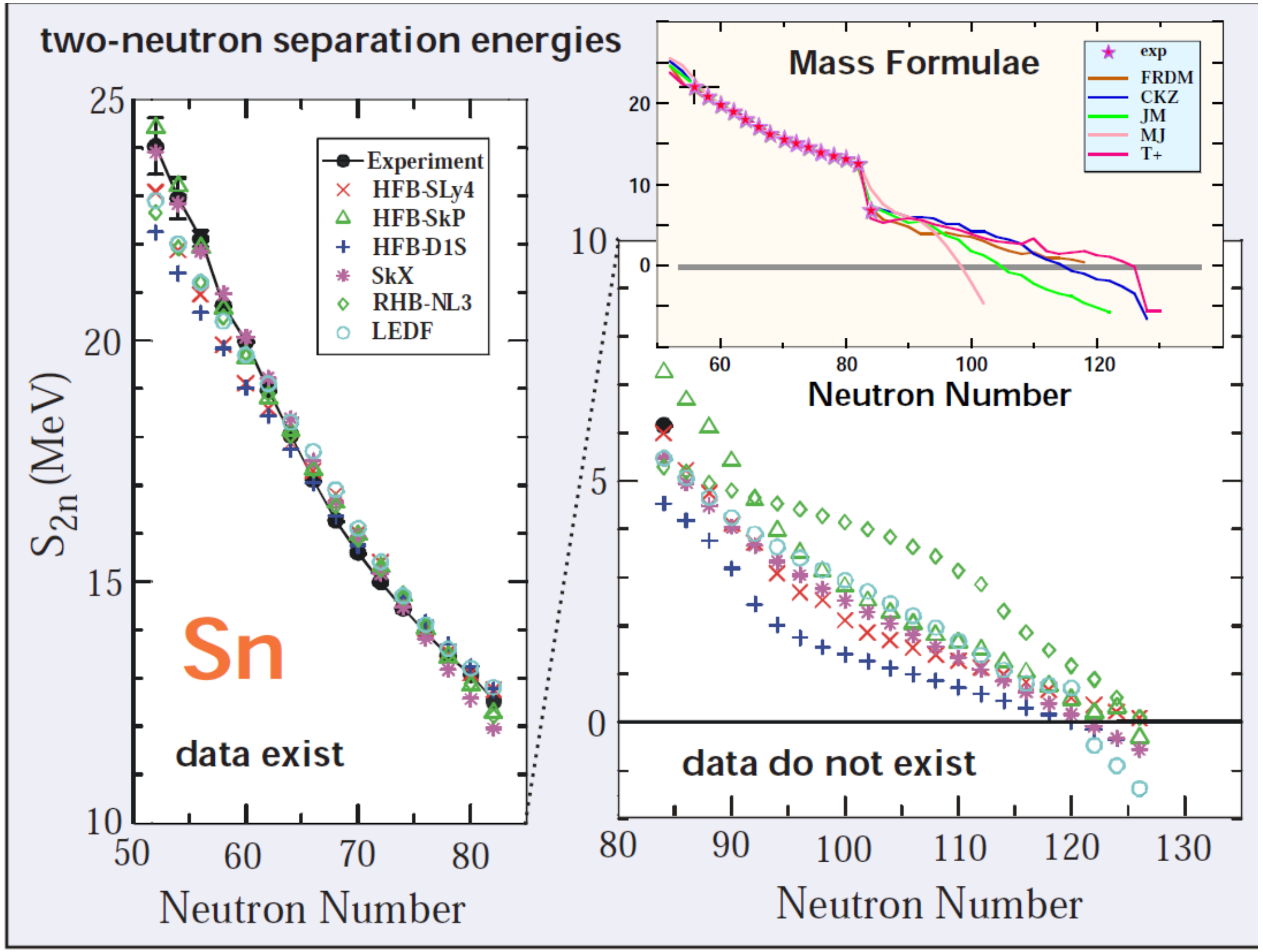
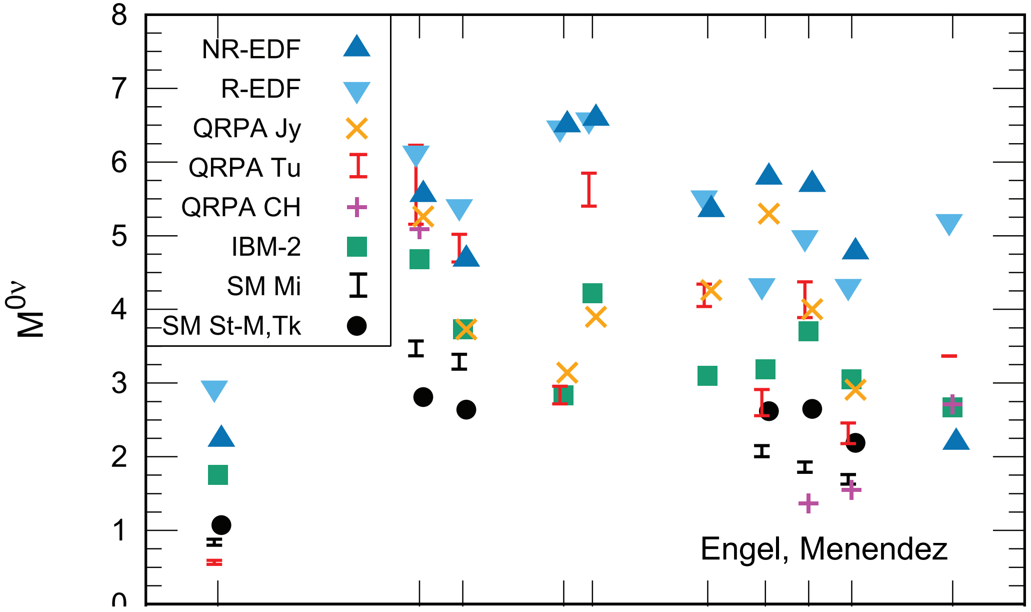
How well can models motivate experiments?



Analogous picture in double beta decay



More billions invested worldwide

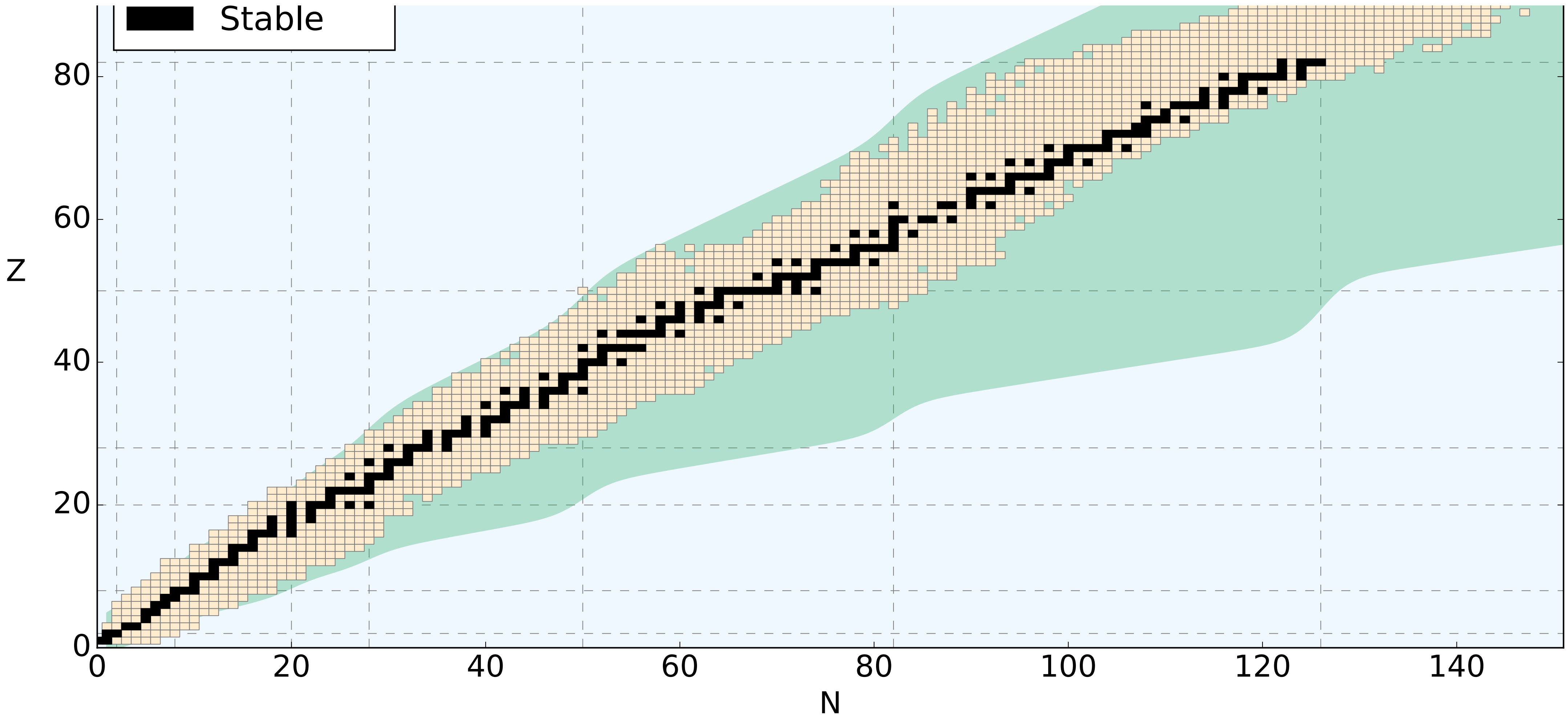
Often extrapolates unreliably

Spread in results = meaningful uncertainty?

Ab Initio Theory for Atomic Nuclei

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

$$H\psi_n = E_n\psi_n$$



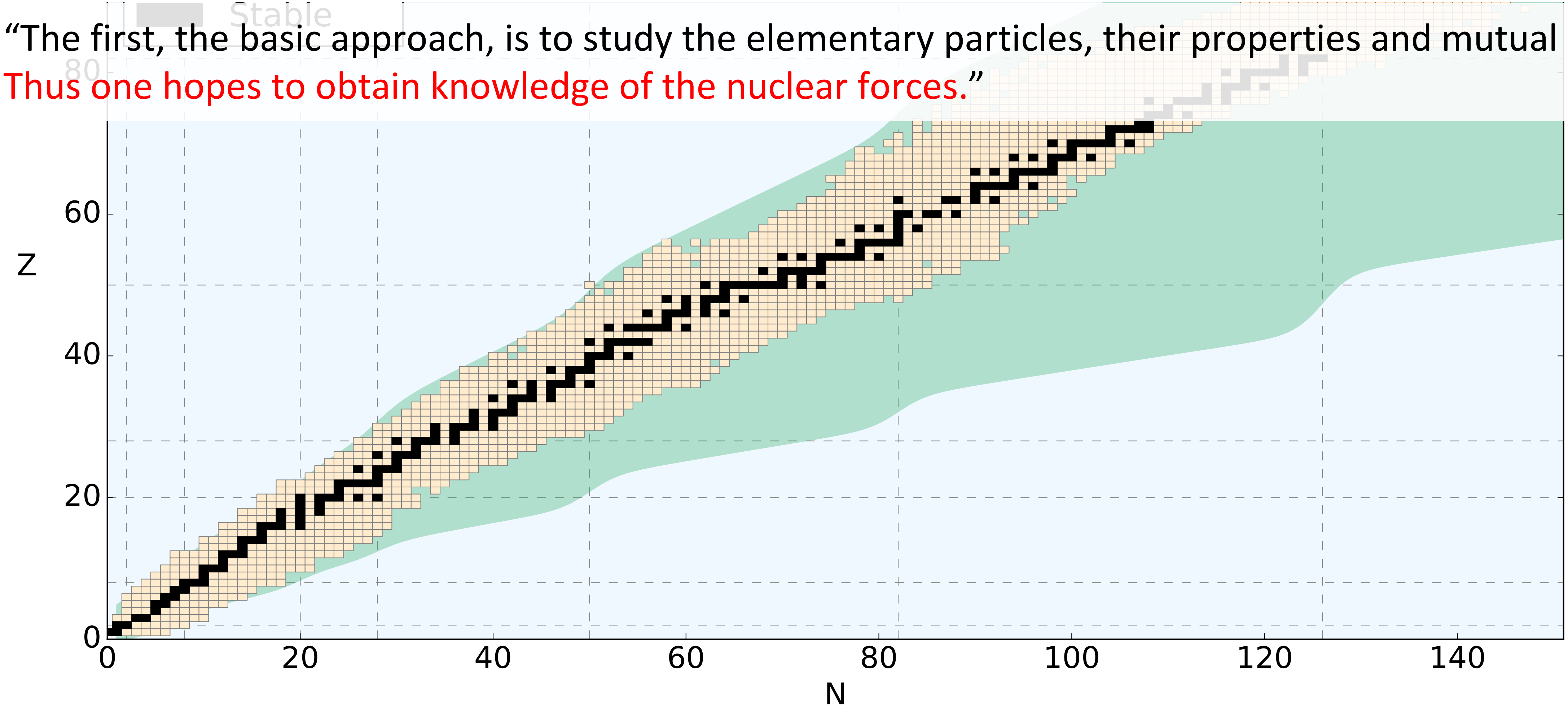
Ab Initio Theory for Atomic Nuclei

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

- Nuclear forces (low-energy QCD)
- Electroweak physics

$$H\psi_n = E_n\psi_n$$

"The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces."



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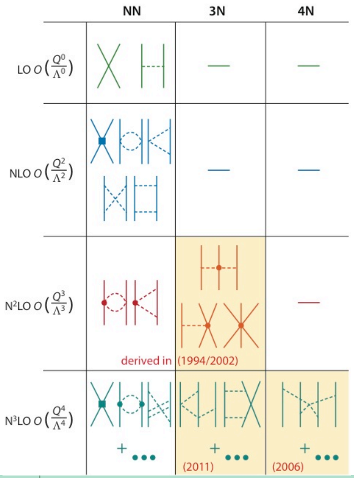
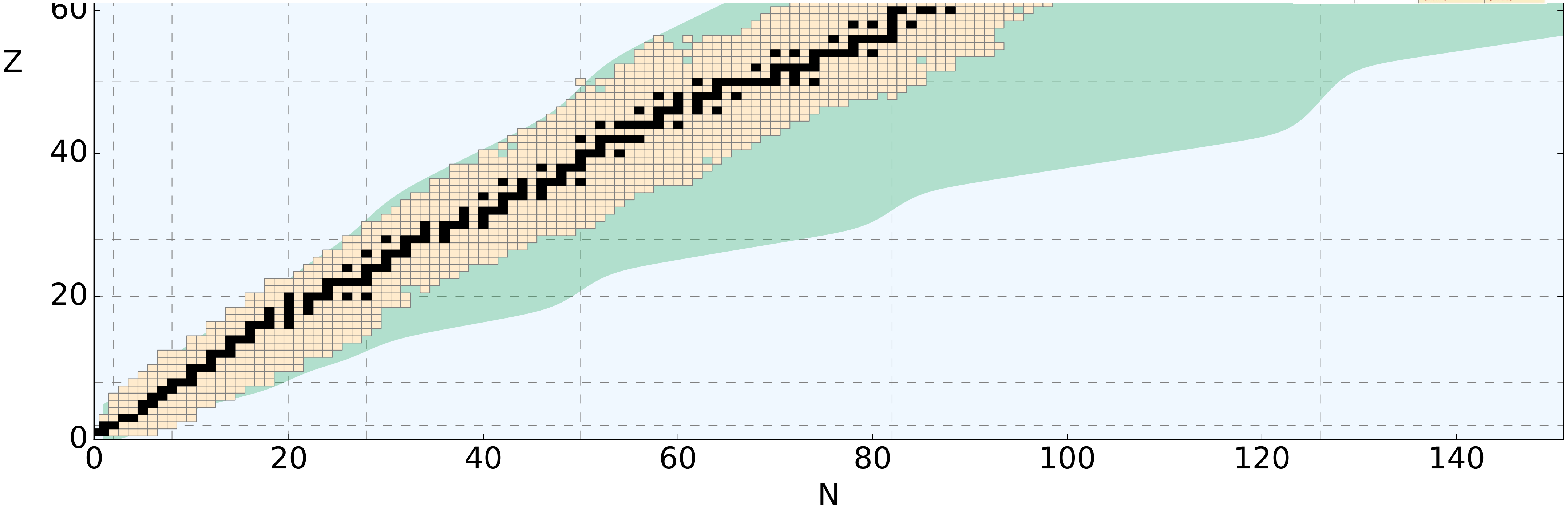


Chiral effective field theory: systematic expansion of nuclear interactions

Consistent 3N forces, electroweak currents

Quantifiable uncertainties possible



Ab Initio Theory for Atomic Nuclei

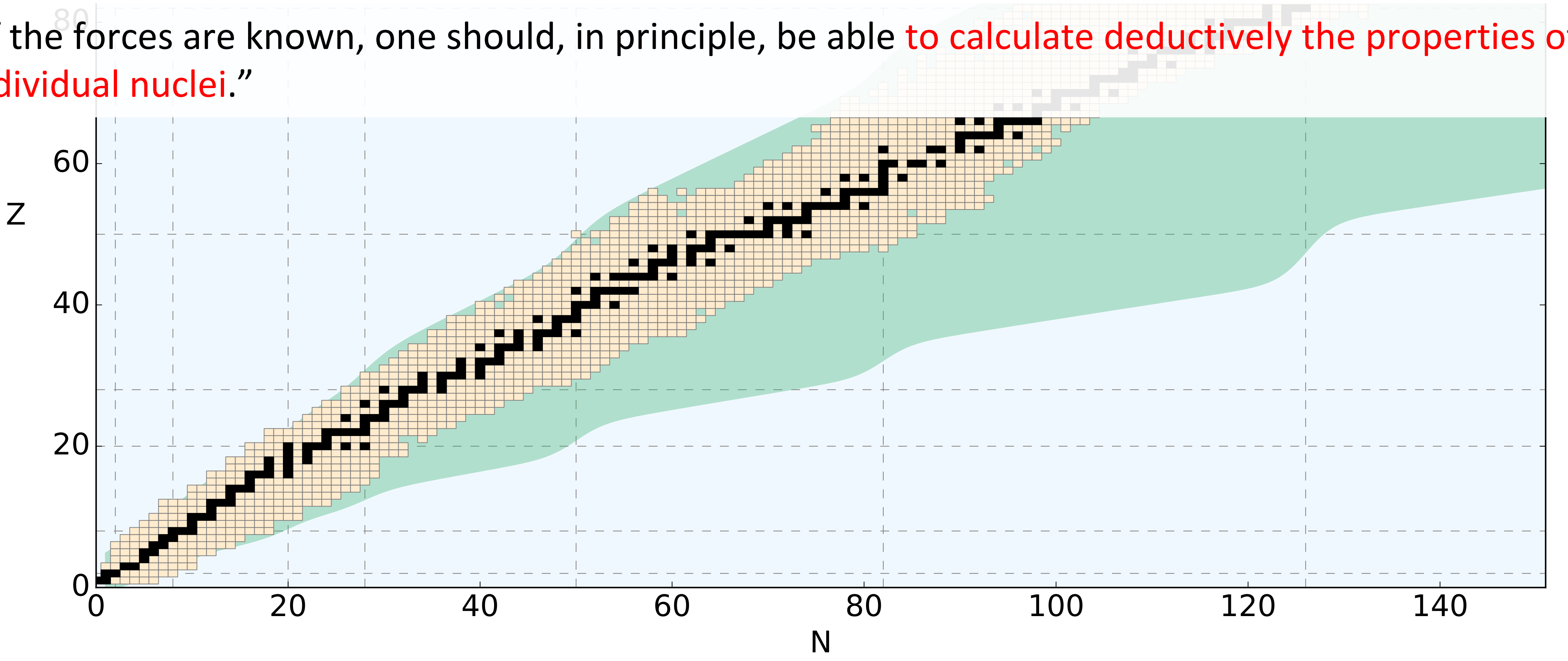
TRIUMF

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

- Nuclear forces (low-energy QCD)
- Electroweak physics
- **Nuclear many-body problem**

$$H\psi_n = E_n\psi_n$$

"If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei."

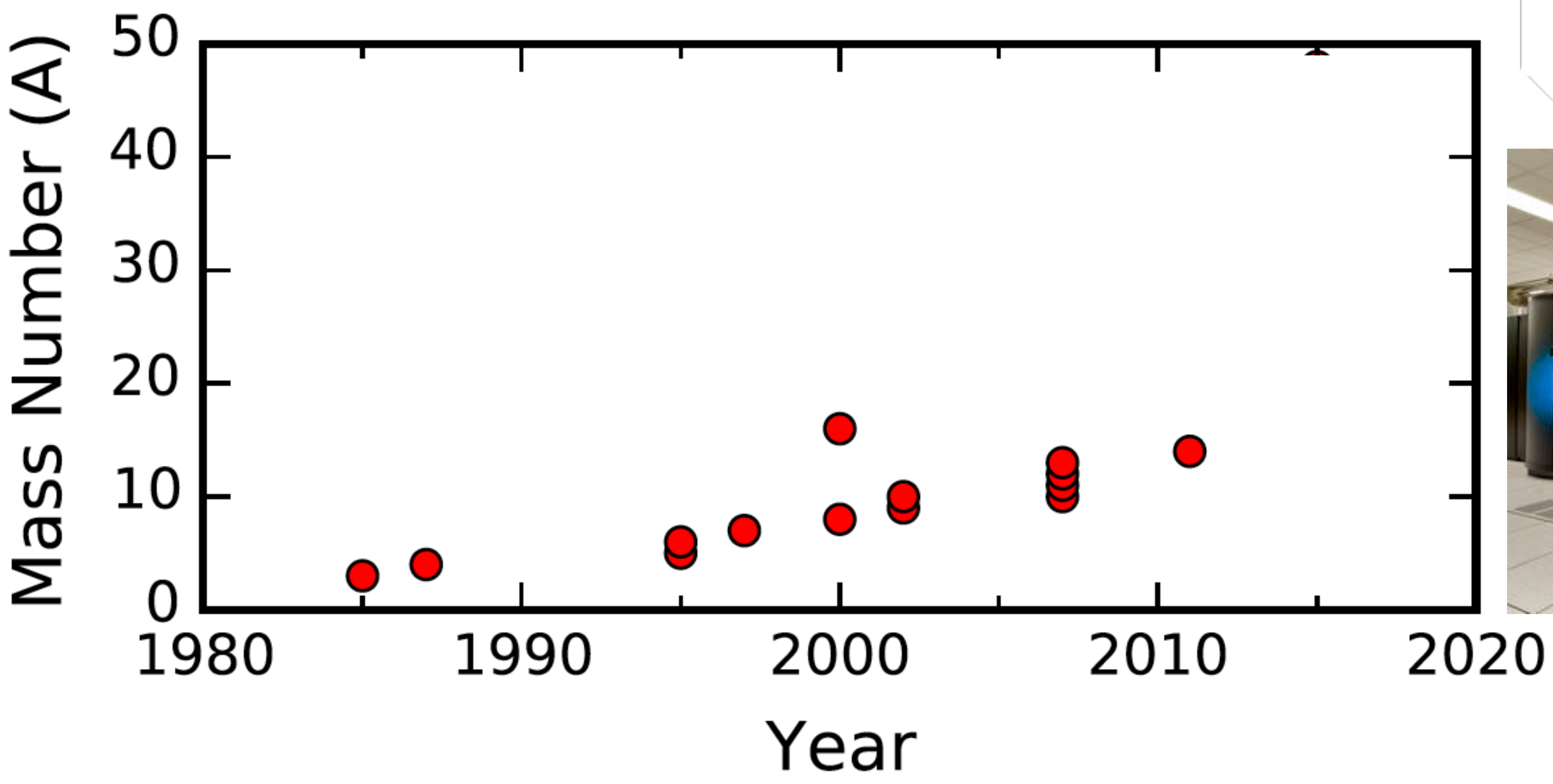


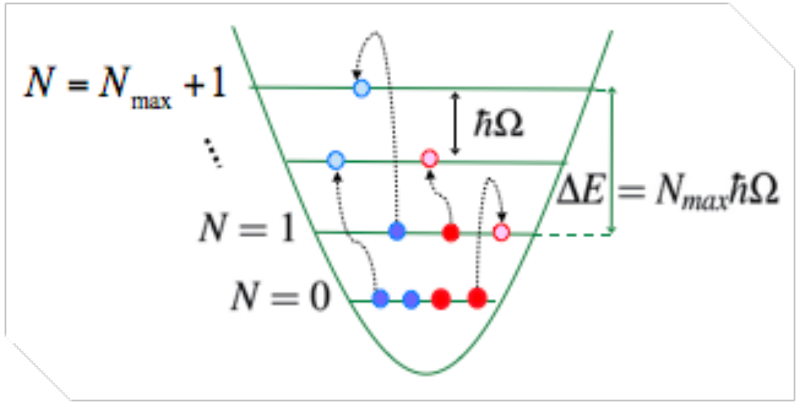
Chronological Reach of Ab Initio Theory

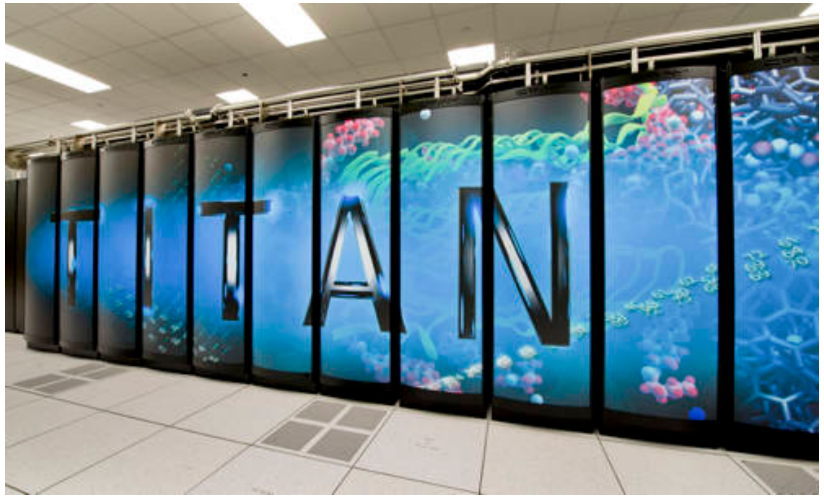
Moore's law: exponential growth in computing power

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

TRIUMF







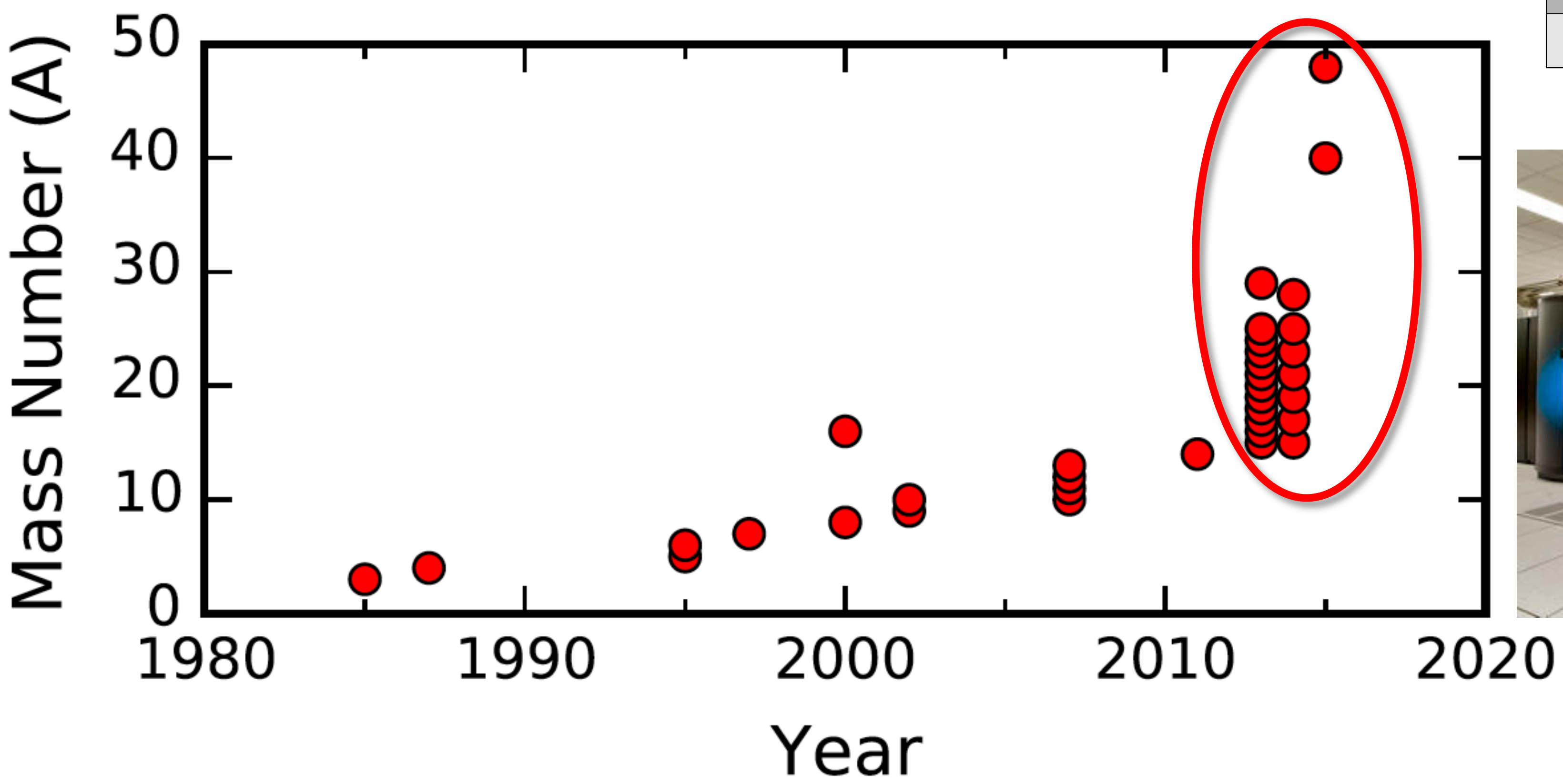
Chronological Reach of Ab Initio Theory

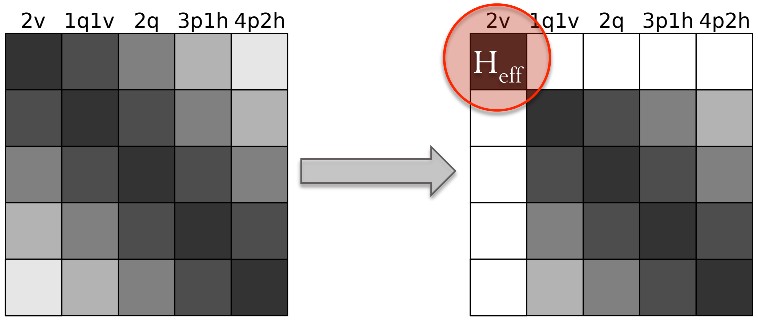
Moore's law: exponential growth in computing power

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

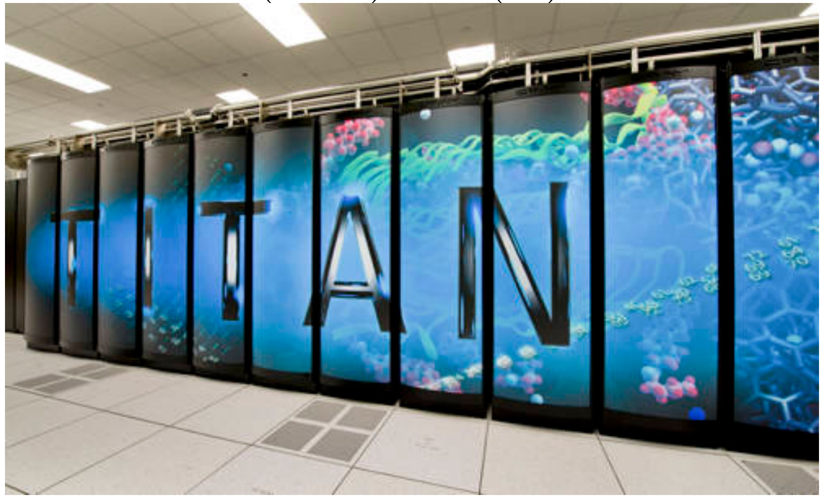
Polynomial scaling methods developed (**CC**, **VS-IMSRG**, SCGF)

Explosion in limits of ab initio theory





$H(s=0) \to H(\infty)$



Chronological Reach of Ab Initio Theory

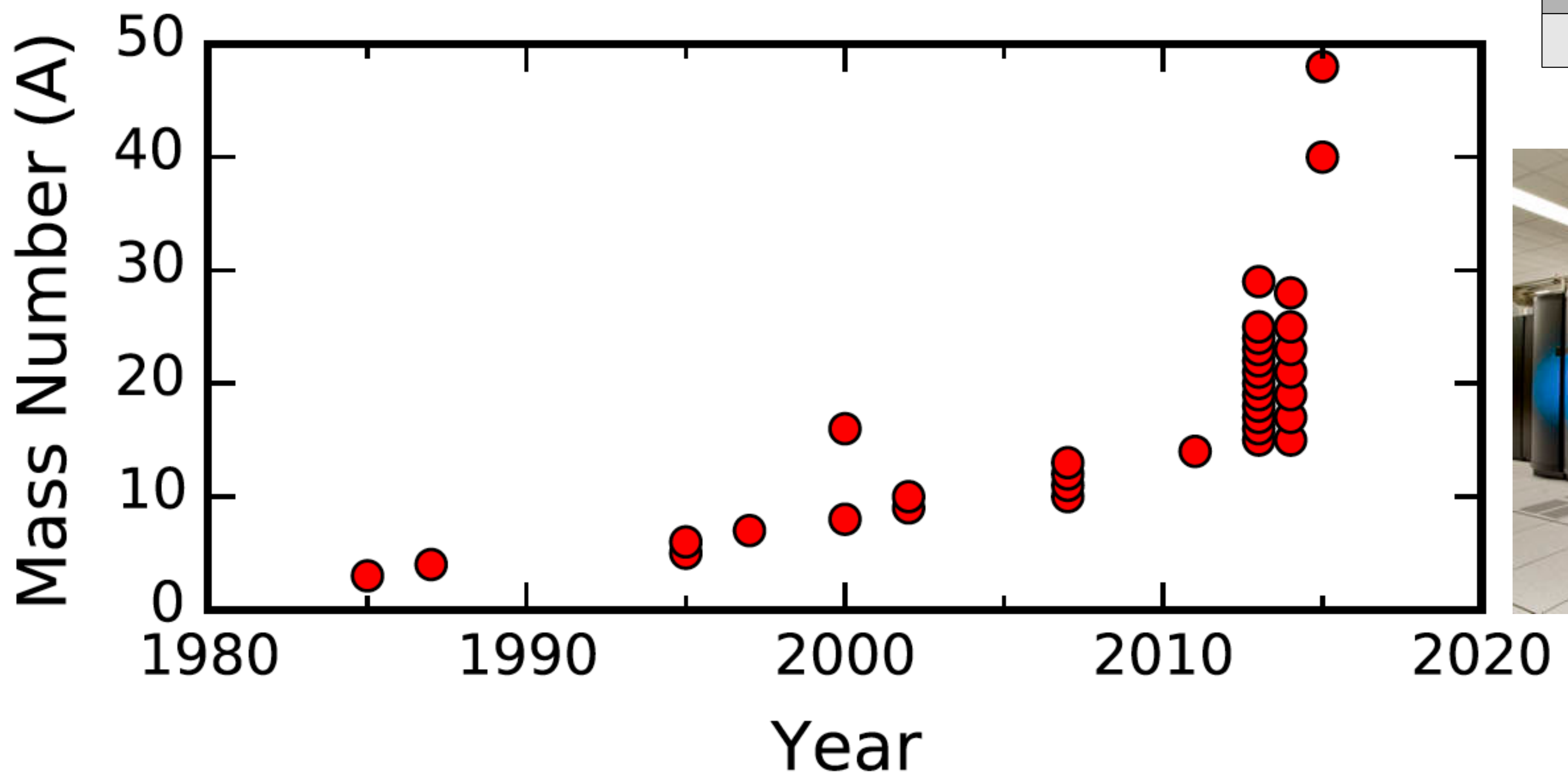
2020: A>100?

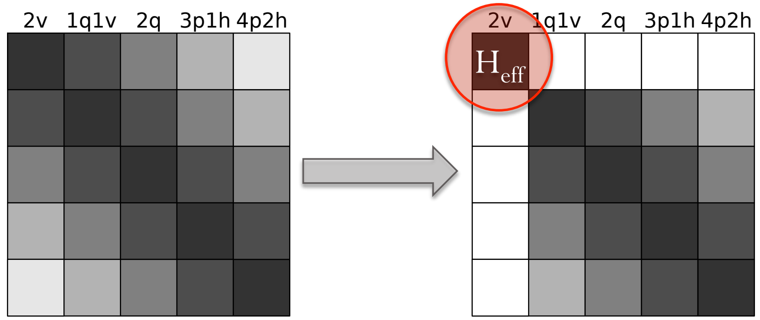
Moore's law: exponential growth in computing power

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

Polynomial scaling methods developed (CC, VS-IMSRG,…)

Explosion in limits of ab initio theory





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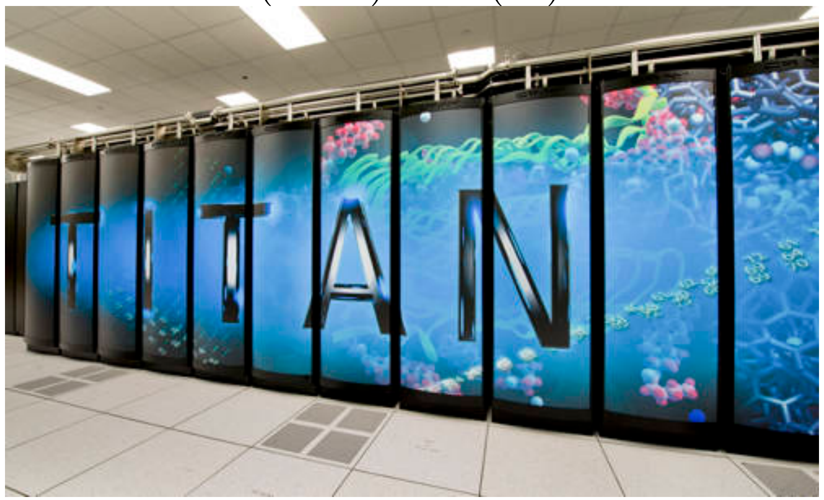
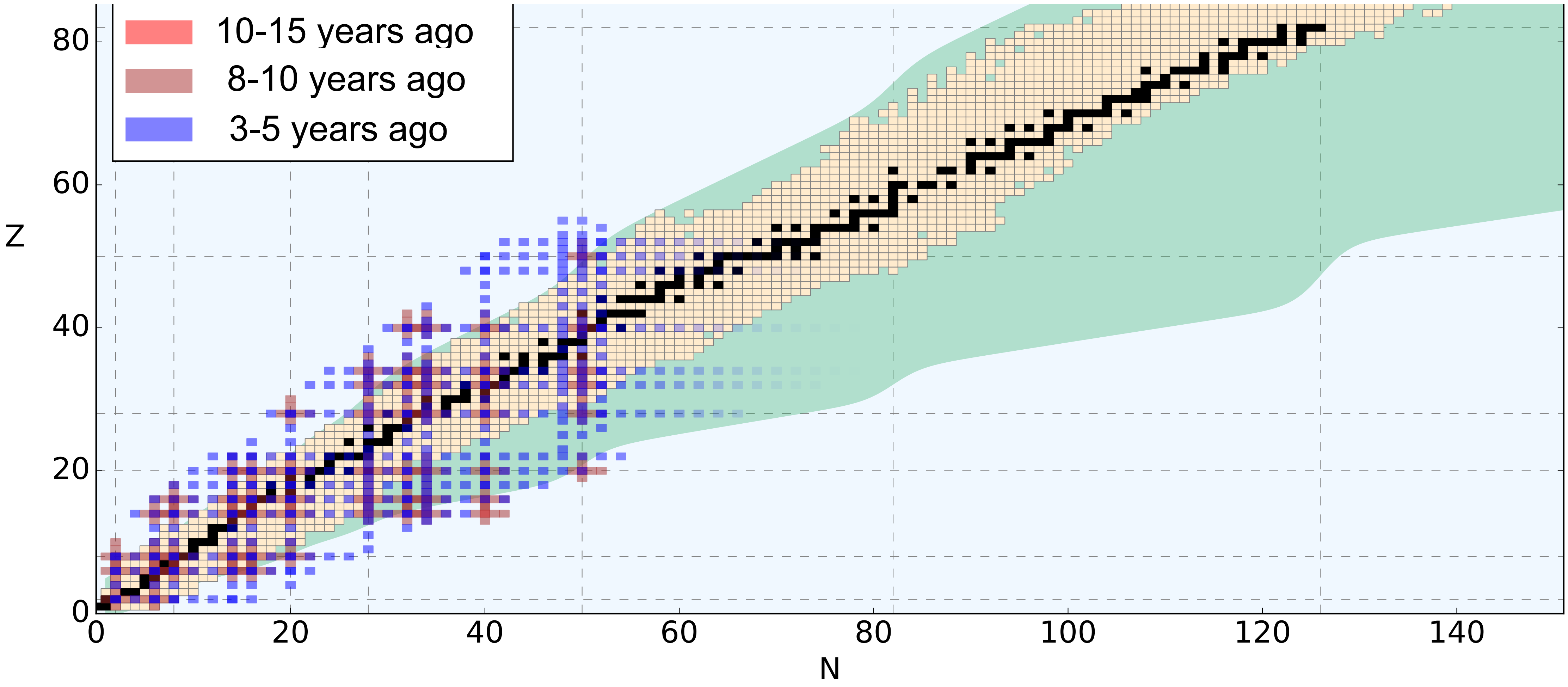


Breadth of Ab Initio Theory

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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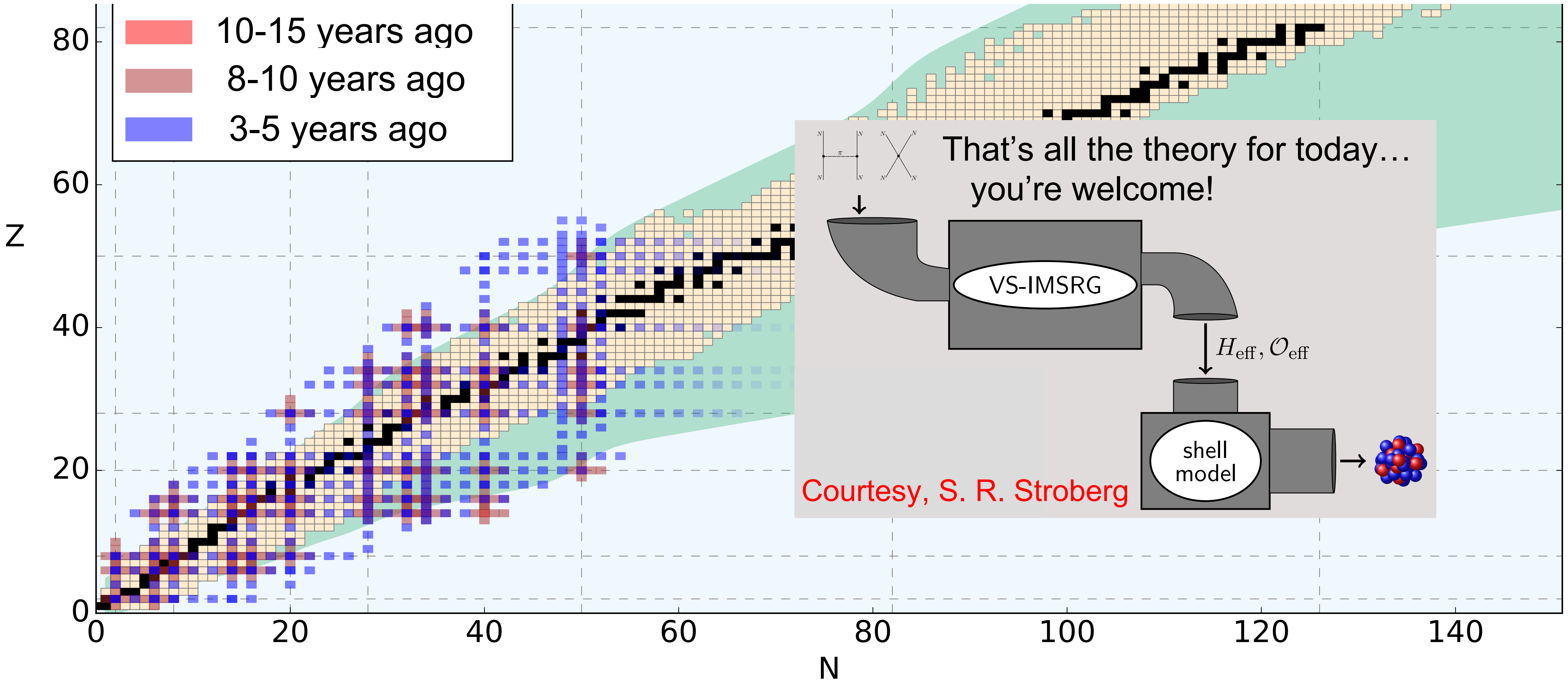

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Towards Global Ab Initio Calculations

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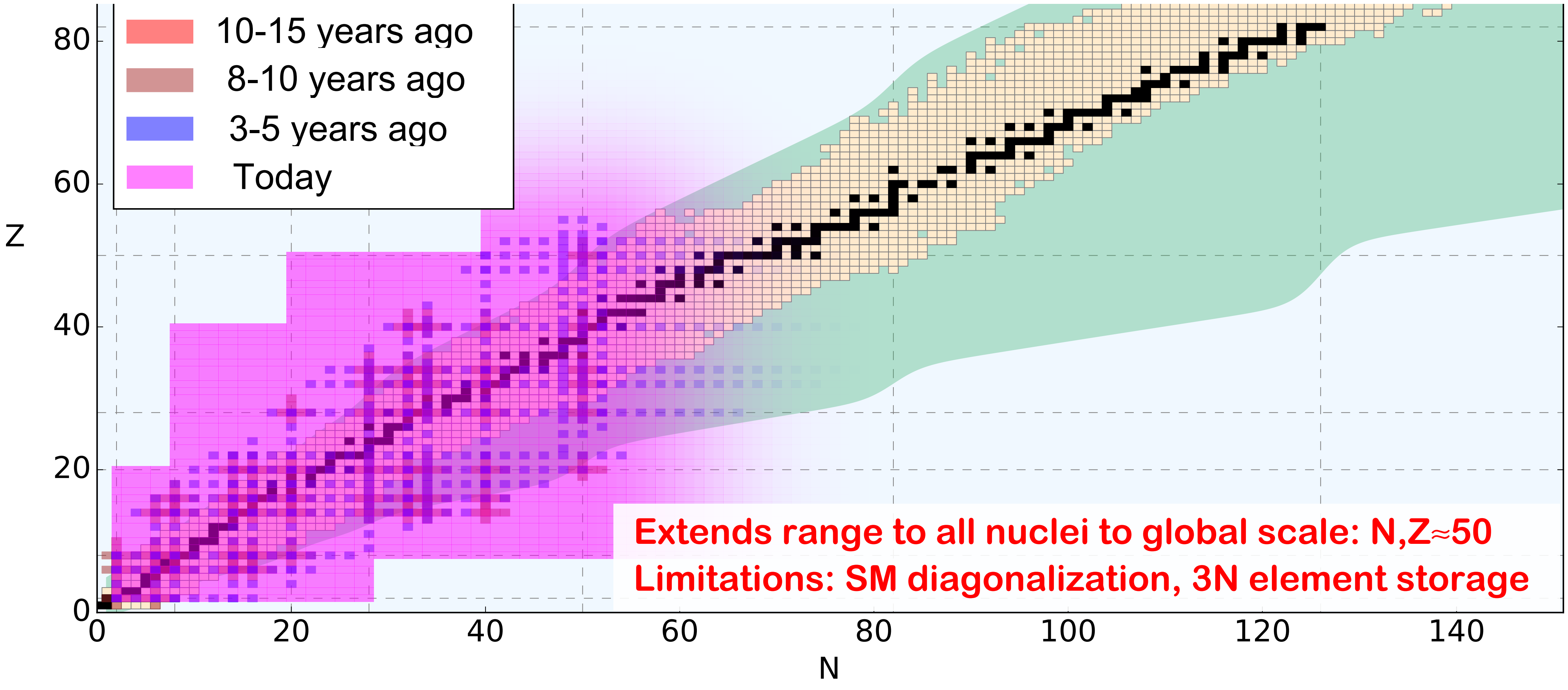

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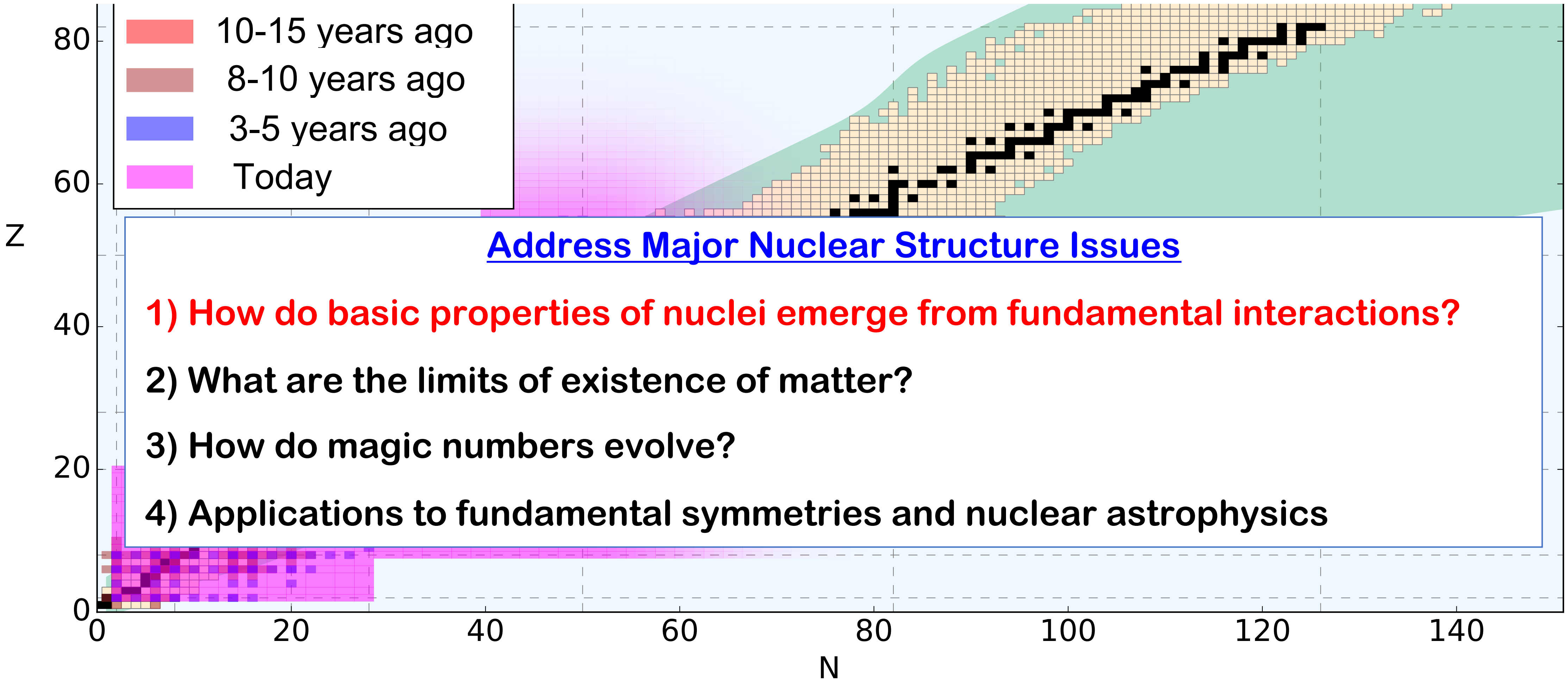

Address Major Nuclear Structure Issues

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) Applications to fundamental symmetries and nuclear astrophysics

Laser Spectroscopy: Charge Radii Across Chains

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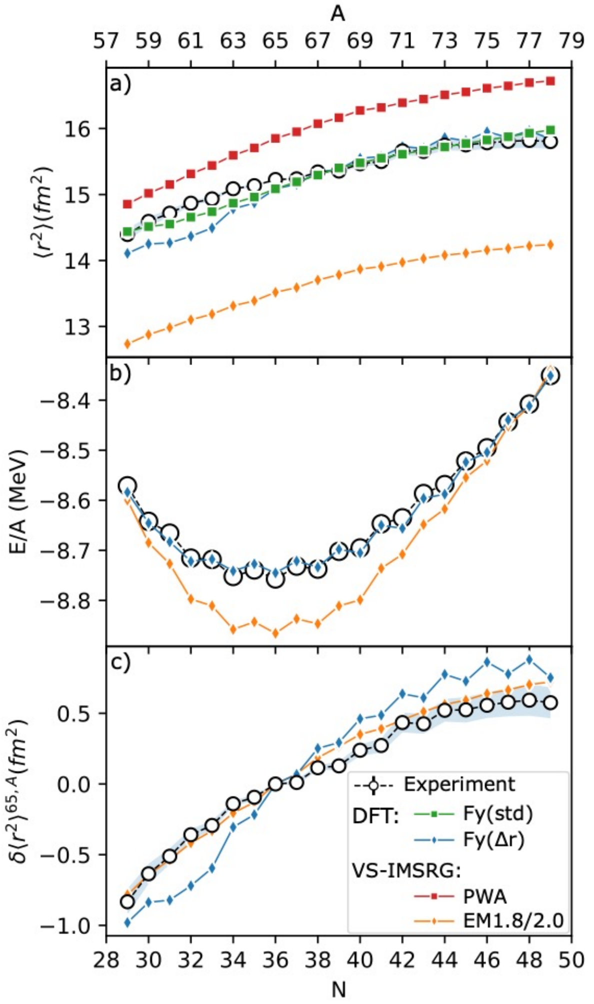
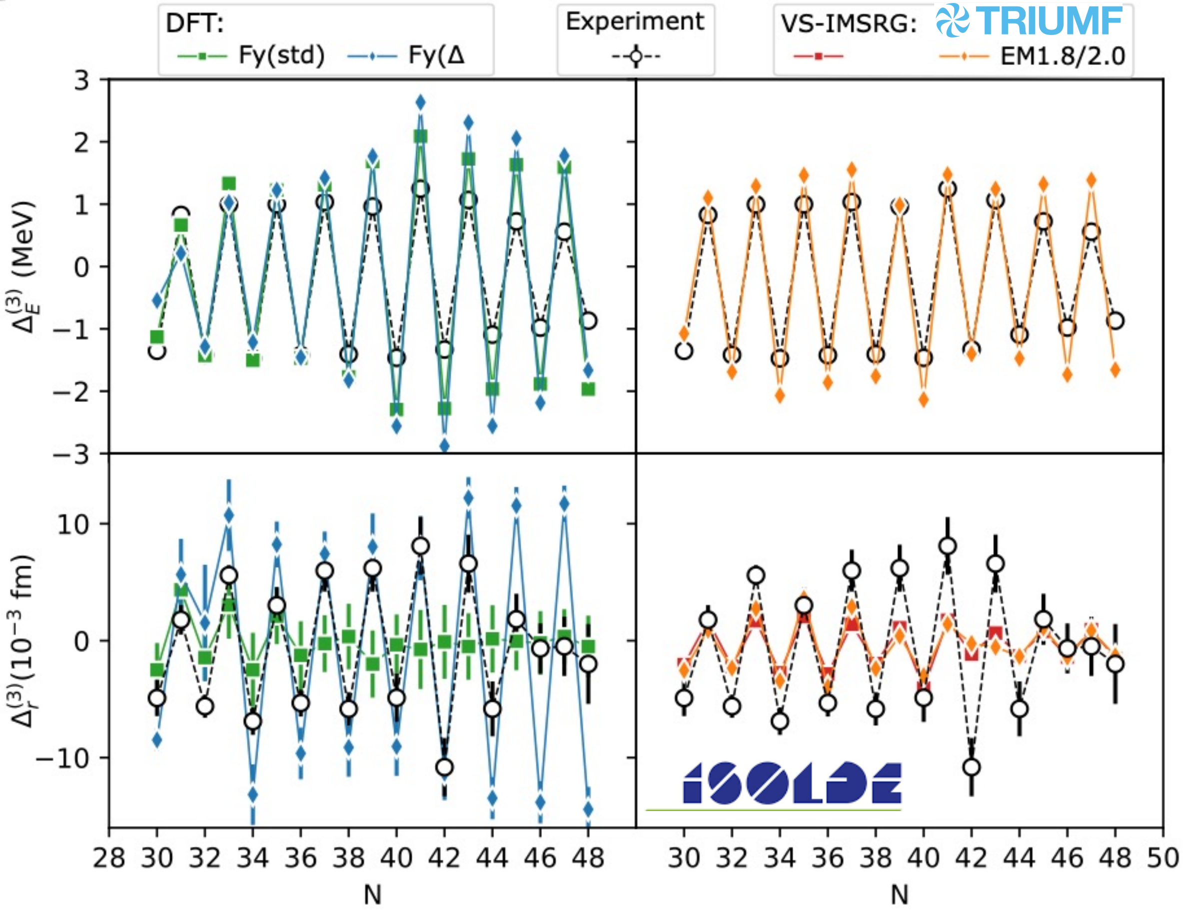
Study odd-even staggering of charge radii across isotopic chains





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

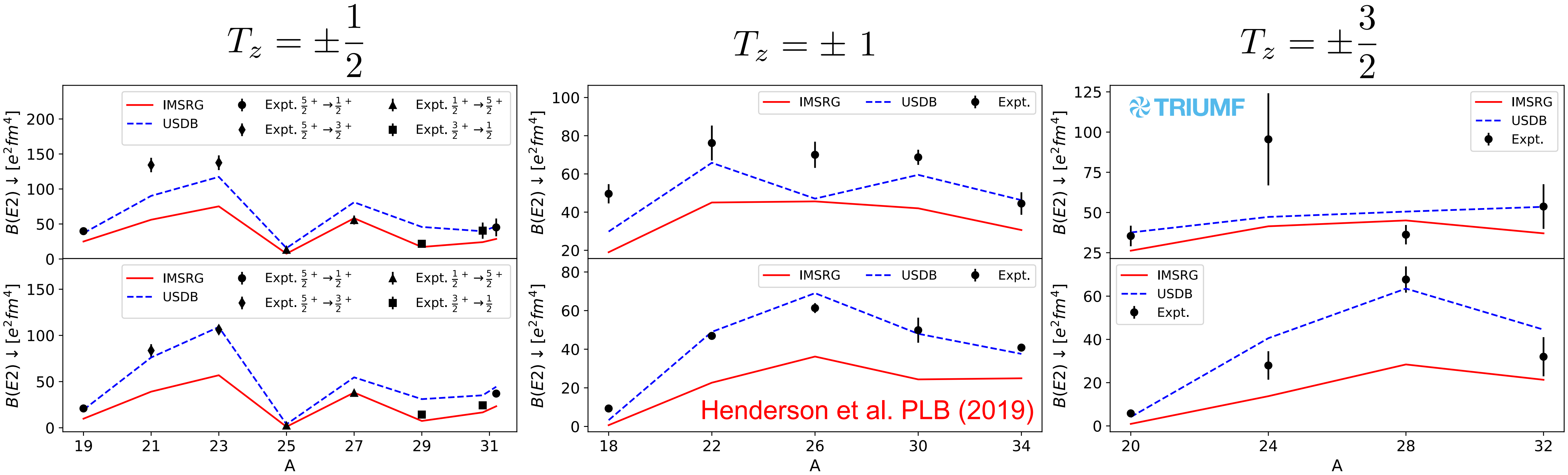
de Groote et al., Nature Phys. (2019)

Cu isotopes, odd-even staggering well reproduced

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

Global Trends in Absolute B(E2): sd Shell

Study charge E2 transitions across sd-shell



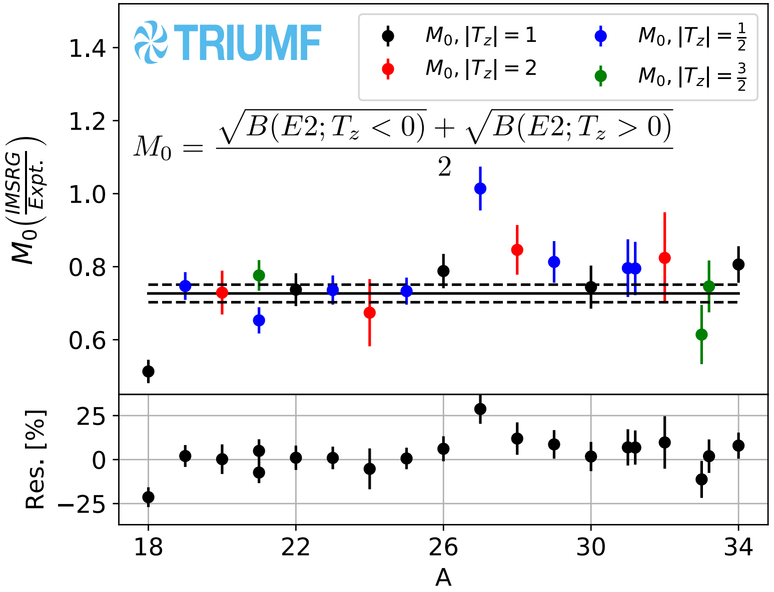
USDB with effective charges typically reproduces absolute values well

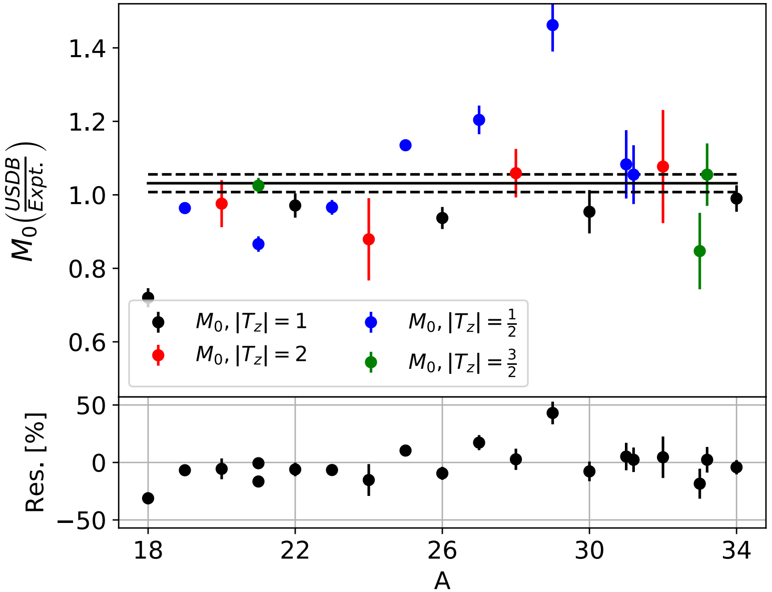
VS-IMSRG (**no effective charges**) typically underpredicts experiment

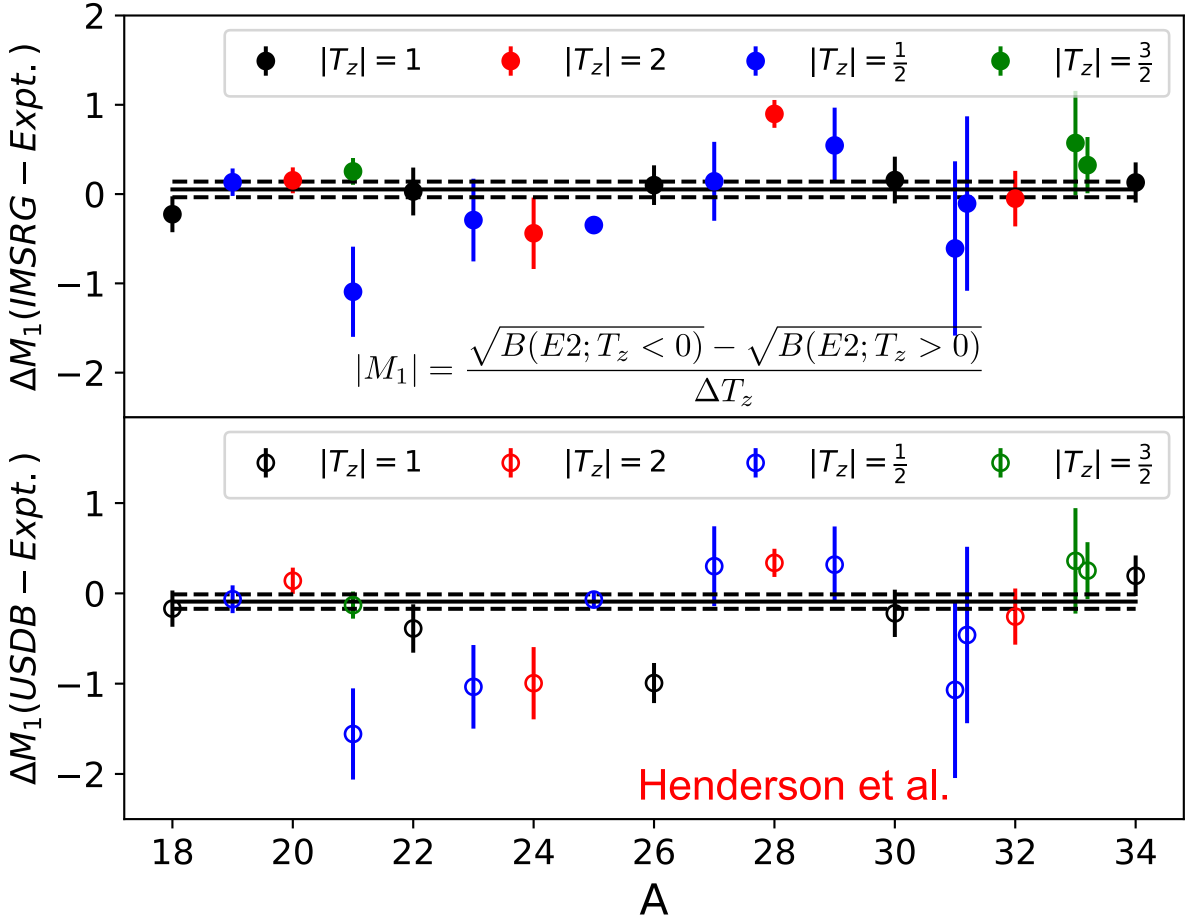
Trends well reproduced in both…

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

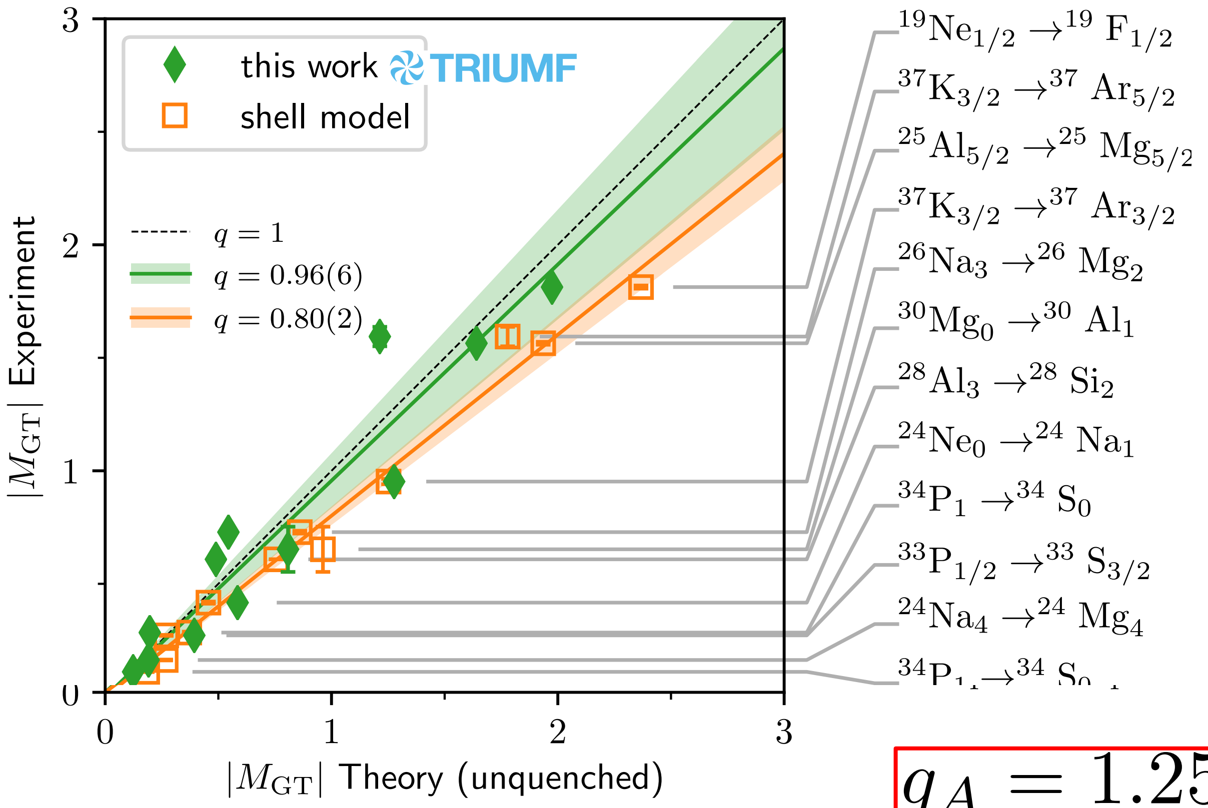
IV: Both agree well

Deficiencies in IS only

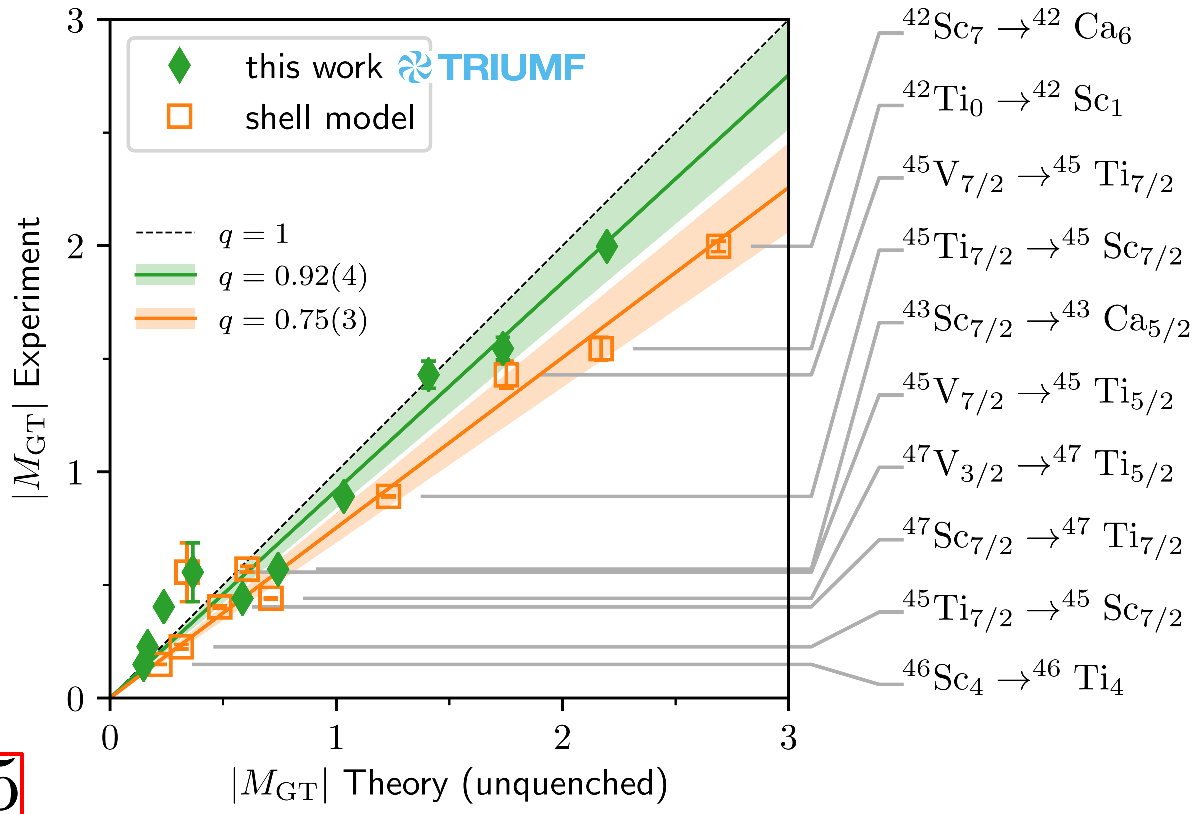
Ab Initio GT Decays in Medium-Mass Region

Comparison to standard phenomenological shell model

Ab initio calculations across the chart explain data with free-space g_A



$g_A = 1.25$



Gysbers et al., Nature Phys. (2019)

Refine results with improvements in forces and many-body methods

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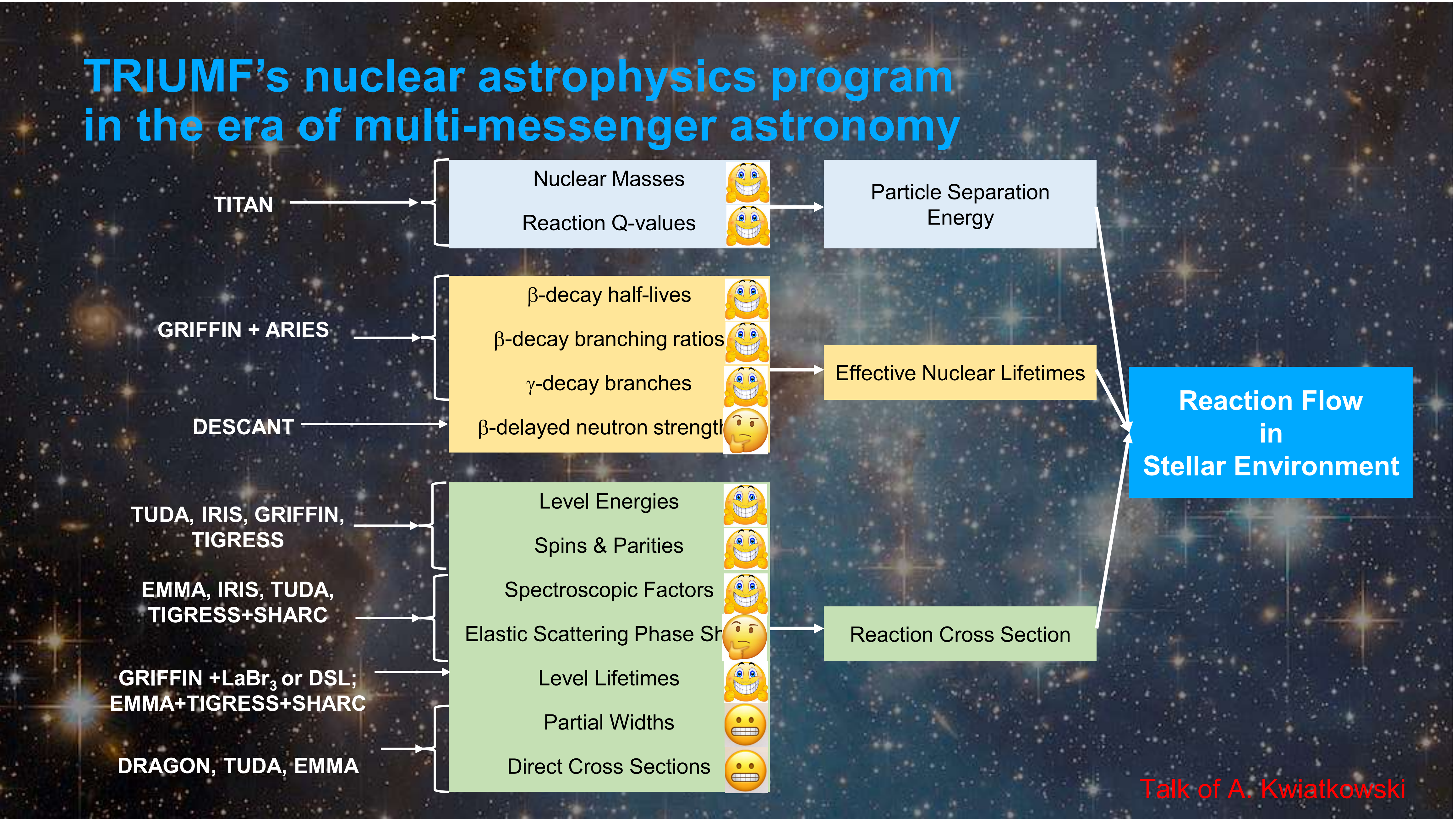
Breadth of Ab Initio: Access to Most Observables



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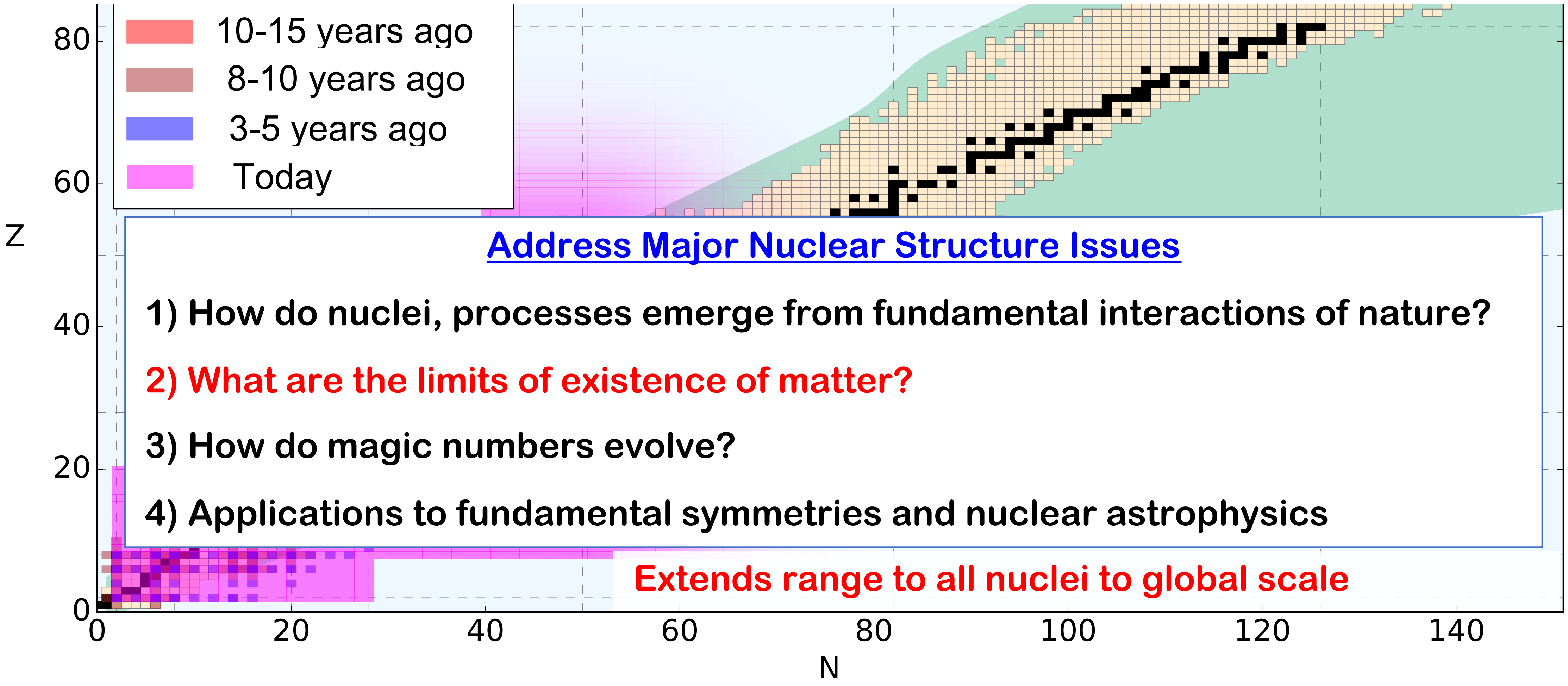


Address Major Nuclear Structure Issues

1) How do nuclei, processes emerge from fundamental interactions of nature?

2) What are the limits of existence of matter?

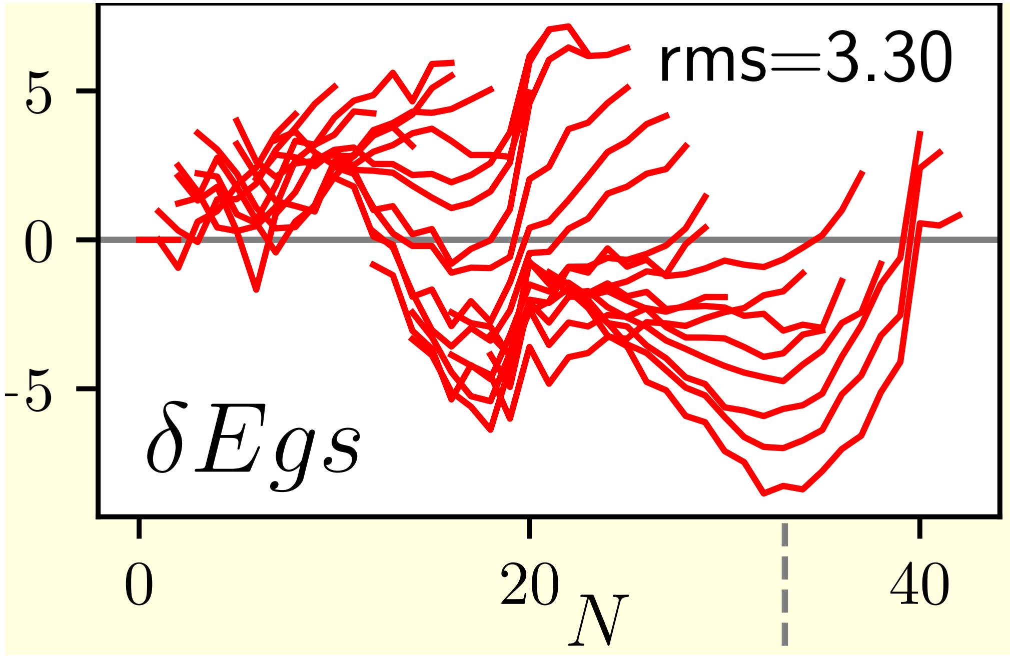
3) How do magic numbers evolve?

4) Applications to fundamental symmetries and nuclear astrophysics

Extends range to all nuclei to global scale

Global Ground-State Energy Residuals

Ab initio calculations of nearly 700 nuclei… how to analyze uncertainties?



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

B-W Mass formula: 3.1MeV Z<28

3.5MeV Z<20

DFT: 0.6-2.0 MeV

Stroberg et al arXiv:1905.10475

rms deviation at level of BW Mass formula, approaching EDF models

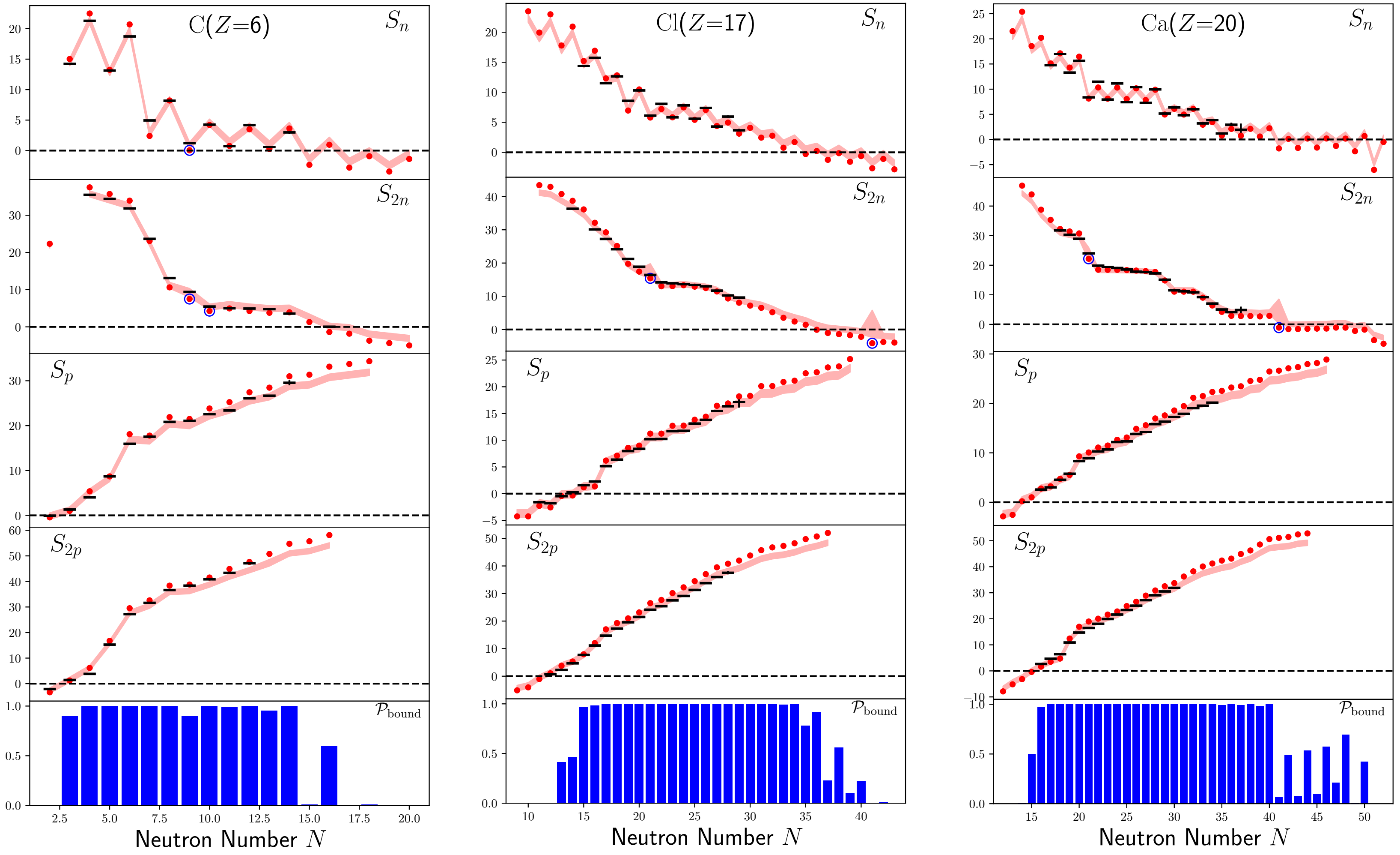
Input Hamiltonians fit to A=2,3,4 – not biased towards known data

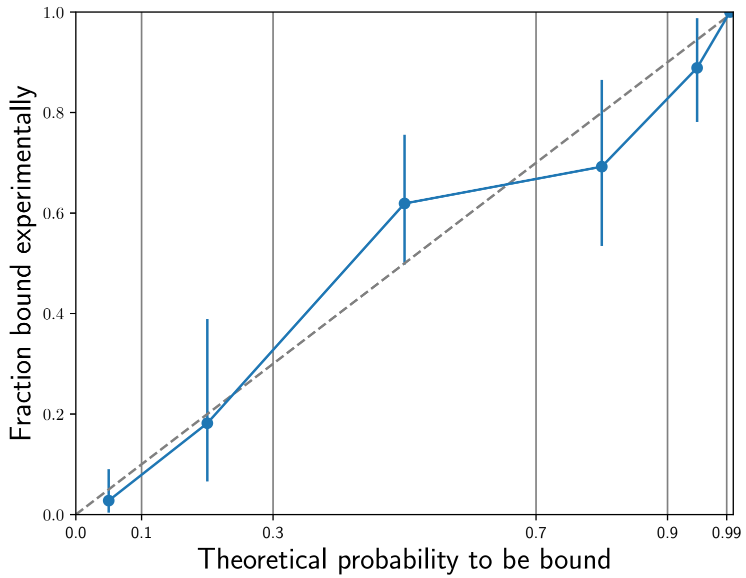
What is deviation for separation energies? **Apply to nuclear driplines**

TRIUMF

Estimating Dripline Uncertainites

Determine rms deviation from experiment – extrapolate this uncertainty beyond data





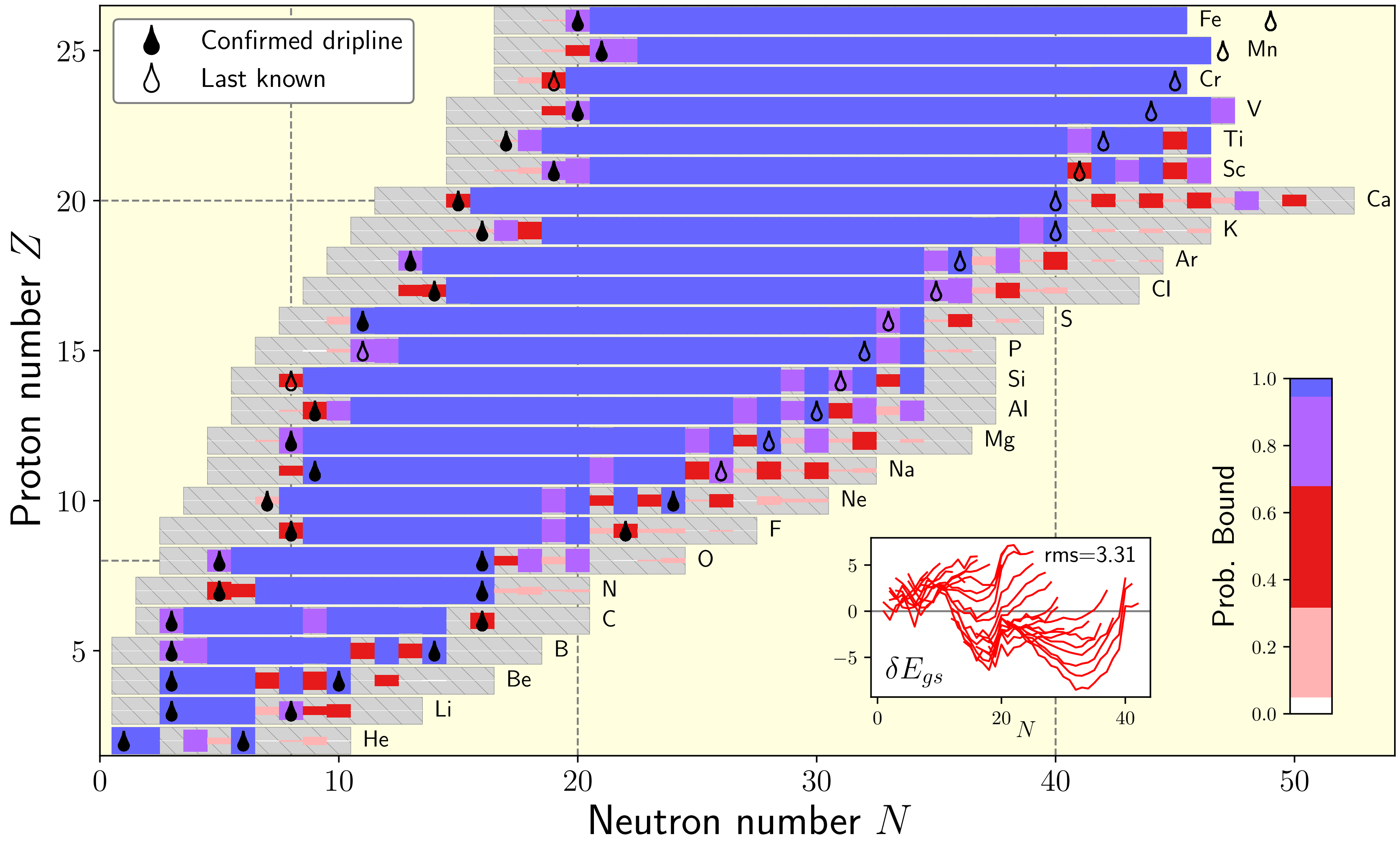
Determine range of likely separation energies reaching 0

Stroberg et al arXiv:1905.10475

Assign probability that a particular nucleus is bound

Dripline Prediction to Iron Isotopes

First predictions of proton and neutron driplines from first principles



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

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

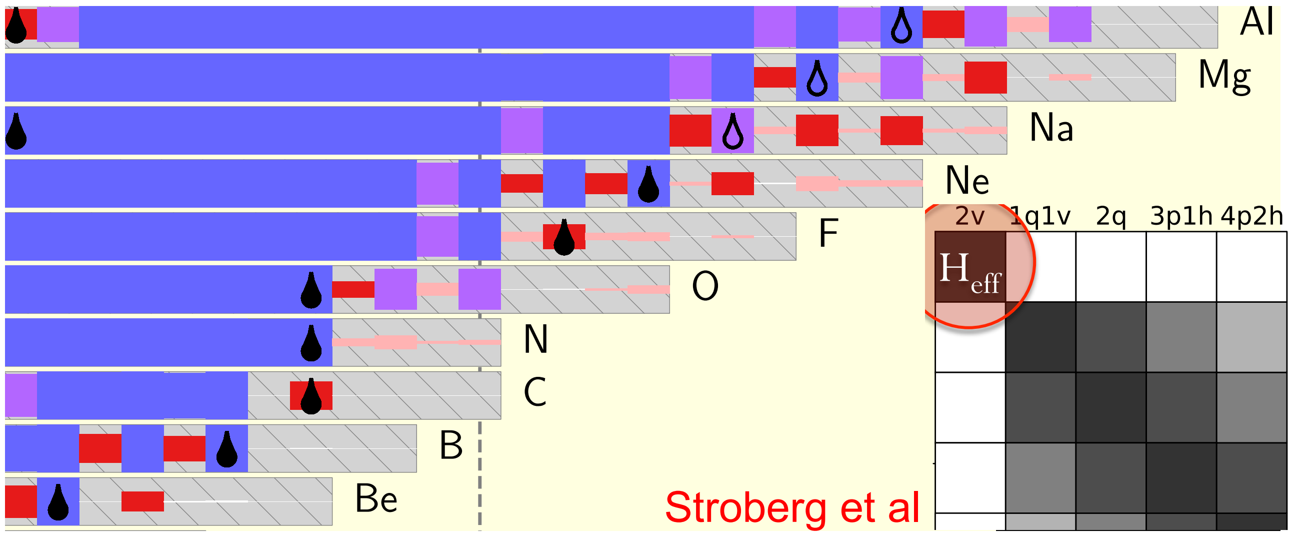
Stroberg et al arXiv:1905.10475

Known drip lines largely predicted within uncertainties (issues remain at shell closures)

Provide ab initio predictions for neutron-rich region

Dripline Flagship RIB Science Motivation

New measurements determine dripline in F and Ne isotopes, extend known Na isotopes



All new measurements agrees well with ab initio predictions

Next-generation RIB aim to extend driplines to Ca!

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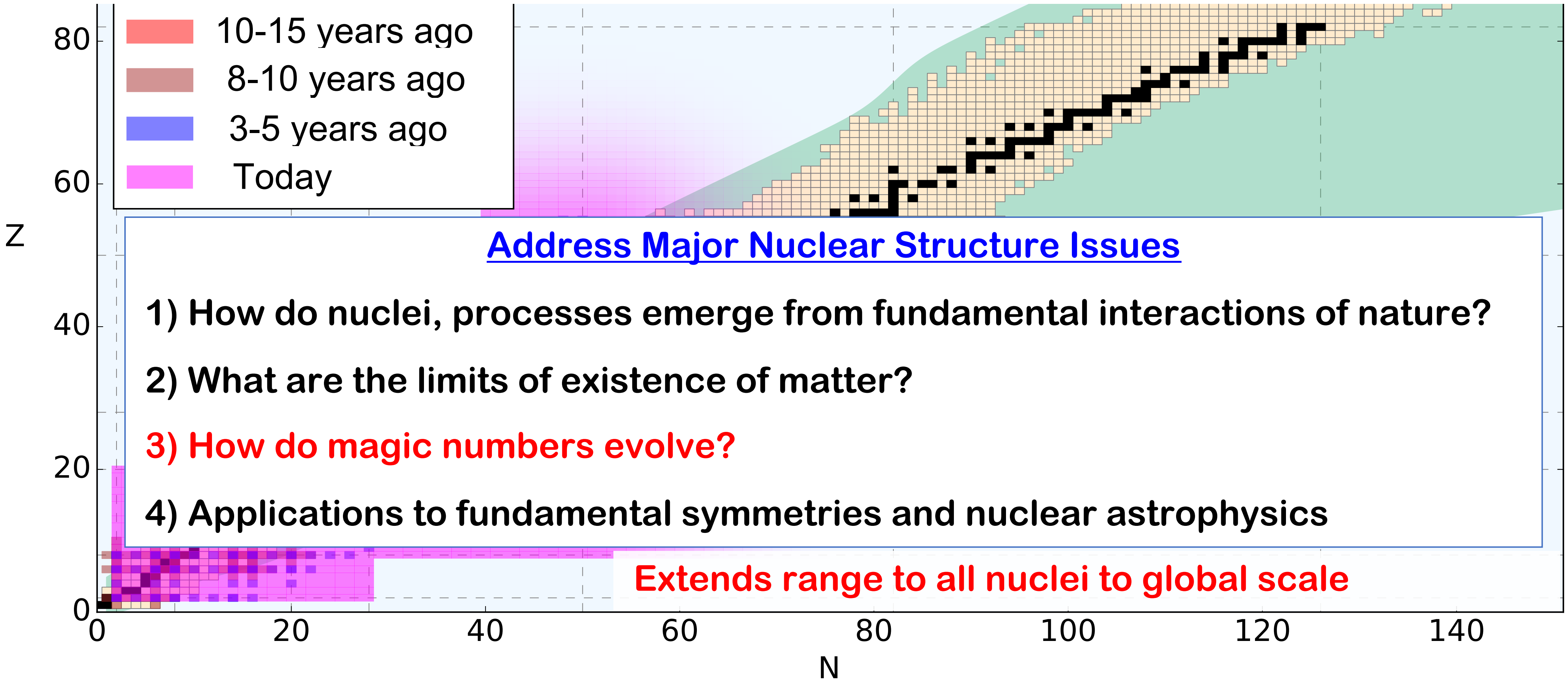

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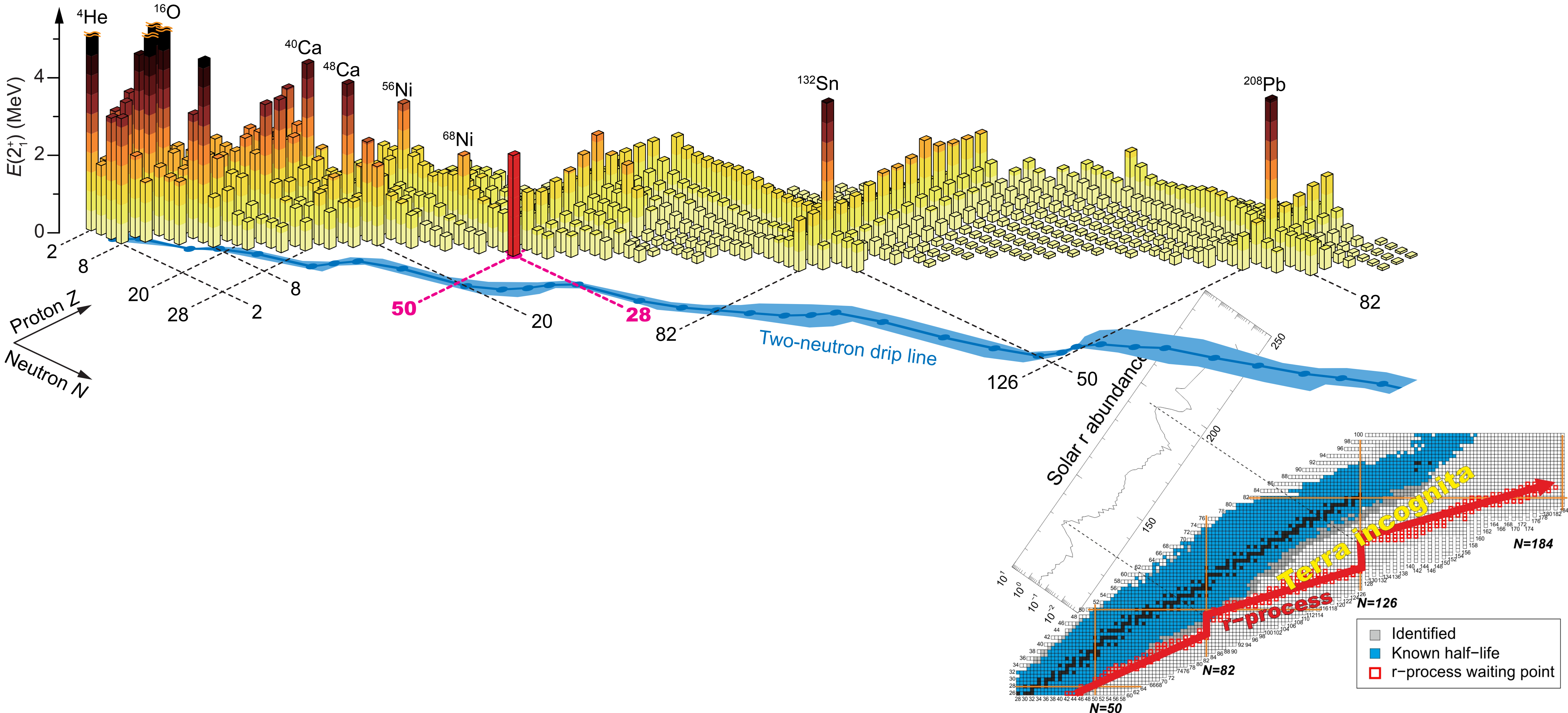
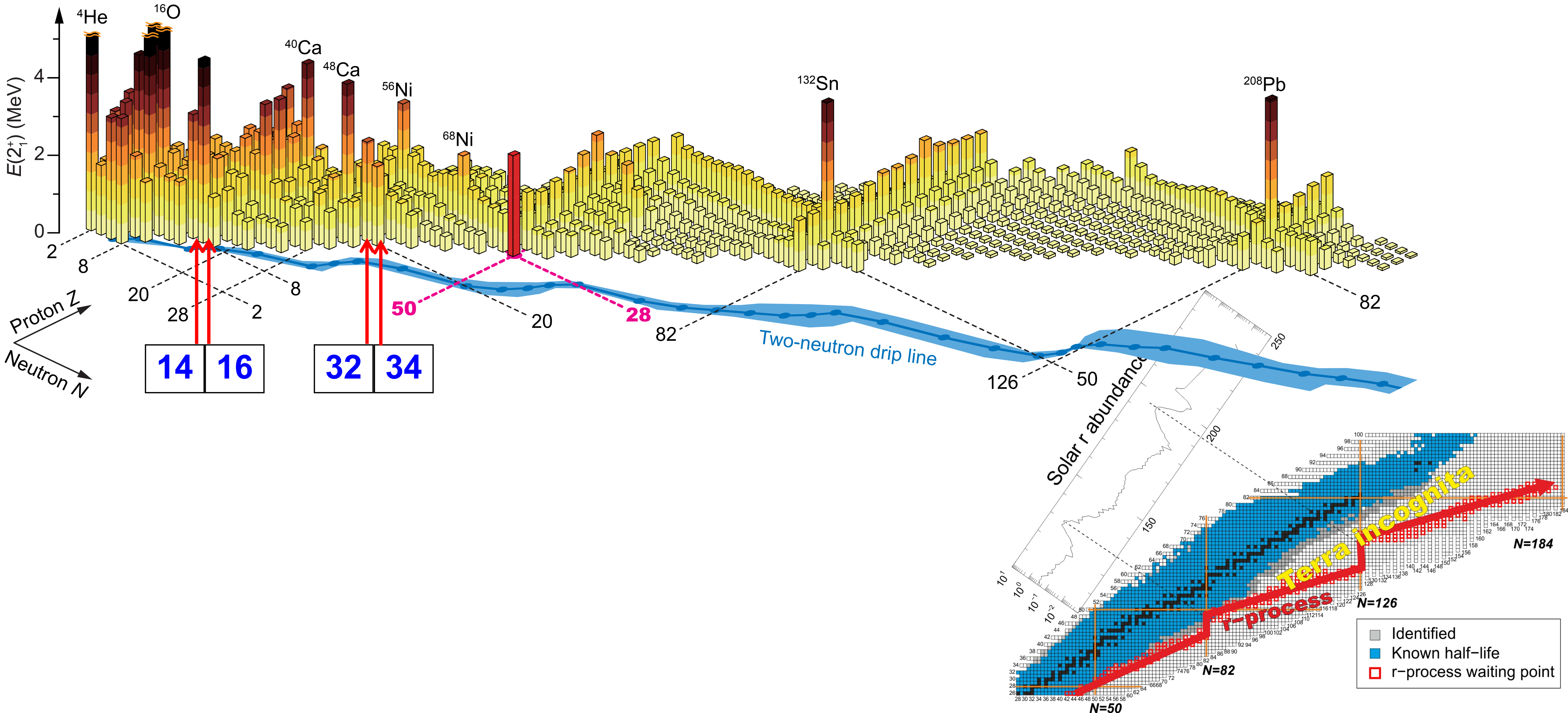
Magic Numbers in Nuclei

Magic numbers: pillars of nuclear structure, vital for r-process nucleosynthesis



Magic Numbers in Nuclei

Magic numbers: pillars of nuclear structure, **novel evolution in exotic nuclei**



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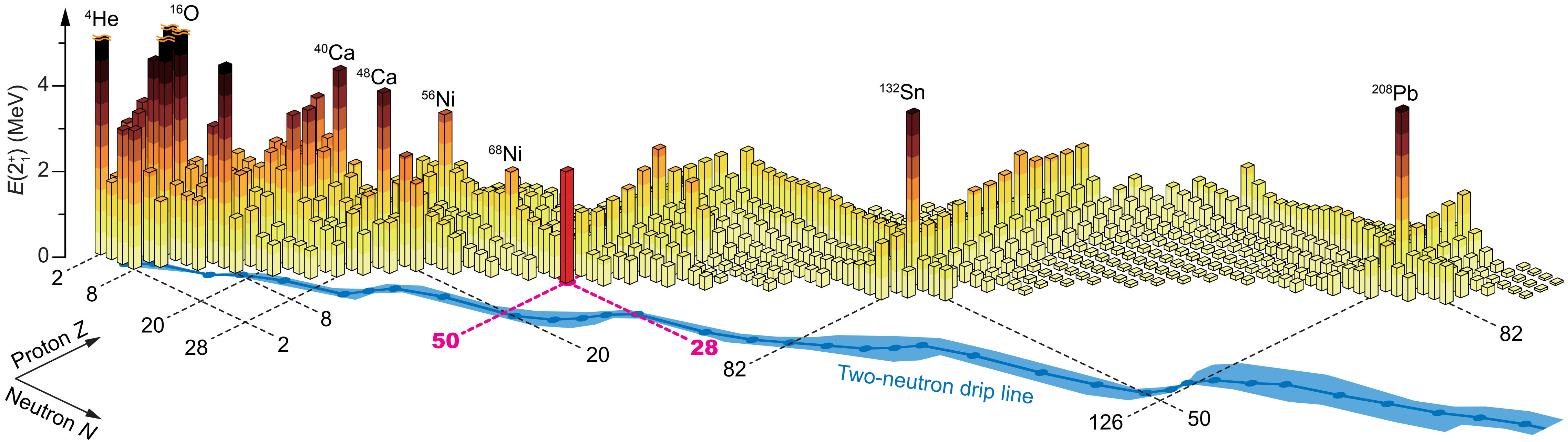


Signatures of Magic Numbers

Sharp decrease in separation energy (masses)

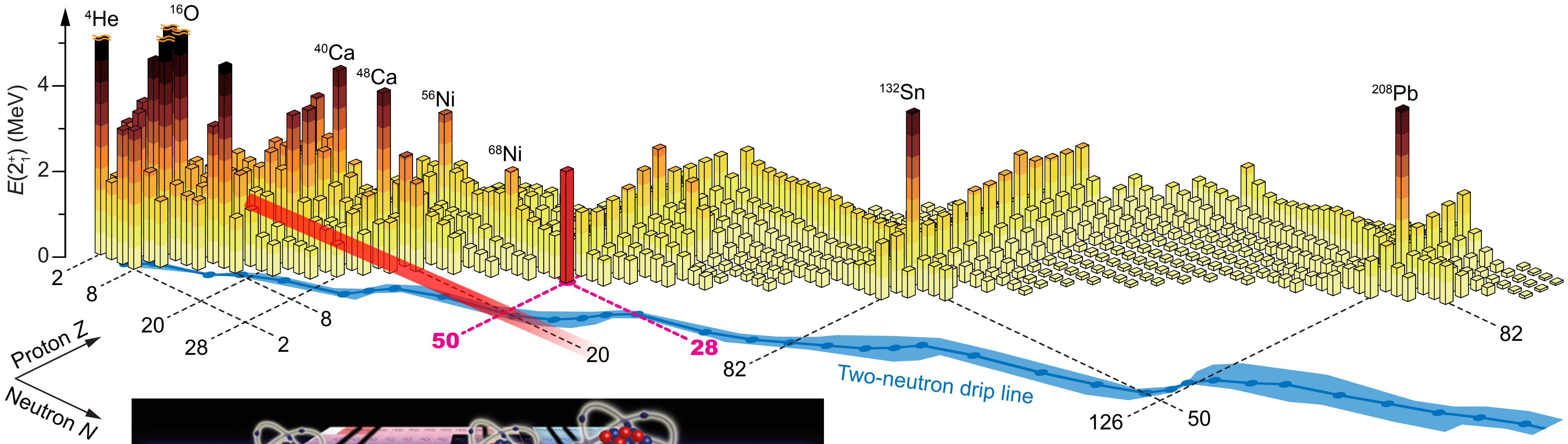
Elevated first excited 2+ energy (spectroscopy)

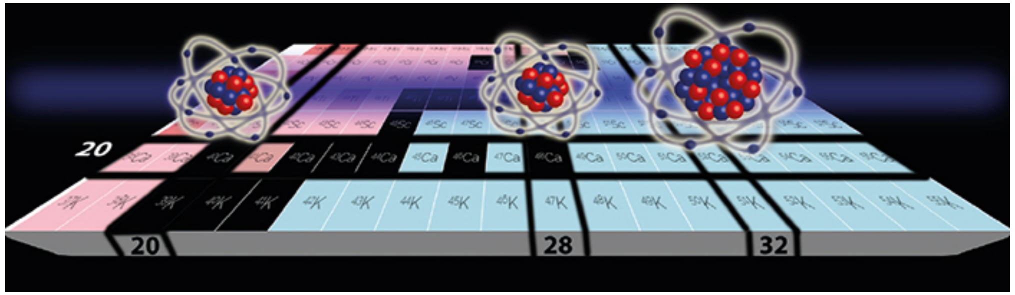
Tightly bound (decreased radii)

Must observe all signatures – many experiments (and calculations) needed!

Evolution of N=32,34 Magic Numbers

Magic numbers: pillars of nuclear structure, novel evolution in exotic nuclei



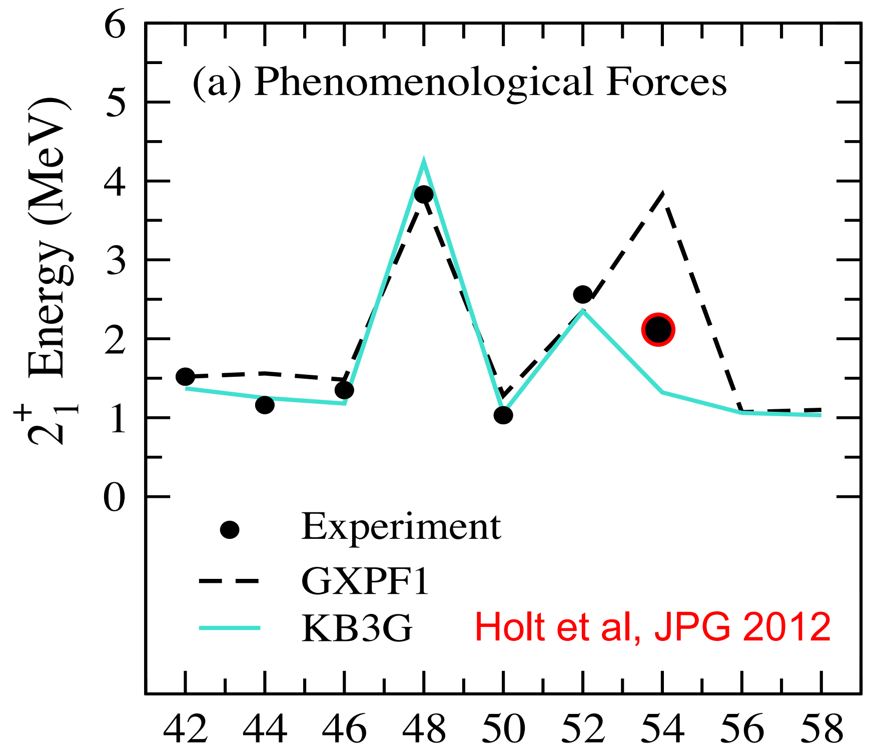


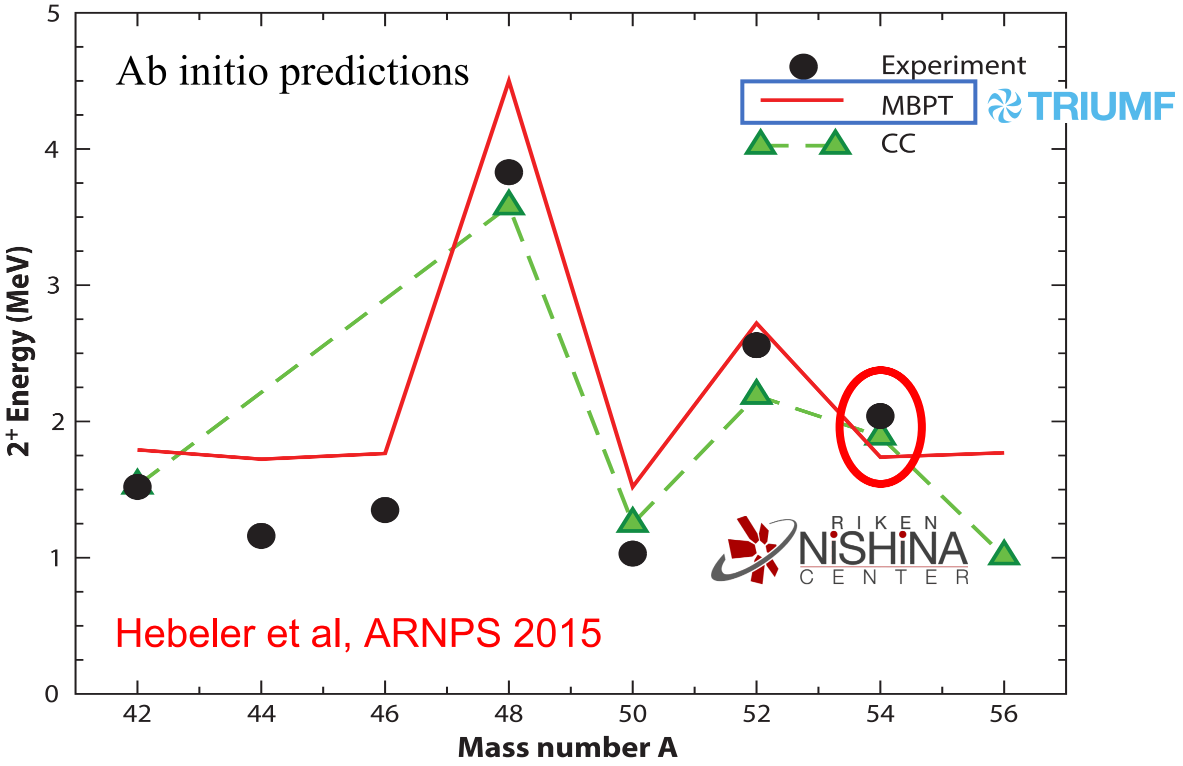
Highlight of TRIUMF theory and experiment:

Discovery and evolution of new N=32,34 magic numbers in calcium region

N=32,34 Magic Numbers: Spectroscopy

2013 potentially new magic numbers from 2^+ energies: N=32,34 – **New ^{54}Ca measurement at RIKEN**





Phenomenological Models

Readjusted to fit new data

Ab initio theories

Correctly predicted excitation energy of N=34!

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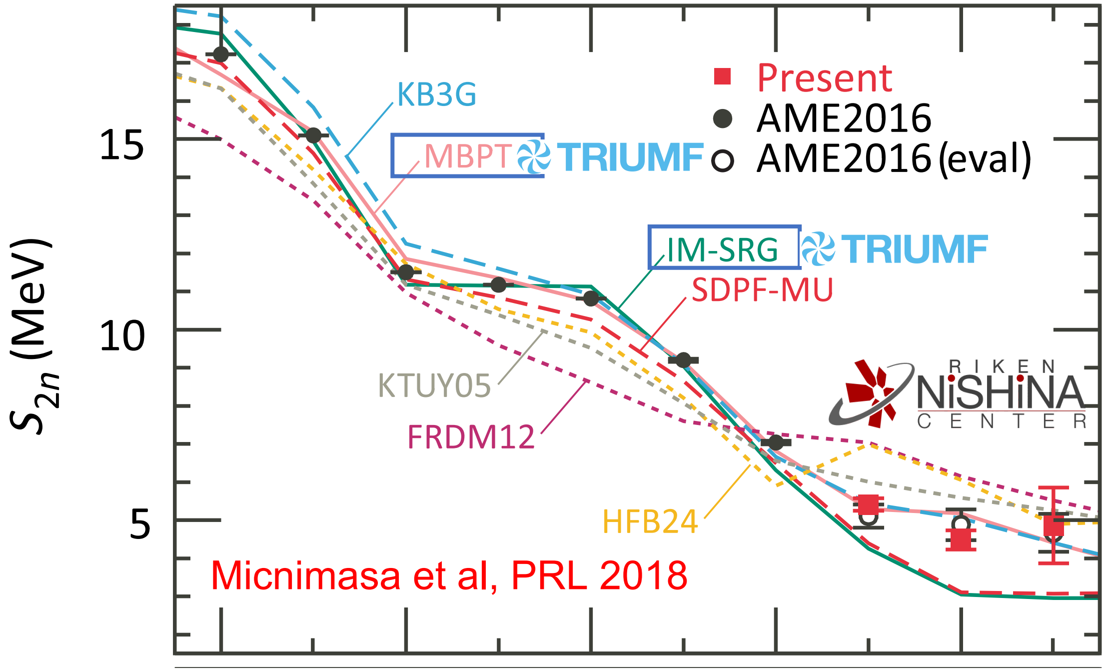
N=32,34 Magic Numbers: Masses

2013-2018 impressive series of experiments; ideal example of theory/exp overlap

Story continues at RIKEN



TITAN @ TRIUMF Measurement

Flat trend from $^{50-52}Ca$

^{52}Ca 1.74 MeV deviation from AME!

ISOLTRAP @ CERN *Measurement*

Sharp decrease from $^{52-54}Ca$

Confirms N=32 magic number

RIBF @ RIKEN Measurement

Modest decrease past ^{54}Ca

Confirms N=34 magic number

Ab Initio

Excellent agreement with RIBF data

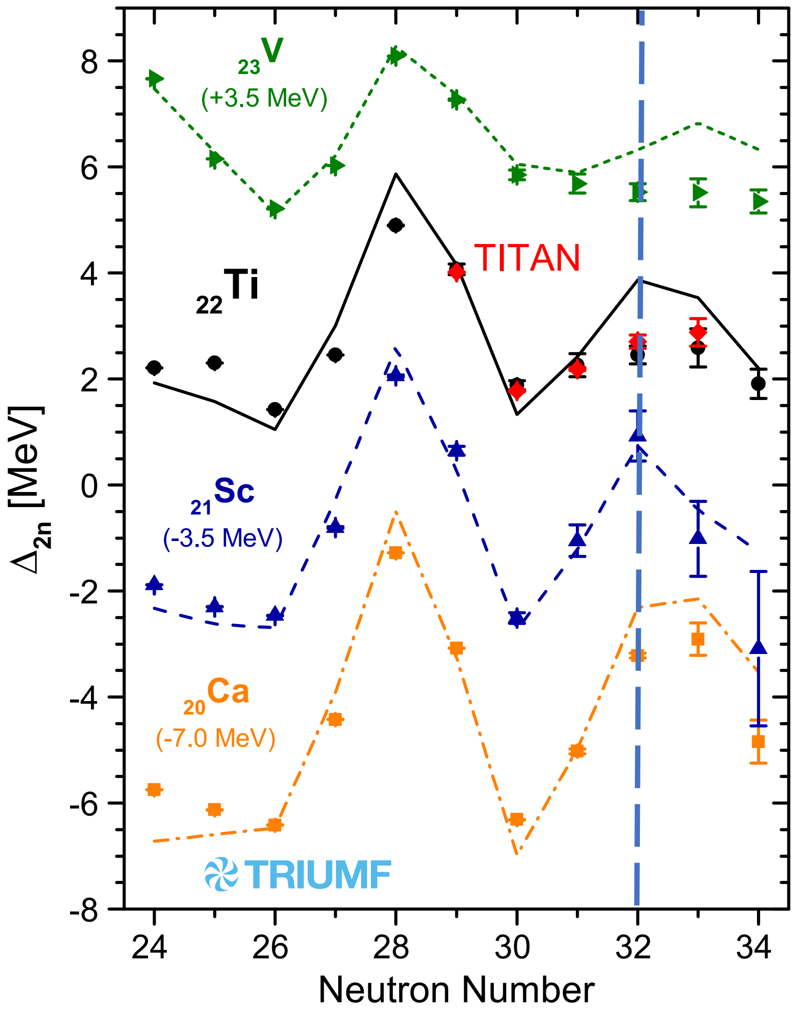
Predicts doubly magic $^{48,52,54}Ca$

TRIUMF

Dawning of N=32 Magic Number: Masses

Further questions: how do magic numbers evolve with proton number?

Current frontier of measurements and theory



Leistenschneider et al, PRL 2018

New TITAN Measurements of Ti masses

Probe “dawning” of N=32 magic number

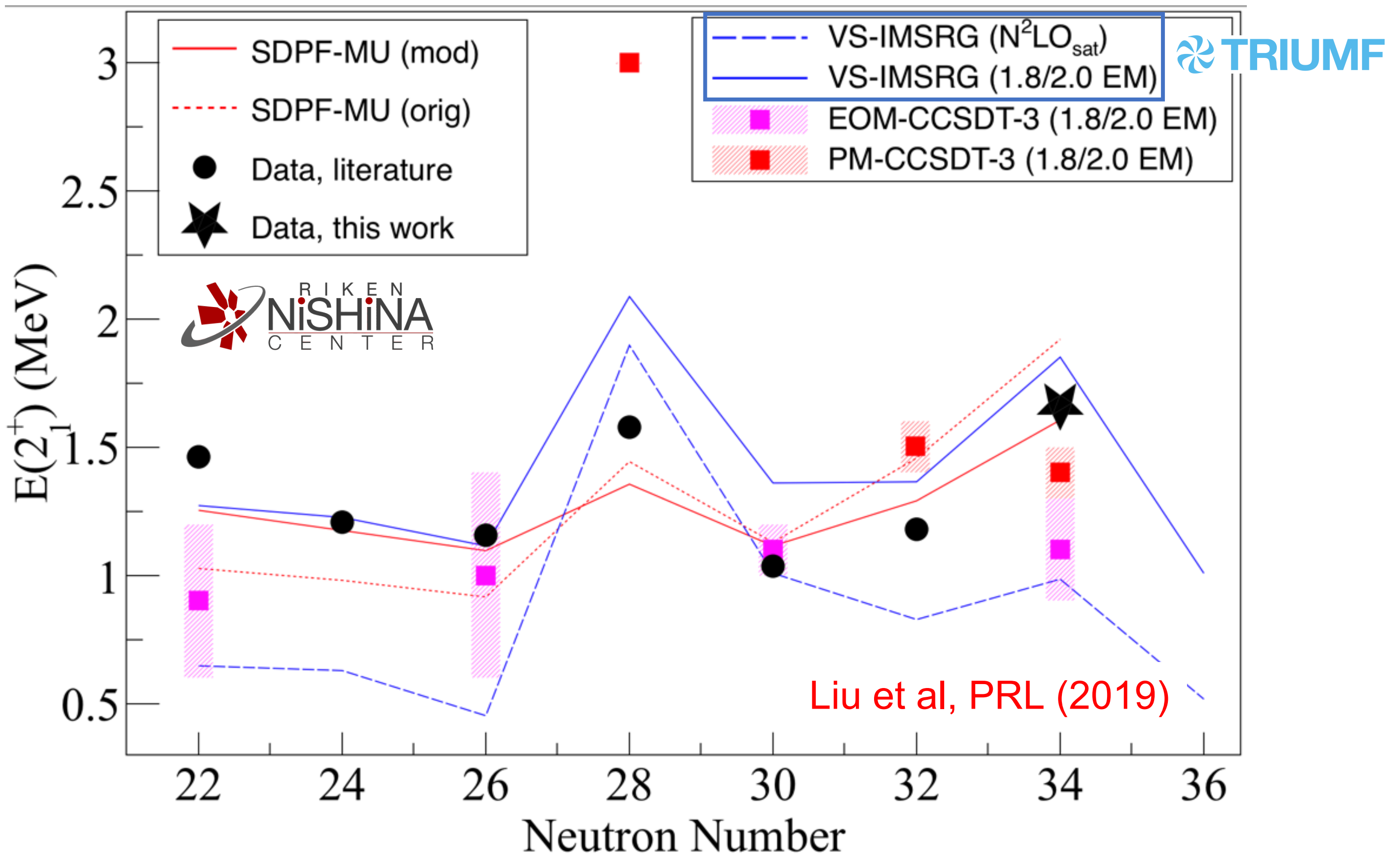
Ab Initio from NN+3N

Generally good agreement, but predicts appearance too early

Future: Evolution to be measured in Ar, Cl

Persistence of N=34 Magic Number Below Ca

New measurement at RIKEN: 2⁺ energy in ^{52}Ar – clear peak at N=34

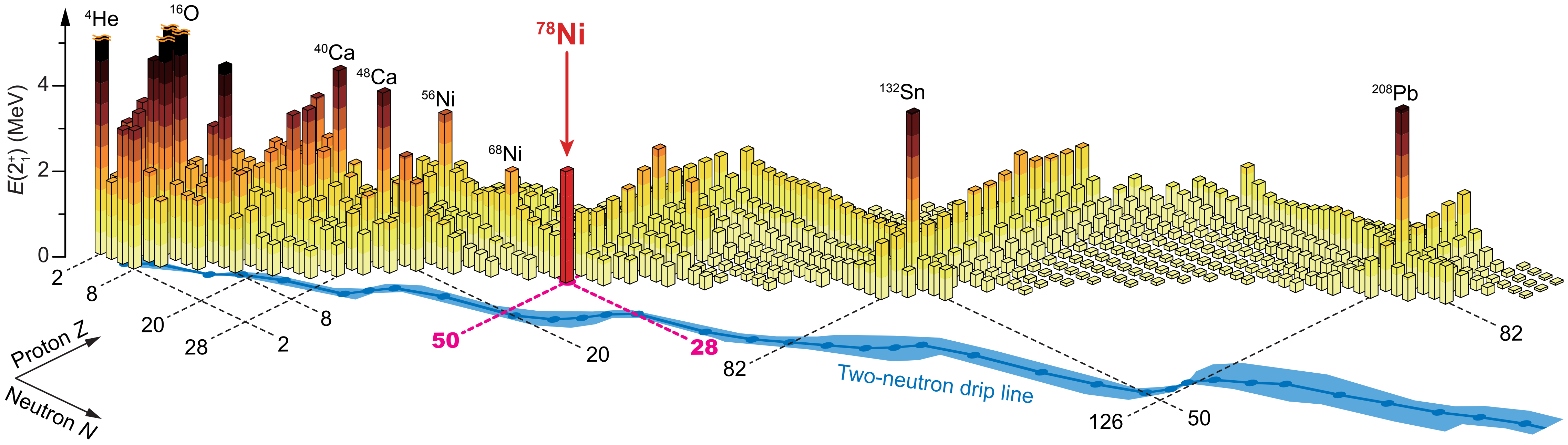


Agreement with IMSRG and other ab initio predictions (coupled cluster theory)

First evidence for persistence of N=34 magic number away from calcium!

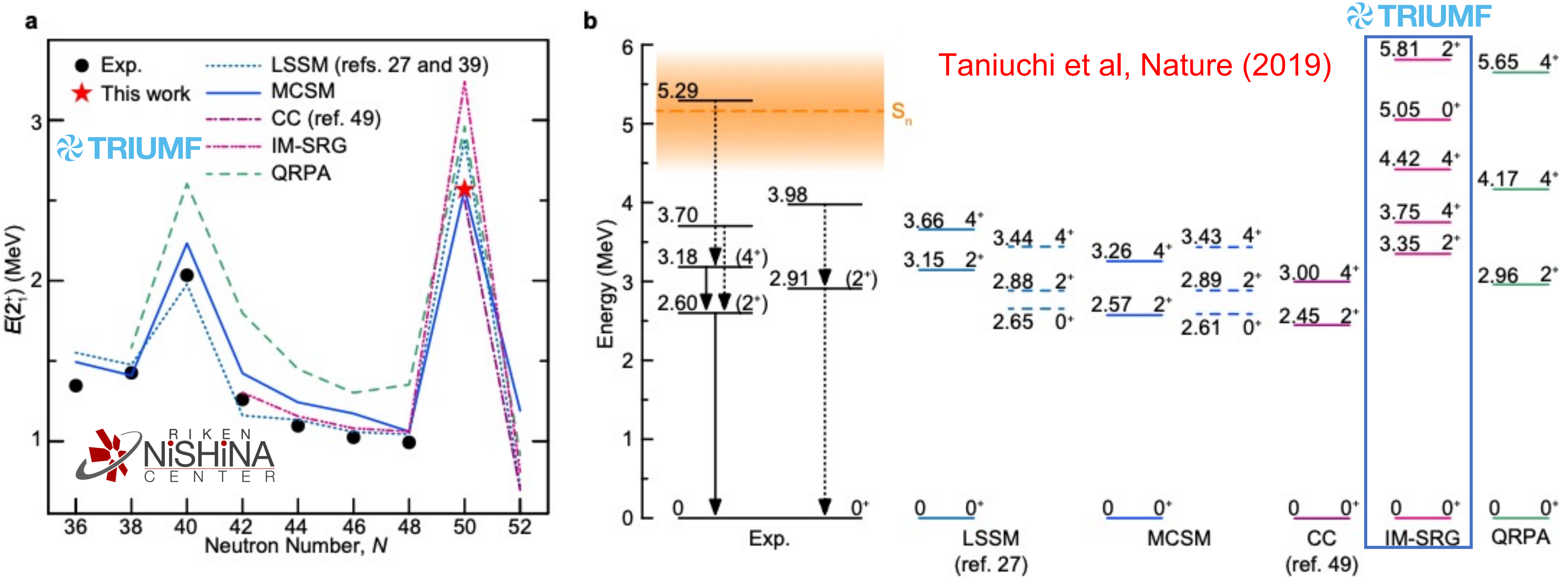
Discovery of Doubly Magic ^{78}Ni

Magic numbers: pillars of nuclear structure, novel evolution in exotic nuclei



Missing Pillar: Magicity of ^{78}Ni?

New measurement at RIKEN 2$^+$ energy in ^{78}Ni – clear peak compared to ^{76}Ni



Peak wrt neighboring systems well predicted by IMSRG (also phenomenology)

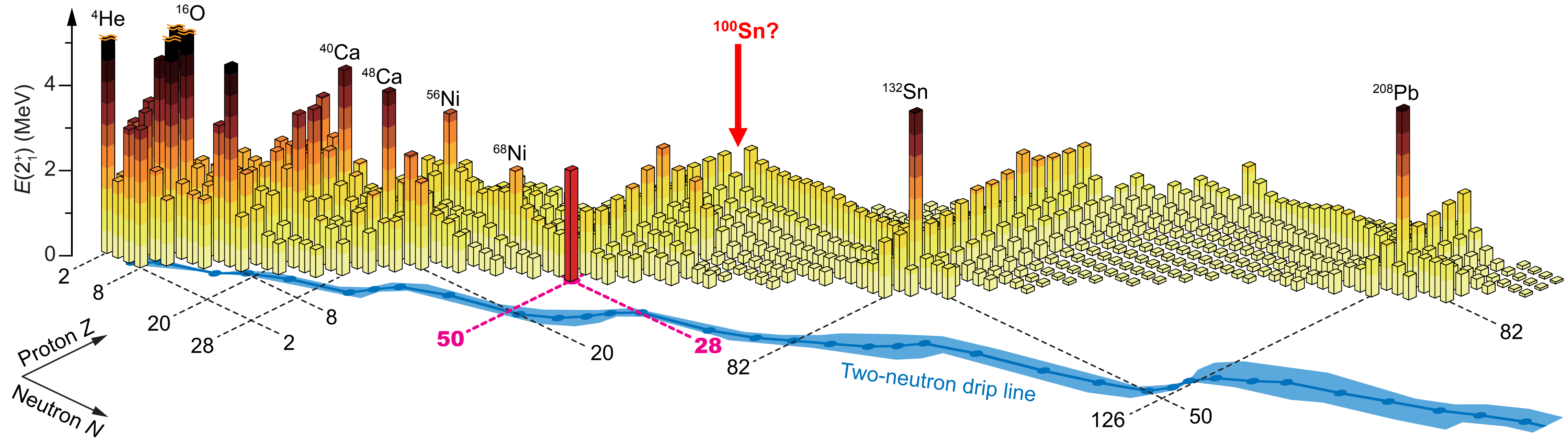
First evidence for the (double) magicity of ^{78}Ni

Next: determine evolution below Z=28

TRIUMF

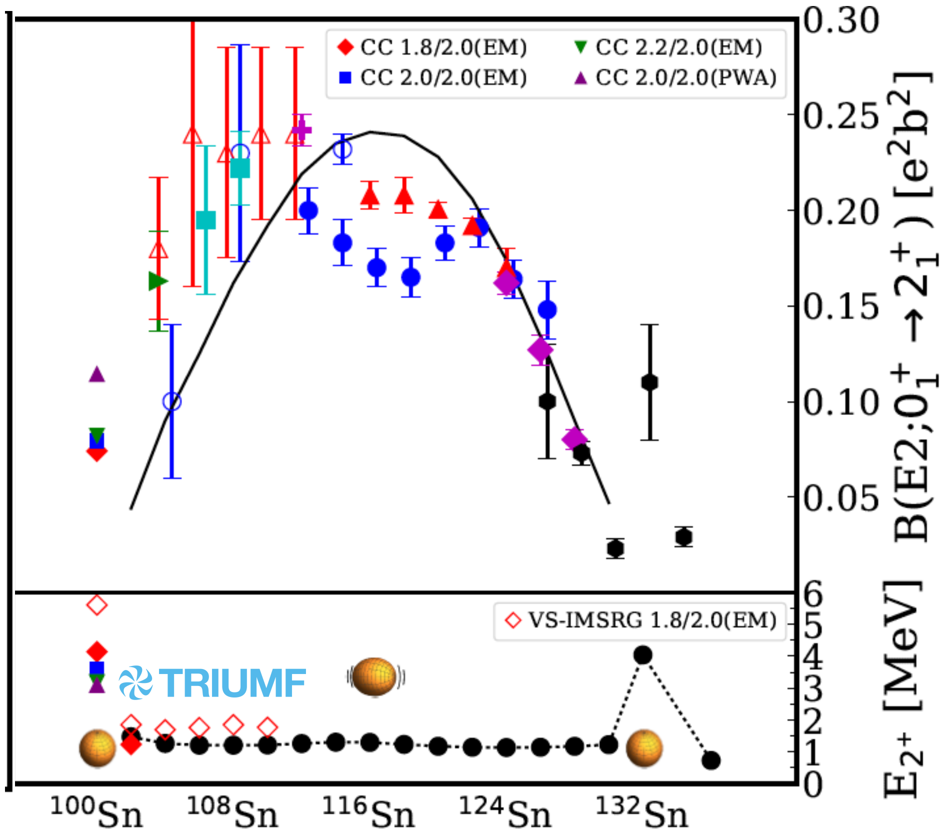
Currently Unmeasured: ^{100}Sn

Magic numbers: pillars of nuclear structure, novel evolution in exotic nuclei

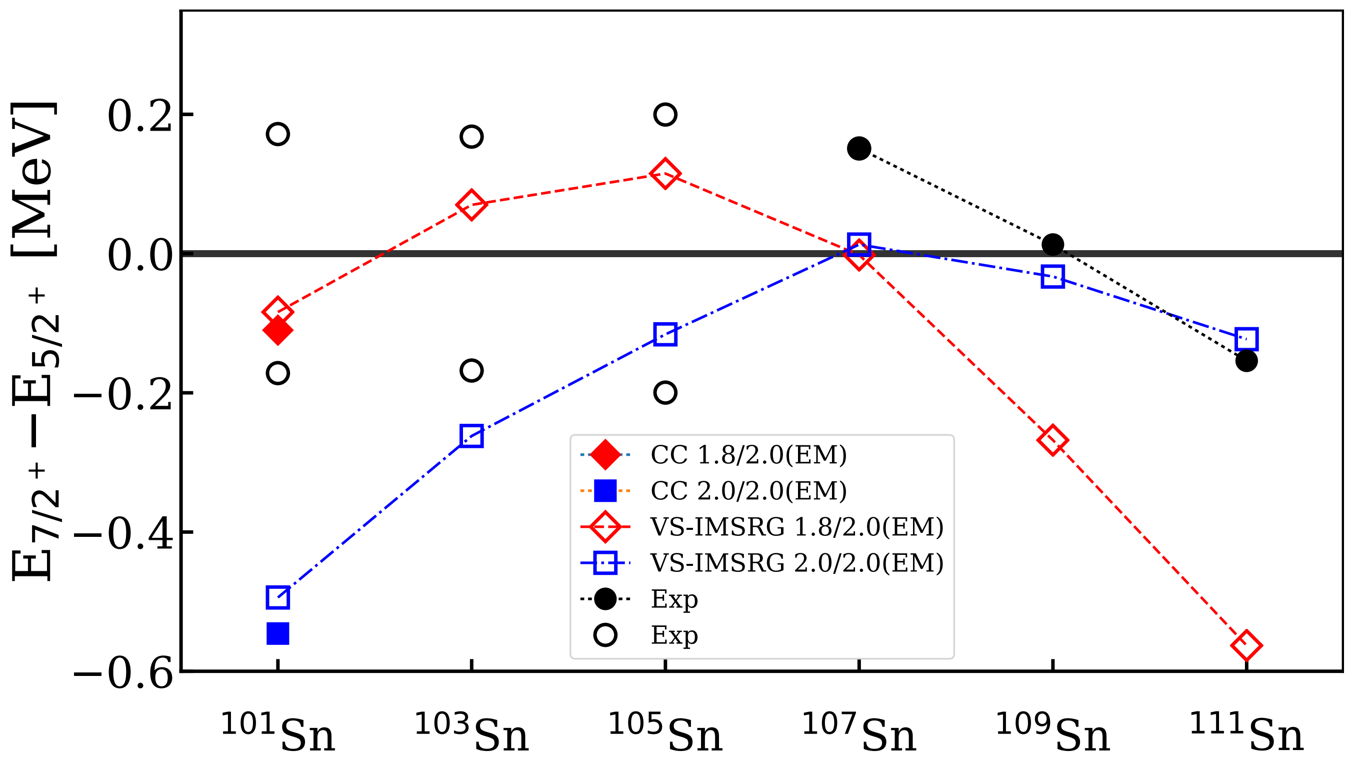


Structure of Light Tin Isotopes

Extend ab initio to heavy-mass region: magicity of ^{100}Sn, controversial level ordering in ^{101}Sn



Morris et al., PRL (2018)



Predicts doubly magic nature from

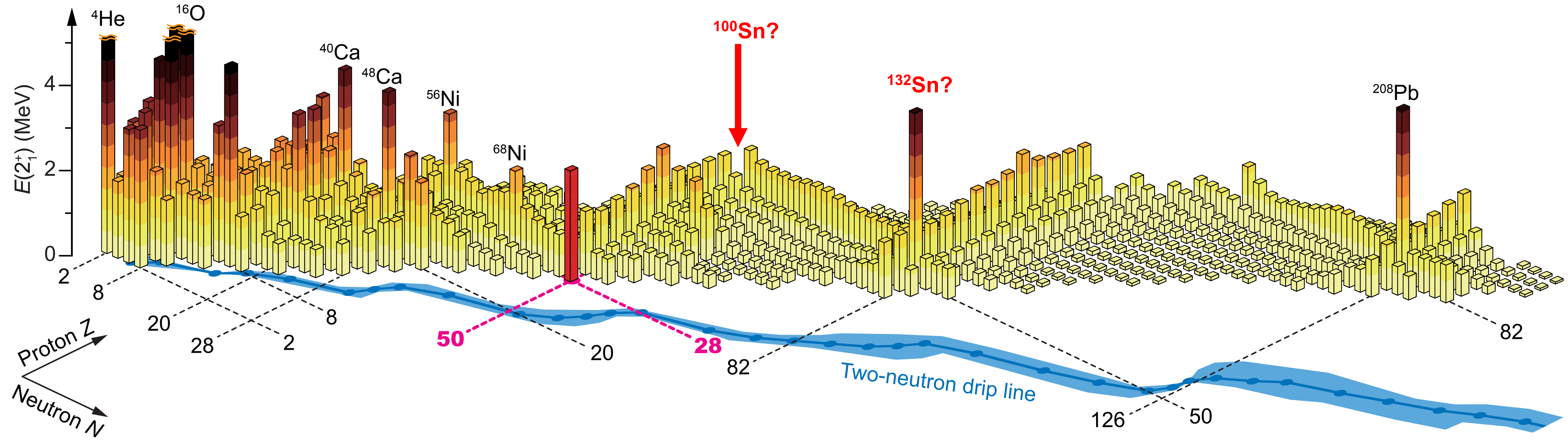
2$^+$ energies and B(E2) systematics

Limits of ab initio theory…

Both calculations predict 5/2+ ground state

Can ab initio Treat Neutron-Rich Tin?

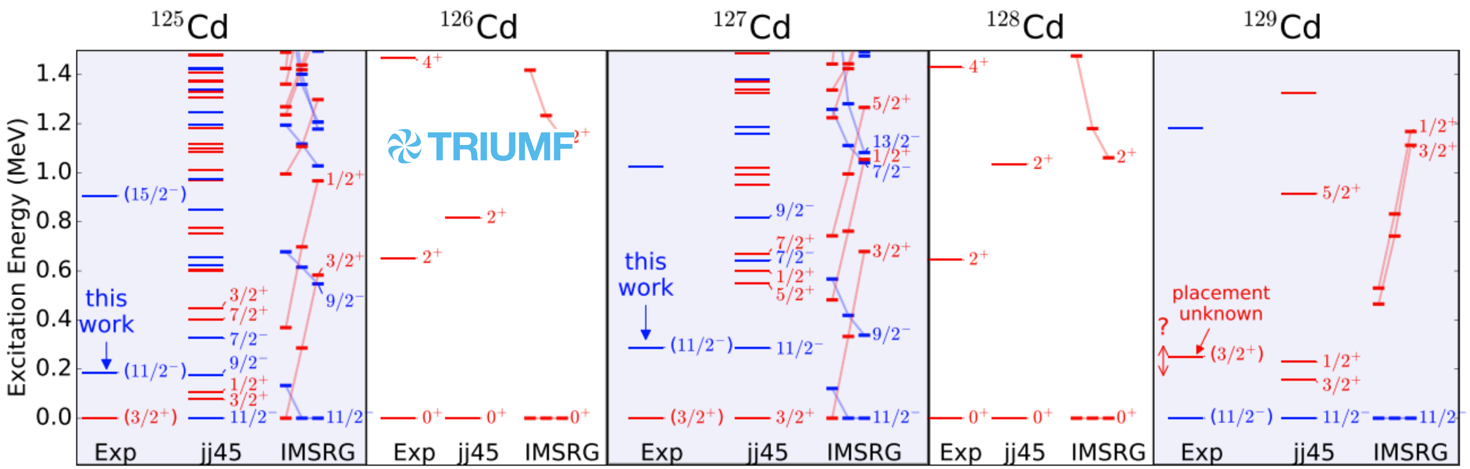
Magic numbers: pillars of nuclear structure, novel evolution in exotic nuclei



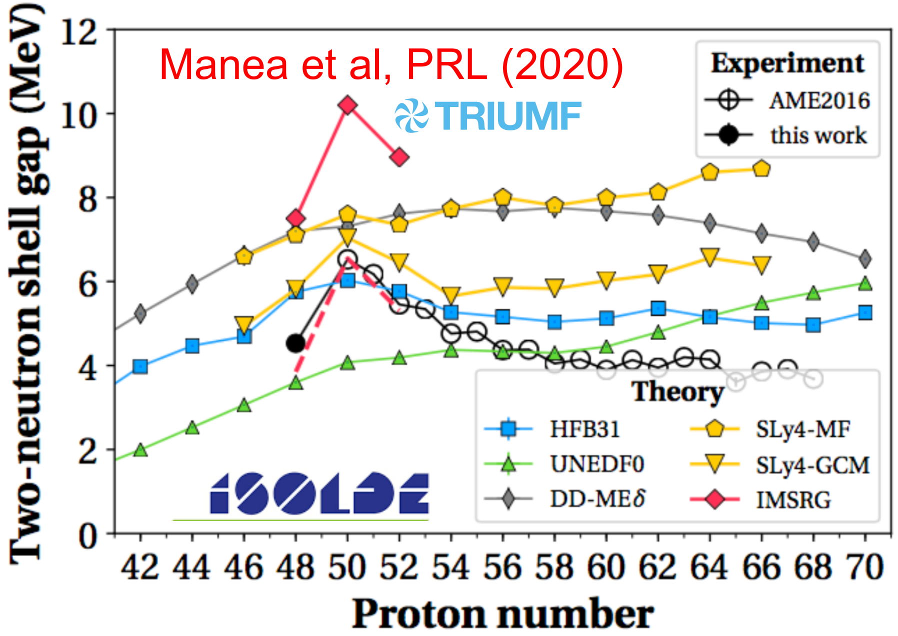
Problematic Convergence of N=70 Gap

TRIUMF

Several studies show N=70 gap clearly not converged wrt E_{3max} – for neutron-rich Sn, In, Cd…



Lascar et al PRC (2017)



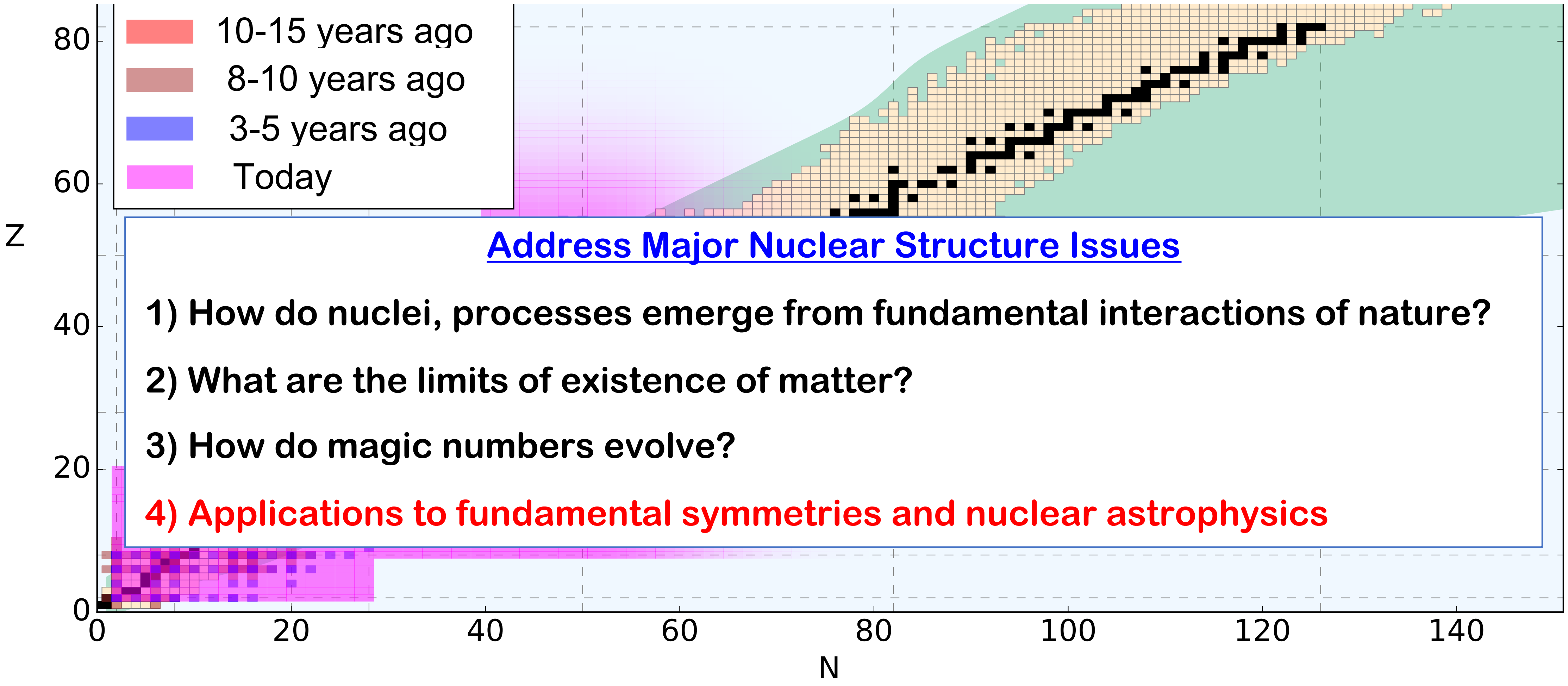
Resorted to unreliable extrapolations…

Towards Global Ab Initio Calculations

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

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

$$H\psi_n = E_n\psi_n$$



Address Major Nuclear Structure Issues

1) How do nuclei, processes emerge from fundamental interactions of nature?

2) What are the limits of existence of matter?

3) How do magic numbers evolve?

4) Applications to fundamental symmetries and nuclear astrophysics

Towards Global Ab Initio Calculations

TRIUMF

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

proton spallation yields in uranium target

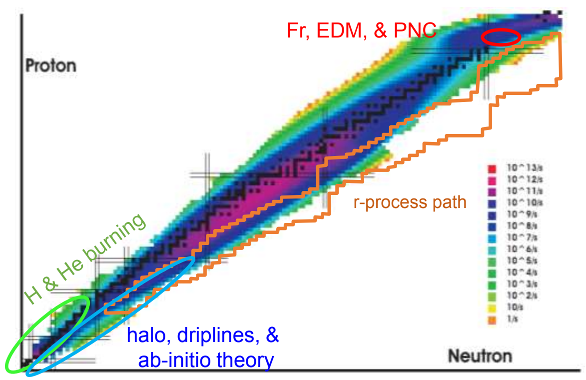
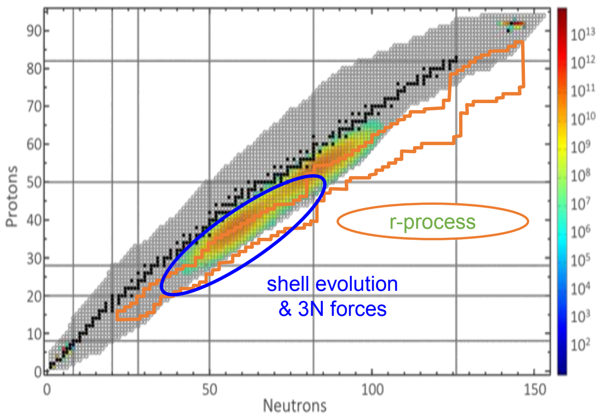
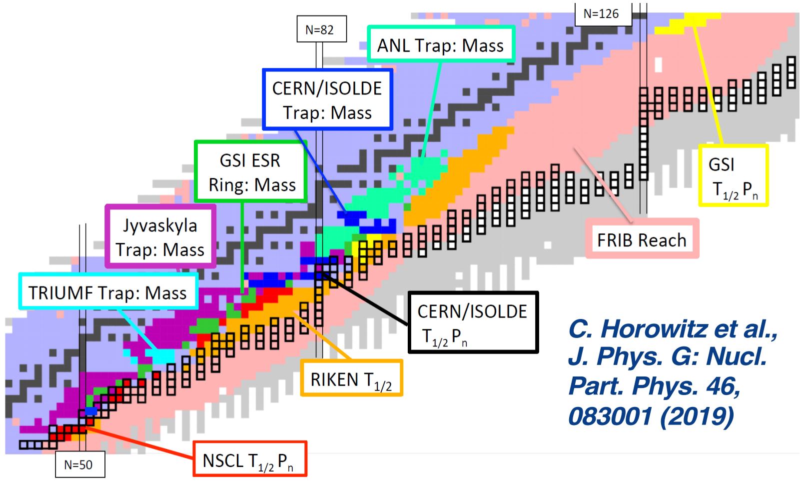


photo-fission yields in uranium target





C. Horowitz et al., J. Phys. G: Nucl. Part. Phys. 46, 083001 (2019)

Address Major Nuclear Structure Issues

1) How do nuclei, processes emerge from fundamental interactions of nature?

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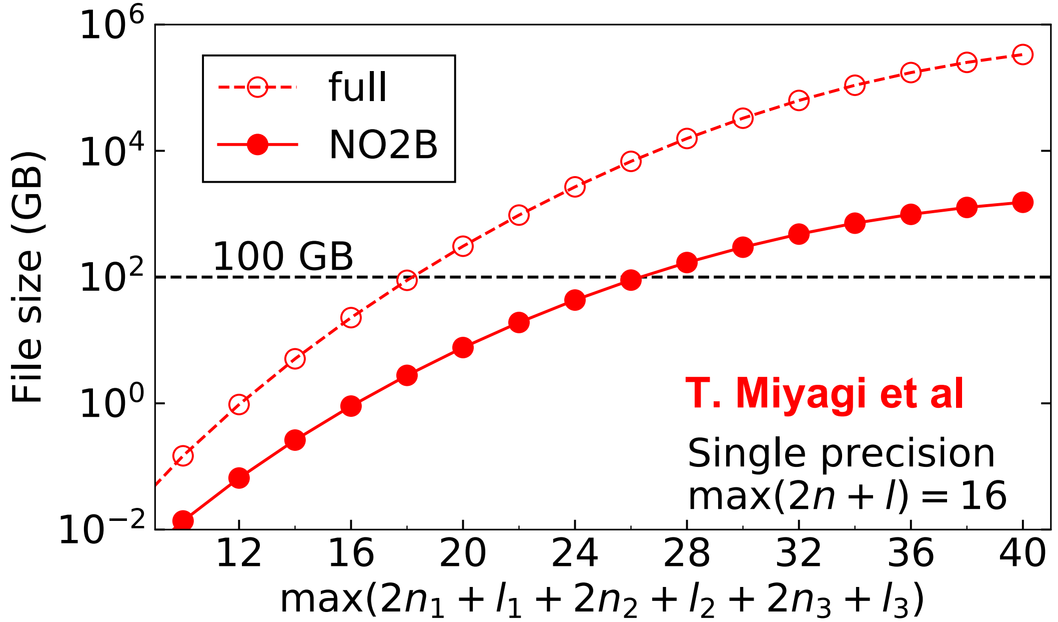
4) Applications to fundamental symmetries and nuclear astrophysics

Extension to heavy nuclei necessary – limited by 3N element storage

TRIUMF

Towards Heavy Nuclei: ^{132}Sn

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



First converged calculations of 132Sn!

Opens new region of chart to ab initio theory

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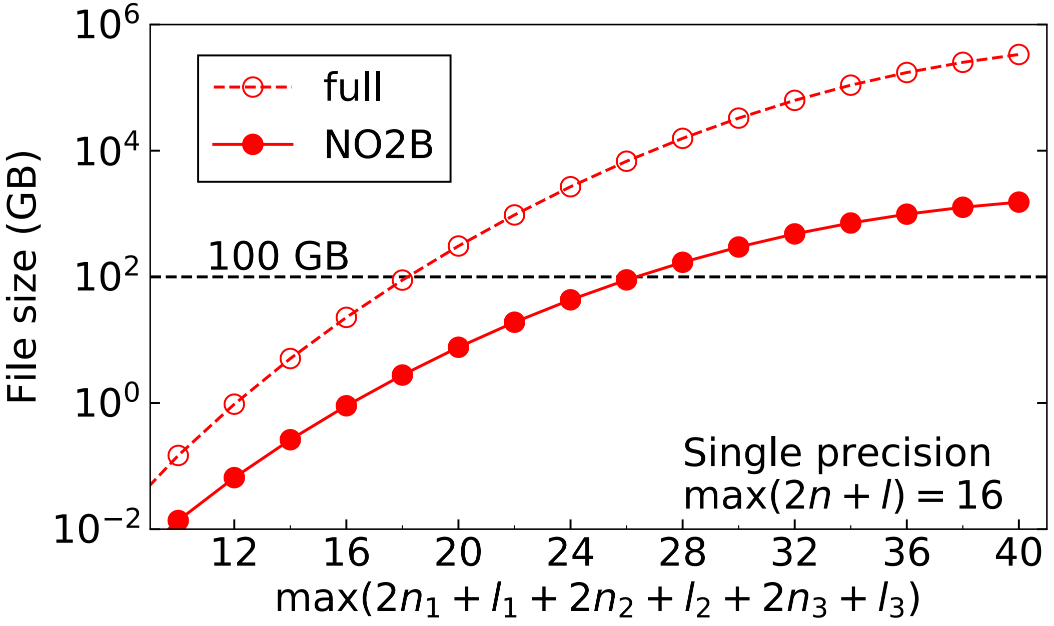
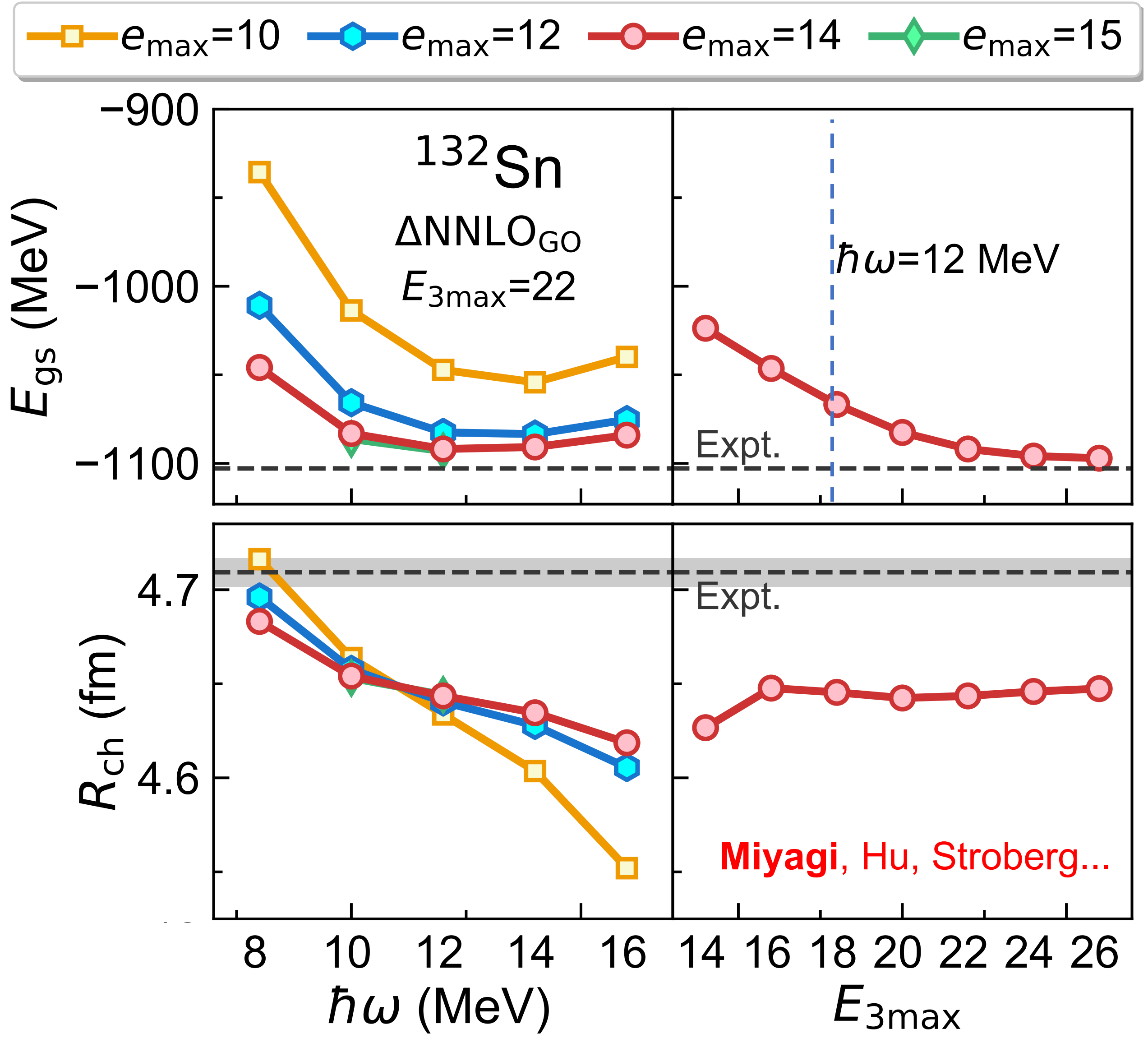


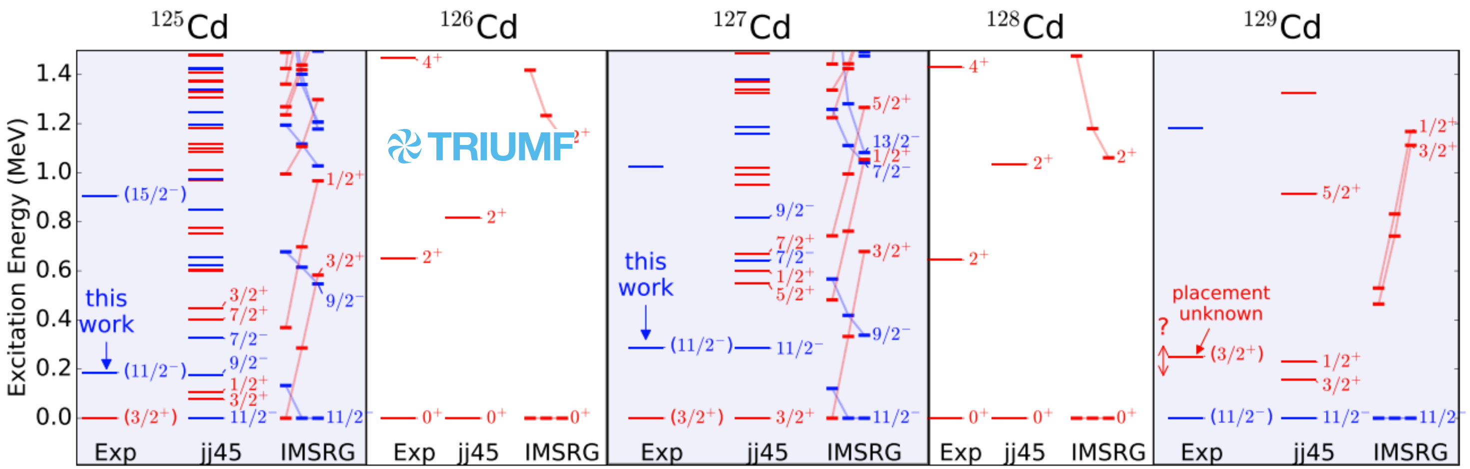


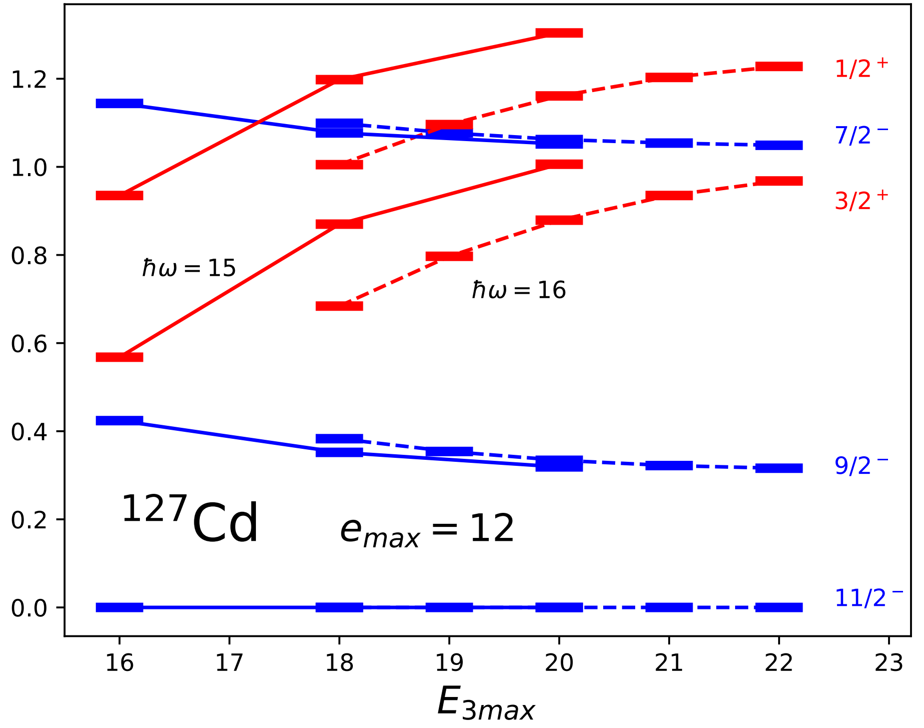
First converged calculations of ^{132}Sn!

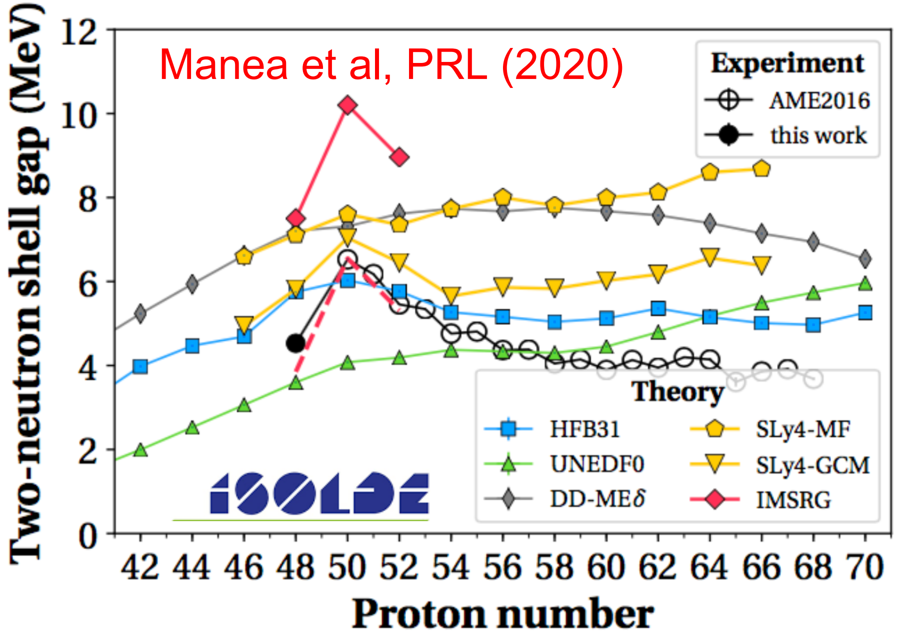
Opens new region of chart to ab initio theory

Convergence of N=82 Gap

Size of N=70 gap clearly not converged wrt E3max – for neutron-rich Sn, In, Cd…







Lascar et al PRC (2017)

Resorted to unreliable extrapolations…

New capabilities: converged spectra in N=82 region!

Explore new physics near ^{132}Sn!

TRIUMF

Towards Global Ab Initio Calculations

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

- Nuclear forces, electroweak physics
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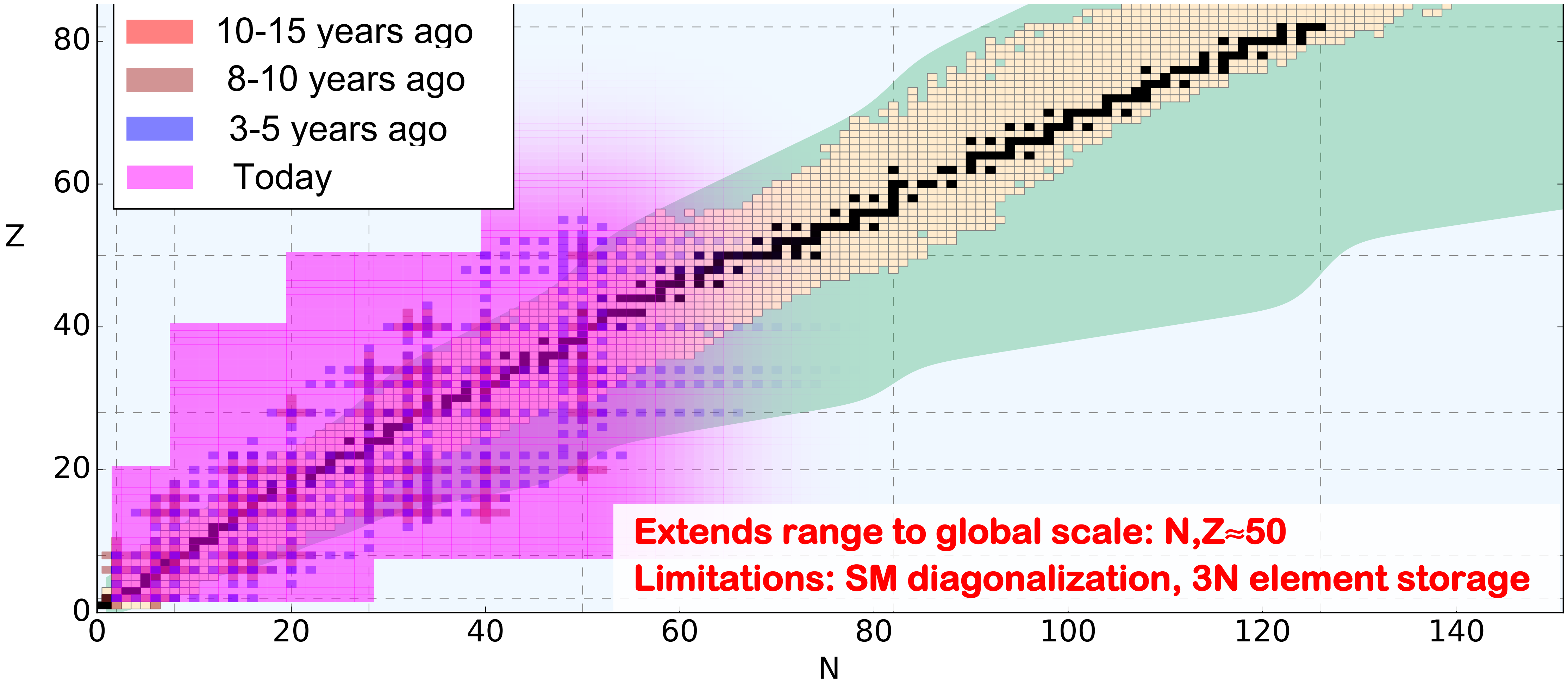

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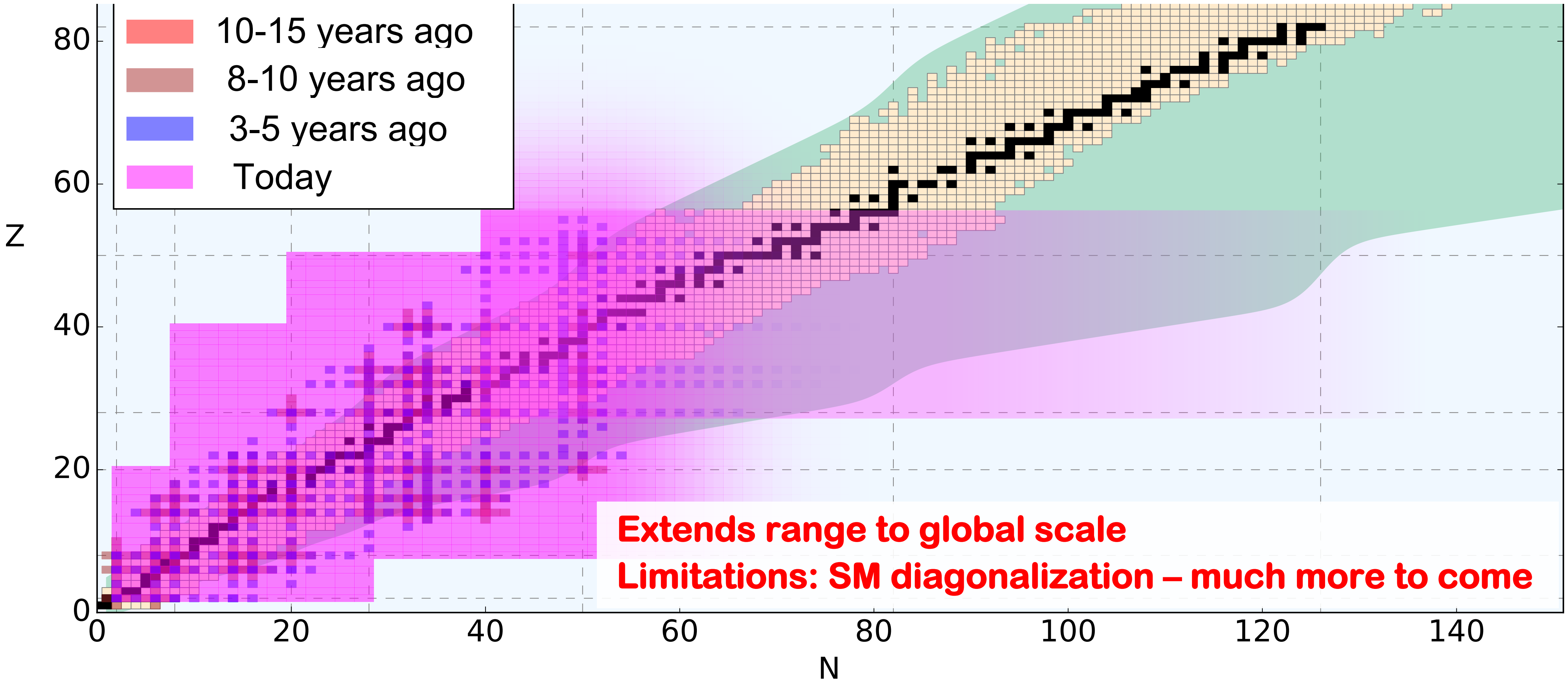

One more thing… Can we go heavier?

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

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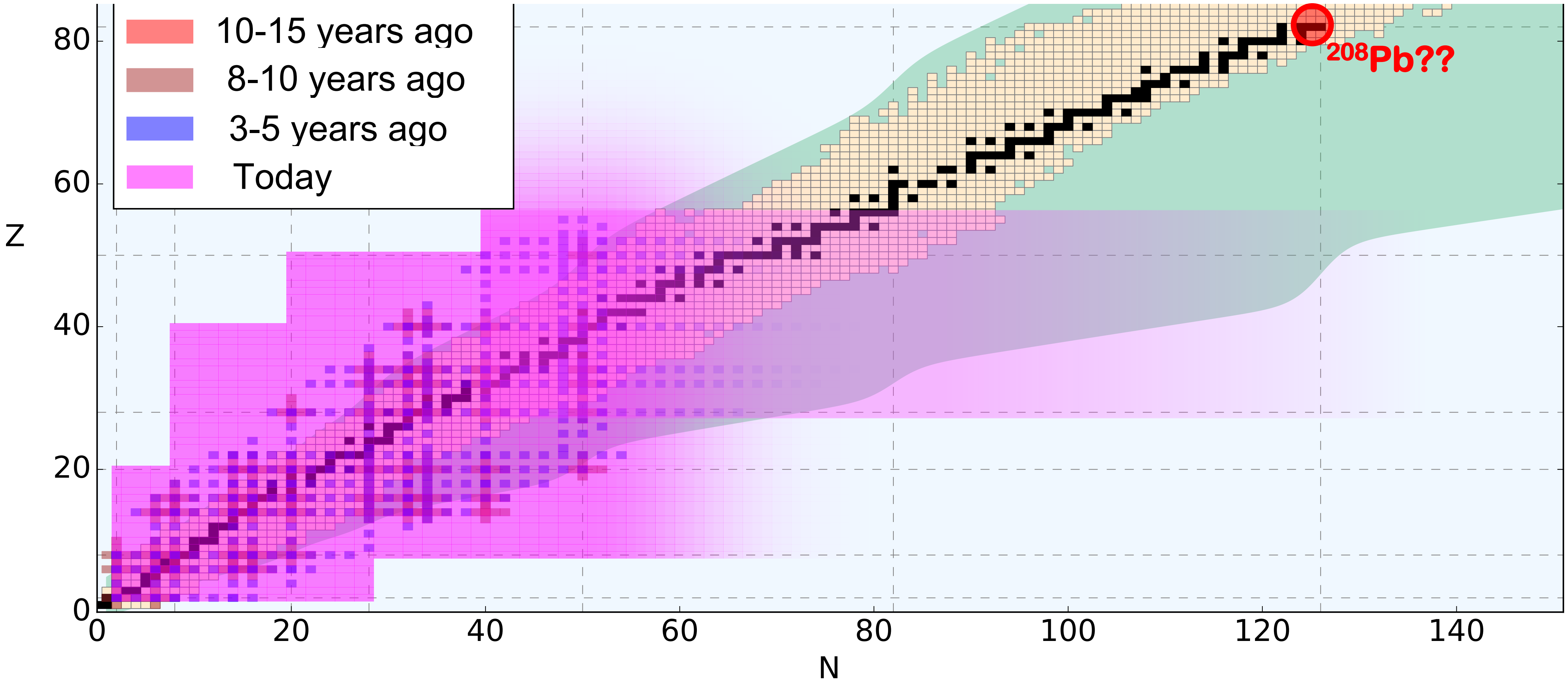
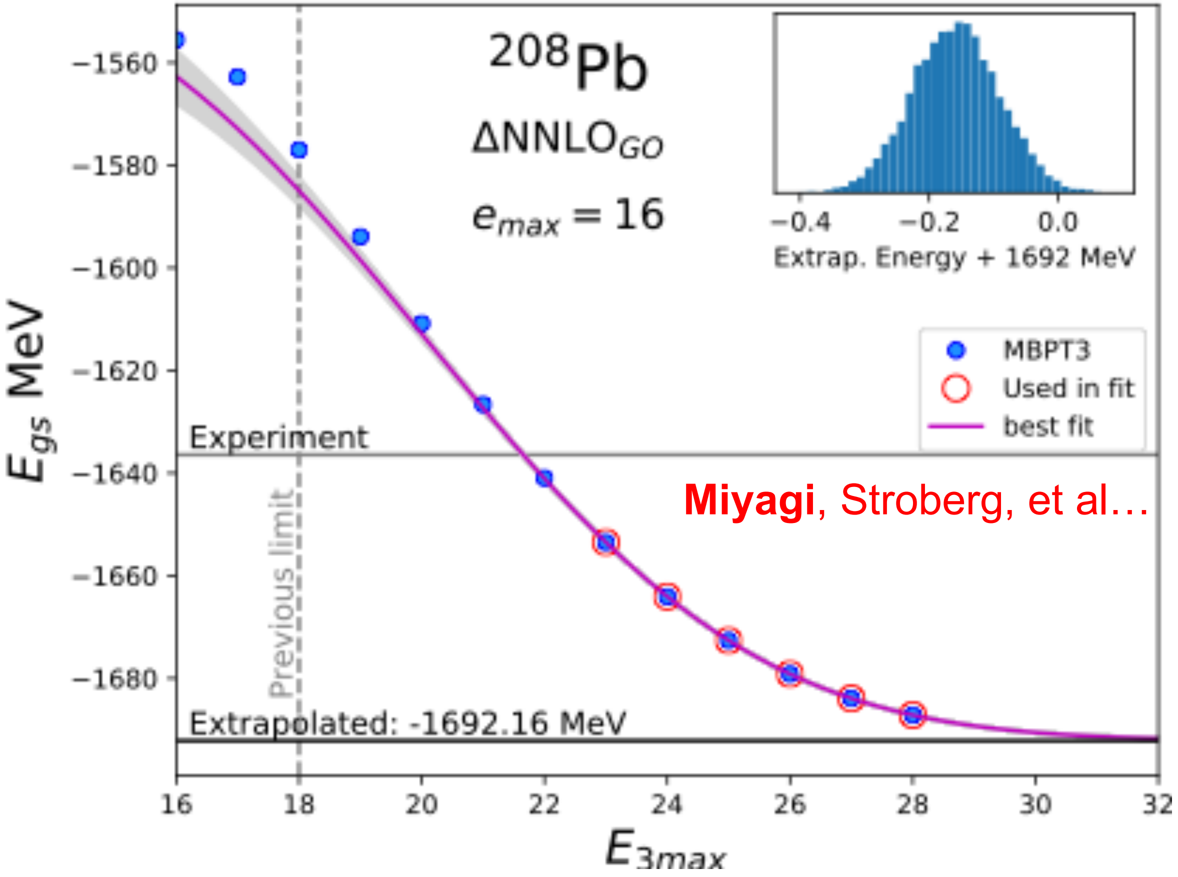


Can We Ever Compute ^{208}Pb?

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

Increased E_{3max} range allows first reliable convergence of ^{208}Pb



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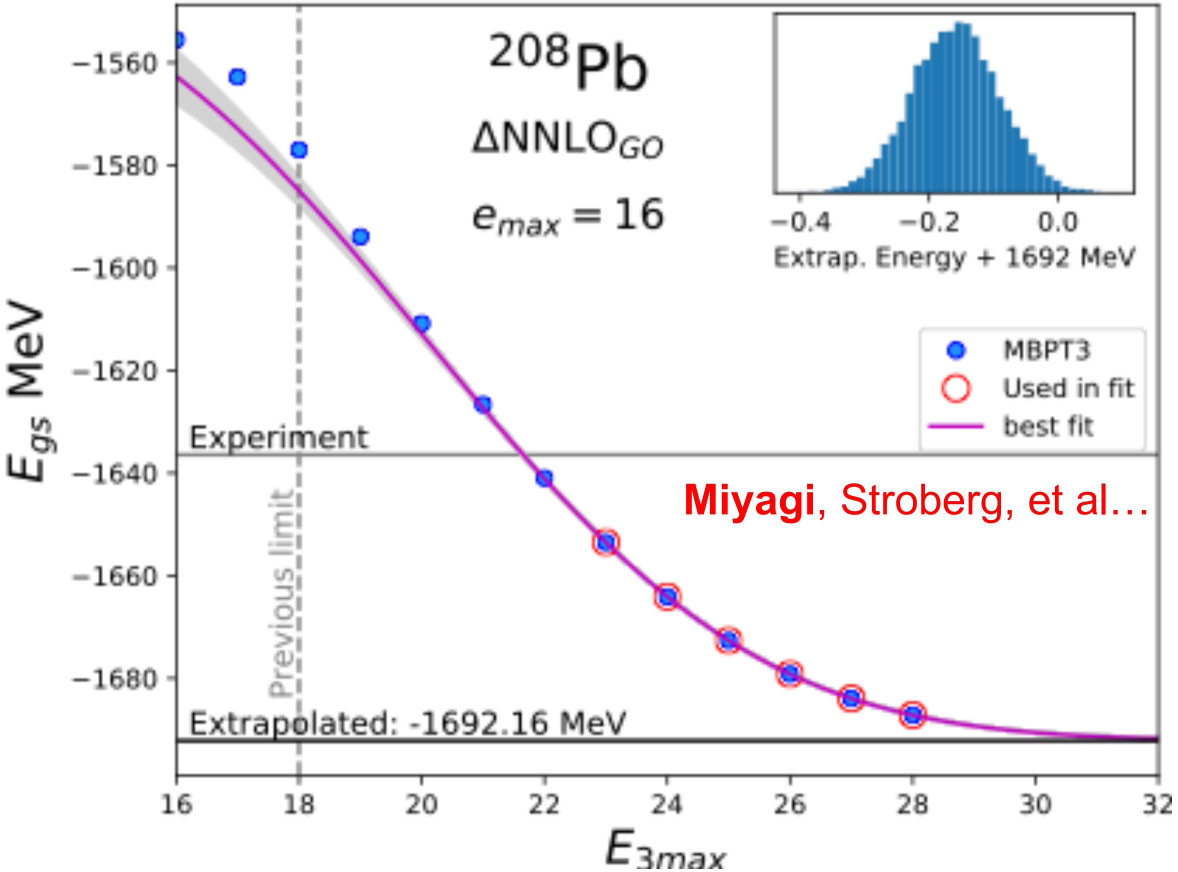

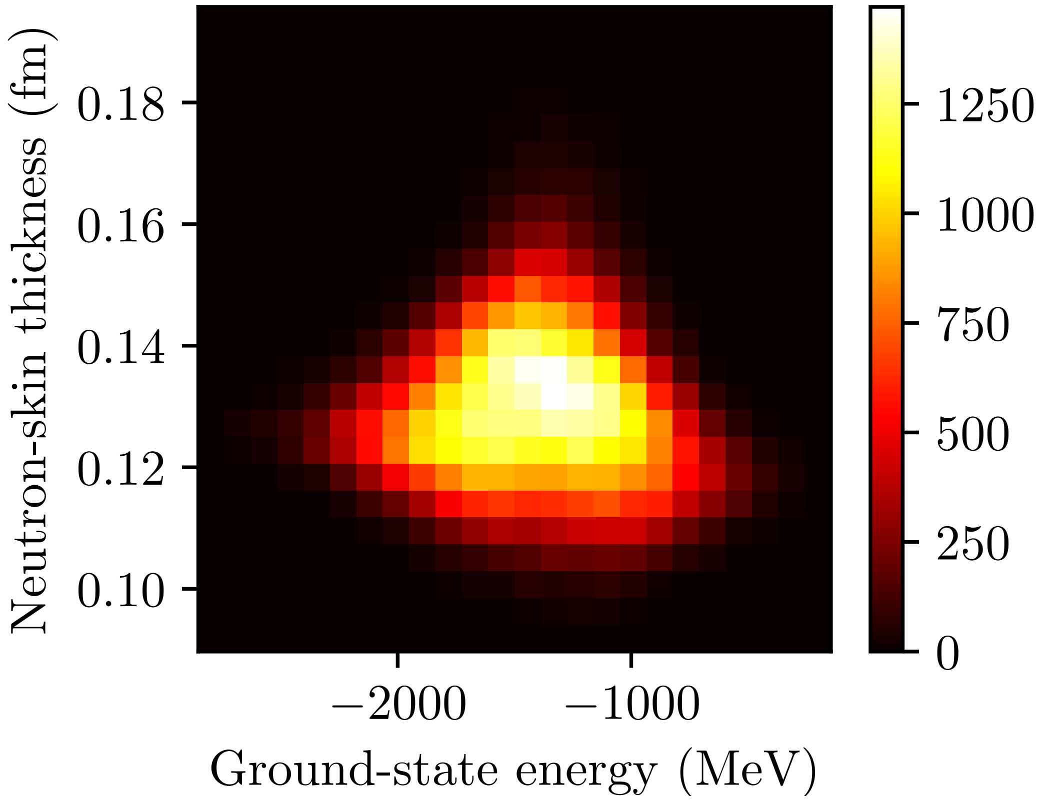

Machine learning algorithms sample "all" chiral interactions: 100 000 ^{208}Pb calculations - billions in progress

Heat map of neutron skin/ground state energy - constraints on equation of state and neutron stars!

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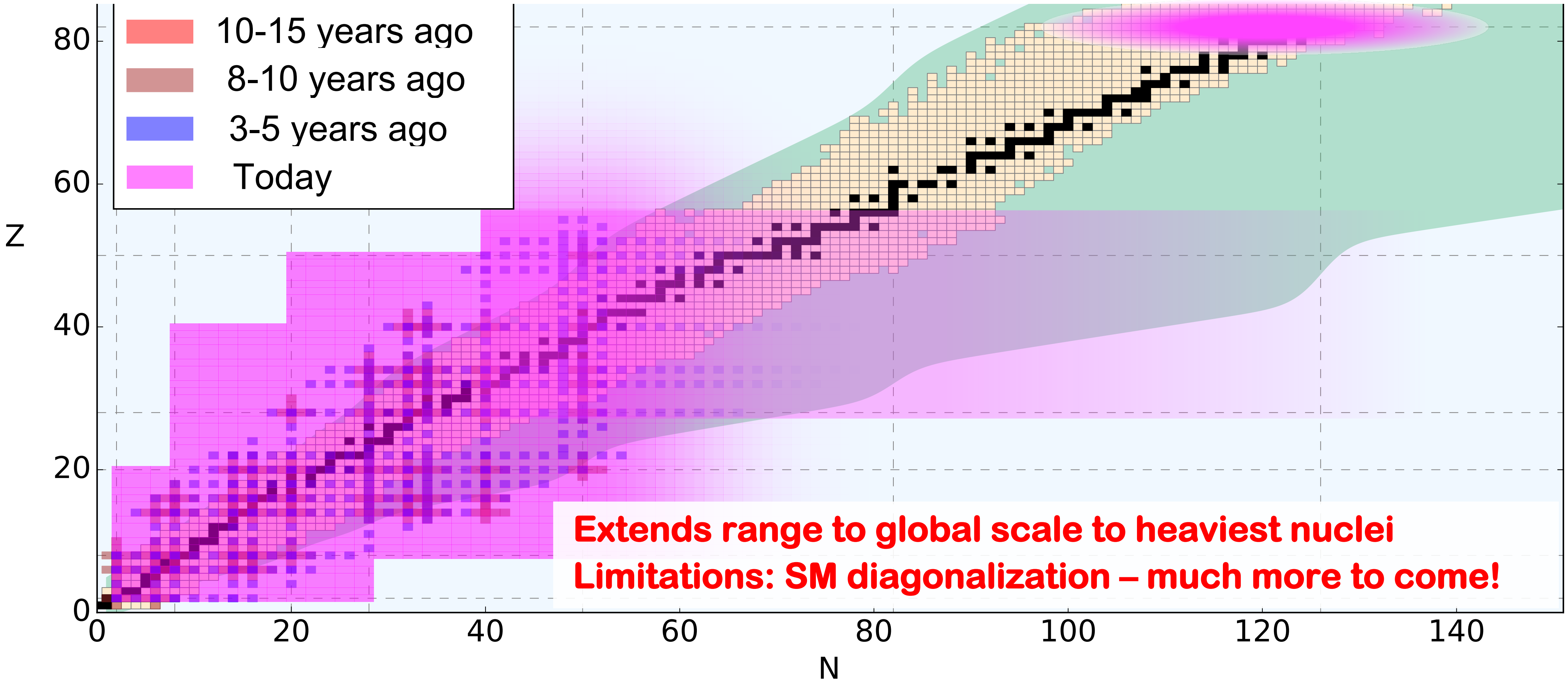


Present and Future

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

Nuclear Structure

Development of forces and currents[1]

Dripline predictions for medium-mass

Evolution of magic numbers from masses, radii, spectroscopy, EM transitions: ^{78}Ni

Multi-shell theory:

- Island of inversion[2]
- Forbidden decays[3]

Atomic systems[4]

Fundamental Symmetries/BSM Physics

Effective electroweak operators: GT quenching

Effective $0\nu\beta\beta$ decay operator[5]

WIMP-Nucleus scattering[6]

Superallowed Fermi transitions[7]

Symmetry-violating moments [molecules][8]

Experimental overlap

Best data for constraining nuclear forces

New measurements of driplines

Data on magic numbers in exotic nuclei

Precision data on GT transitions

TRIUMF, THE UNIVERSITY OF BRITISH COLUMBIA, McGill UNIVERSITY:
S. R. Stroberg*
T. Miyagi[2,3,4,7,8]
B. Hu
C. Gwak[3,8]
G. Tenkila[4]
D. Livermore[4]
A. Belley[5]
C. Payne[5]
J. Padua[6]
S. Leutheusser[6]

THE UNIVERSITY of TENNESSEE KNOXVILLE: T. Morris, G. Hagen, T. Papenbrock

TECHNISCHE UNIVERSITÄT DARMSTADT: A. Schwenk

東京大学 THE UNIVERSITY OF TOKYO: J. Menéndez

MICHIGAN STATE UNIVERSITY: H. Hergert, S. Bogner

THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL: J. Engel

JGU: J. Simonis[1]

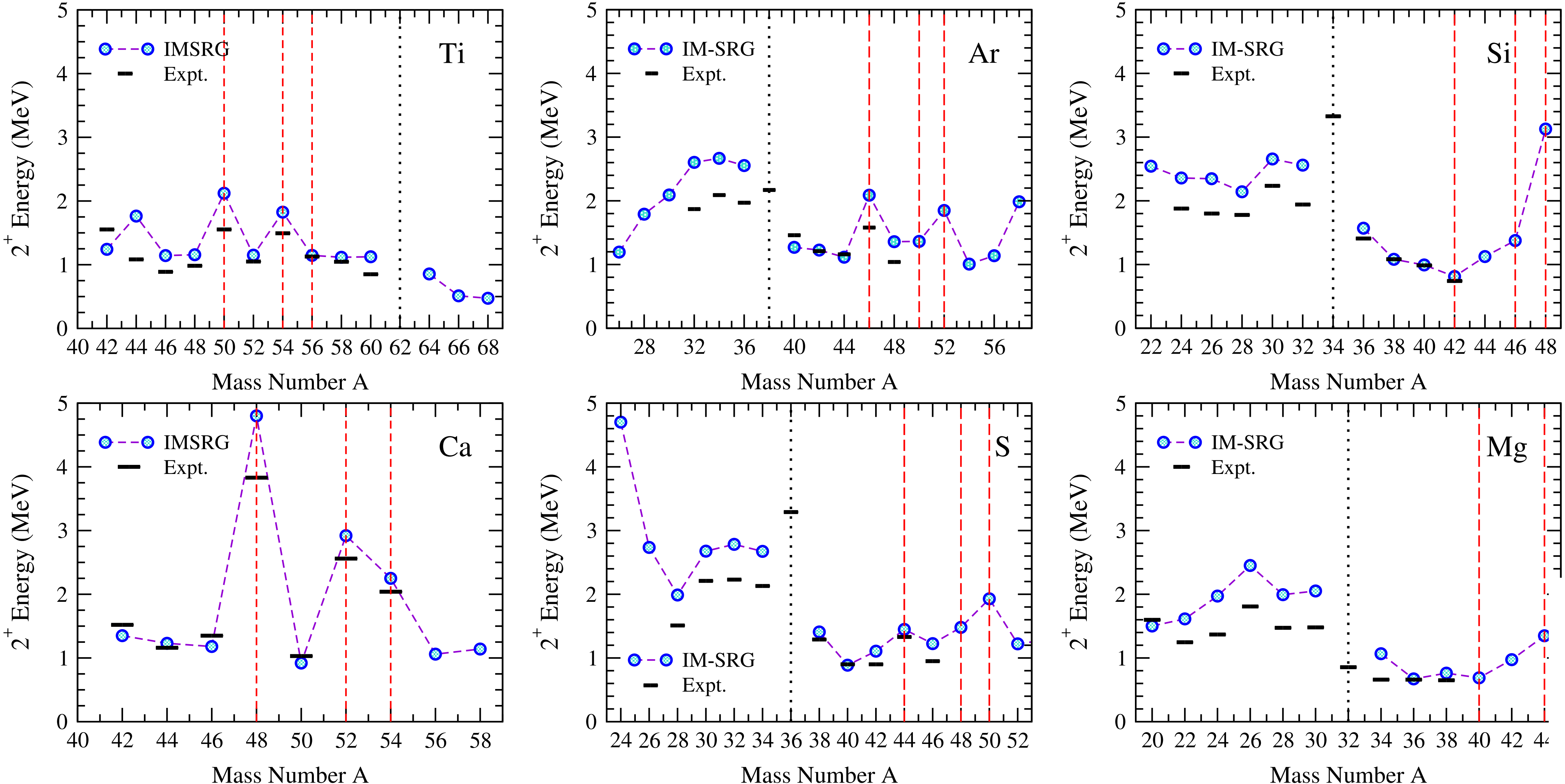
COLORADO SCHOOL OF MINES: M. Martin[7], K. G. Leach

Massachusetts Institute of Technology: R. F. Garcia-Ruiz[8]

TRIUMF

Future: Evolution of N=28,32,34 Magic Numbers

Ab initio predictions from above calcium towards oxygen – **persistence of N=34**



Large-Scale Efforts for Ab Initio GT Transitions

Calculate **large GT matrix elements**

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

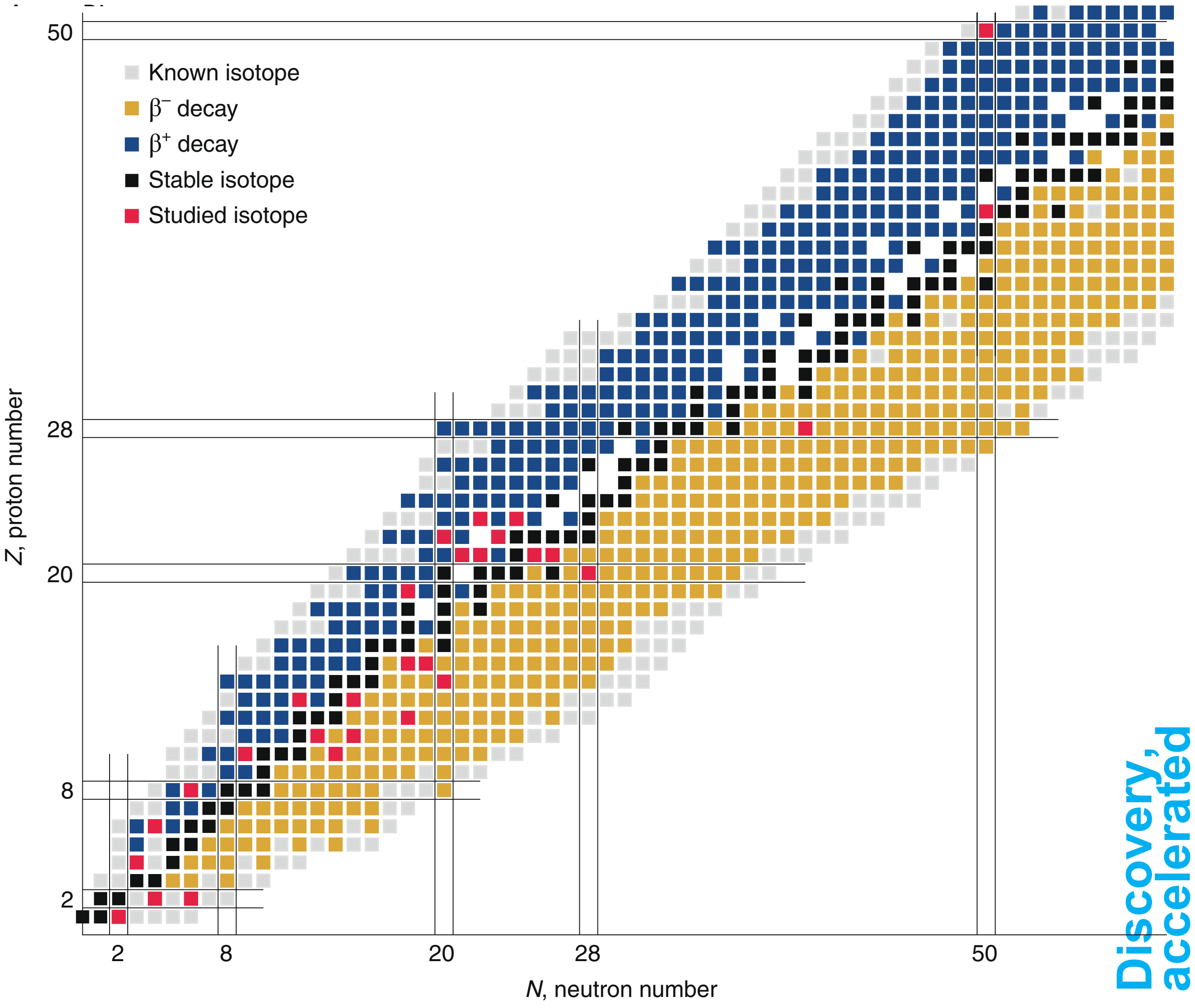
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

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

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.



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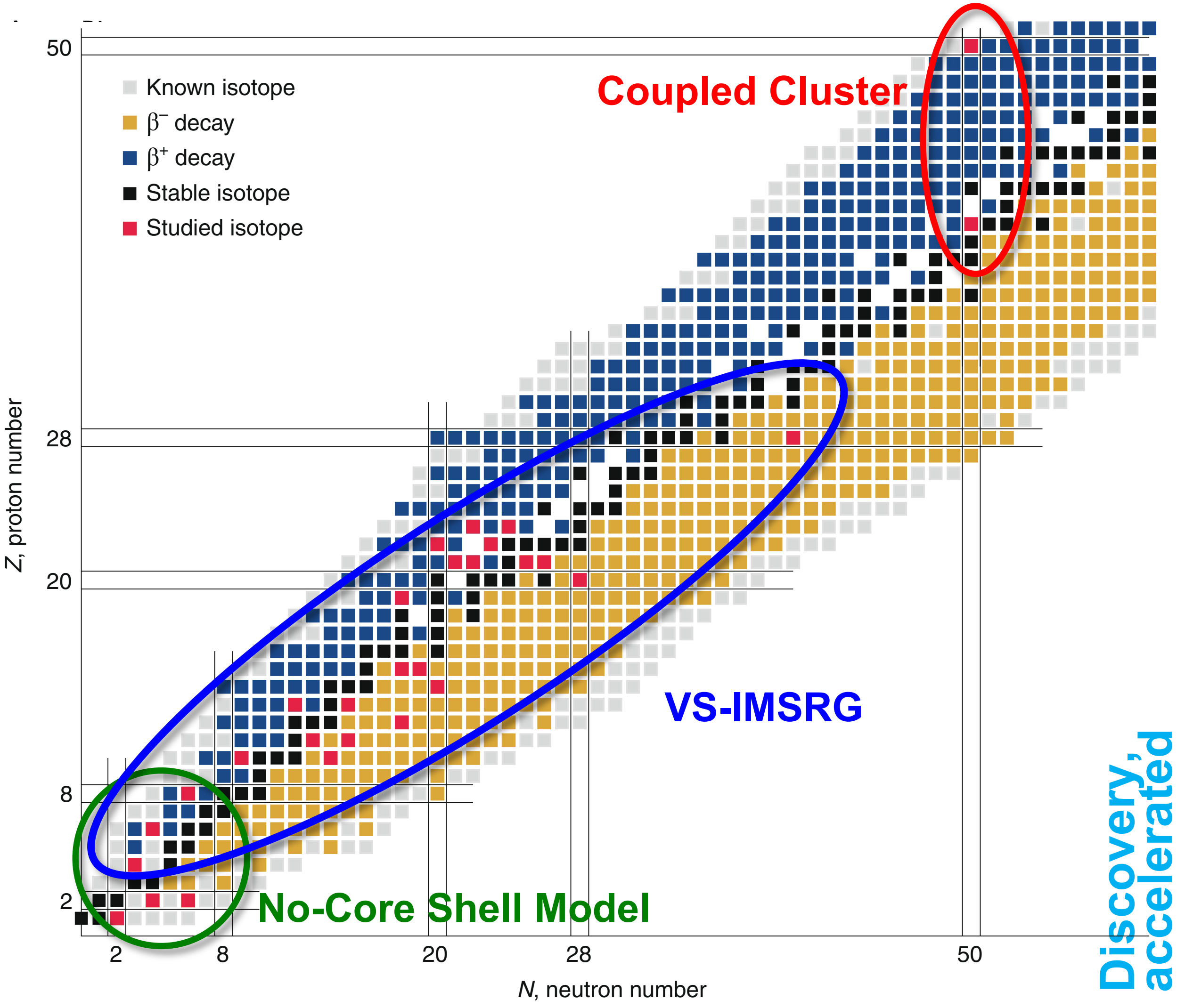
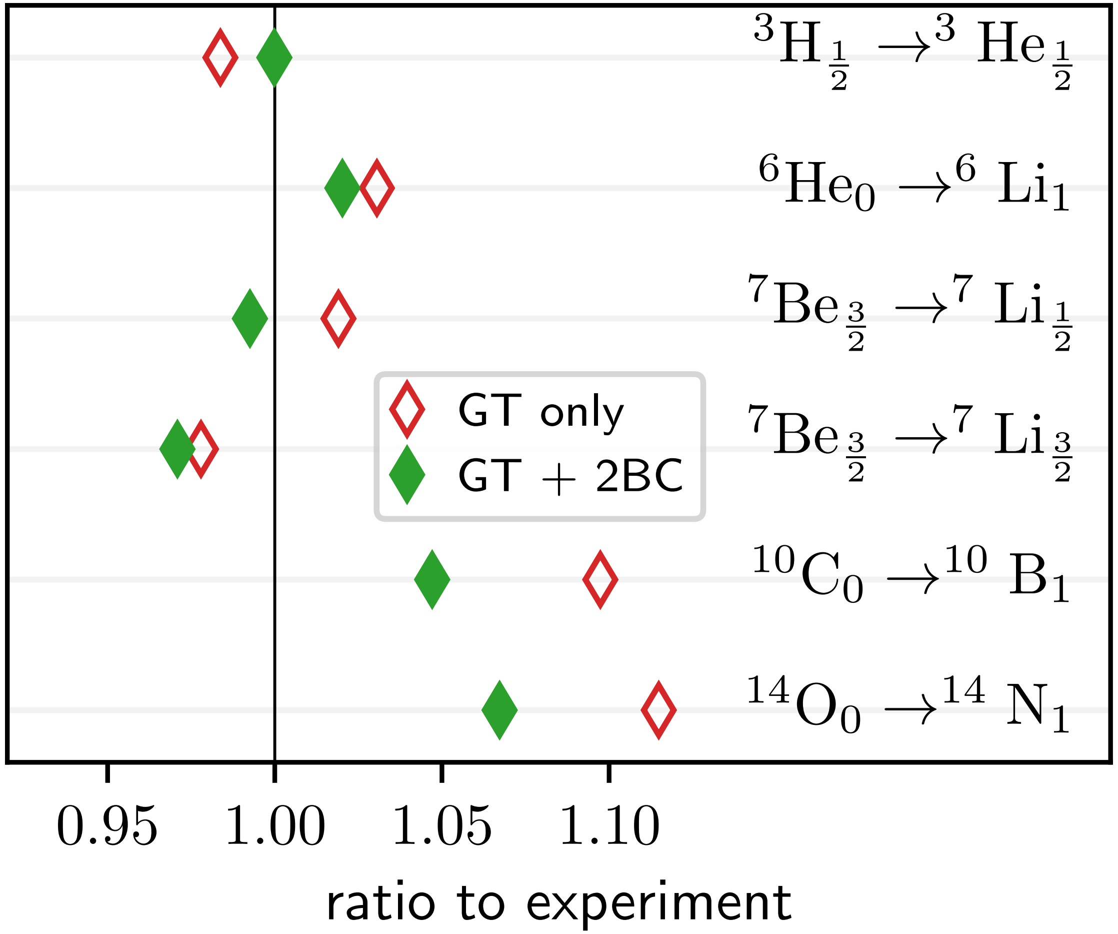
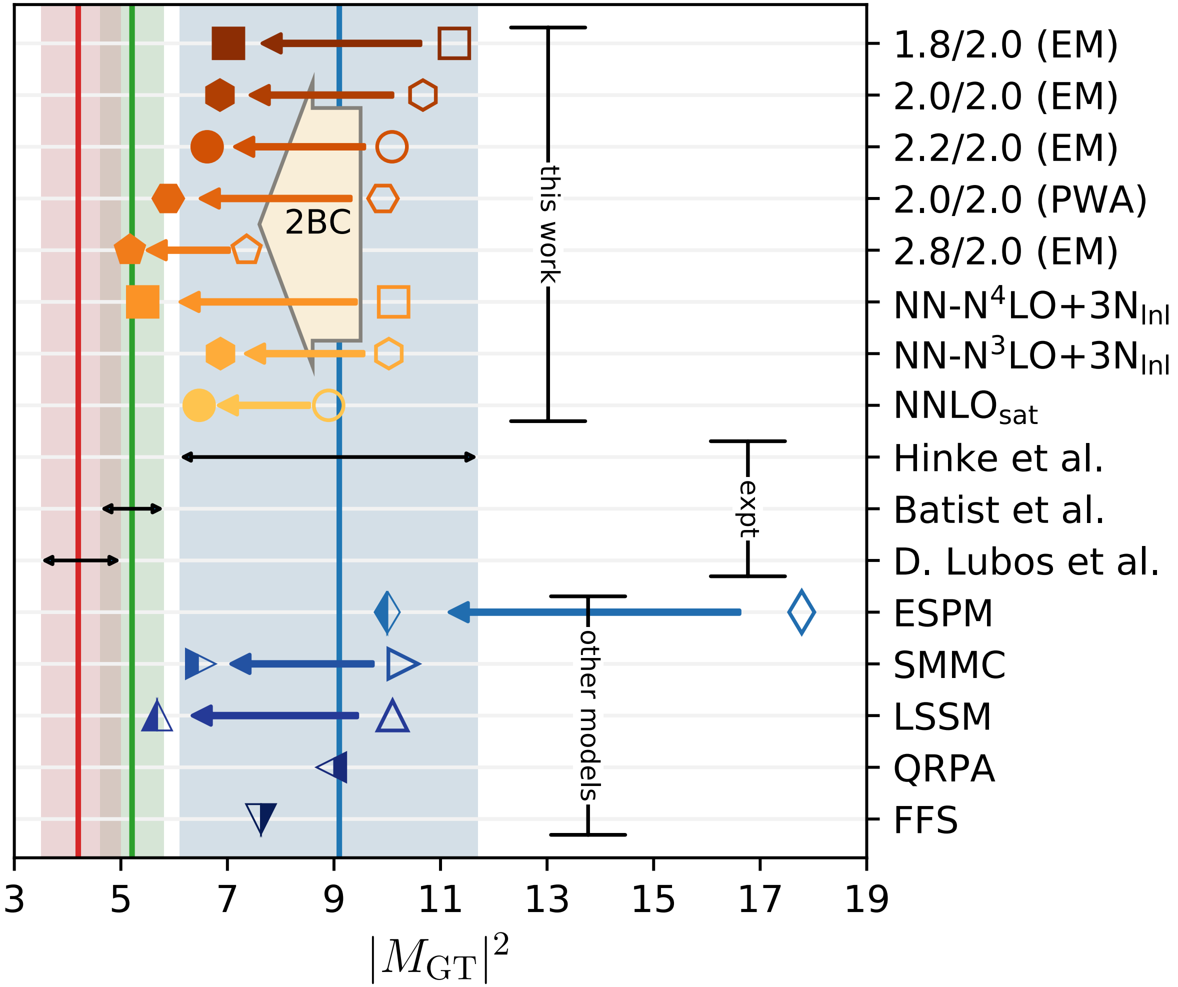


Discovery, accelerated

GT Transitions in Light nuclei and ^{100}Sn

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





Gysbers et al., Nature Phys. (2019)

Large quenching effect from correlations

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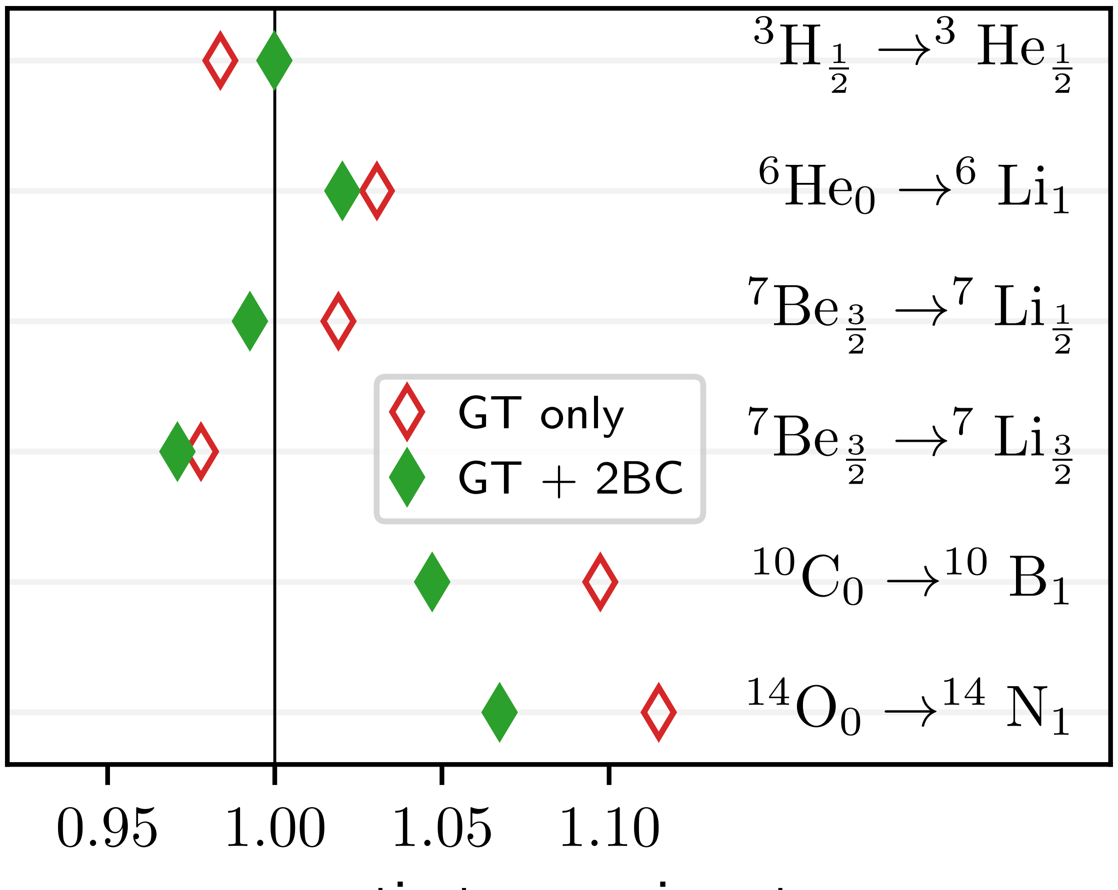

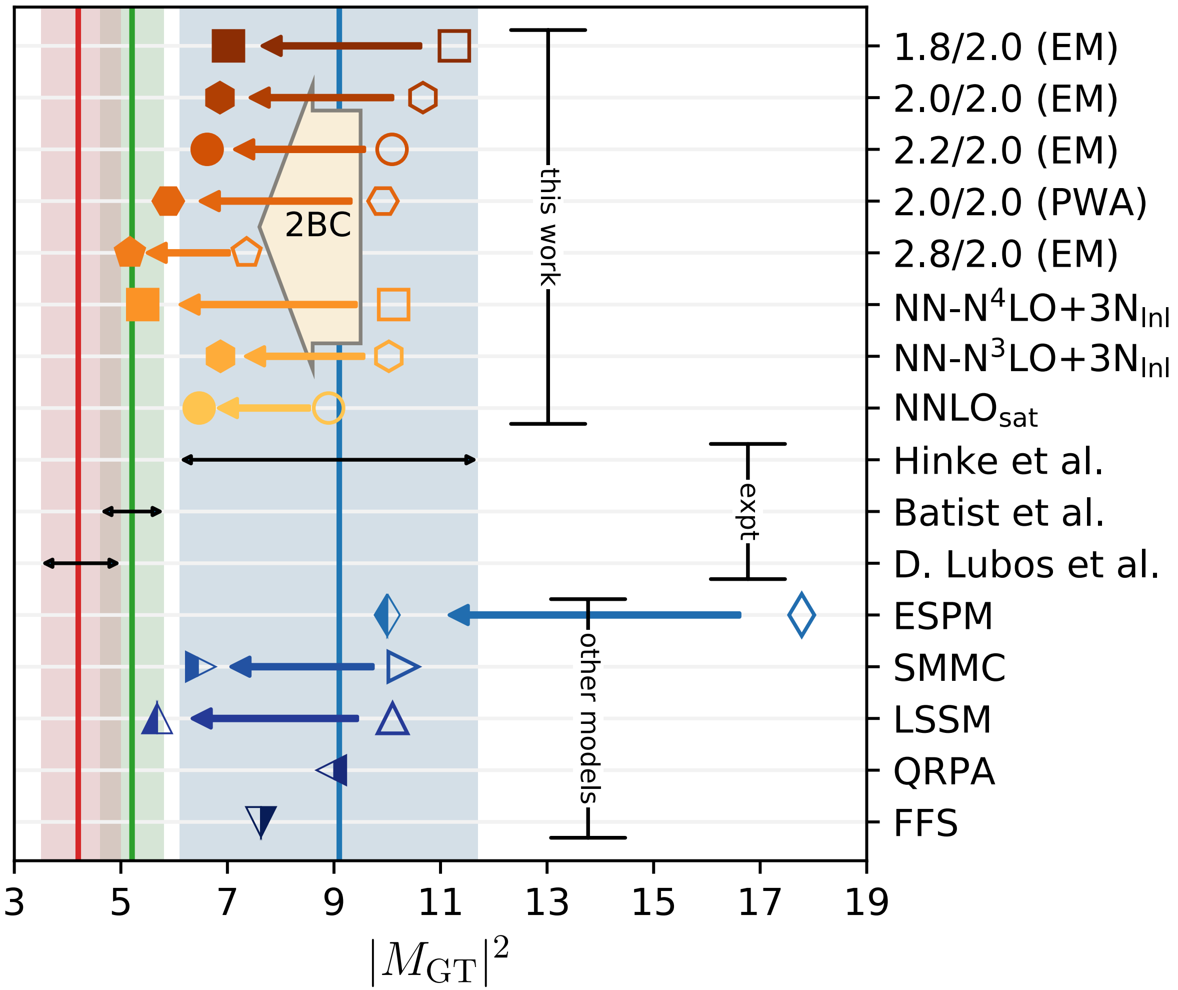

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Large quenching effect from correlations

Addition of 2BC further quenches and reduces spread in results

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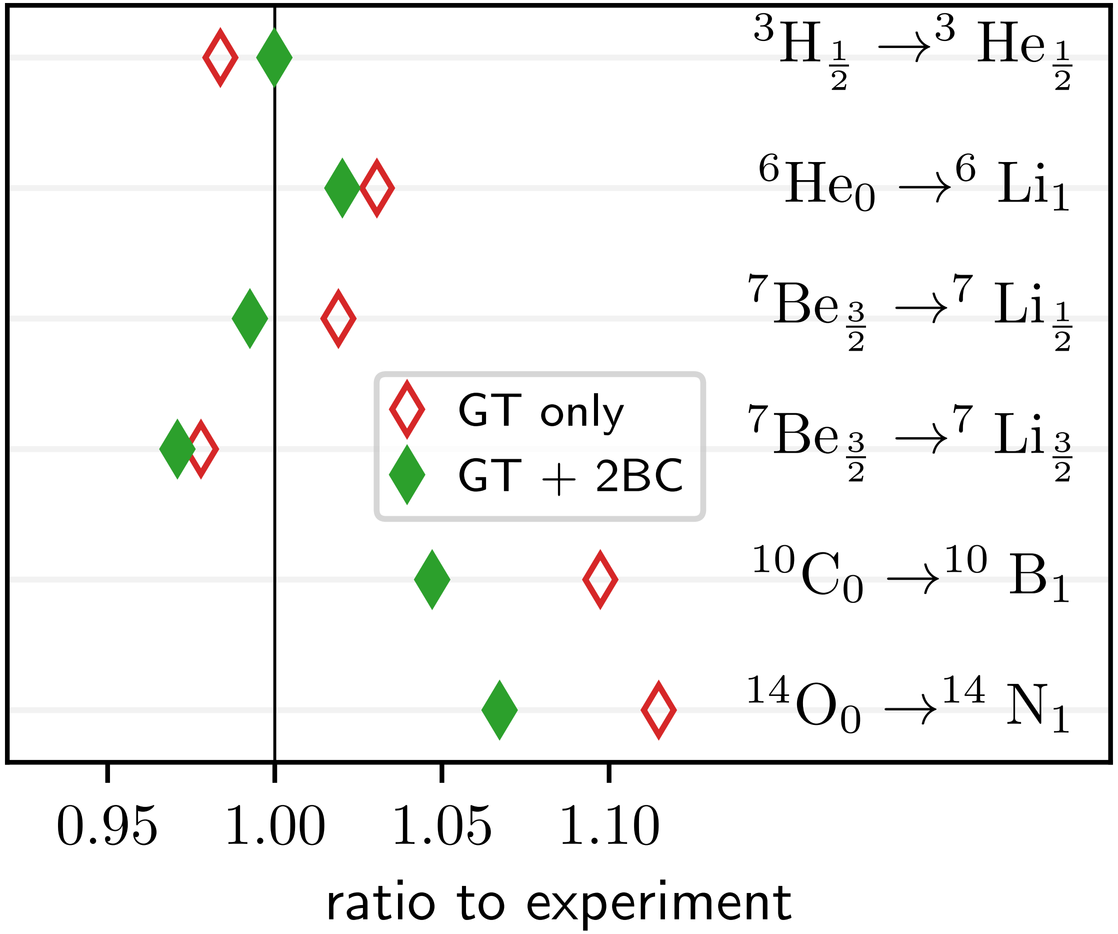

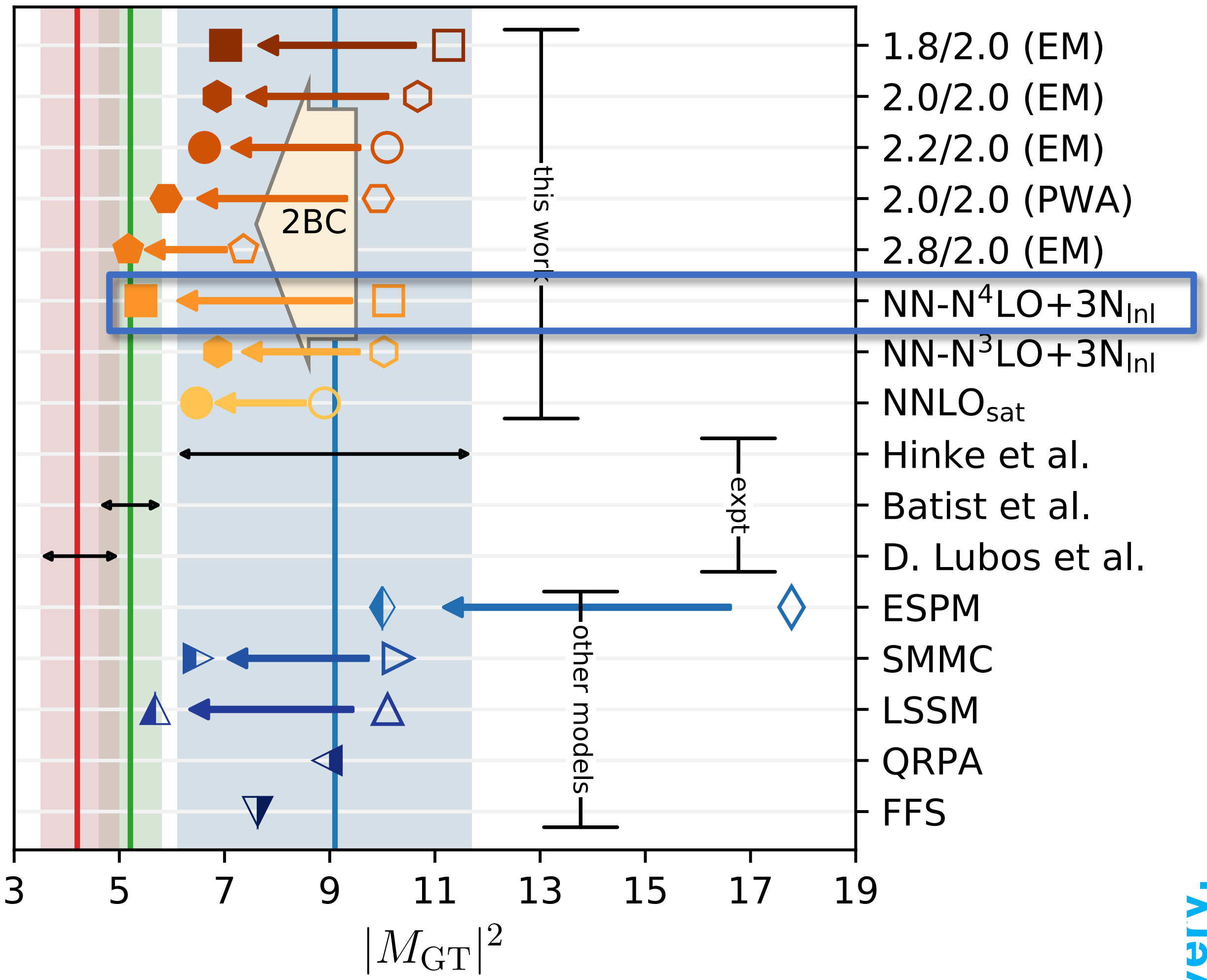

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Gysbers et al., Nature Phys. (2019)

Addition of 2BC further quenches and reduces spread in results

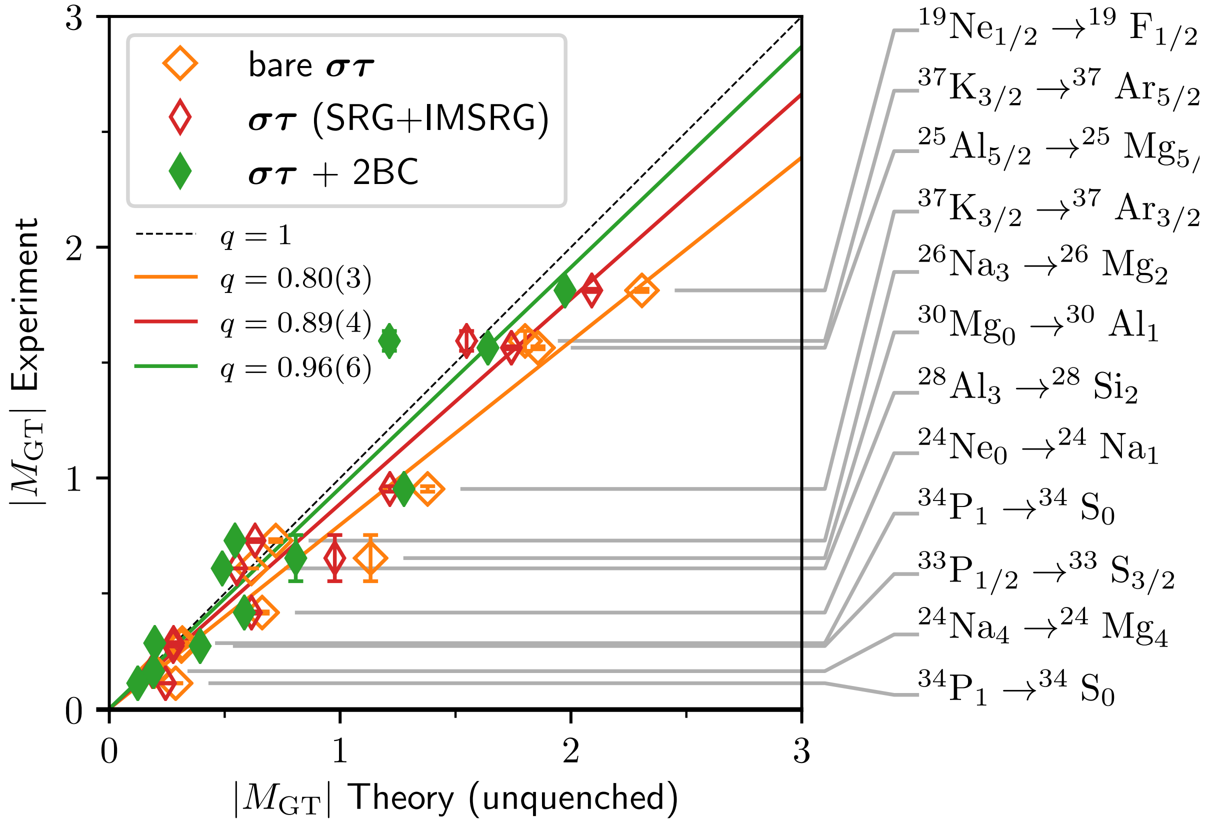
TRIUMF

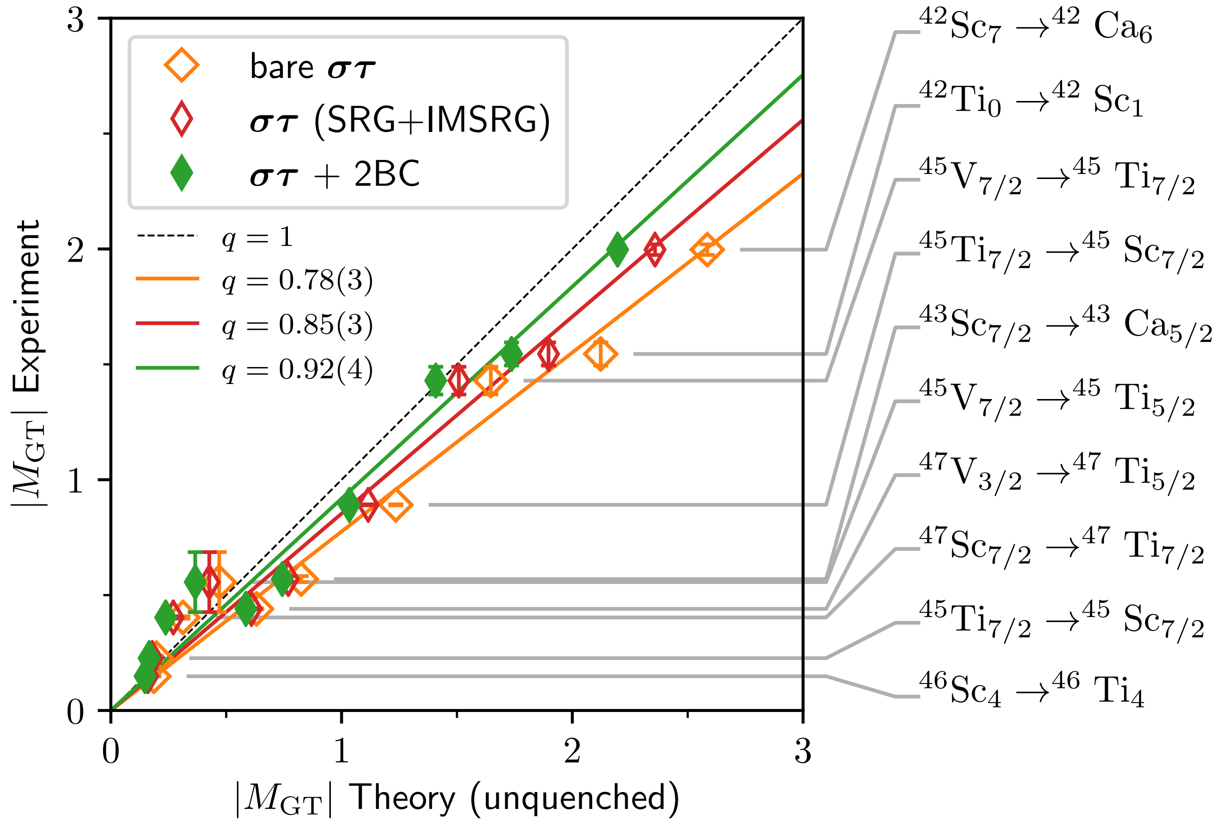
Ab Initio GT Decays in Medium-Mass Region

Ab initio calculations of **large** GT transitions in *sd*, *pf* shells

Bare operator similar to phenomenological shell model

Modest quenching from consistent ab initio wavefunctions and operators





Gysbers et al., Nature Phys. (2019)

Further modest quenching from 2BC

Disc accelerated

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

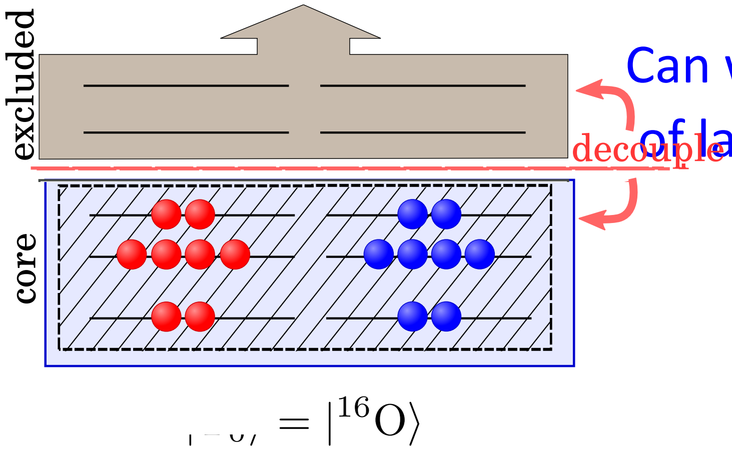
$$U = e^{\Omega} = e^{\eta_n} \ldots e^{\eta_1} \qquad \eta = \frac{1}{2}\arctan\left(\frac{2H_{\text{od}}}{\Delta}\right) - \text{h.c.}$$

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

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

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

Step 1: Decouple core



Can we achieve accuracy of large-space methods?

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

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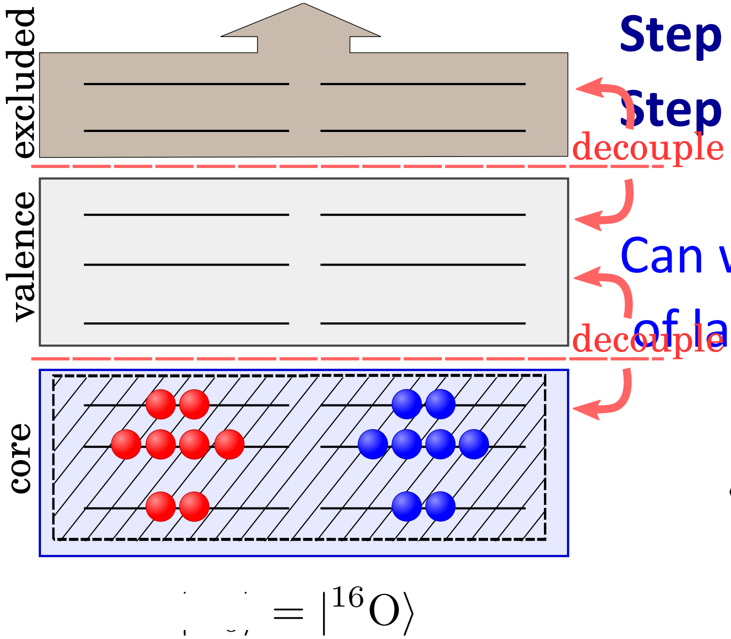

Step 1: Decouple core

Step 2: Decouple valence space

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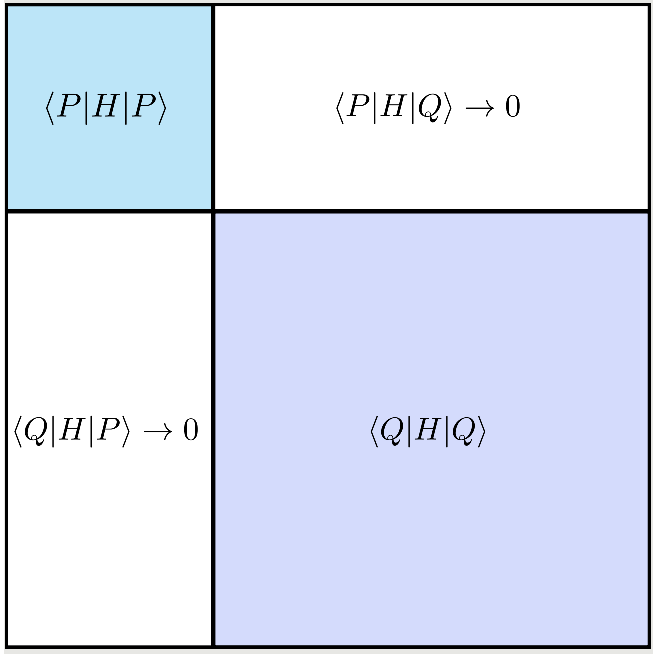

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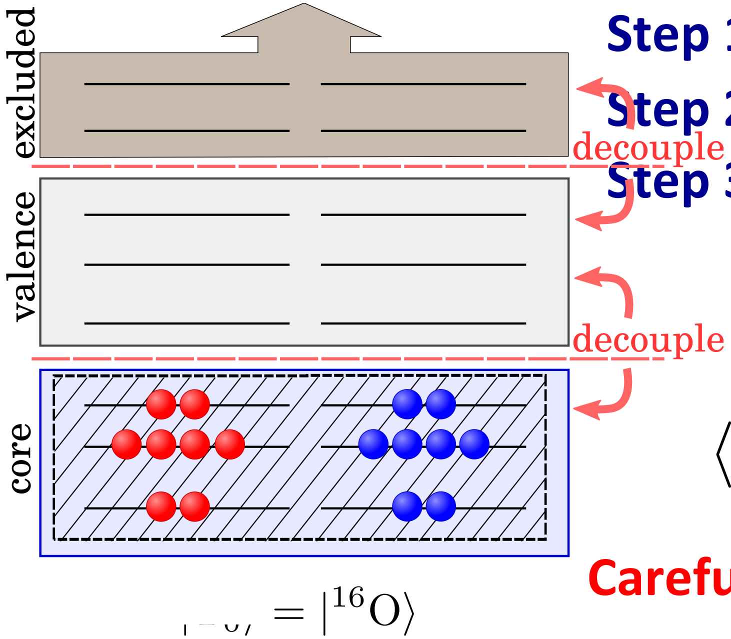
$$\tilde{\mathcal{O}} = e^{\Omega} \mathcal{O} e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2}[\Omega, [\Omega, \mathcal{O}]] + \cdots$$



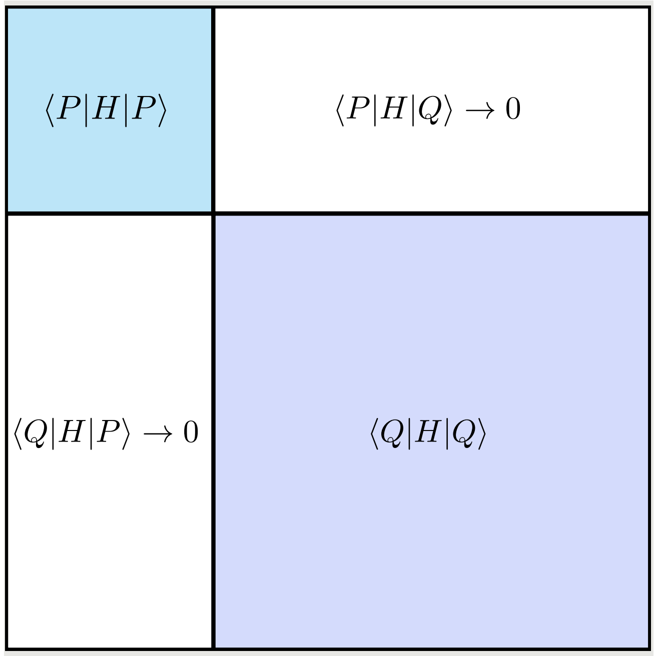
Step 1: Decouple core

Step 2: Decouple valence space

Step 3: Decouple additional operators

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

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

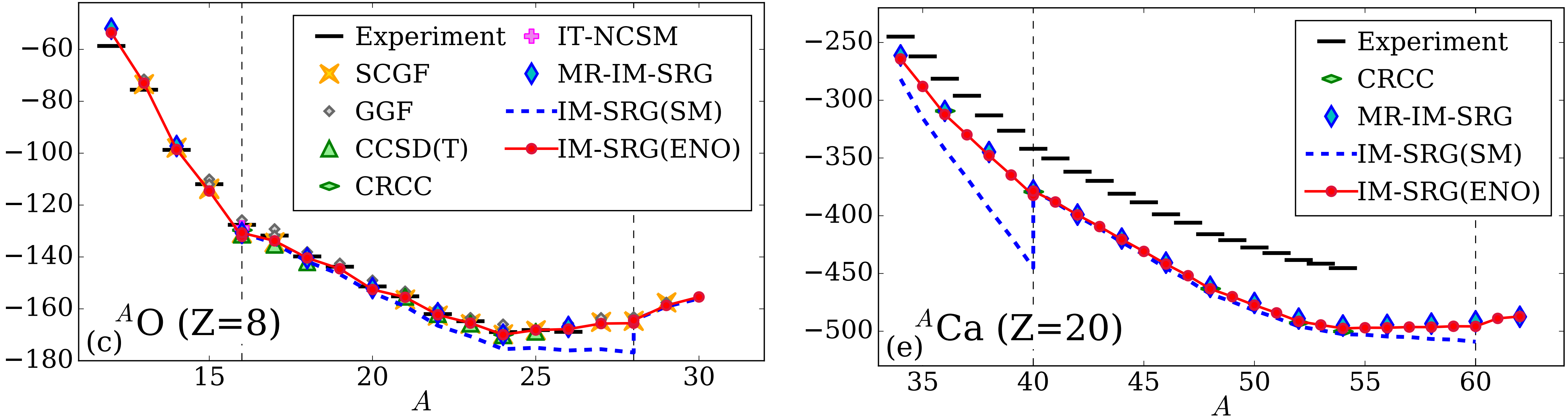


Careful benchmarking essential

TRIUMF

Valence-Space IMSRG: From Oxygen to Calcium

New approach accesses *all* nuclei: agrees to 1% with large-space methods



Stroberg et al., PRL (2017)

Agreement with *experiment* deteriorates for heavy chains (due to input Hamiltonian)

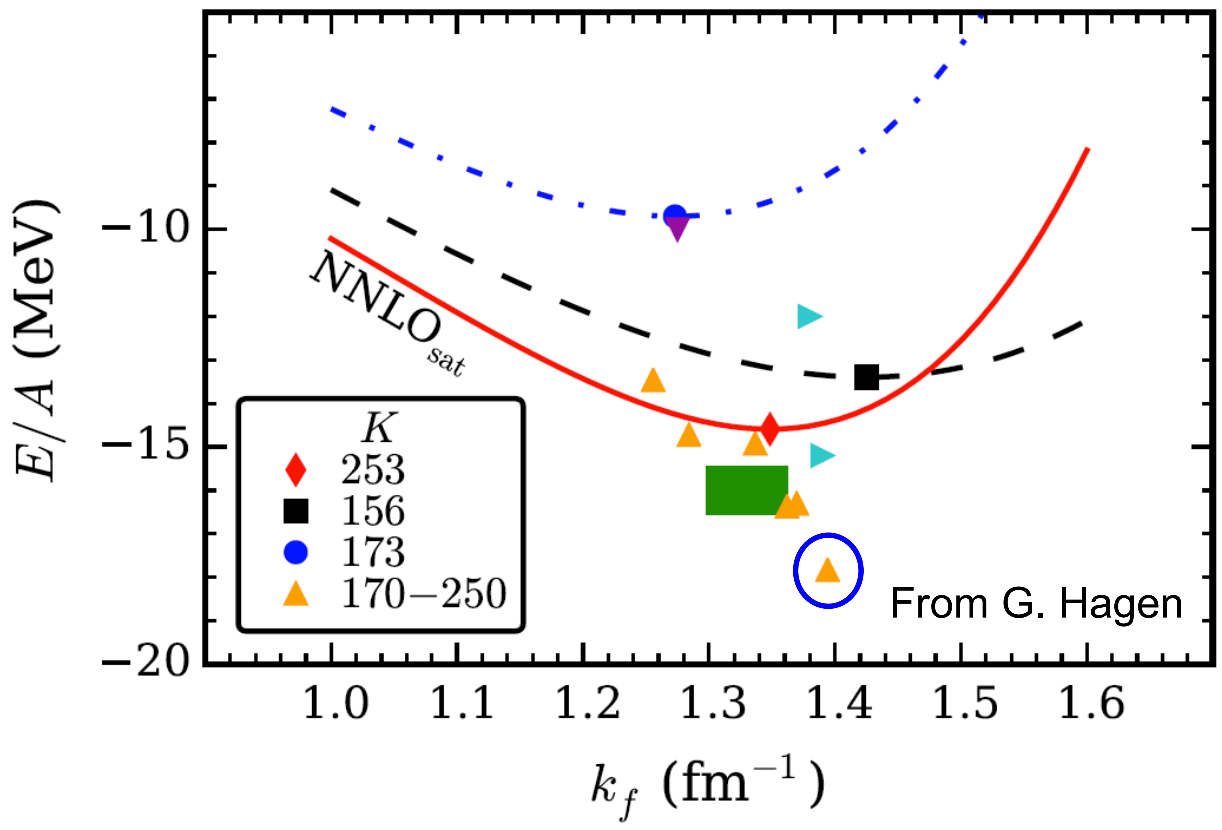
Significant gain in applicability with little/no sacrifice in accuracy

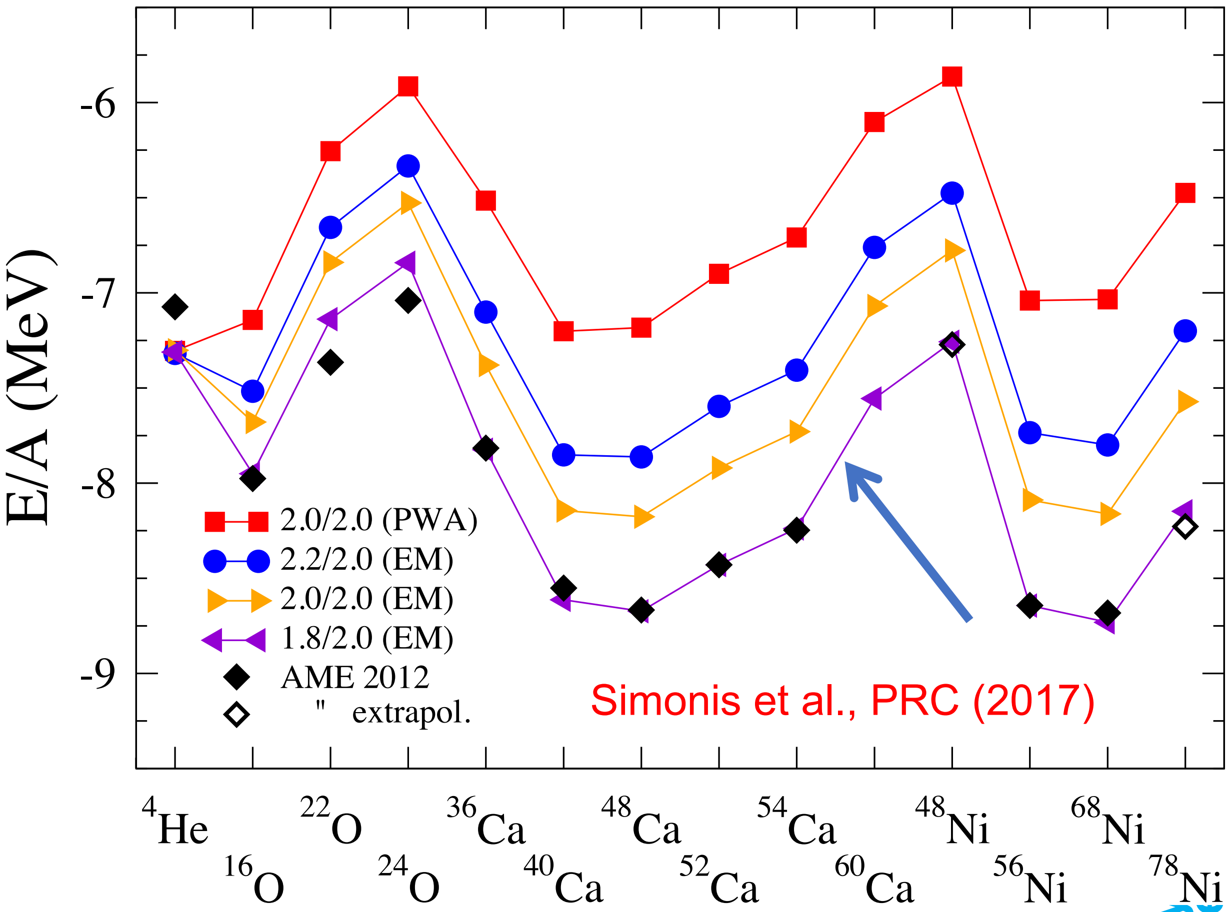
Low computational cost: ~1 node-day/nucleus

Discovery, accelerated

Connection to Infinite Matter: Saturation as a Guide

NN+3N force with good reproduction of ground-state energies (but poor radii)





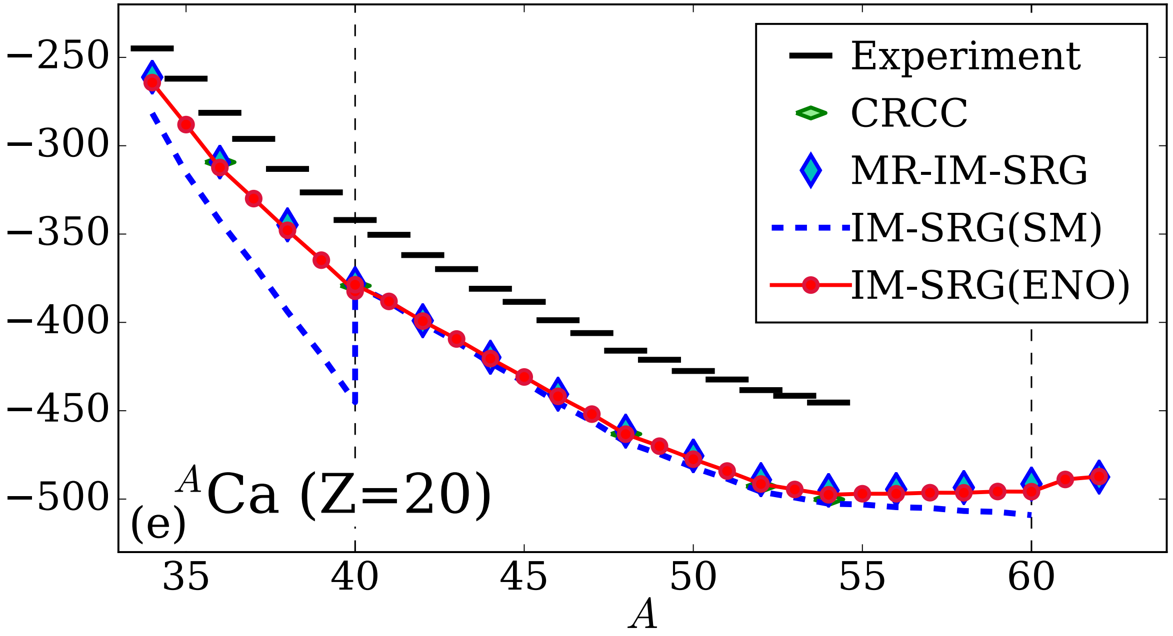
1.8/2.0 (EM) reproduces ground-state energies through ^{78}Ni

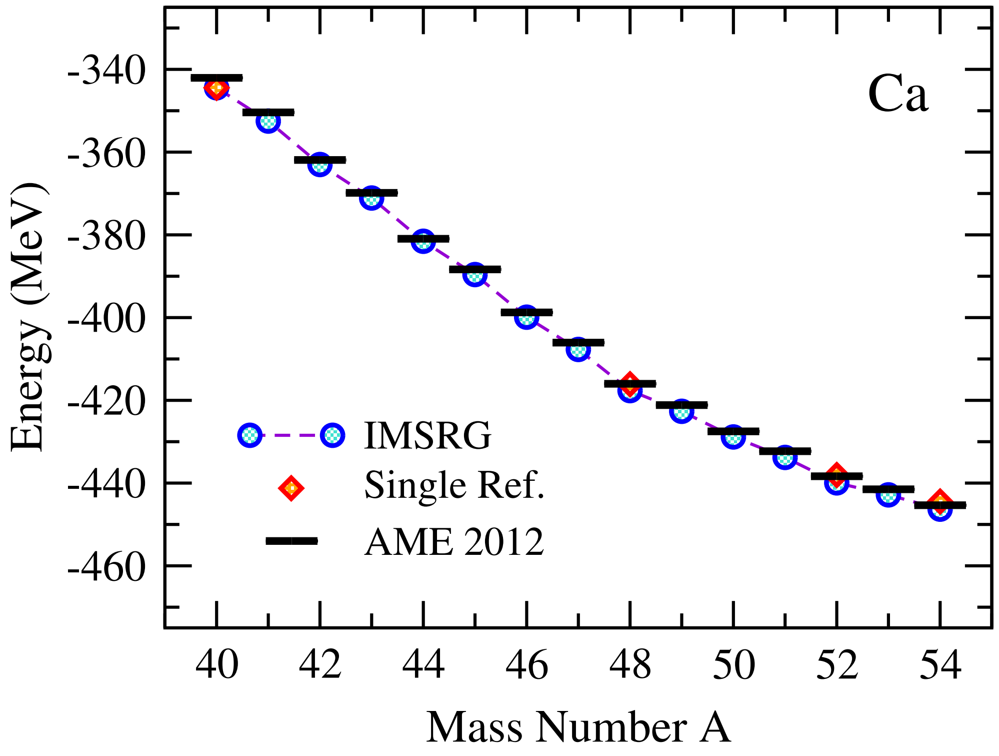
Slight underbinding for neutron-rich oxygen

NN+3N Forces with Good Saturation Properties

TRIUMF

Dramatic improvement with respect to experimental data





Opens possibility for reliable ab initio predictions across the nuclear chart!

Accesses **all** properties of **all** nuclei:

- Ground states, excited states, radii, electroweak transitions…

Discovery, accelerated