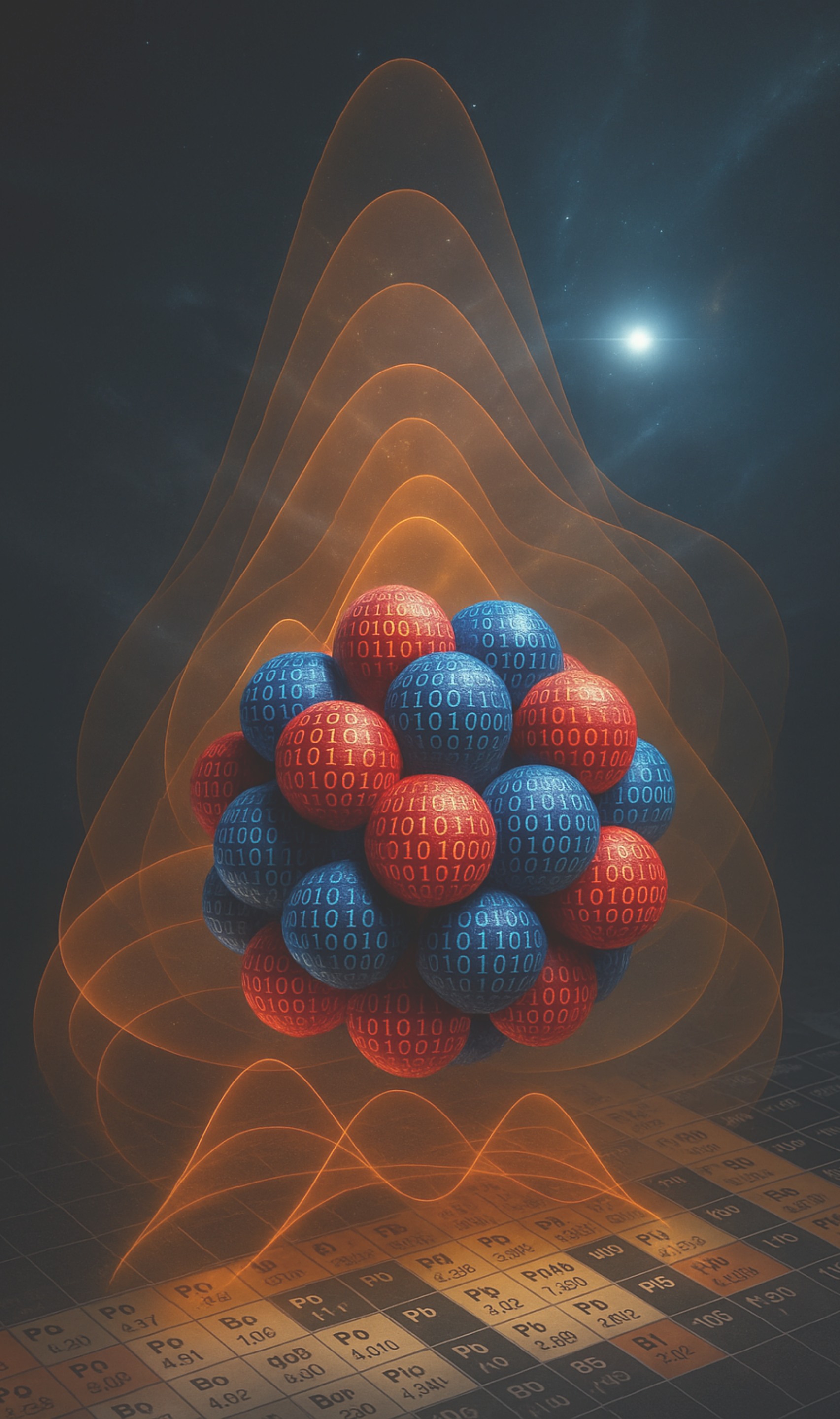




Ab initio in nuclear theory — what, why, and how —

Andreas Ekström
Chalmers University of Technology



CHALMERS
UNIVERSITY OF TECHNOLOGY

European Nuclear Physics Conference 2025, Caen, France



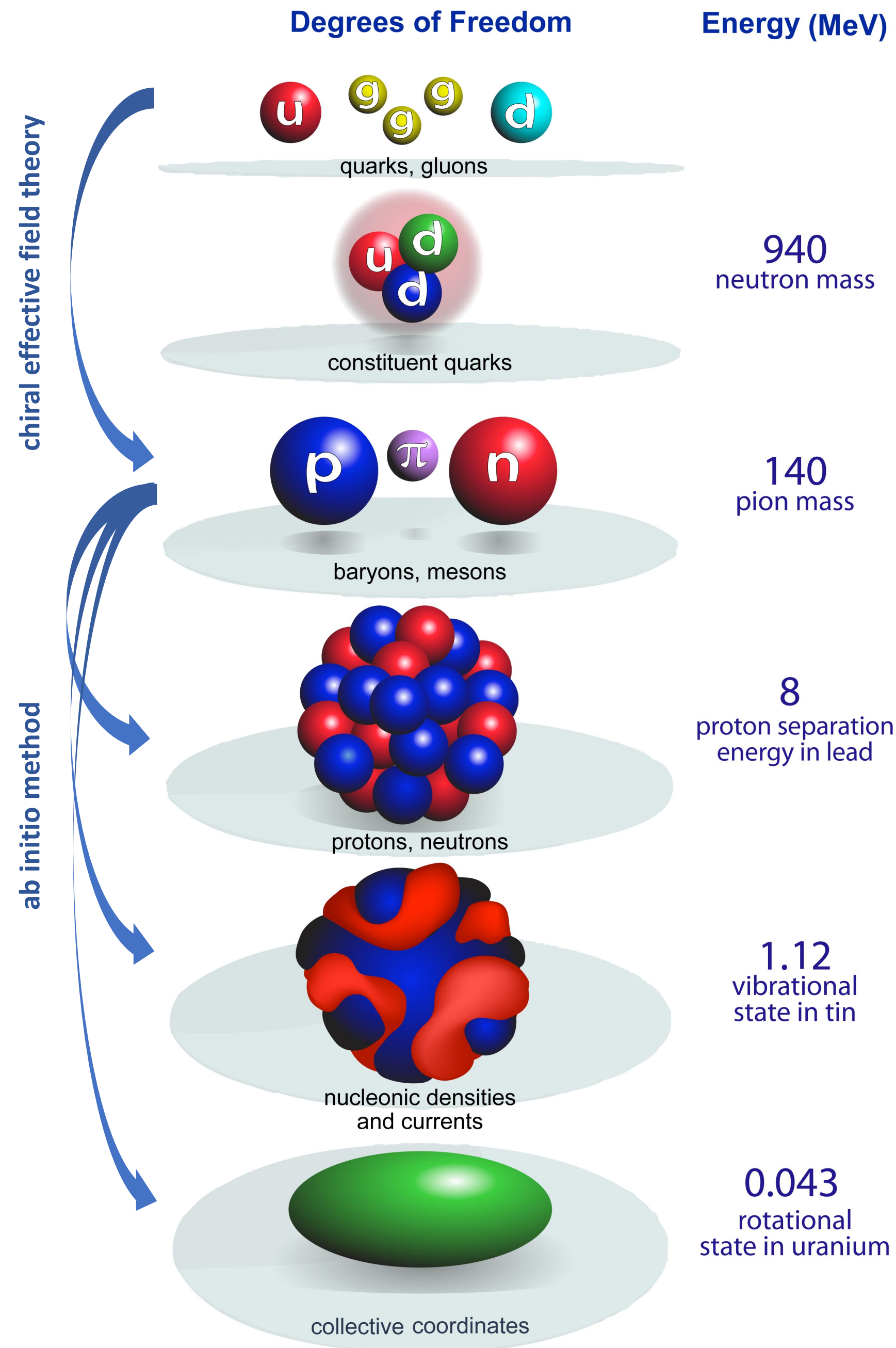
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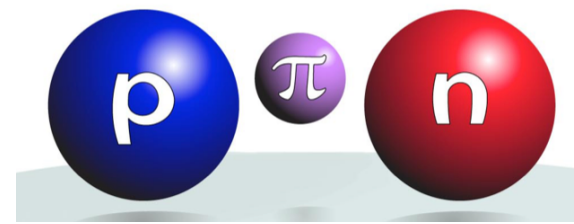
Swedish
Research
Council



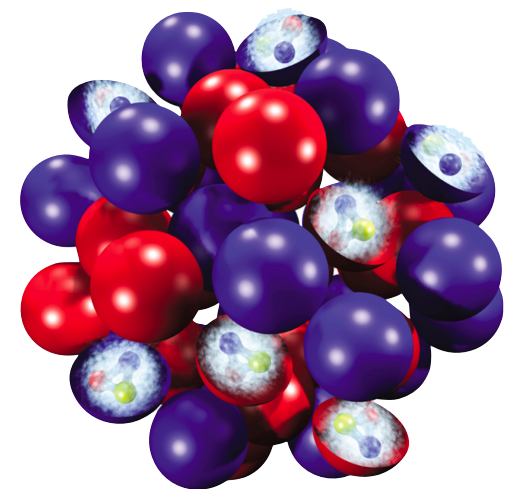
Overview

- **A long-standing challenge** in nuclear physics is to simultaneously describe nuclear phenomena across a wide range of energies and mass numbers starting from nuclear forces with roots in quantum chromodynamics.
- **In this talk**, I will highlight some recent developments in *ab initio* nuclear structure calculations, focusing on the use of Bayesian methods for uncertainty quantification. I will also discuss some of the challenges that we are facing.

Main takeaways



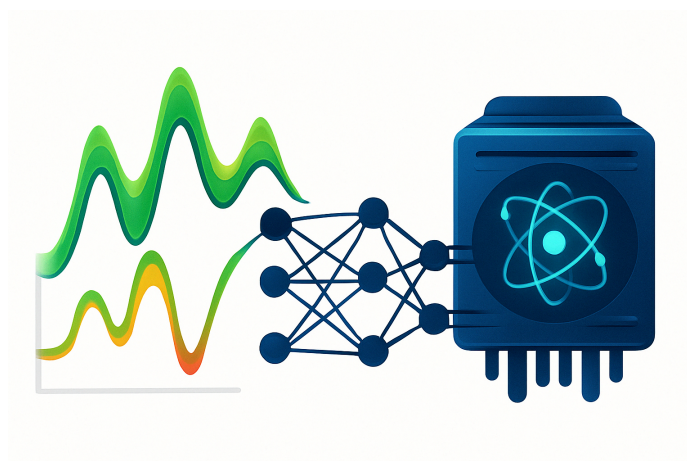
- We put forward an interpretation of ***ab initio*** in **nuclear theory**. This approach is making impressive strides towards heavier-mass and deformed nuclei.



- The nucleus is a complex **quantum many-body system**. Exact quantitative nuclear models do not exist. We are uncertain about their predictions.

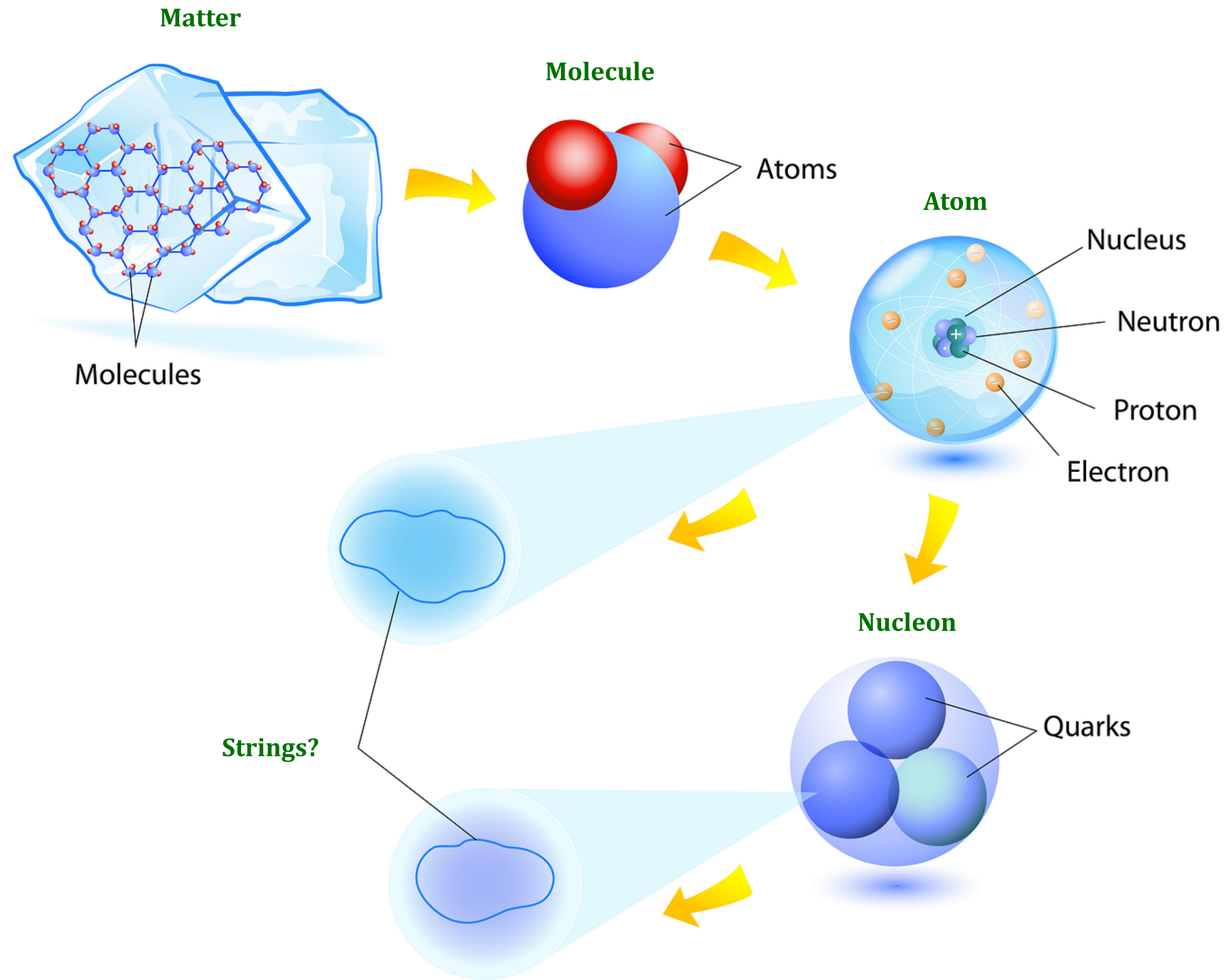


- Uncertainty quantification informs your **decision making**, and Bayesian statistics provides a powerful and principled approach. Can we better guide where to make future measurements?



- It's an exciting time in nuclear science—our challenges meet new tools from computational statistics and applied mathematics; e.g. **Bayesian inference & Emulators**.

Ab initio (latin adv. & adj. from the beginning)



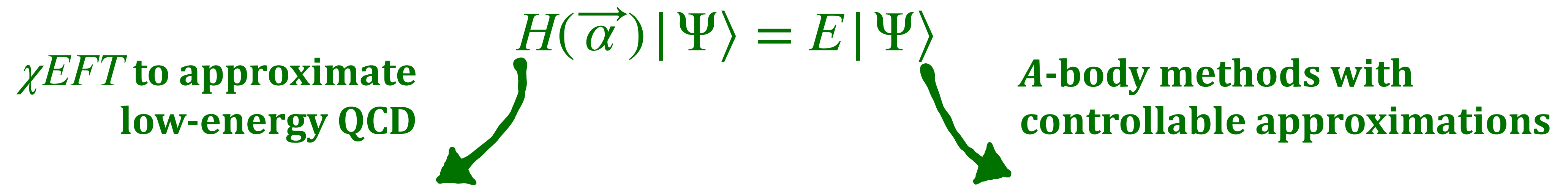
The history of physics tells us that we do not need to know everything to describe something.

Renormalization methods grant us some freedom in choosing the starting point.

Ab initio: we put forward our interpretation

Nuclear *ab initio*: a *systematically improvable* approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.

we therefore let nucleons define the beginning



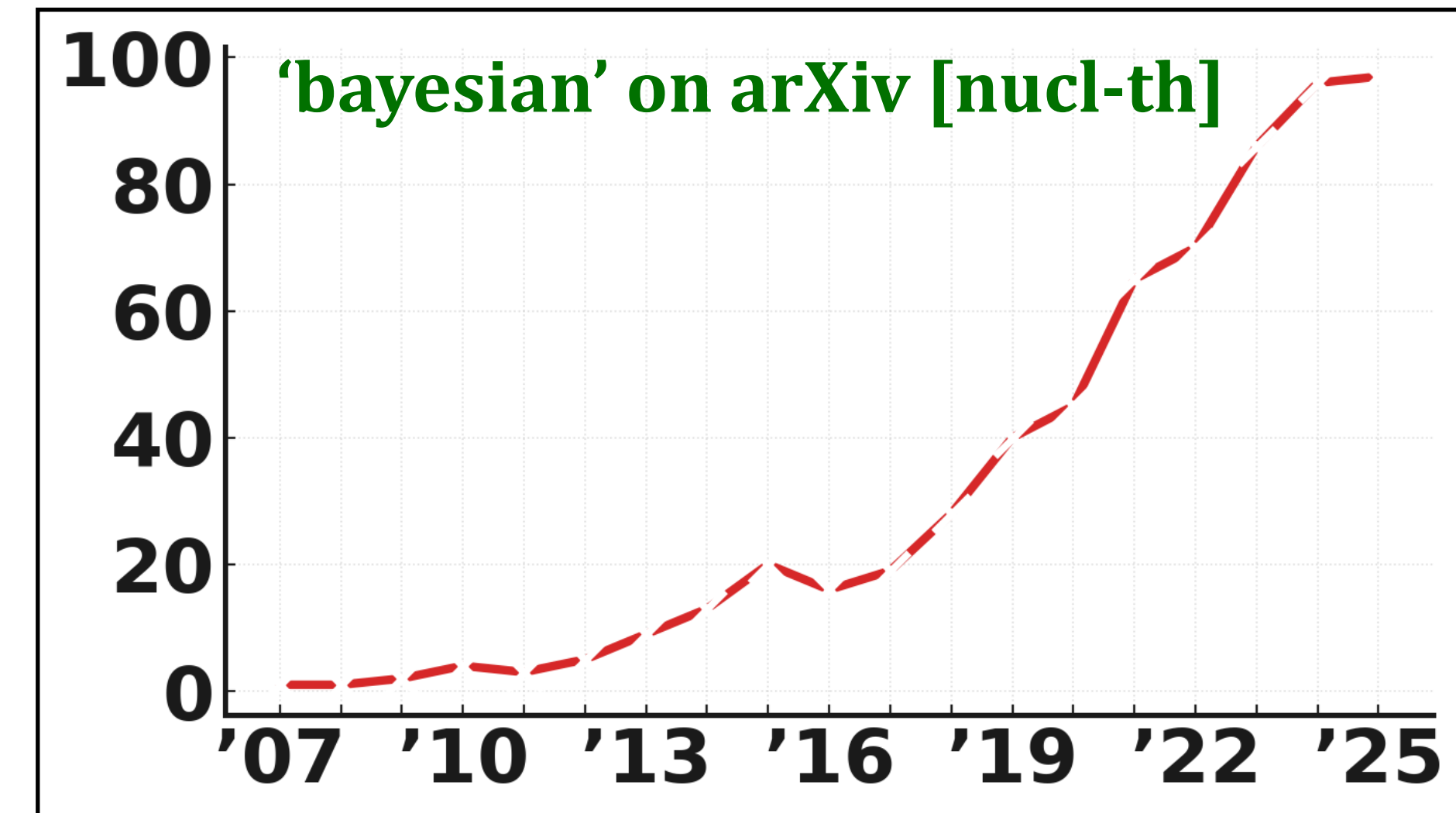
$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \dots \quad |\Psi\rangle = |\Phi^{(0)}\rangle + |\Phi^{(1)}\rangle + |\Phi^{(2)}\rangle + \dots$$

This systematicity creates an *inferential advantage*. We can test our assumptions about the model and the model discrepancy as we increase the model fidelity.

$$y_{\text{exp}}(\vec{x}) = \underbrace{y_{\text{th}}(\vec{\alpha}; \vec{x}) + \delta y_{\text{th}}(\vec{\alpha}; \vec{x})}_{\text{'Model'}} + \delta y_{\text{exp}}(\vec{x})$$

Why uncertainty quantification?

- Predicting future data $\tilde{y}$ from past data y is uncertain.
- Quantifying this uncertainty with probability:
 - enhances transparency and communication of results
 - informs decision-making and helps model assessment



Why Bayesian inference?

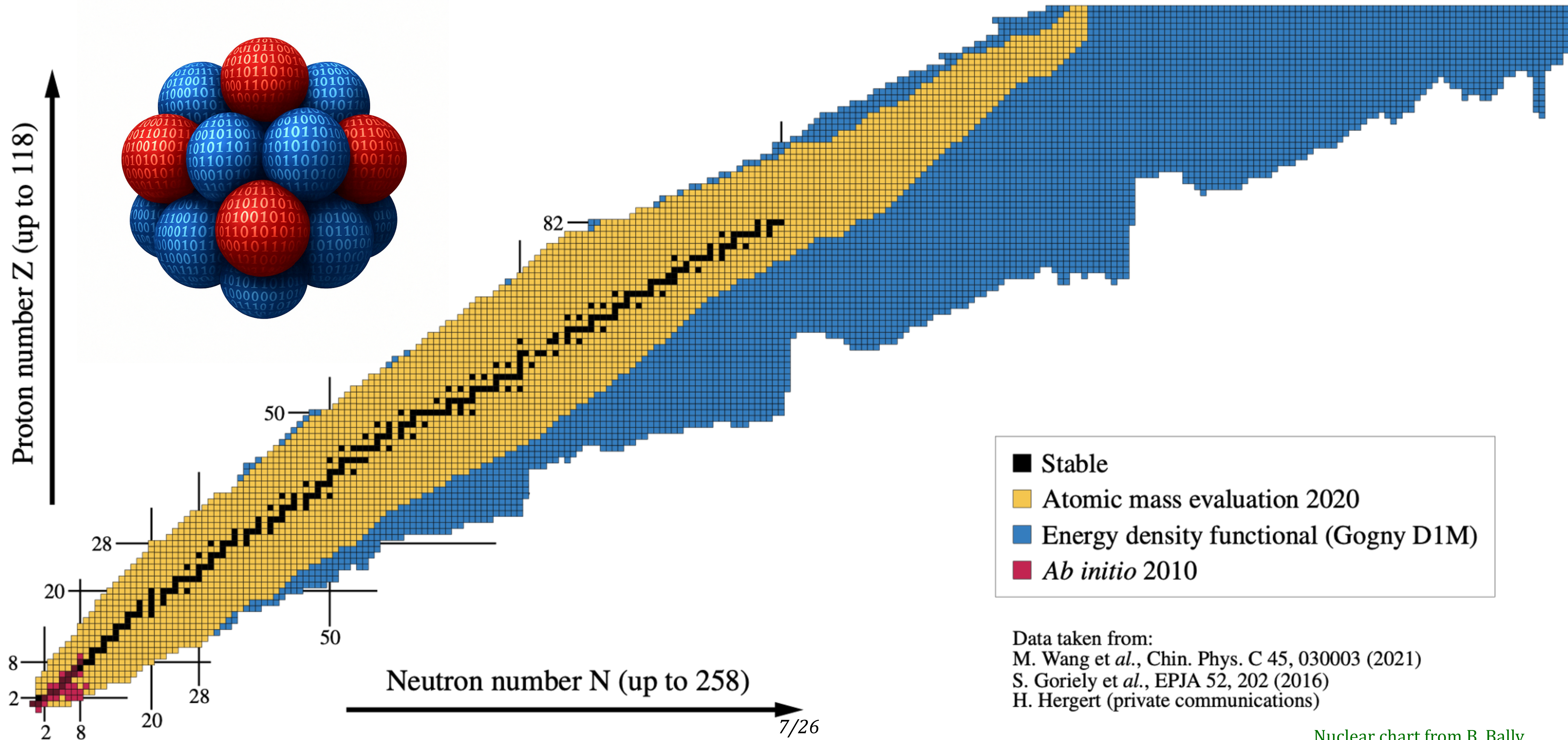
The probability for $\tilde{y}$ given y is called the *posterior predictive distribution*, and this quantity is central to Bayesian inference.

$$p(\tilde{y} | y, I)$$

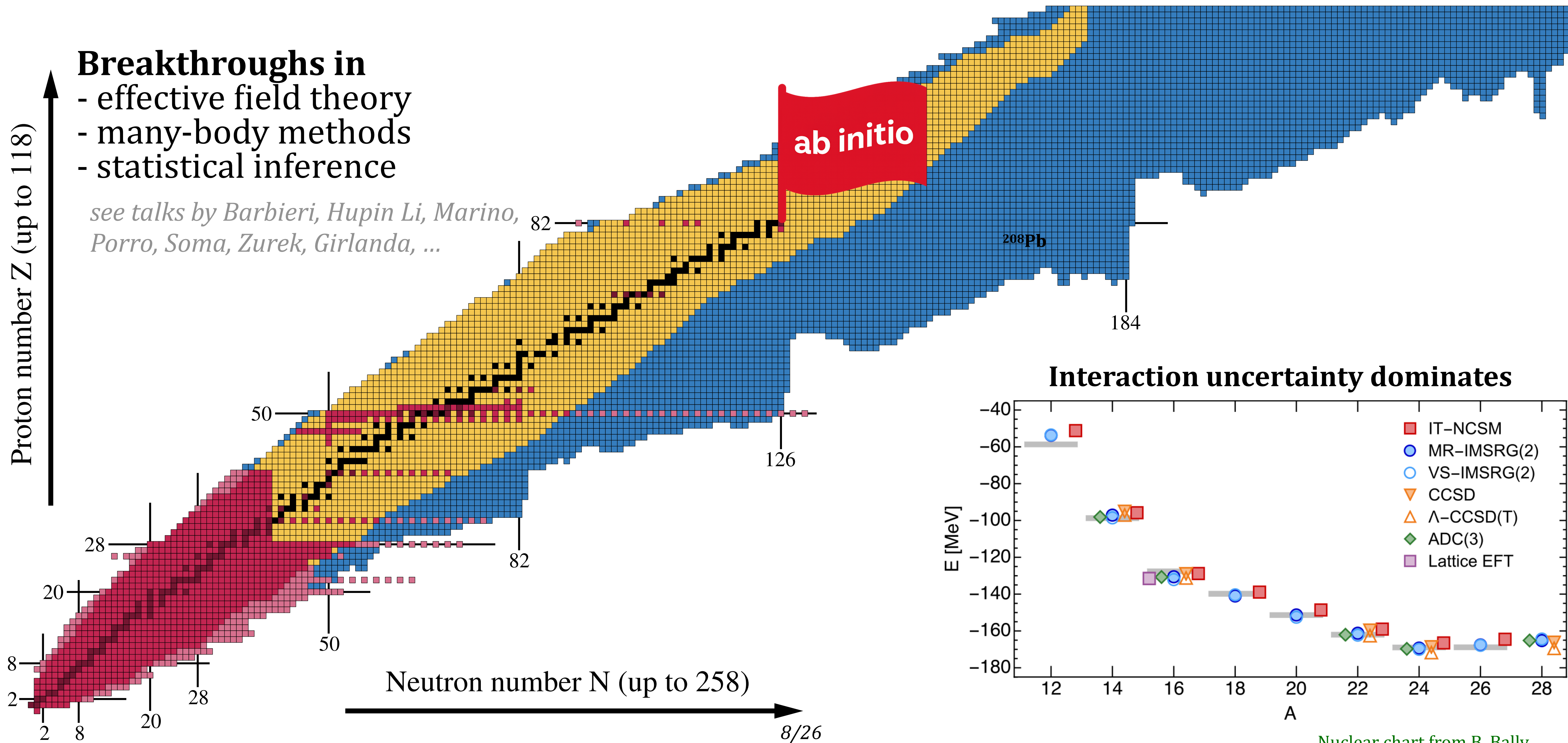
Here, I denotes *your* background knowledge. To enable quantitative statements, we construct a *model* M . Any model comes with uncertain parameters $\vec{\alpha}$.

$$p(\tilde{y} | y, M, I) = \int p(\tilde{y} | \vec{\alpha}, M, I) p(\vec{\alpha} | y, M, I) d\vec{\alpha}$$

Progress in *ab initio* predictions (2010)



Progress in *ab initio* predictions: 15 years later

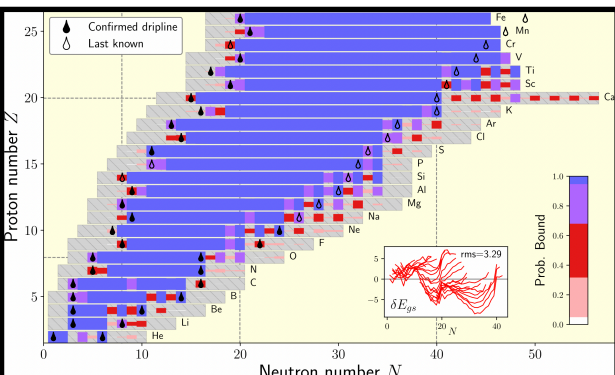
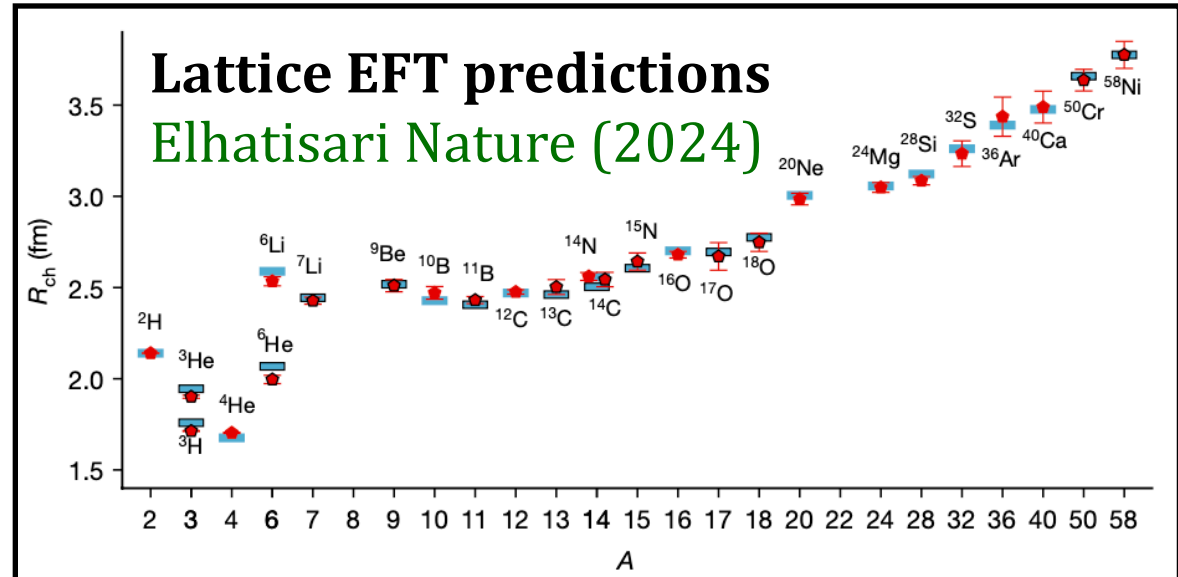


Progress in *ab initio* predictions: 15 years later

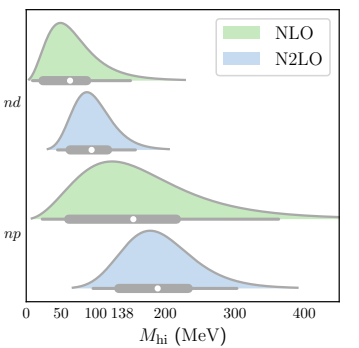
Proton number Z (up to 118)

Breakthroughs in

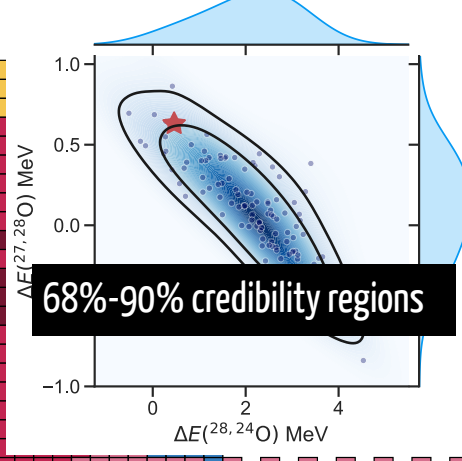
- effective field theory
- many-body methods
- statistical inference



He-Fe: (~700 isotopes)
Stroberg *et al.*, PRL (2021)

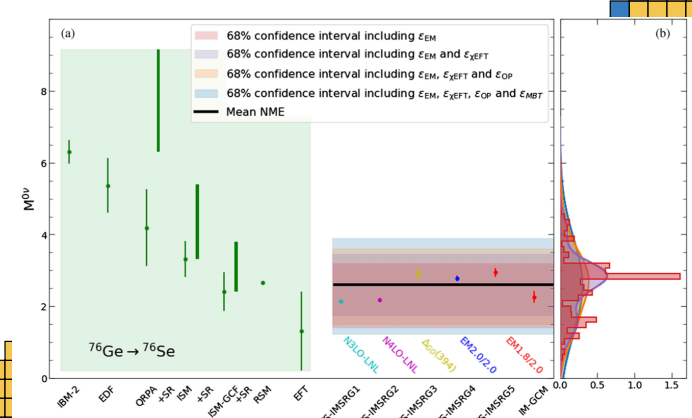
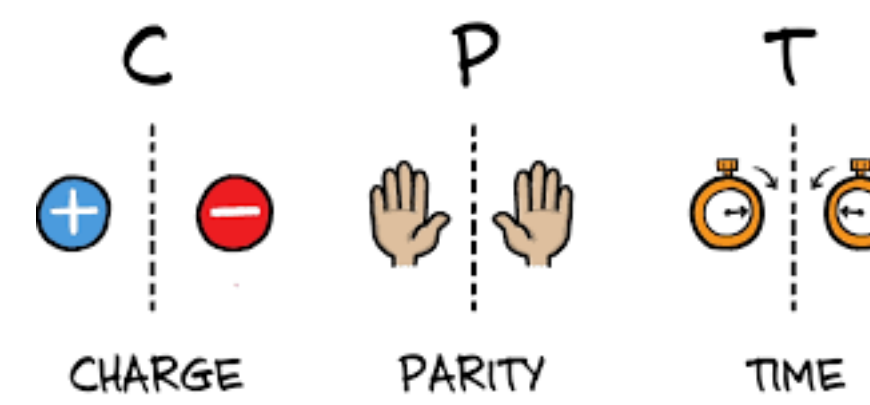


π EFT Breakdown
Ekström and Platter PLB&PRC(L)(2025)



²⁸O Kondo *et al.*,
Nature (2023)

A lens to explore symmetries
Engel Annu. Rev. Nucl. Part. Sci. (2025)

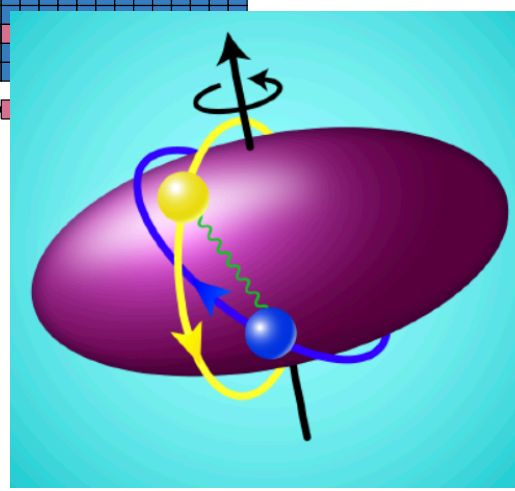


UQ fo $0\nu\beta\beta$ decay: Belley PRL (2024)

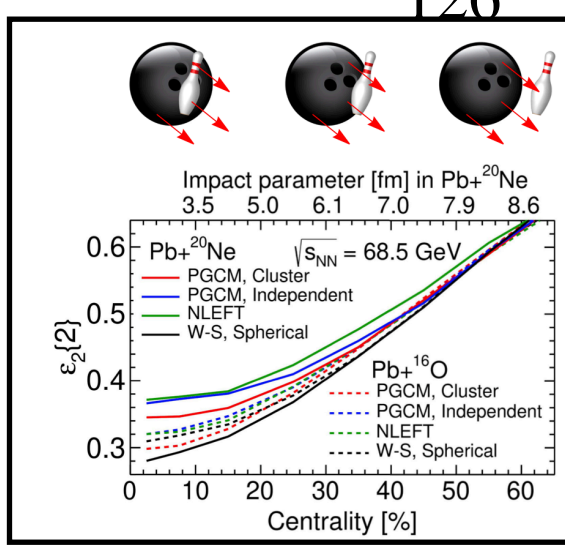
138 Xe: Arthuis *et al.*, PRL (2020)

100-170 Sn: Tichai *et al.*, PLB (2024)

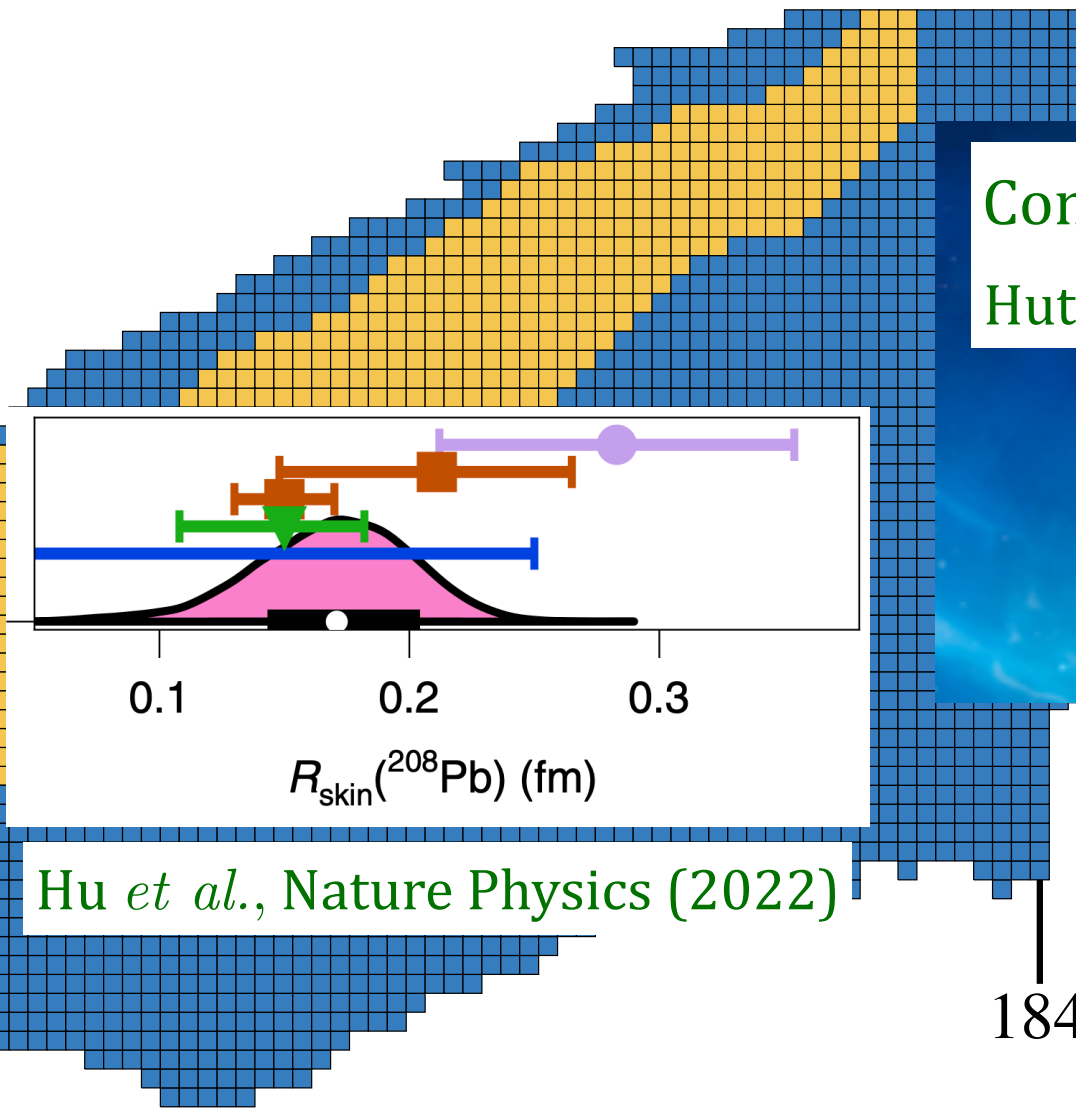
Miyagi *et al.*, PRC (2022)



Multiscale Sun *et al.*, PRX (2024) ($u_F \approx 250$)



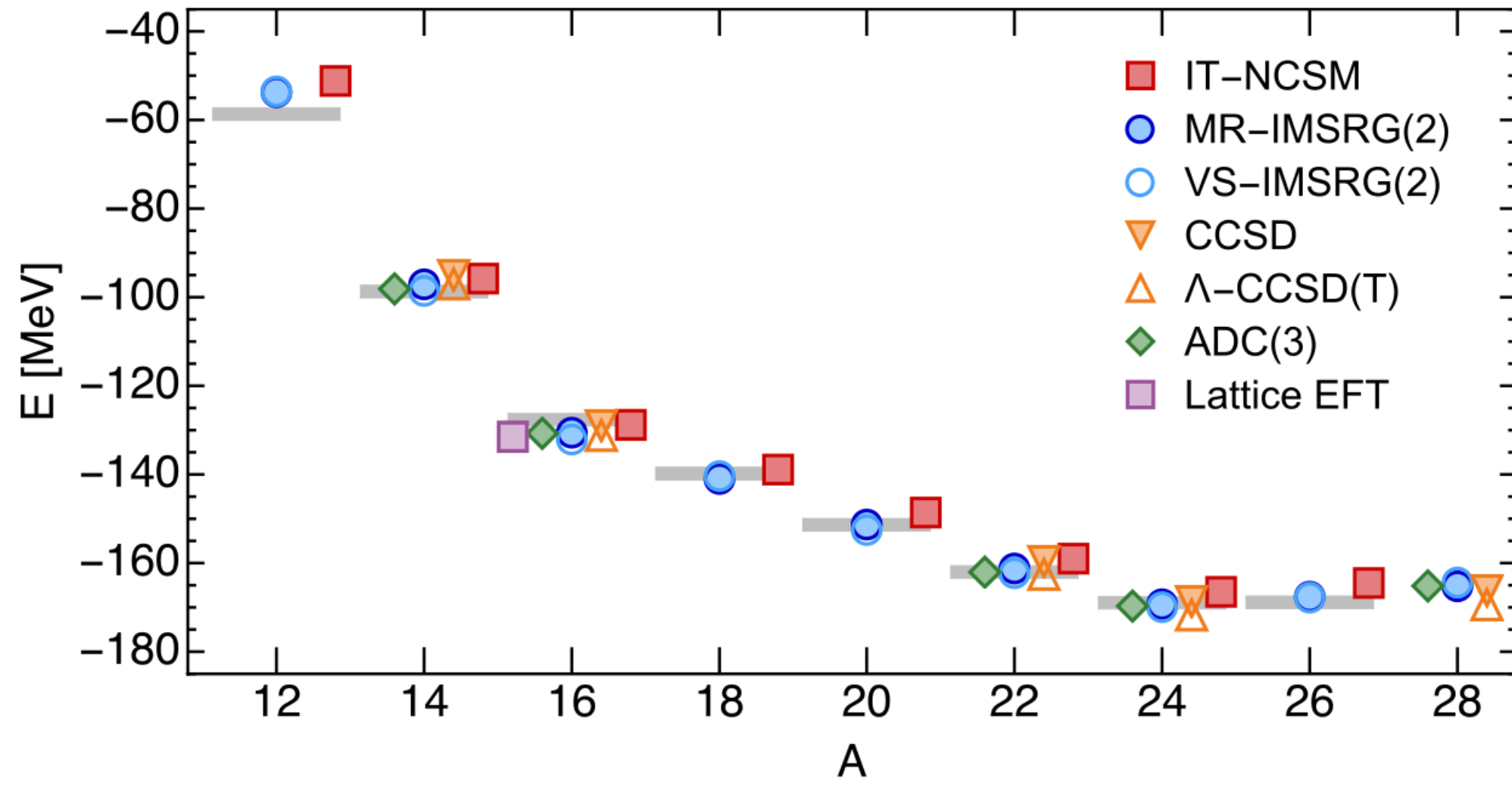
Ab initio & HIC
G. Giacalone *et al.*, PRL (2025)



Hu *et al.*, Nature Physics (2022)

Constraining neutron star matter
Huth, Pang, Tews, Le Fèvre, Schwenk, et al Nature (2022)

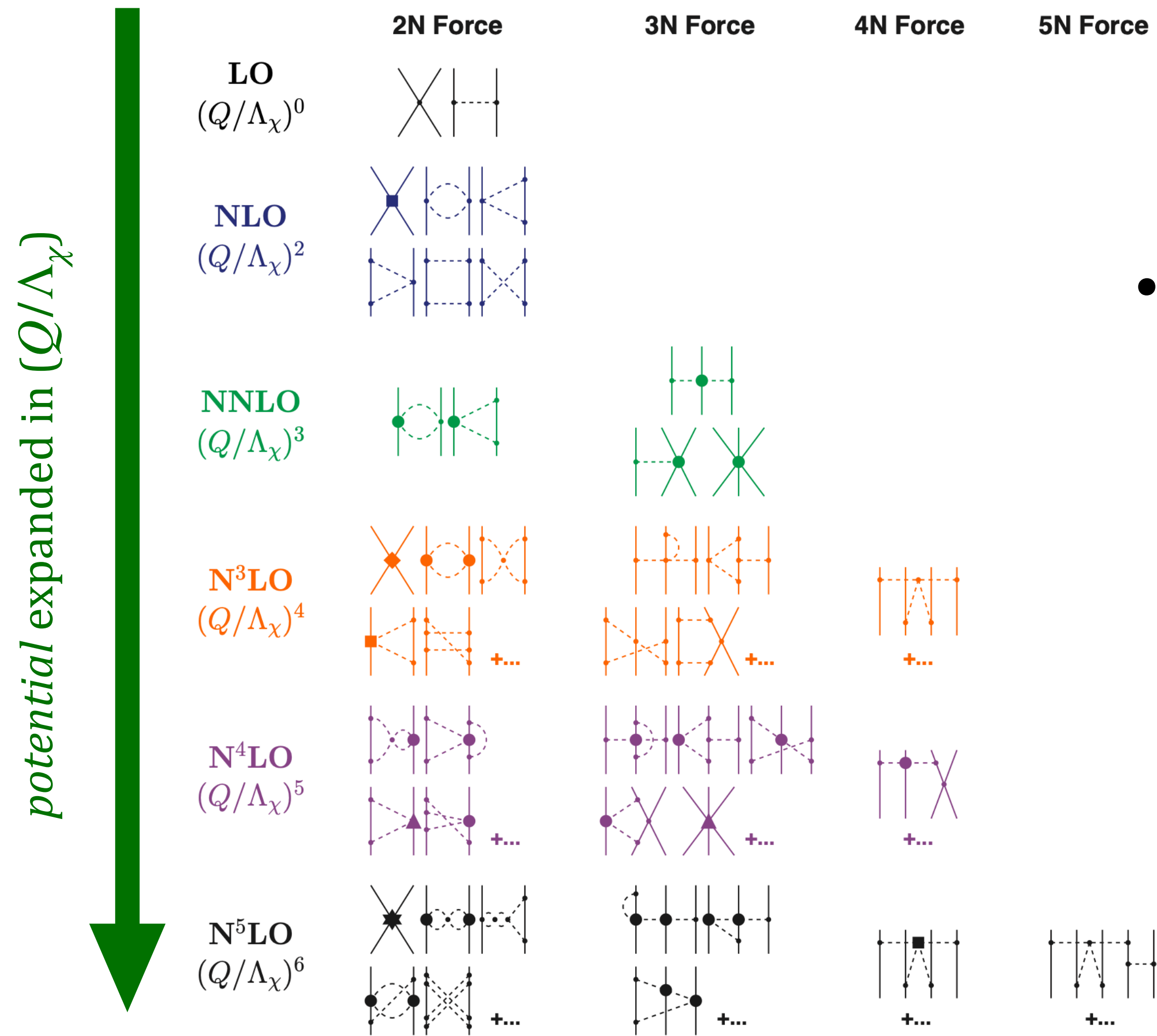
Interaction uncertainty dominates



Nuclear chart from B. Bally

Chiral effective field theory (χ EFT)

- Weinberg power counting (WPC)



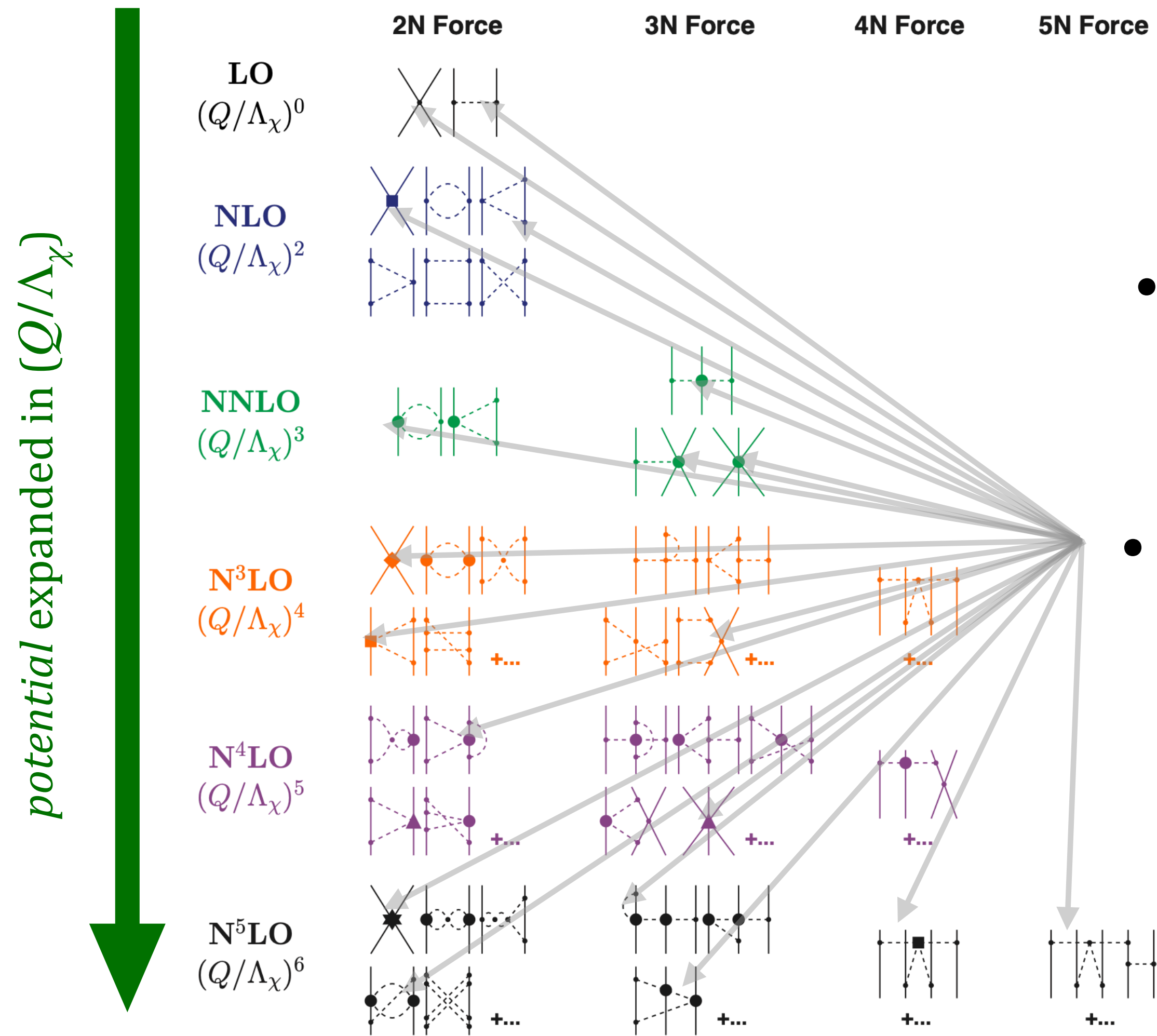
$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \dots$$

EFTs promise a very useful systematicity

- **Order-by-order expansion** in a dimensionless ratio (Q/Λ_χ) constructed from the separation of scales. A soft scale ($Q \sim m_\pi$) and a hard scale ($\Lambda_\chi \sim m_N$), separating the resolved and unresolved dynamics of the nuclear interaction.

Chiral effective field theory (χ EFT)

- Weinberg power counting (WPC)



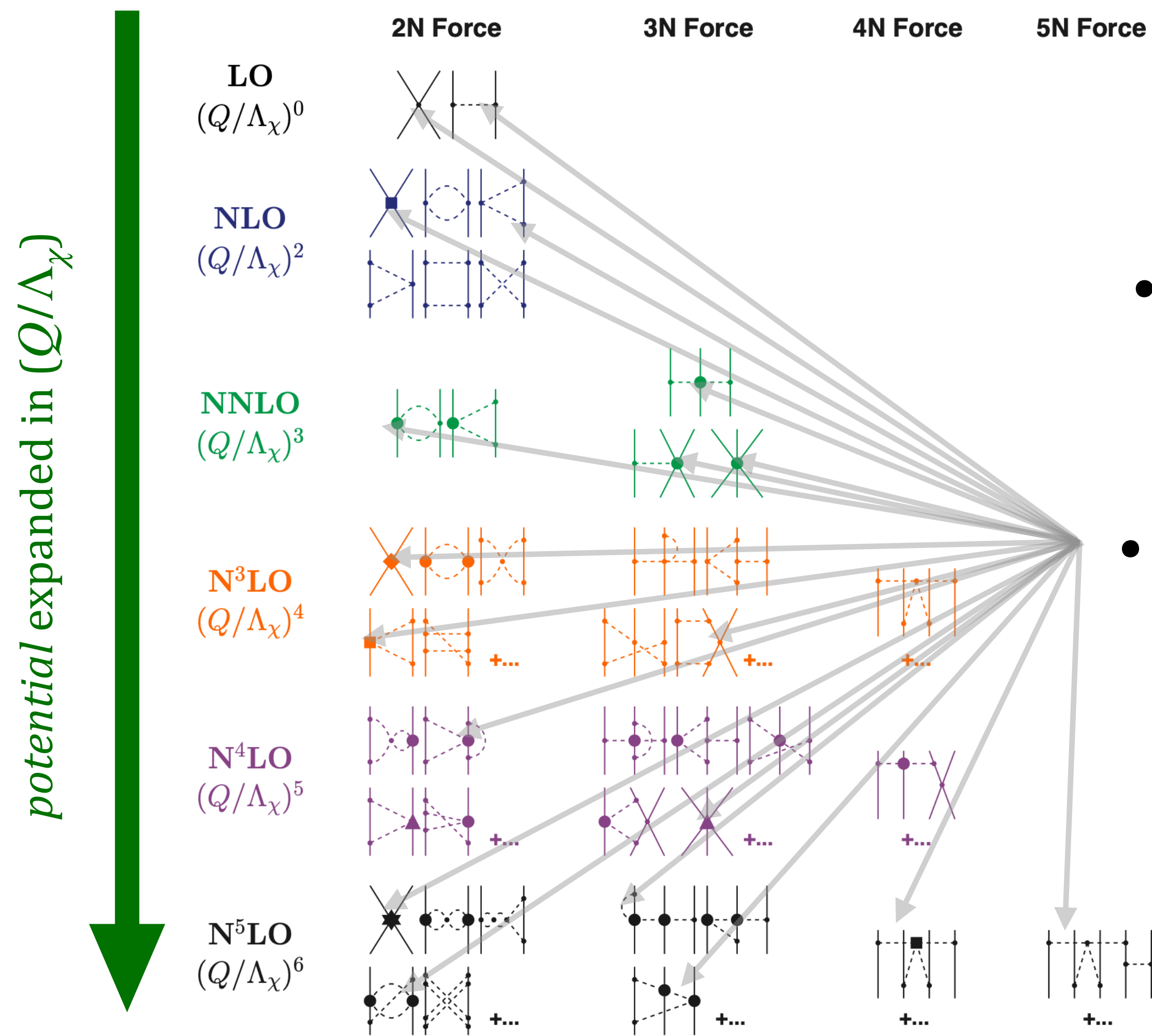
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- $\sim (15 - 30)$ **Low-energy** constants to be inferred from data.

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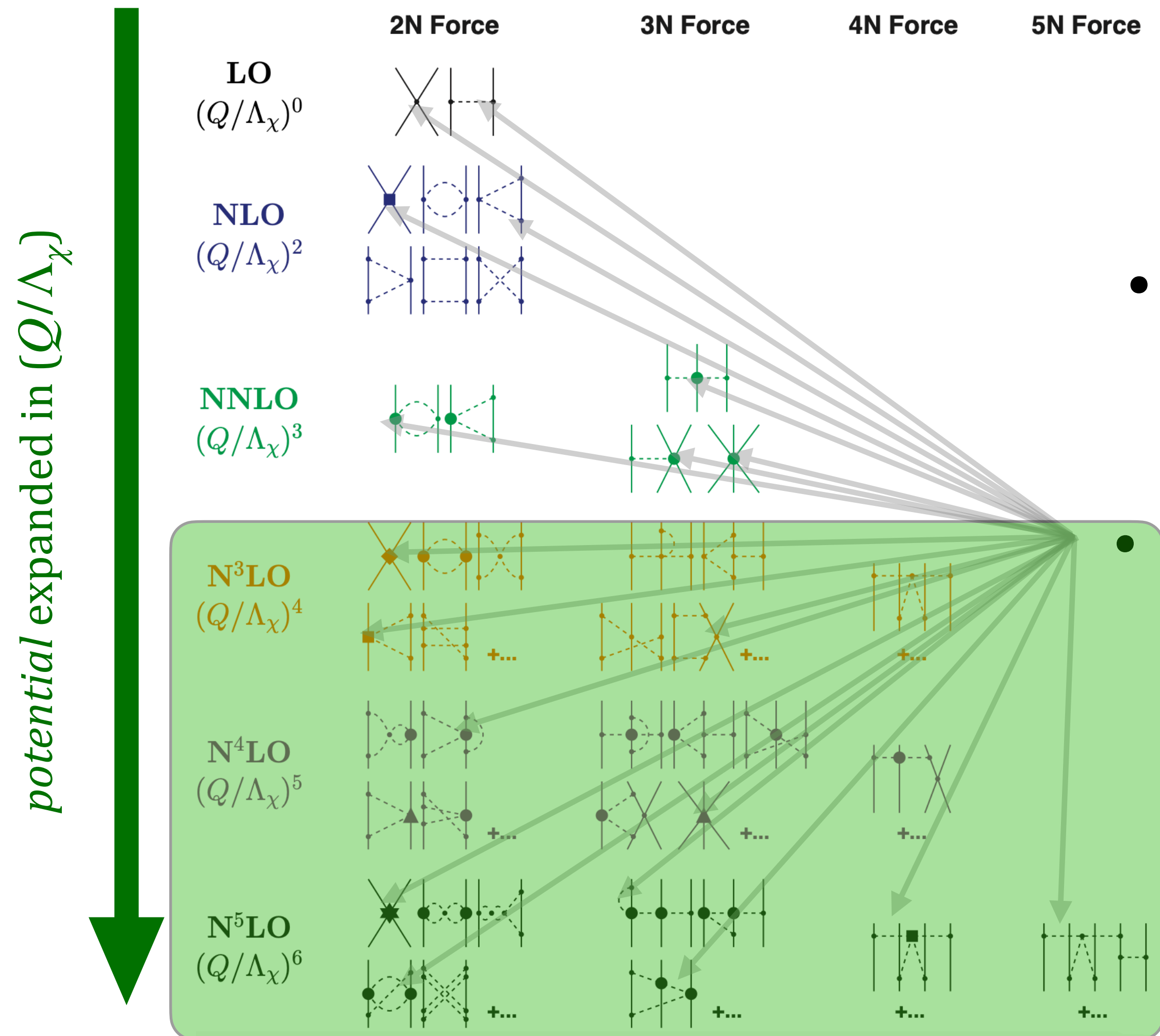
$$y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=0}^k c_\nu \left(\frac{Q}{\Lambda_\chi} \right)^\nu \quad \text{and} \quad \delta y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=k+1}^{\infty} c_\nu \left(\frac{Q}{\Lambda_\chi} \right)^\nu$$

EFT prediction

EFT truncation error

Chiral effective field theory (χ EFT)

- Weinberg power counting (WPC)



$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \dots$$

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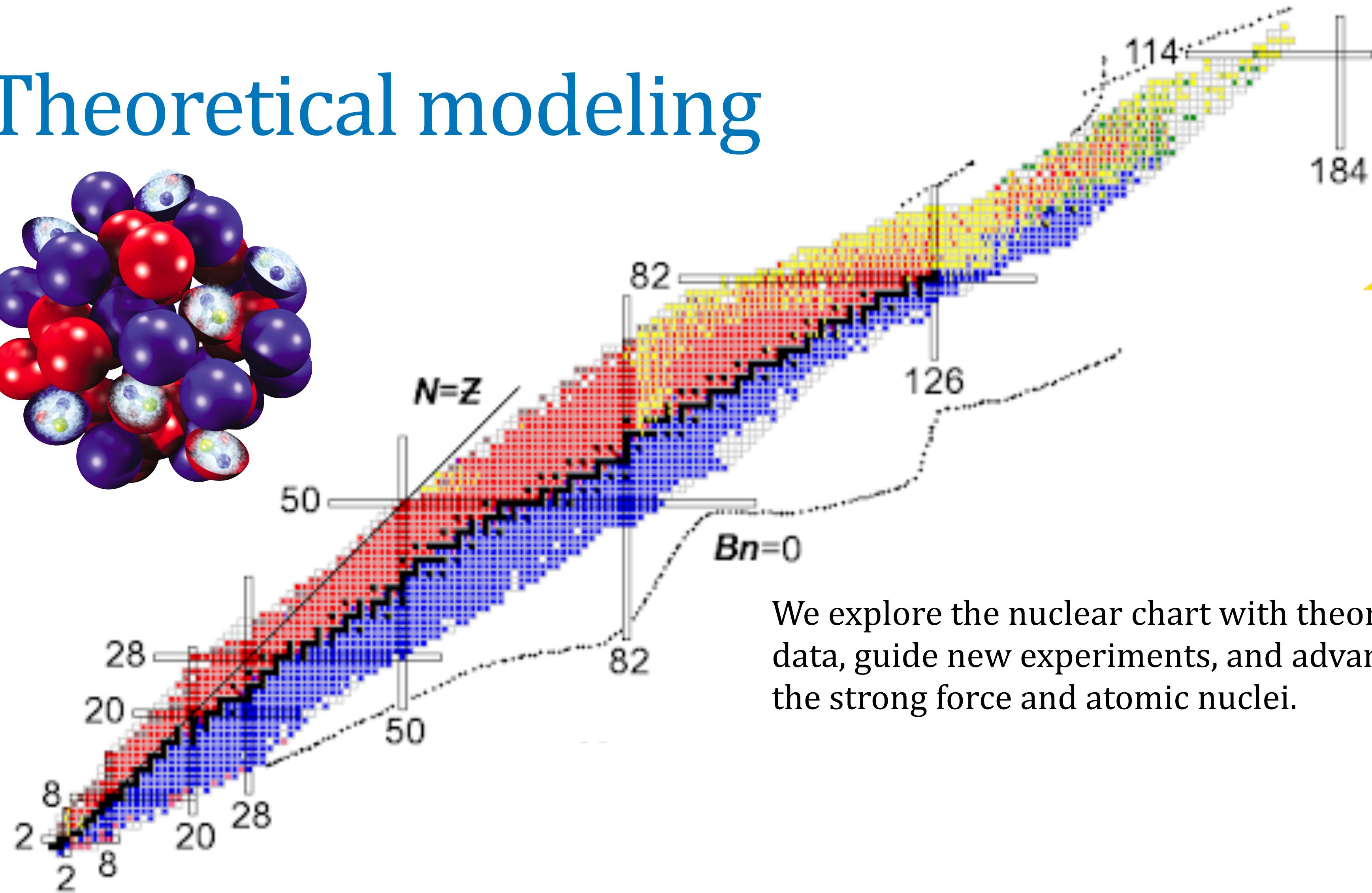
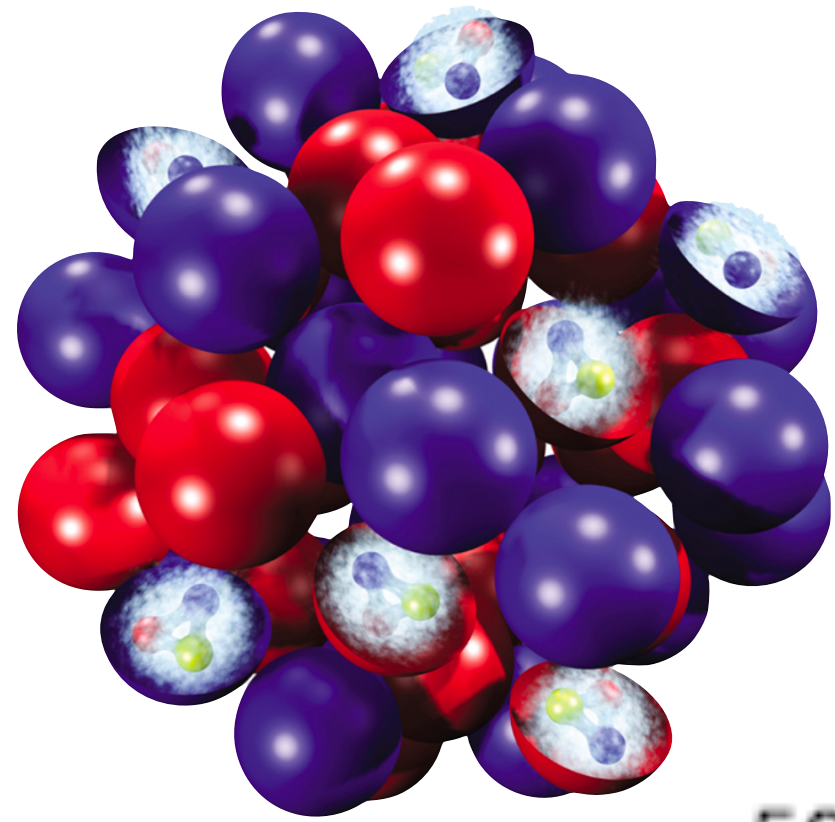
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EFT prediction

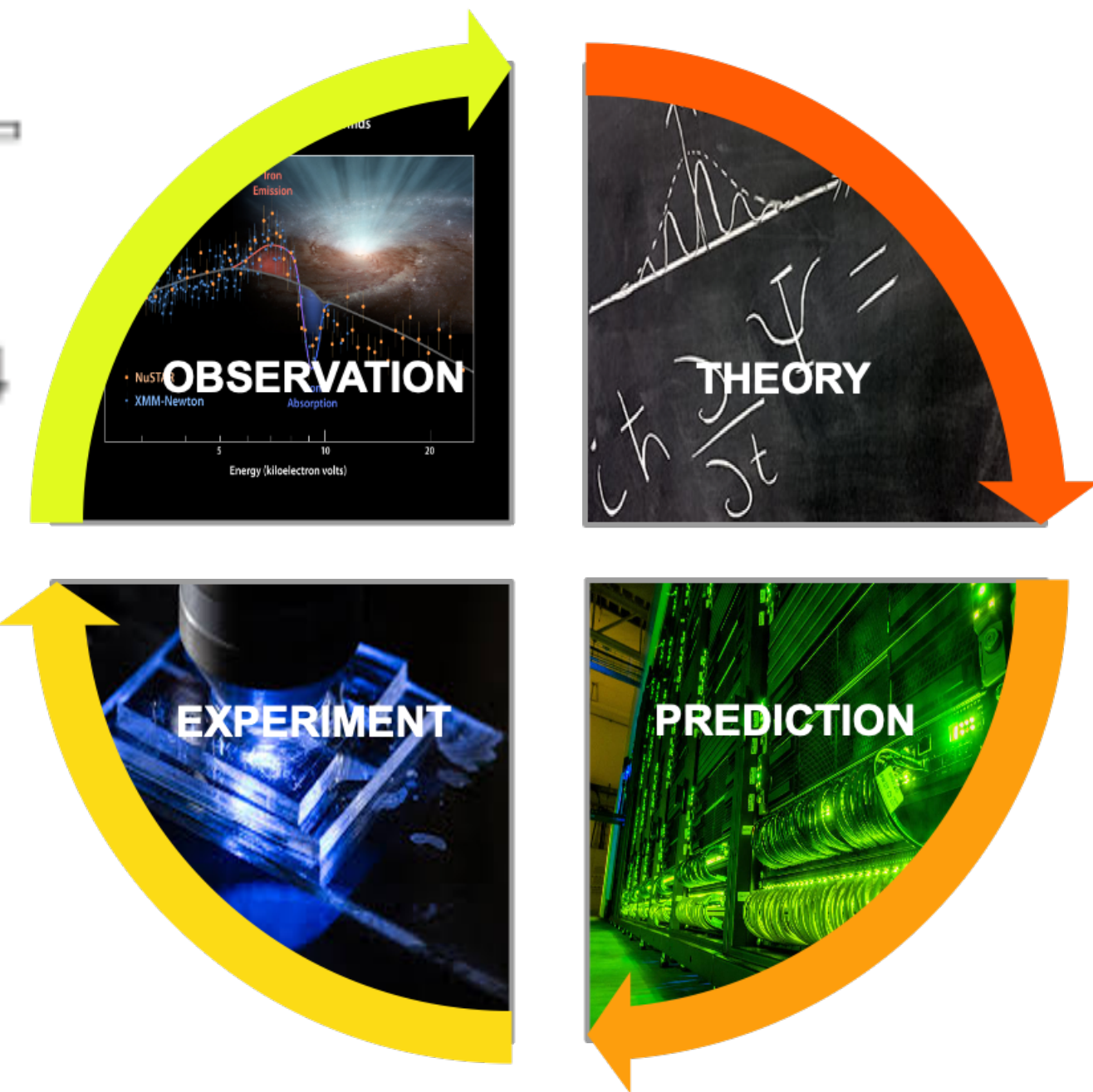
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EFT truncation error

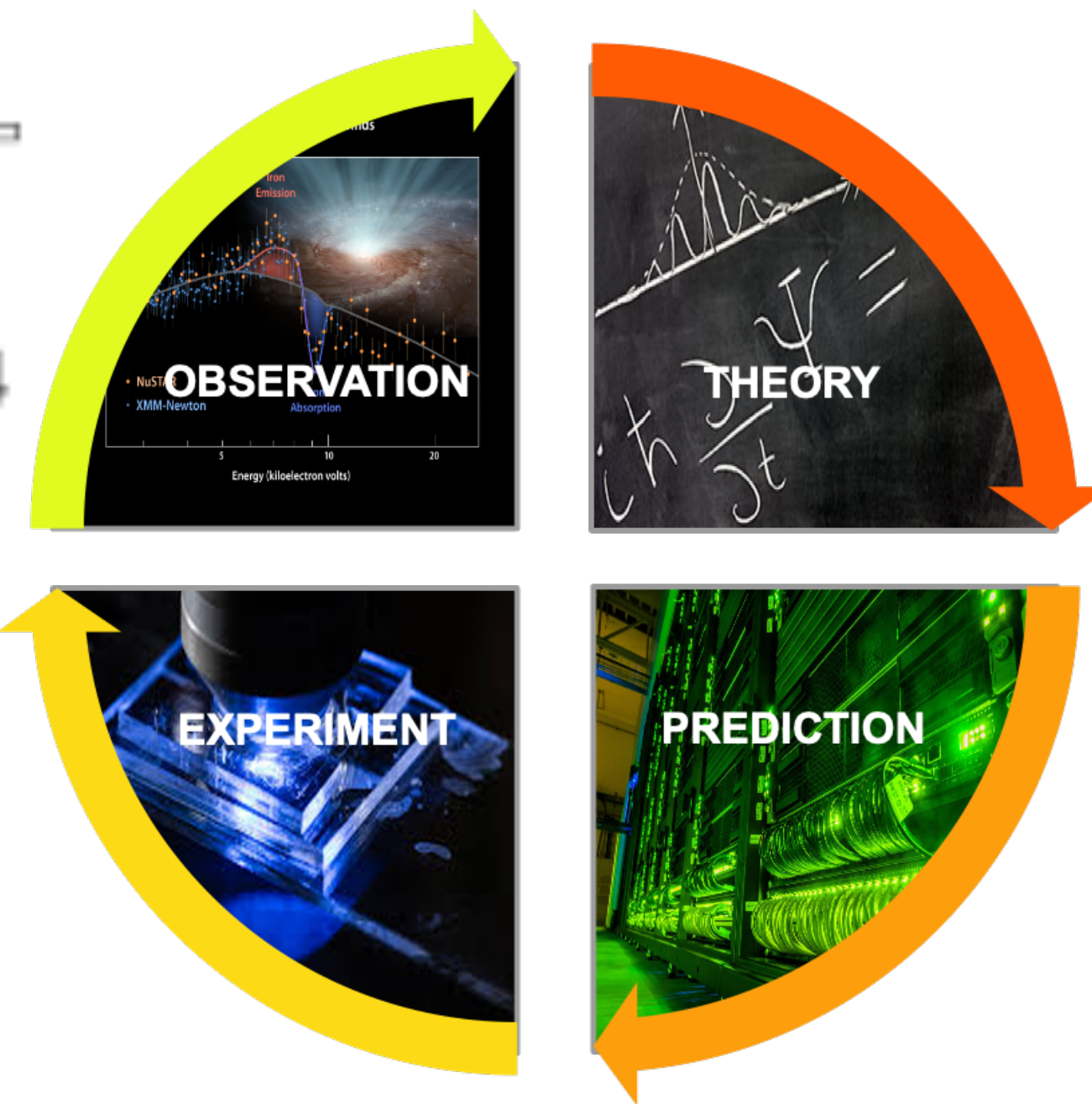
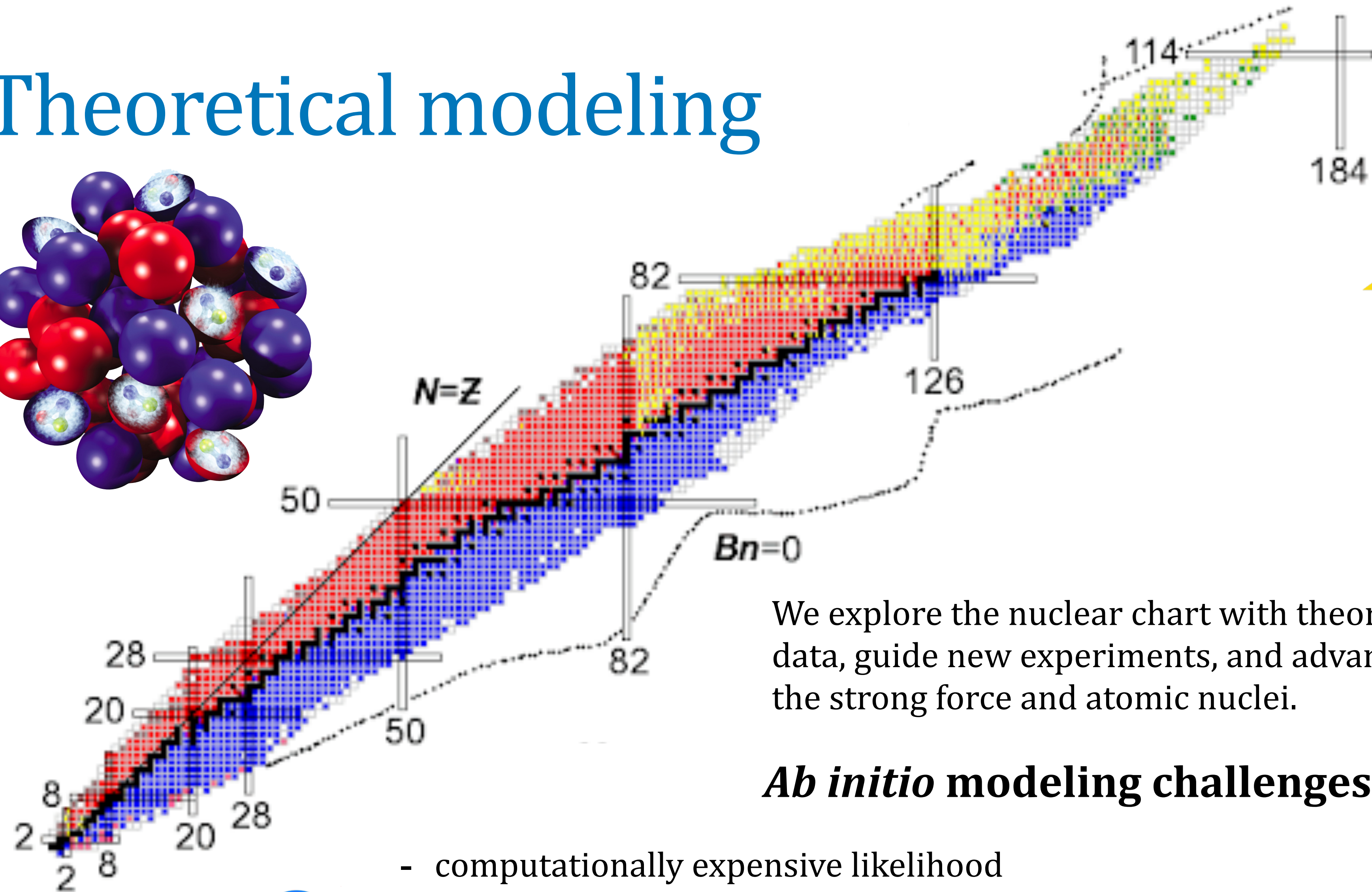
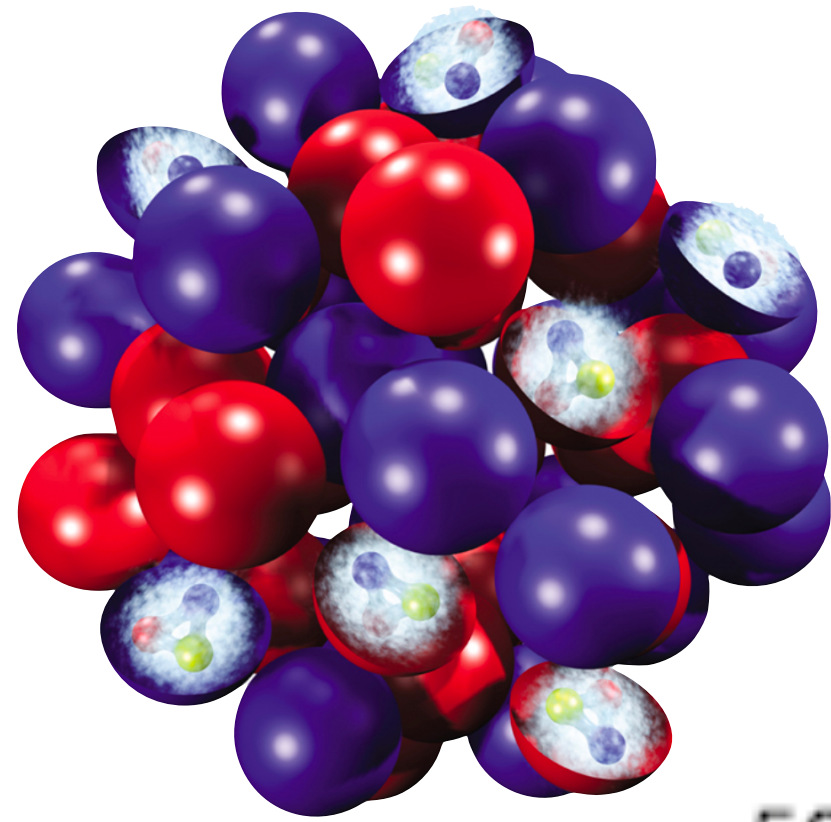
Theoretical modeling



We explore the nuclear chart with theoretical models to learn from data, guide new experiments, and advance our understanding of the strong force and atomic nuclei.



Theoretical modeling



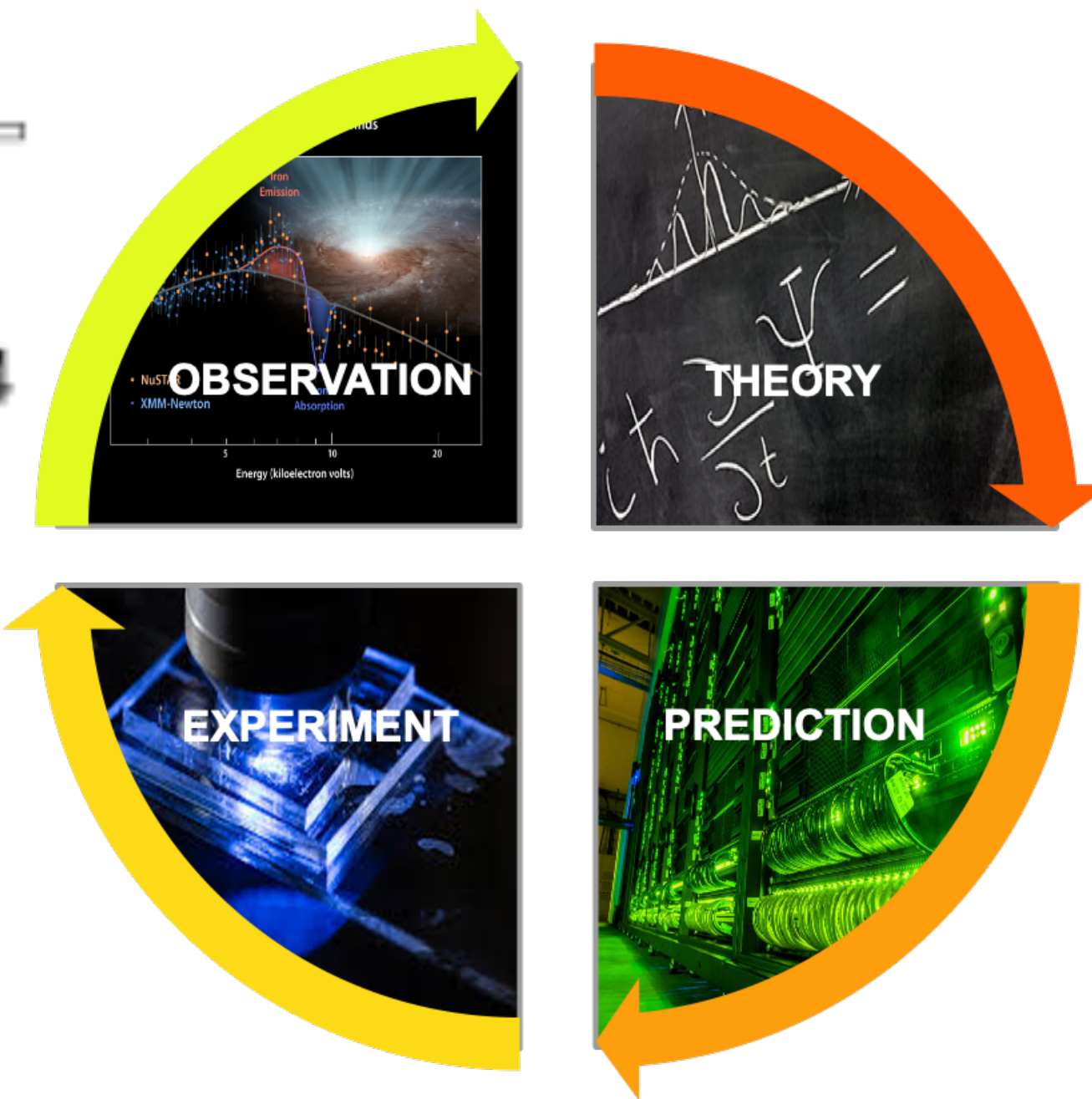
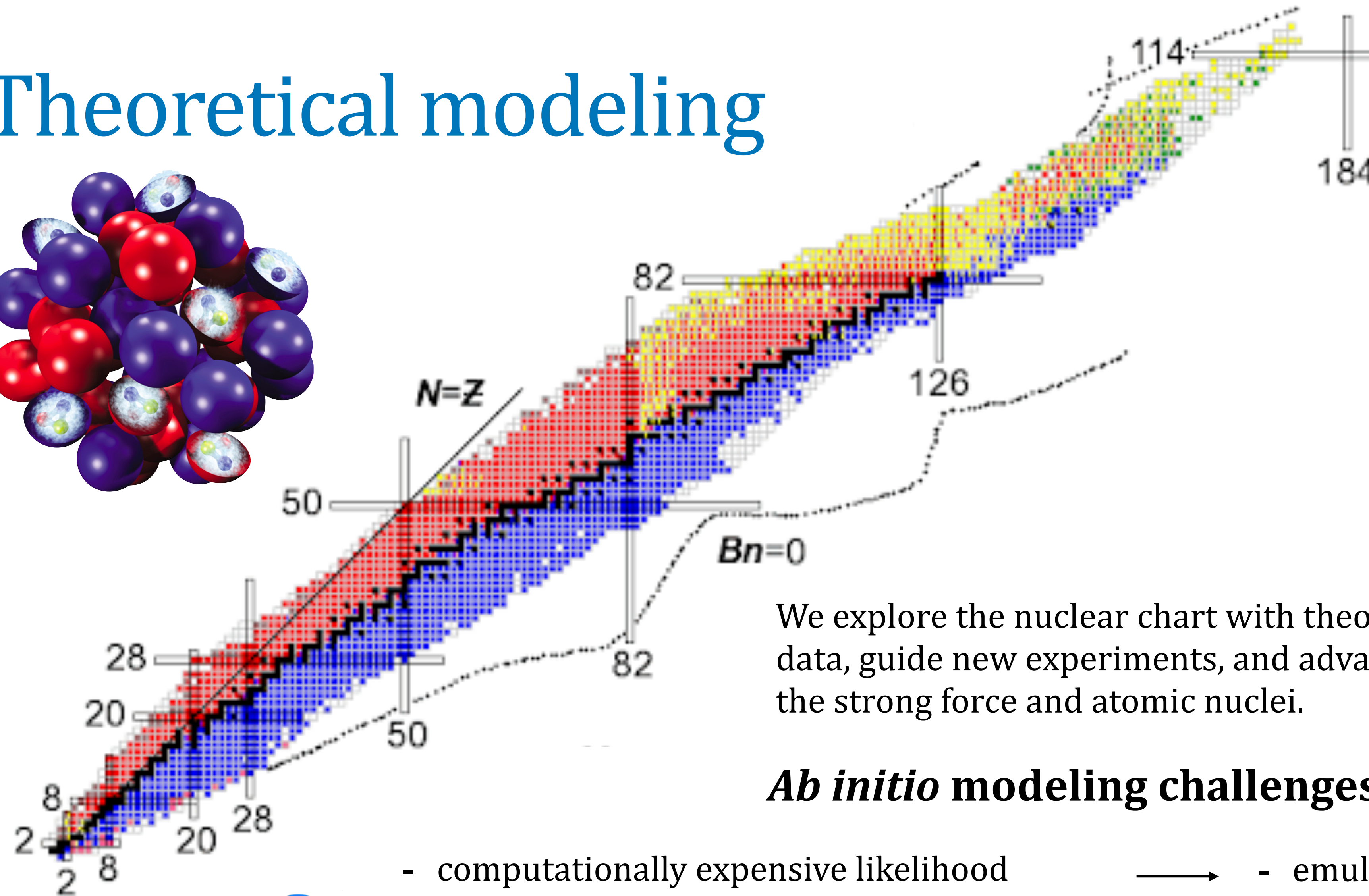
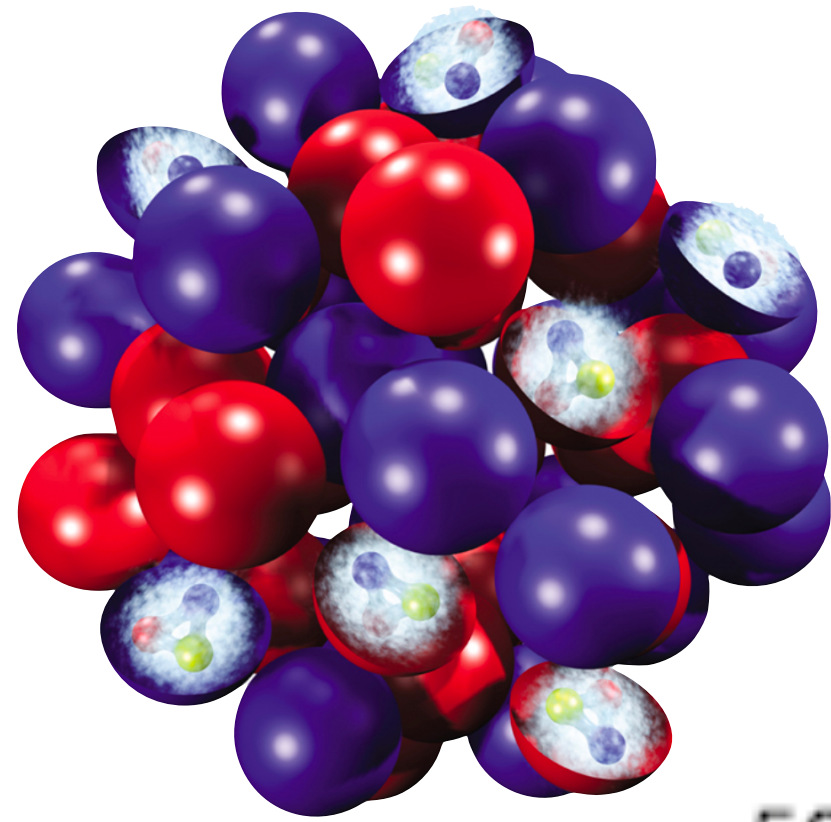
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Ab initio modeling challenges:

- computationally expensive likelihood
- multimodal and high-D parameter space
- *ab initio* method errors difficult to quantify
- χ EFT in Weinberg PC not renormalizable



Theoretical modeling



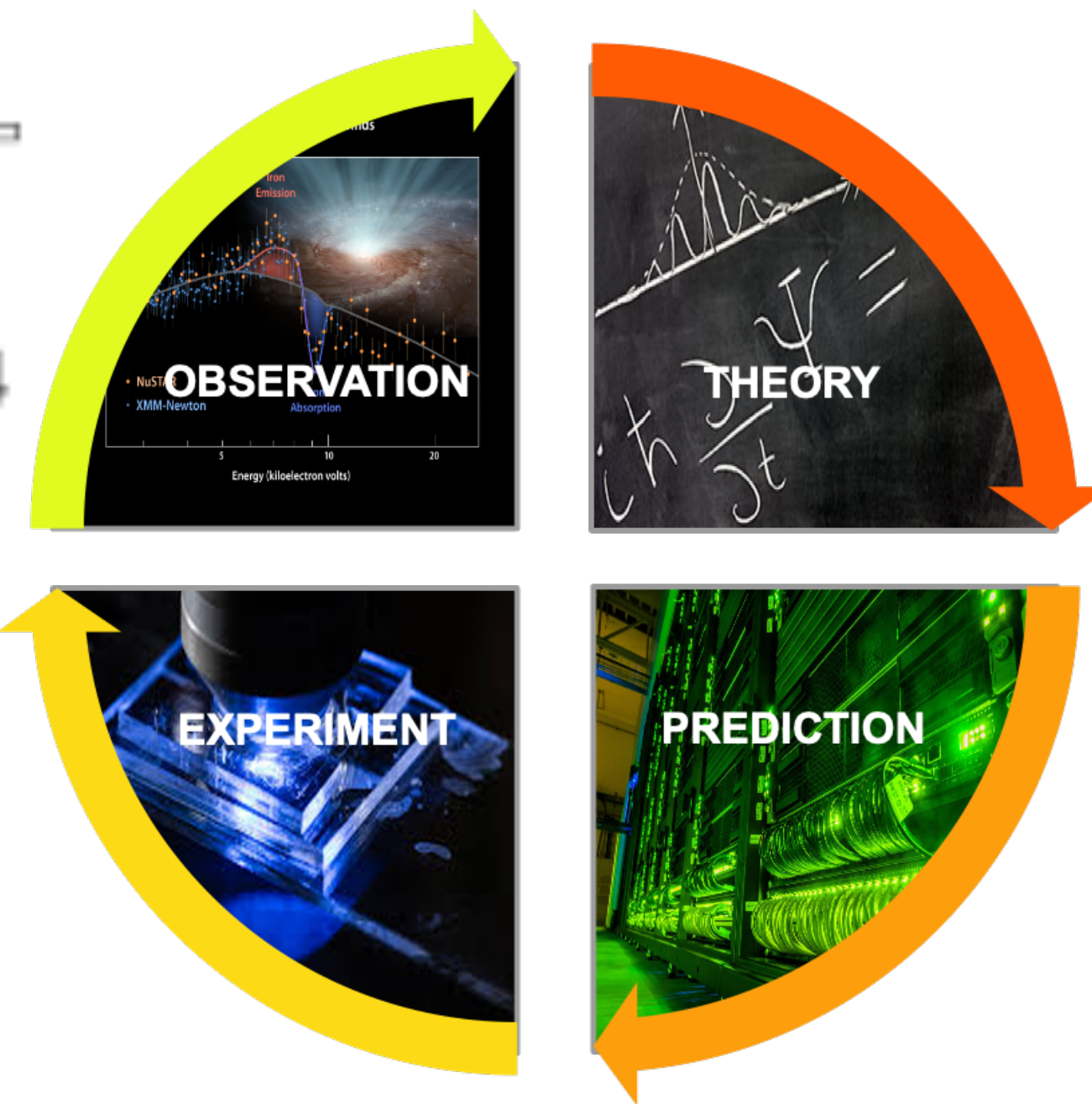
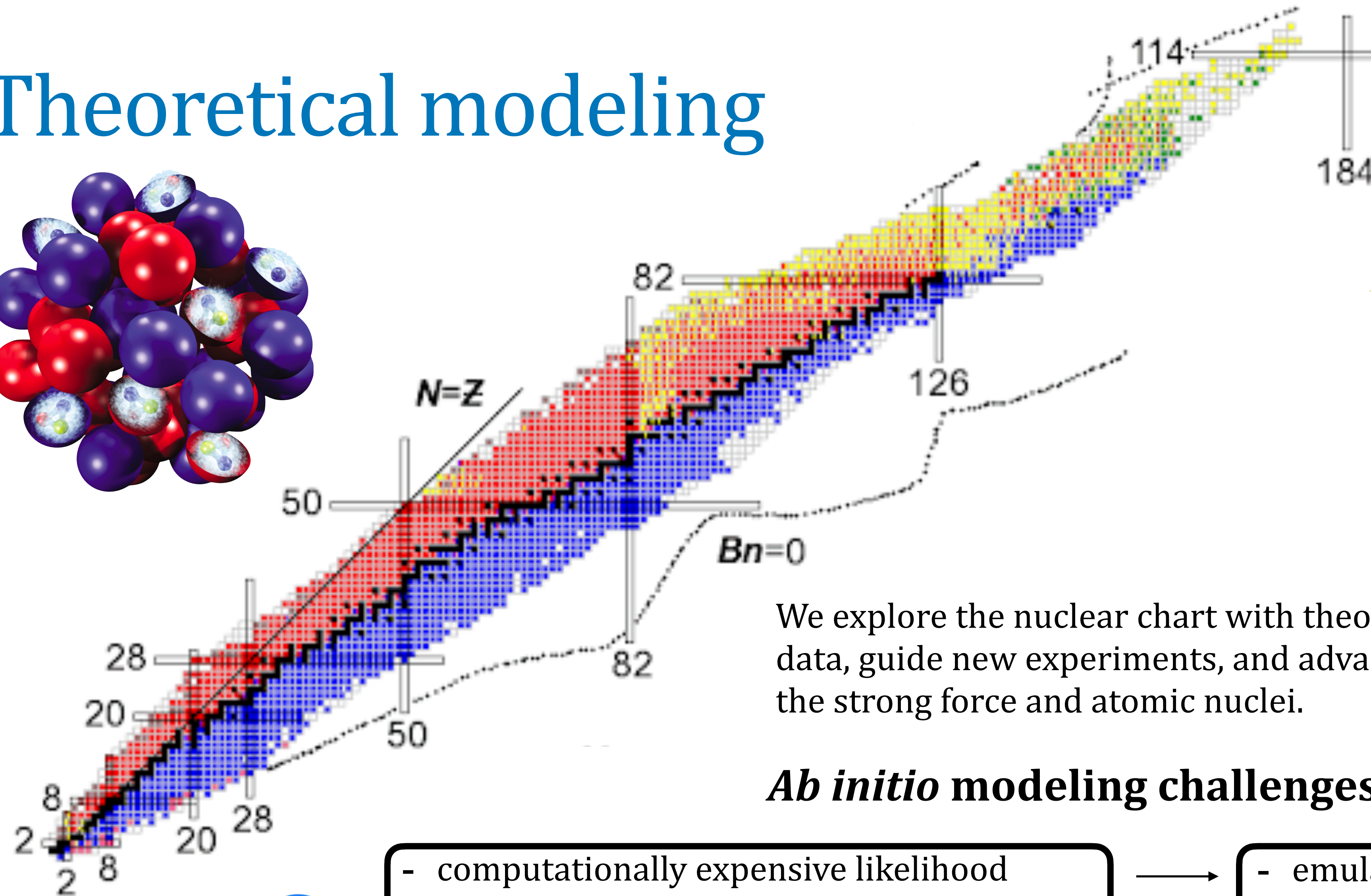
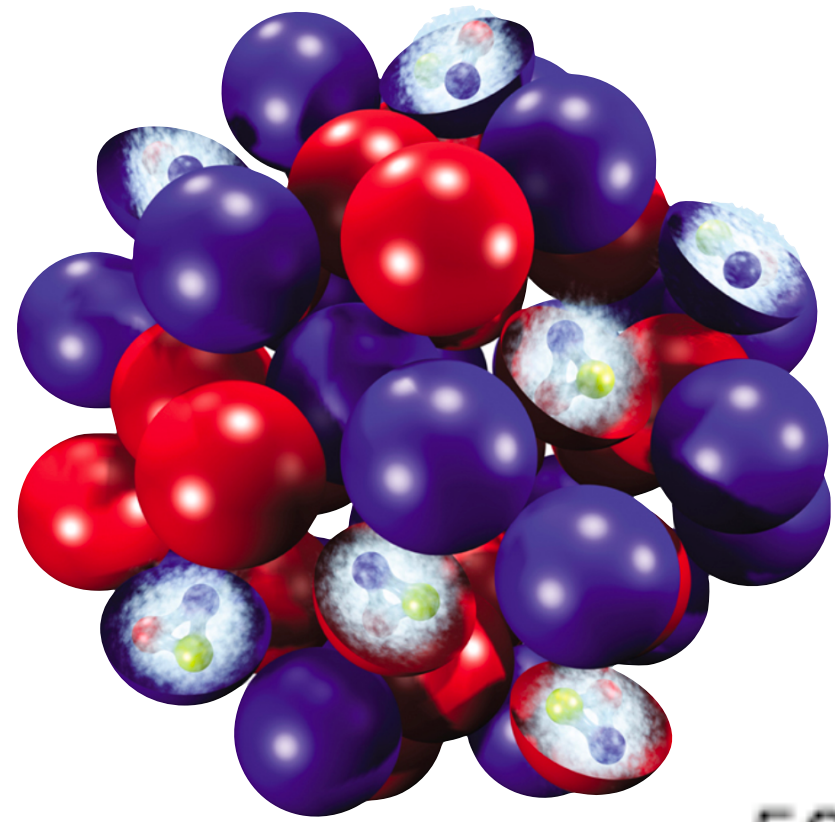
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Ab initio modeling challenges:

- | | | |
|--|---|--------------------------|
| - computationally expensive likelihood | → | - emulators |
| - multimodal and high-D parameter space | → | - history matching / HMC |
| - <i>ab initio</i> method errors difficult to quantify | → | - method comparisons |
| - χ EFT in Weinberg PC not renormalizable | → | - RG-invariant proposals |
- see O. Thim talk (Tuesday)*



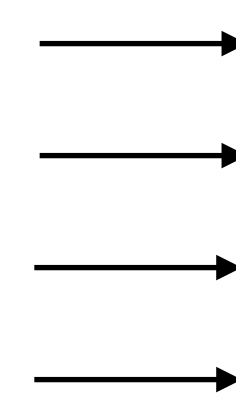
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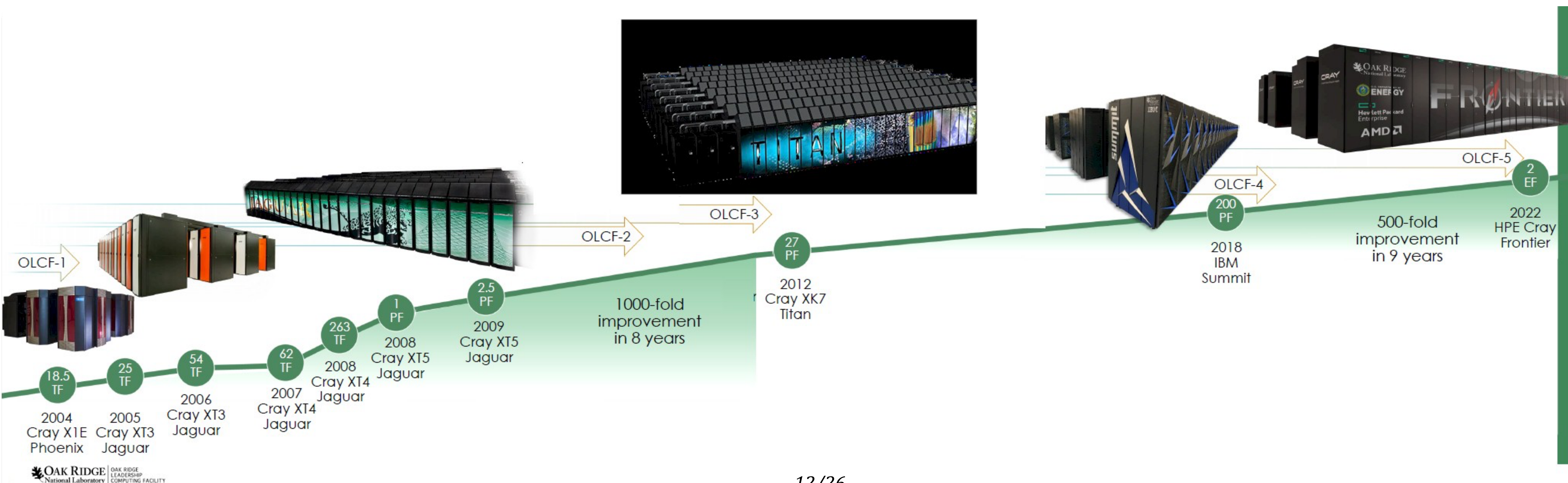
- emulators
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see O. Thim talk (Tuesday)



Computing nuclei: a computationally expensive problem

Solving the Schrödinger equation for many nucleons requires substantial computing resources that grows exponentially with nucleon number and basis size. Polynomially scaling methods exist but are still computationally expensive.

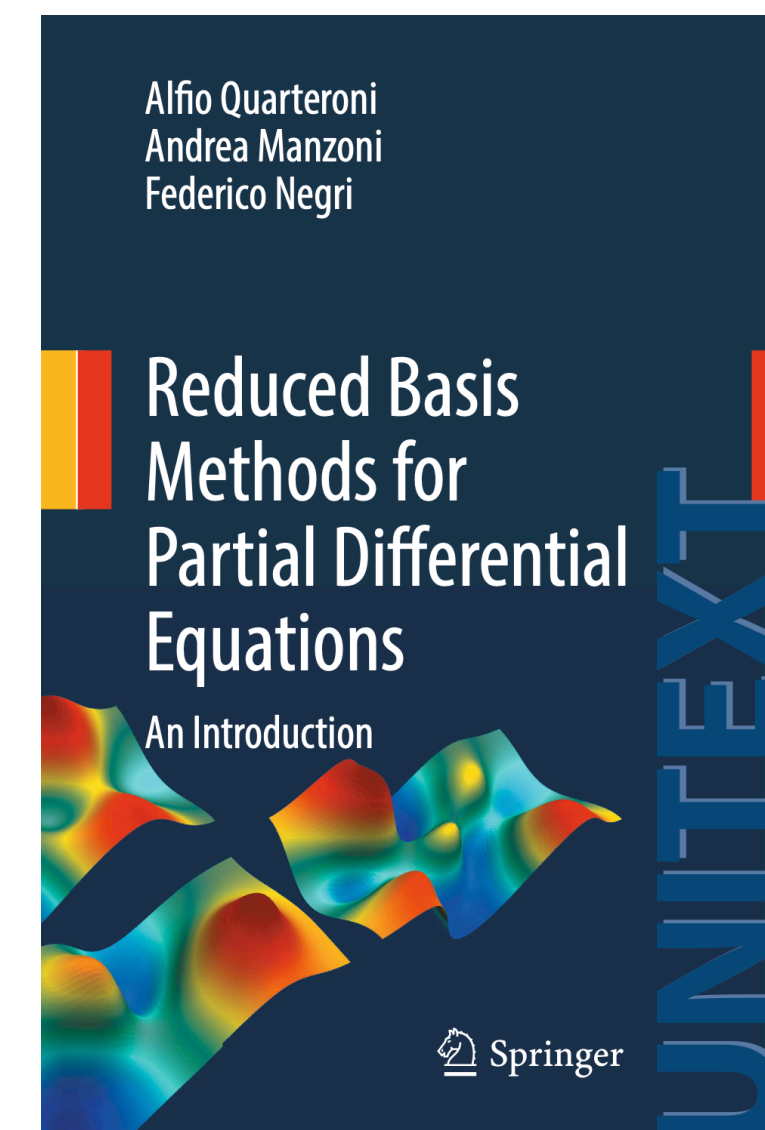


Eigenvector continuation

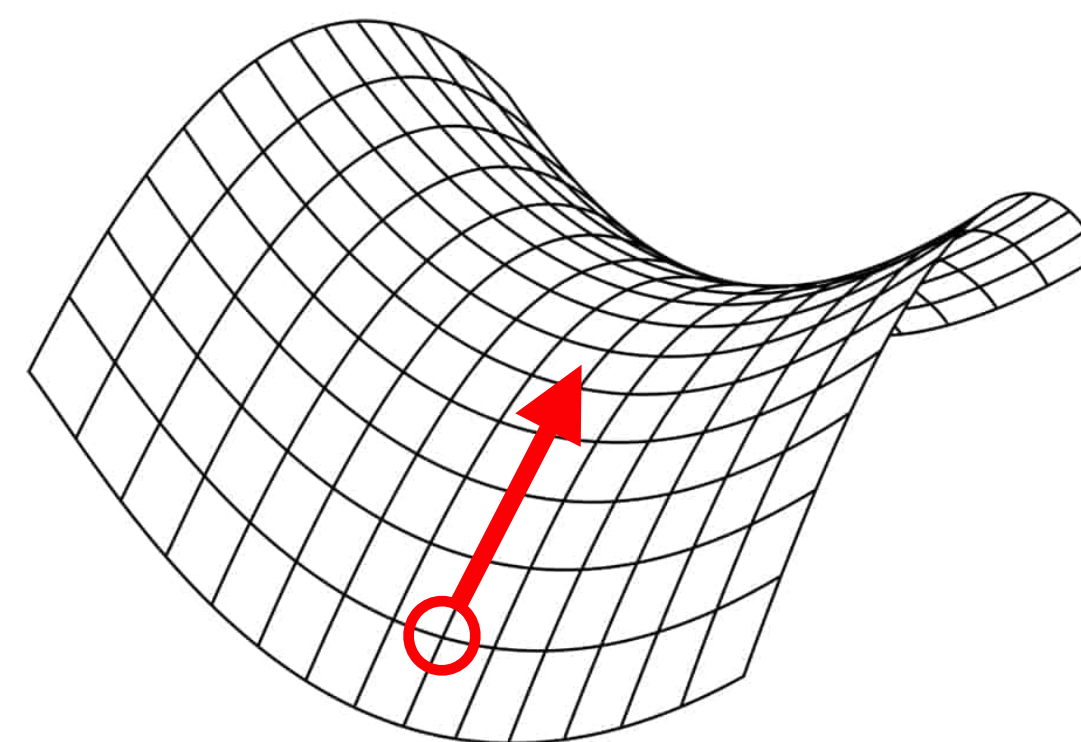
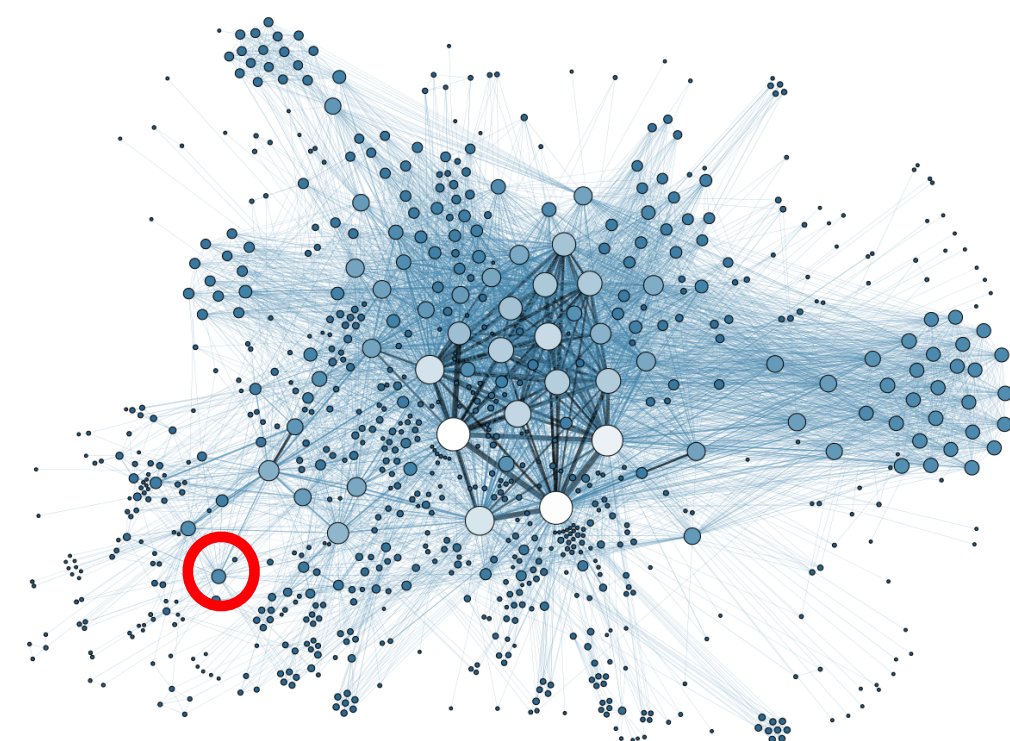
a reduced basis method (RBM)

$$H(\alpha) = H_0 + \alpha H_1$$

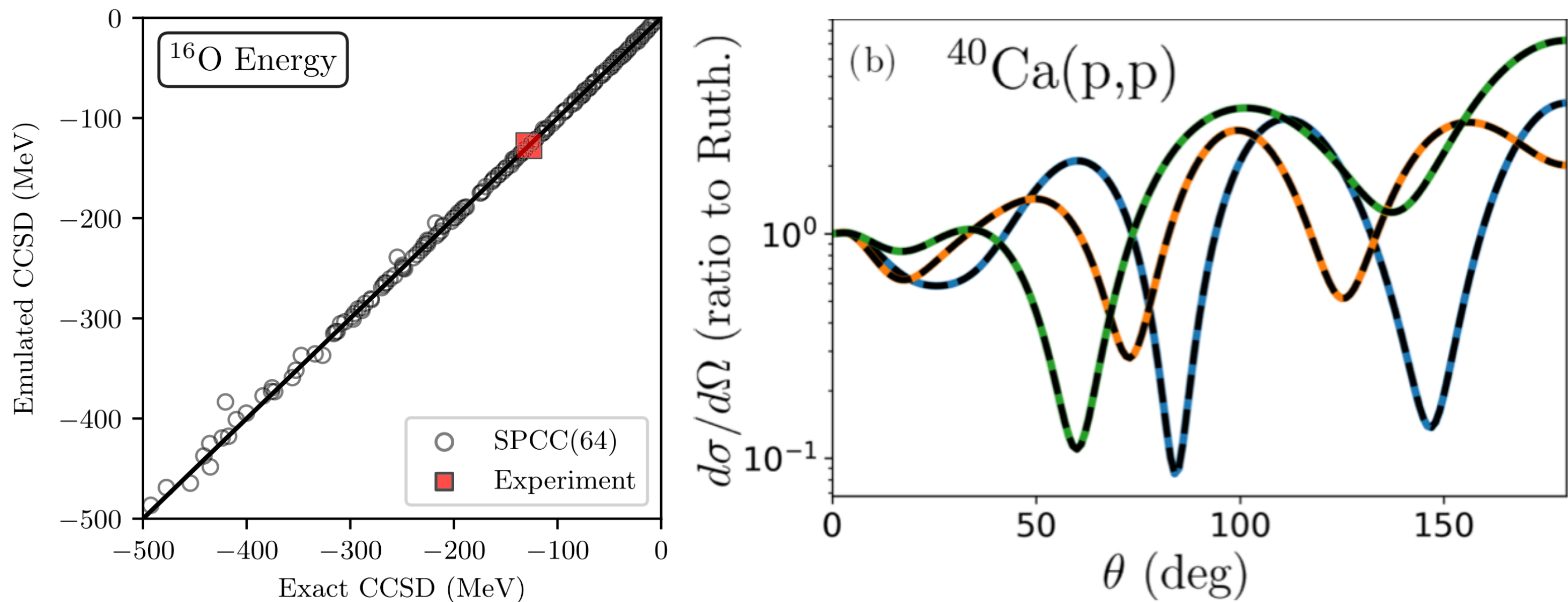
continuous parameter



The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold in many applications.

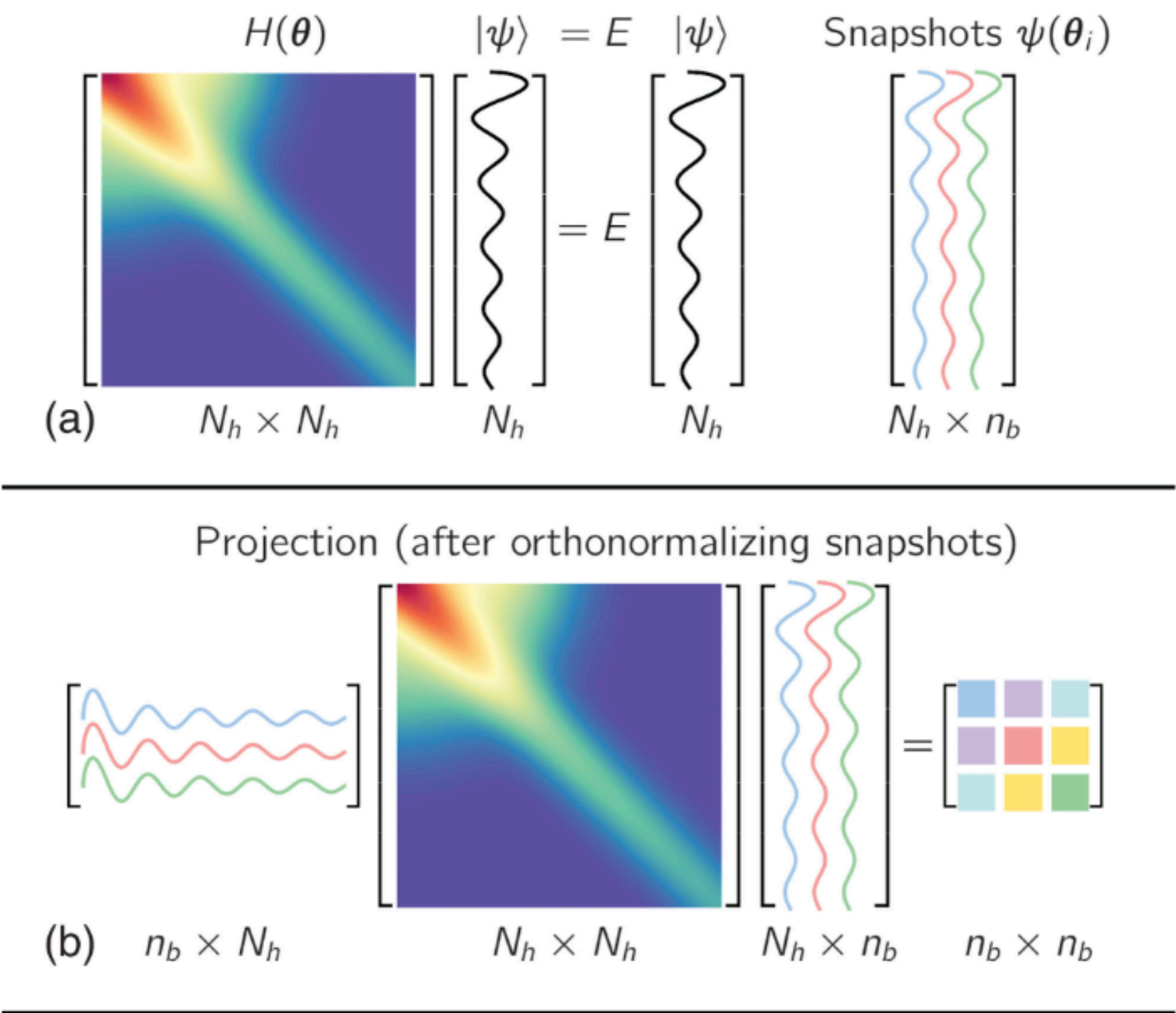


RBM emulators for bound & scattering states!



A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

D. Odell et al Phys. Rev. C **109**, 044612 (2024)
ROSE code



Recent development:

Article

<https://doi.org/10.1038/s41467-025-61362-4>

Parametric matrix models

Received: 27 January 2025

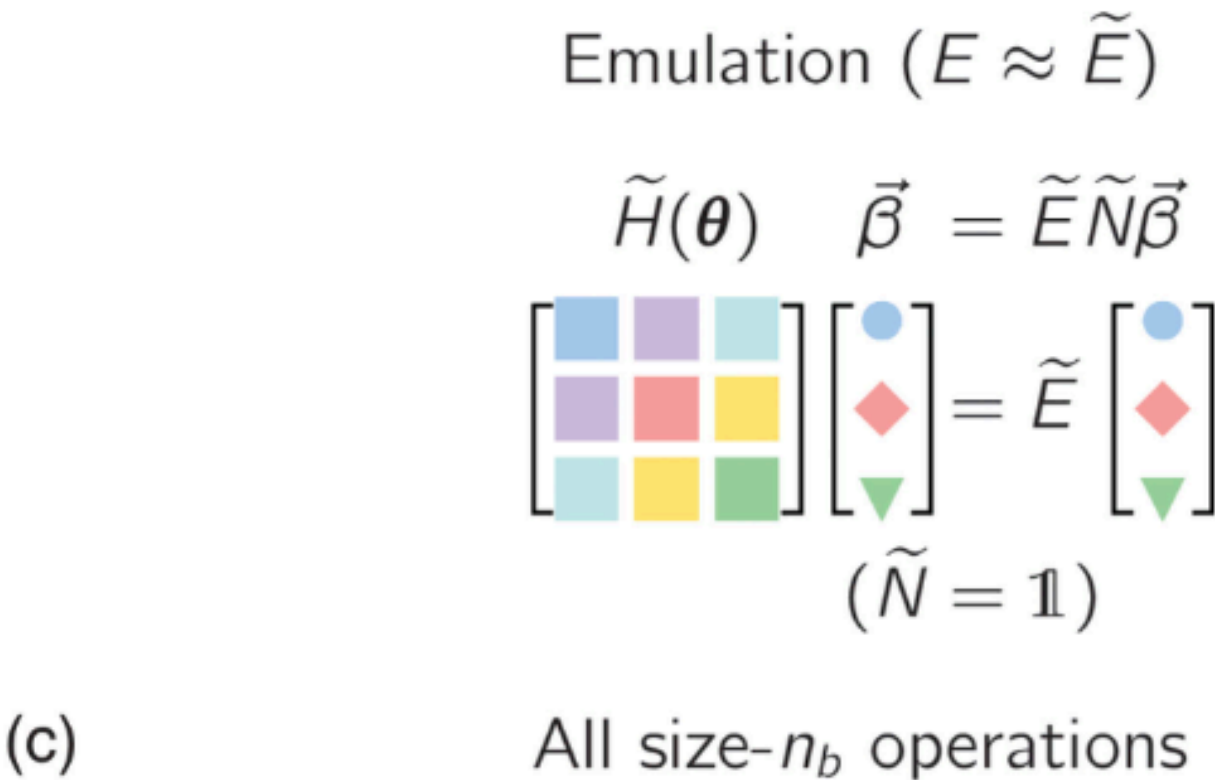
Accepted: 18 June 2025

Published online: 01 July 2025

[Check for updates](#)

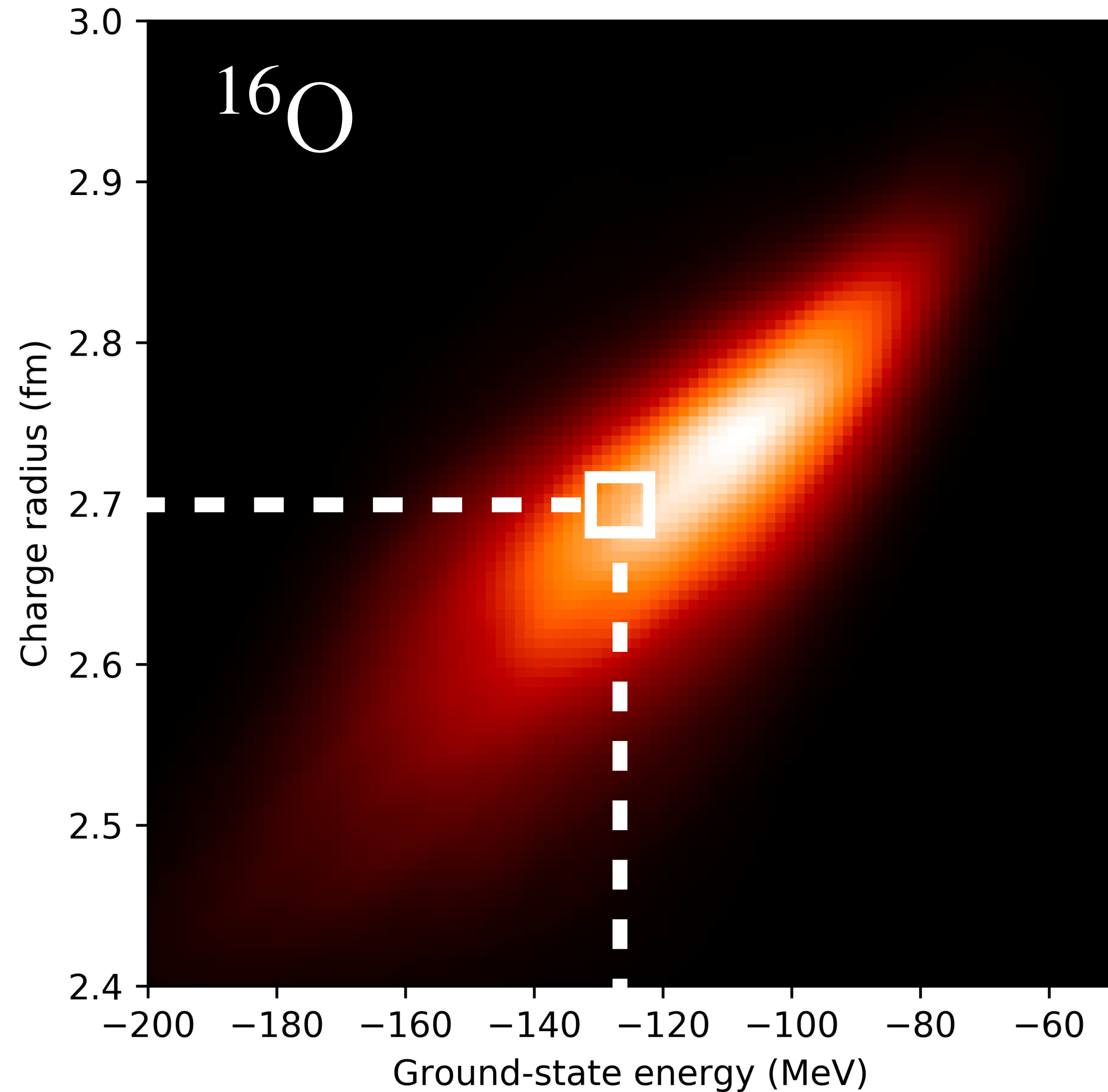
Patrick Cook ^{1,2,5}, Danny Jammooa ^{1,2,5}, Morten Hjorth-Jensen ^{1,2,3}, Daniel D. Lee ⁴ & Dean Lee ^{1,2} ✉

We present a general class of machine learning algorithms called parametric matrix models. In contrast with most existing machine learning models that imitate the biology of neurons, parametric matrix models use matrix equations that emulate physical systems. Similar to how physics problems are usually solved, parametric matrix models learn the governing equations that lead to



C. Drischler, et al. Front. Phys. 10:1092931 (2023)
tutorials at <https://dr.ascsn.net>

Emulator speedup: 20 years vs 1 hour!

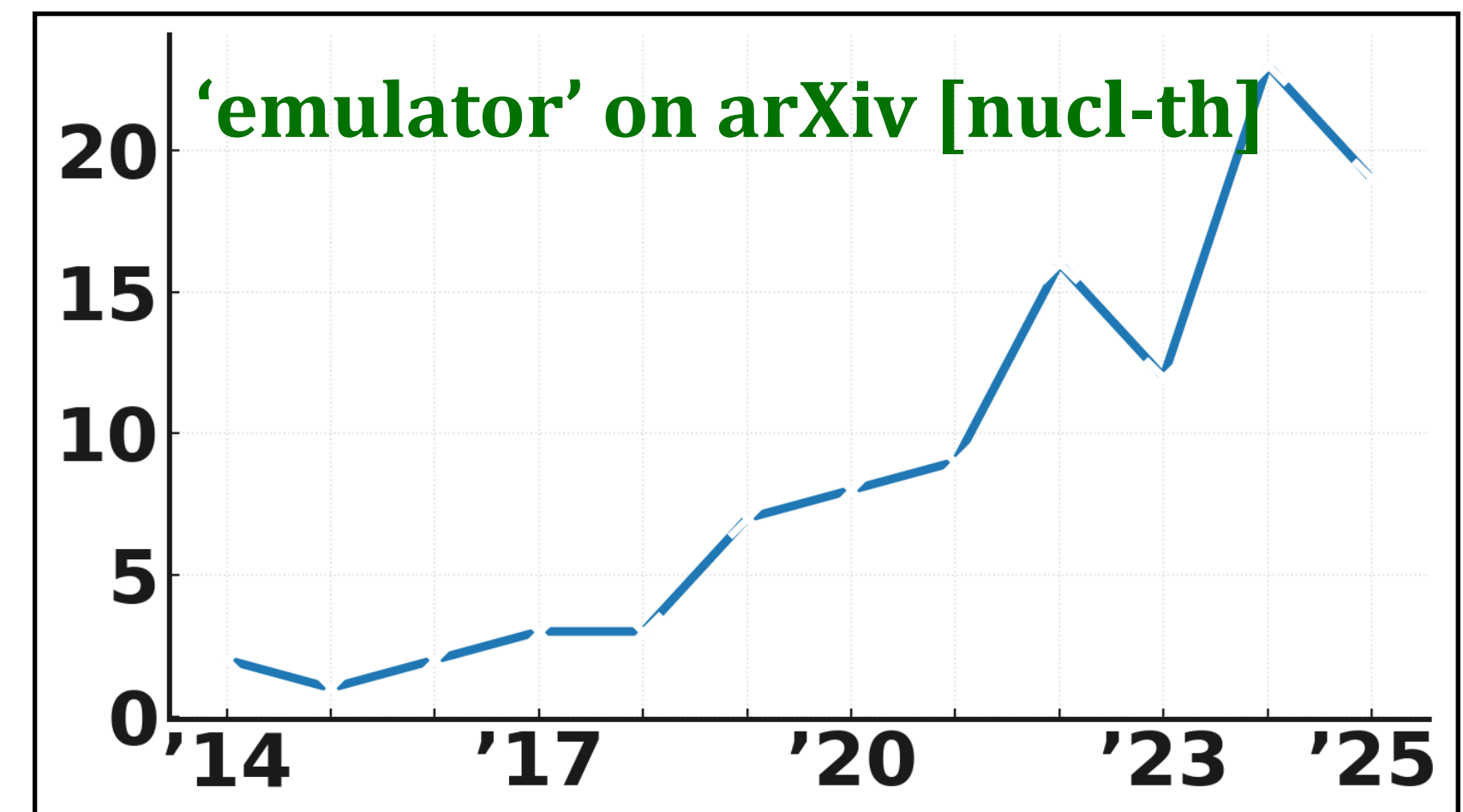


Plot of 100,000 predictions of the radius & energy of ^{16}O for different LEC values of a chiral NNLO interaction.

Using emulators, we generated the results on a laptop in just a few minutes.

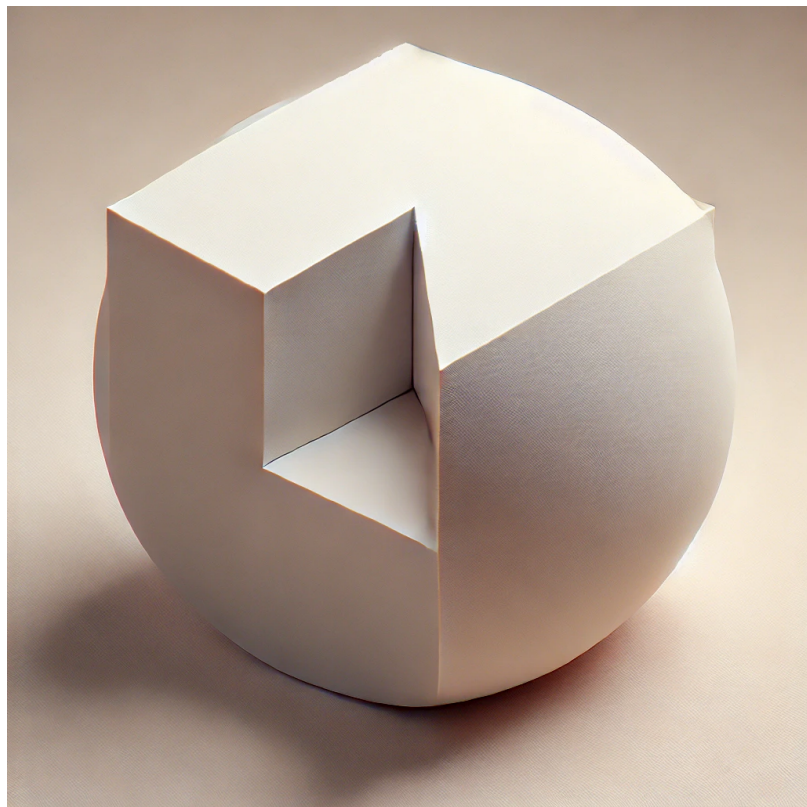
Dashed lines show experimental data.

Emulator error is 1%.



History matching: exploring the parameter space

- excluding parts of parameter space that do not reproduce data



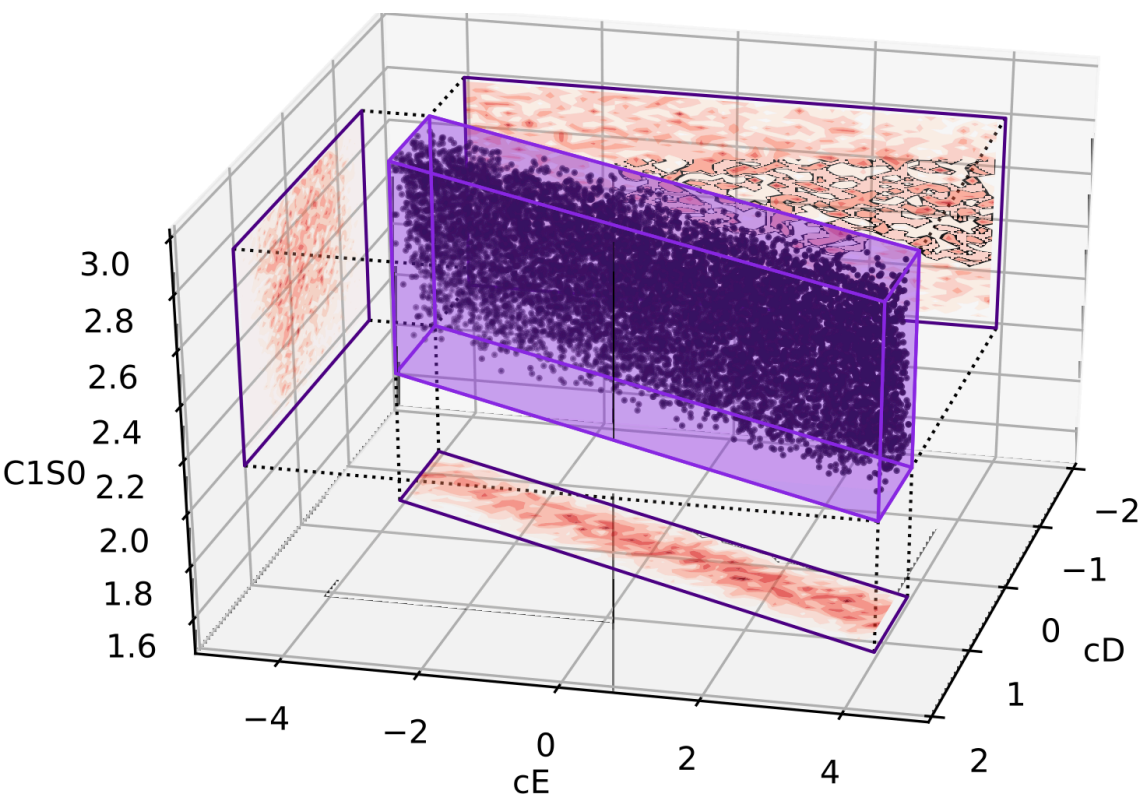
Easier to claim implausibility than to quantify posterior probability

$$p(\vec{\alpha} \mid y, M, I) \text{ vs. } \Theta(\vec{\alpha}), \text{ where } \Theta(\vec{\alpha}) = \begin{cases} 1 & \text{implausible} \\ 0 & \text{non - implausible} \end{cases}$$

Implausibility measure:

$$I^2(\vec{\alpha}) = \max_{y_{\text{exp}}^{(i)} \in y} \frac{|\mathbb{E}[y_{\text{th}}^{(i)}(\vec{\alpha})] - y_{\text{exp}}^{(i)}|^2}{\text{Var}[y_{\text{th}}^{(i)}(\vec{\alpha}) - y_{\text{exp}}^{(i)}]}$$

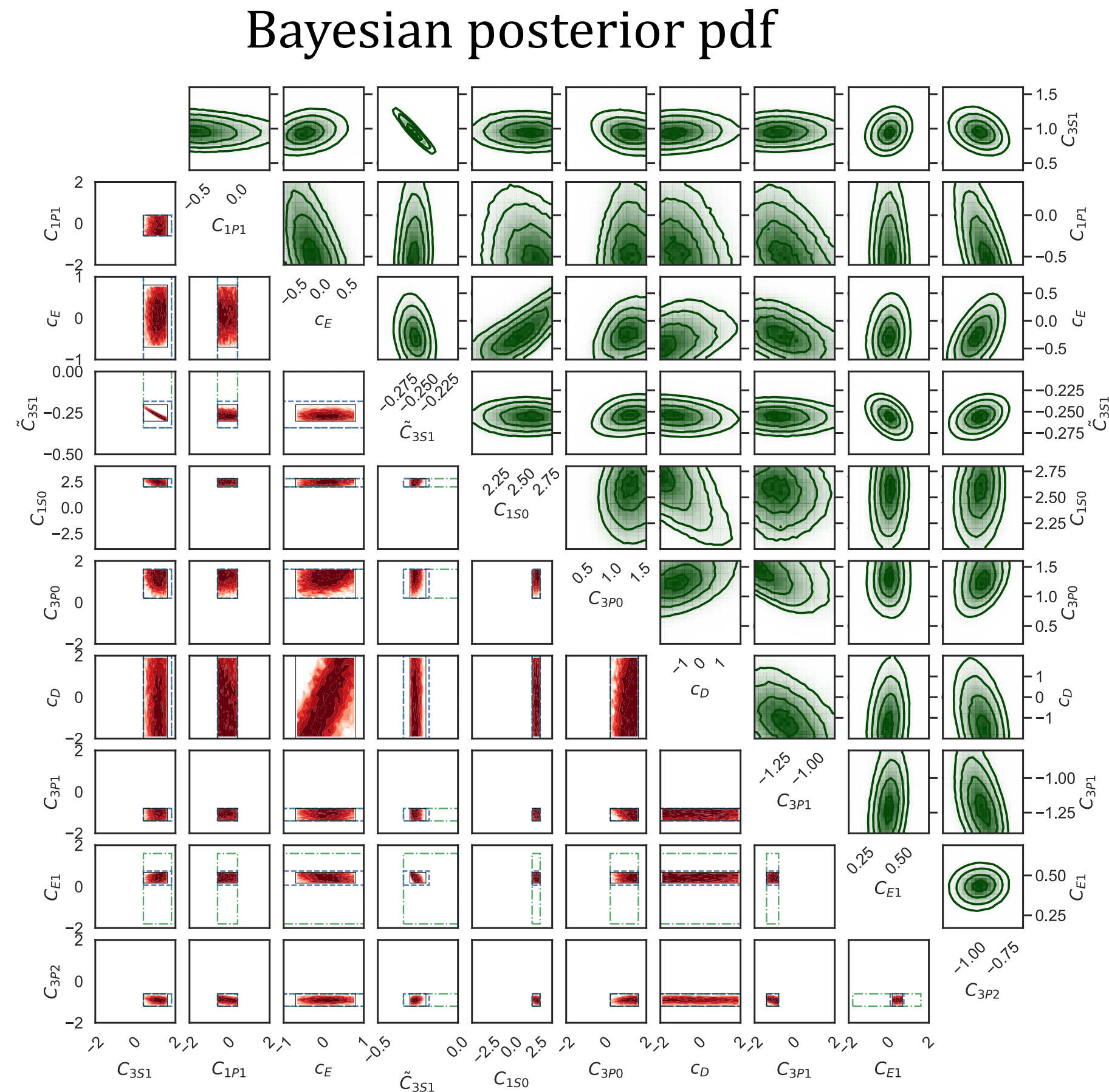
Iteratively rule out $\vec{\alpha}$ for $I(\vec{\alpha}) > 3$
(Pukelsheim)



y	y _{exp}	ε _{exp}	ε _{model}	ε _{method}
E(² H)	-2.2298	0.0	0.05	0.0005
r _p ² (² H)	3.9030	0.0	0.02	0.0005
Q(² H)	0.27	0.01	0.003	0.0005
E(³ H)	-8.4818	0.0	0.17	0.0005
E(⁴ He)	-28.2956	0.0	0.55	0.0005
r _p ² (⁴ He)	2.1176	0.0	0.045	0.0005
E(¹⁶ O)	127.62	0.0	0.75	1.5
r _p ² (¹⁶ O)	6.660	0.0	0.16	0.05
ΔE(²² , ¹⁶ O)	-34.41	0.0	0.4	0.5
ΔE(²⁴ , ²² O)	-6.35	0.0	0.4	0.5
E ₂₊ (²⁴ O)	4.79	0.0	0.5	0.25
ΔE(²⁵ , ²⁴ O)	0.77	0.02	0.4	0.25

Sampling the posterior predictive distribution

Analyzing the first observation of the ^{28}O energy



- **History matching** identifies the parameter region where we expect the LEC posterior distribution to reside.
- **MCMC + emulators** to draw 10^8 samples of the LEC posterior at ΔNNLO with NN+3N interaction.
- We assume uniform prior + uncorrelated normal likelihood

$$p(\vec{\alpha}|A = 2 - 24)$$

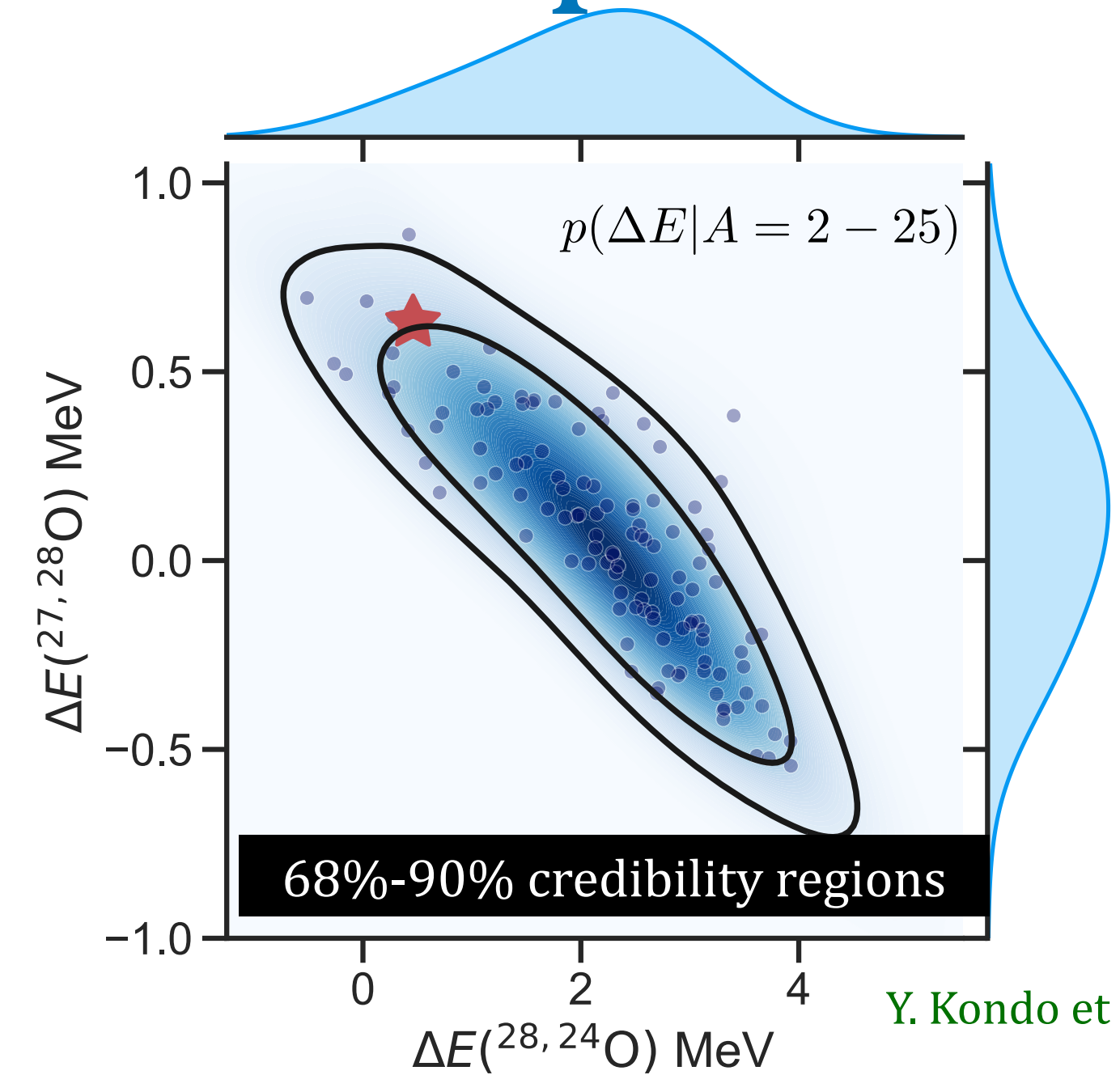
- Informative to update the parameter posterior with $\Delta E(250,240)$. Subsequently draw 121 parameter samples that we employ in our prediction of oxygen-27/28.

$$\vec{\alpha} \sim p(\vec{\alpha}|A = 2 - 25)$$

Posterior predictive distributions for complex nuclei

^{28}O separation energies

- From theory, we claim with 98% certainty that ^{28}O is unbound with respect to ^{24}O :
- The experimental data point (red star) is away from the posterior maximum. This suggests that only a few finely-tuned chiral interactions are able to reproduce low-energy and exotic oxygen structure

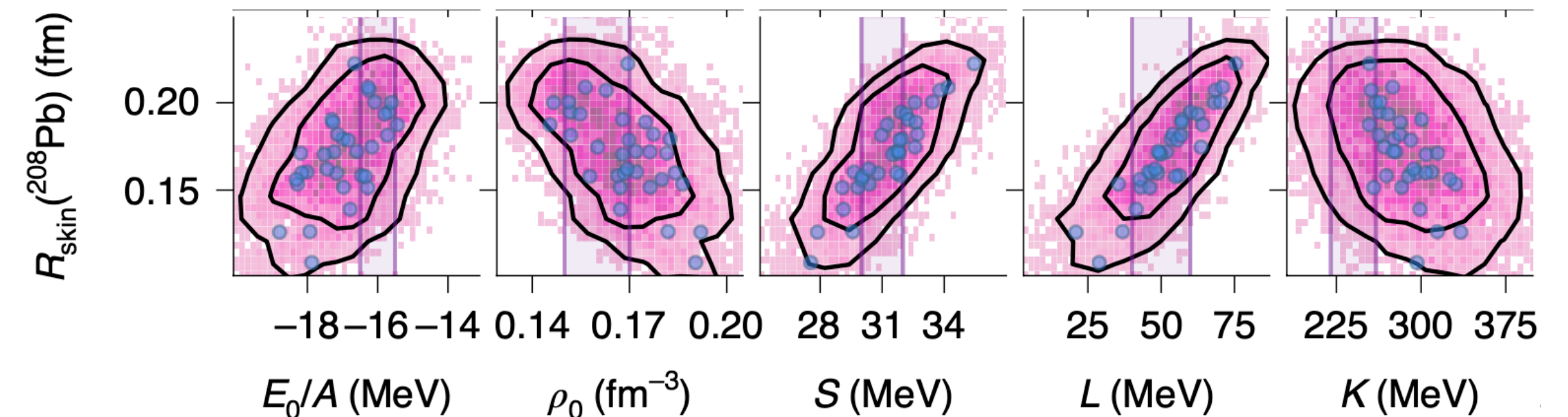
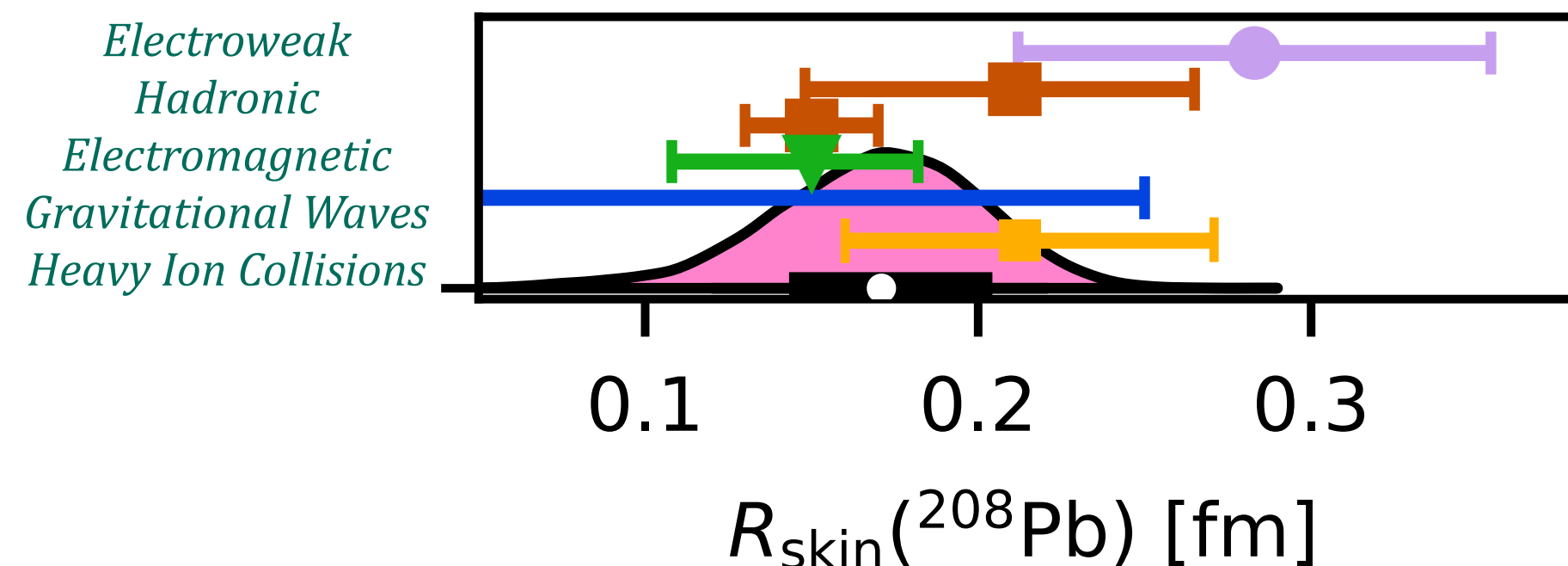


Y. Kondo et al. Nature (2023)

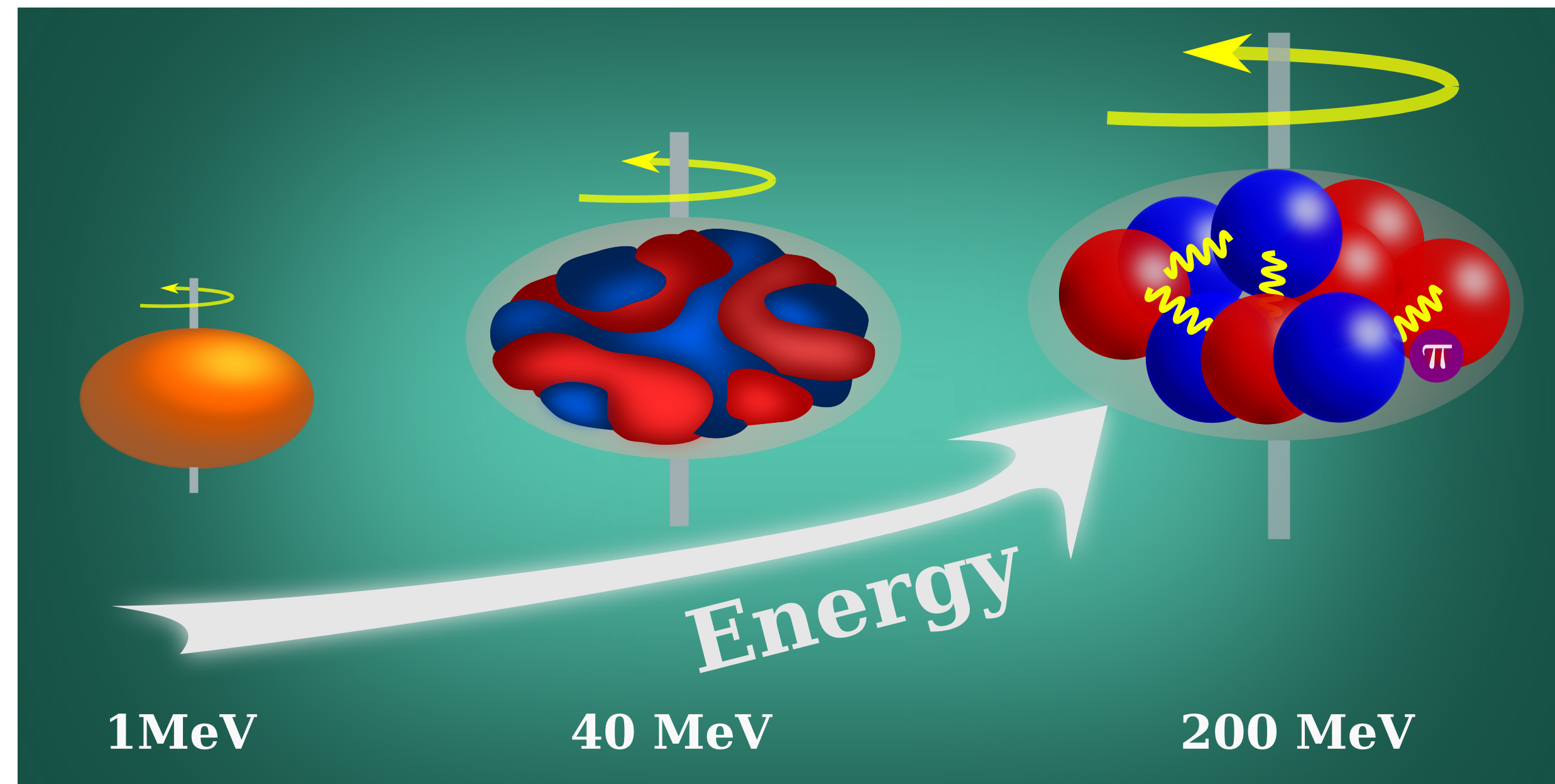
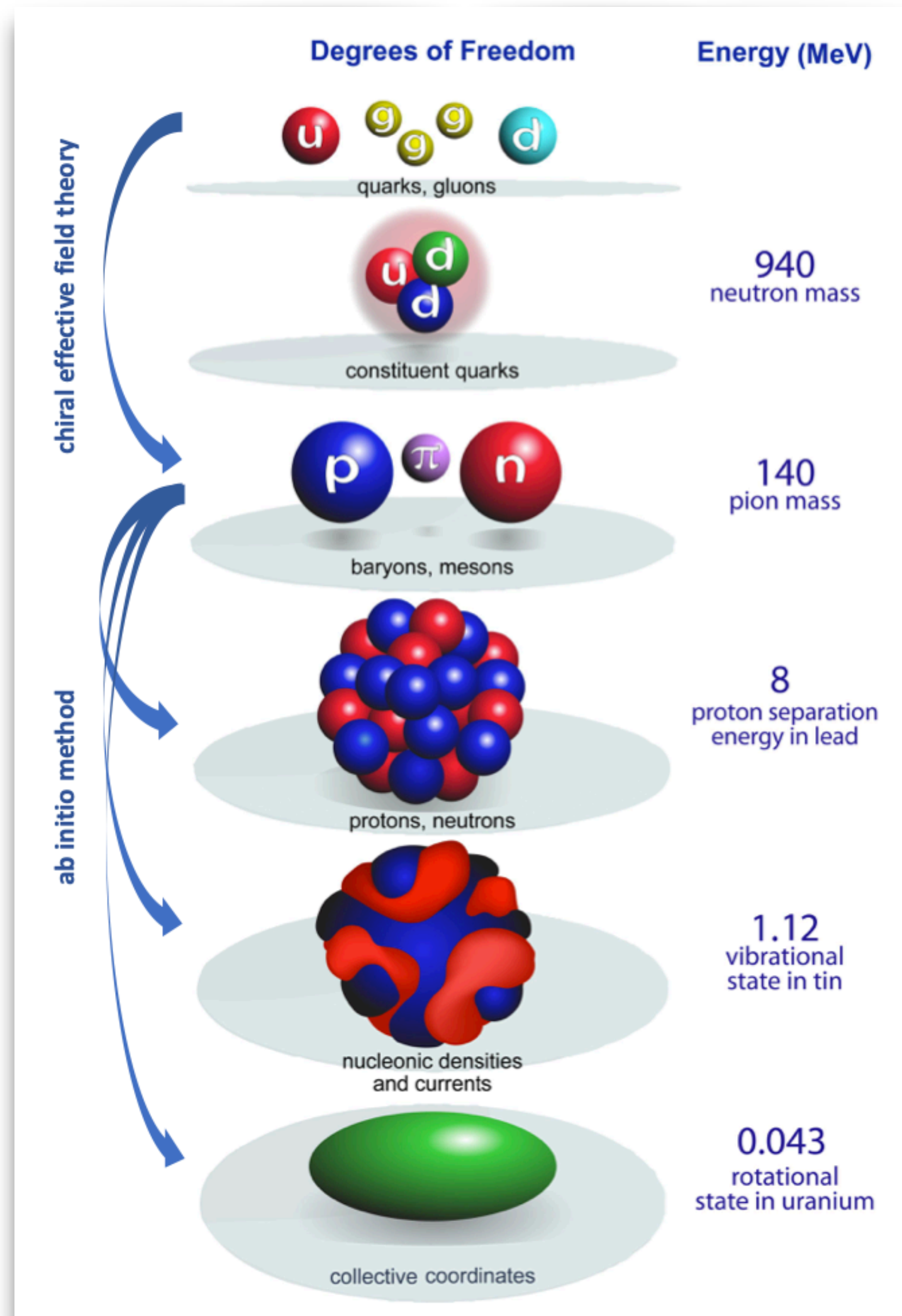
^{208}Pb neutron skin-thickness

n.b. similarly curated history matching data

- We predict a small skin thickness 0.14-0.20 fm in mild (1.5σ) tension with electroweak (PREX) measurement.

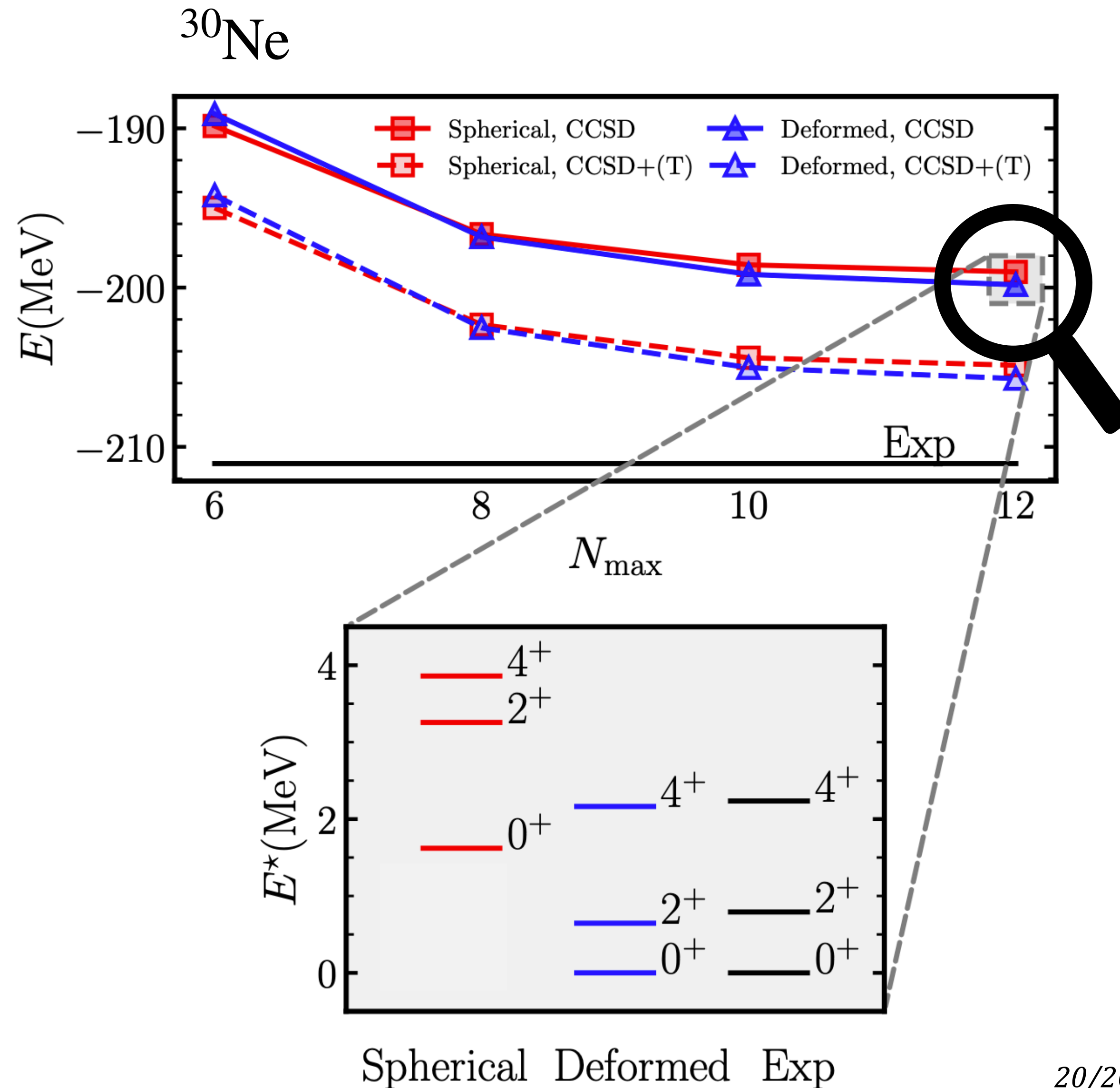


The challenge of *ab initio* multiscale nuclear physics



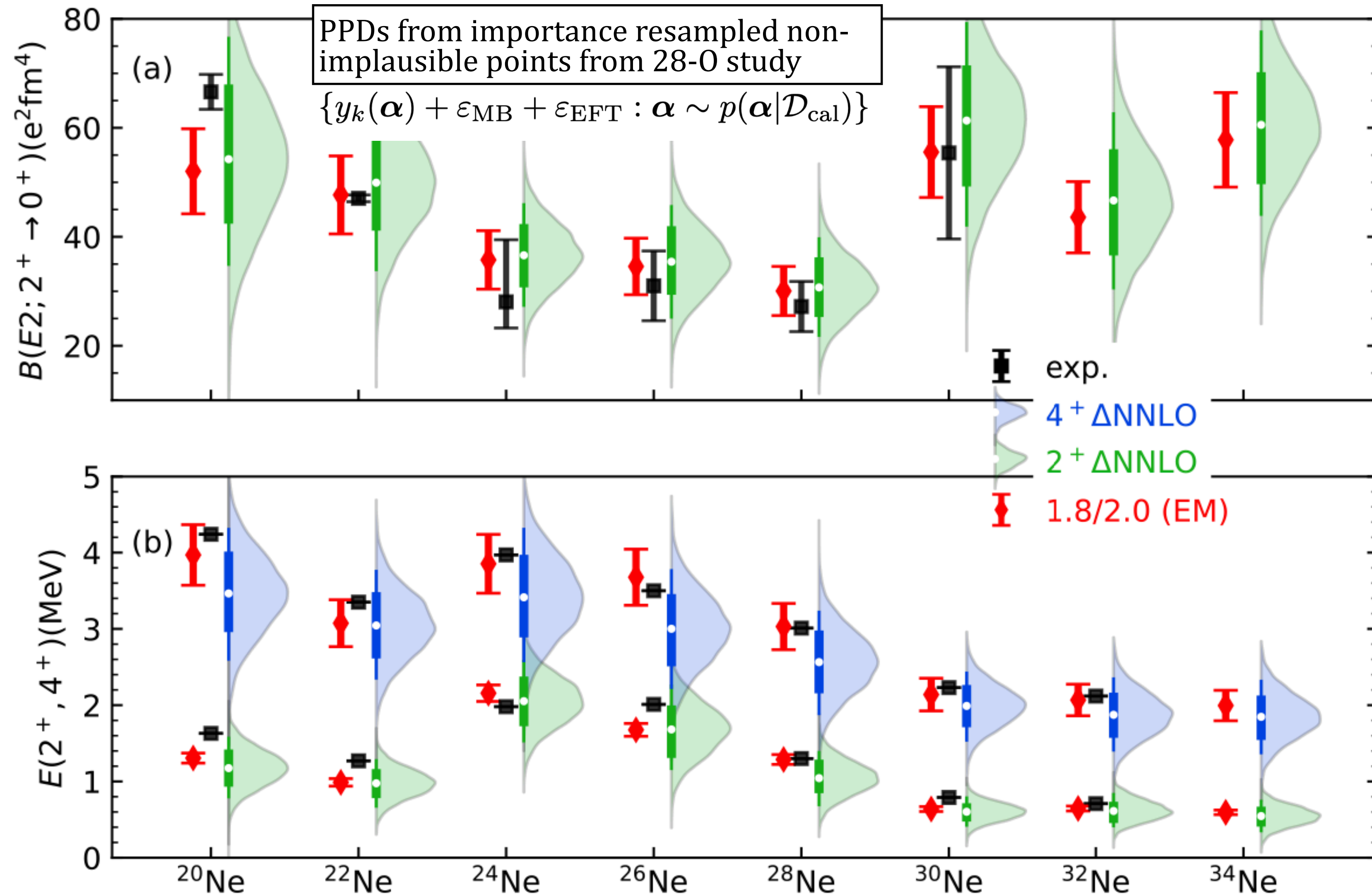
- Deformation is a collective effect and allows rotation.
- Rotational energies are minuscule (sub-%) on the scale of nuclear binding, and collective modes are built from many-particle-many-hole excitations.

Ab initio can capture multiscale nuclear physics



- Symmetry-breaking Hartree-Fock plus few-particle–few-hole excitations using coupled-cluster theory to capture the bulk of the binding energy.
- Symmetry projection adds long-range (static) correlations via many-particle–many-hole excitations, essential for collective structures. Contributes little to the binding energy.
- We predict shape coexistence in ^{30}Ne

Reproduction of data without effective charges

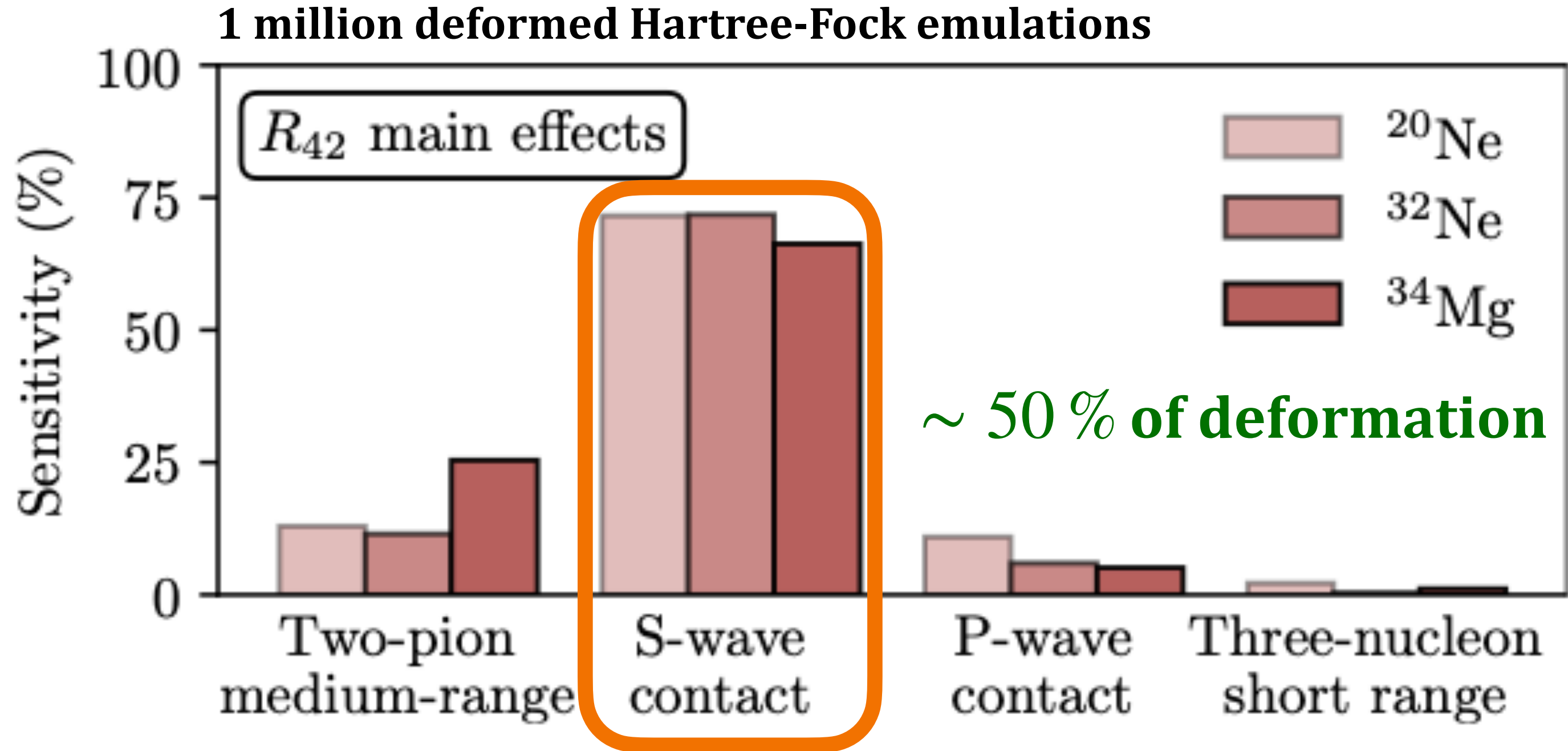


We predict $^{32,34}\text{Ne}$
 $B(E2)$ with quantified
theory uncertainties

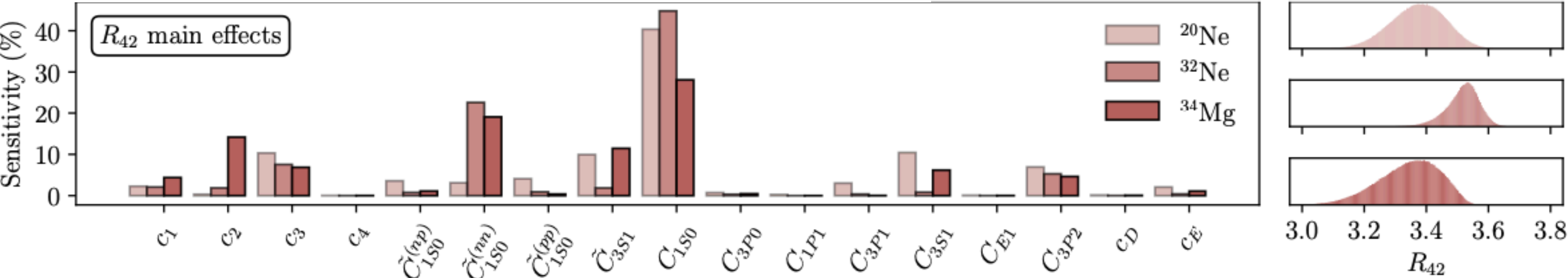
Rigid rotor $R_{42} = 10/3$

$$E(J) = \frac{J(J+1)}{2I}$$

Linking deformation and chiral nuclear forces



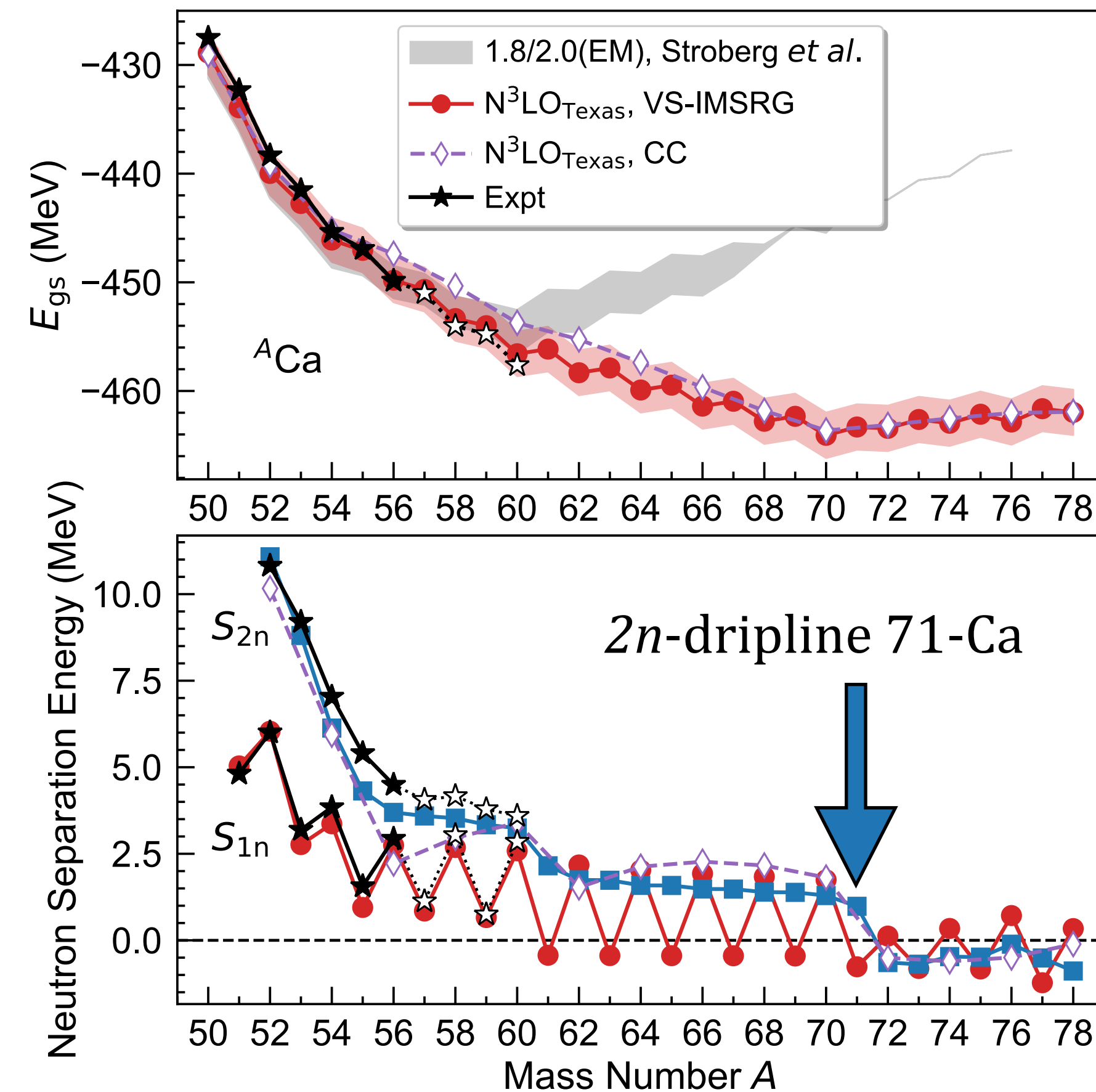
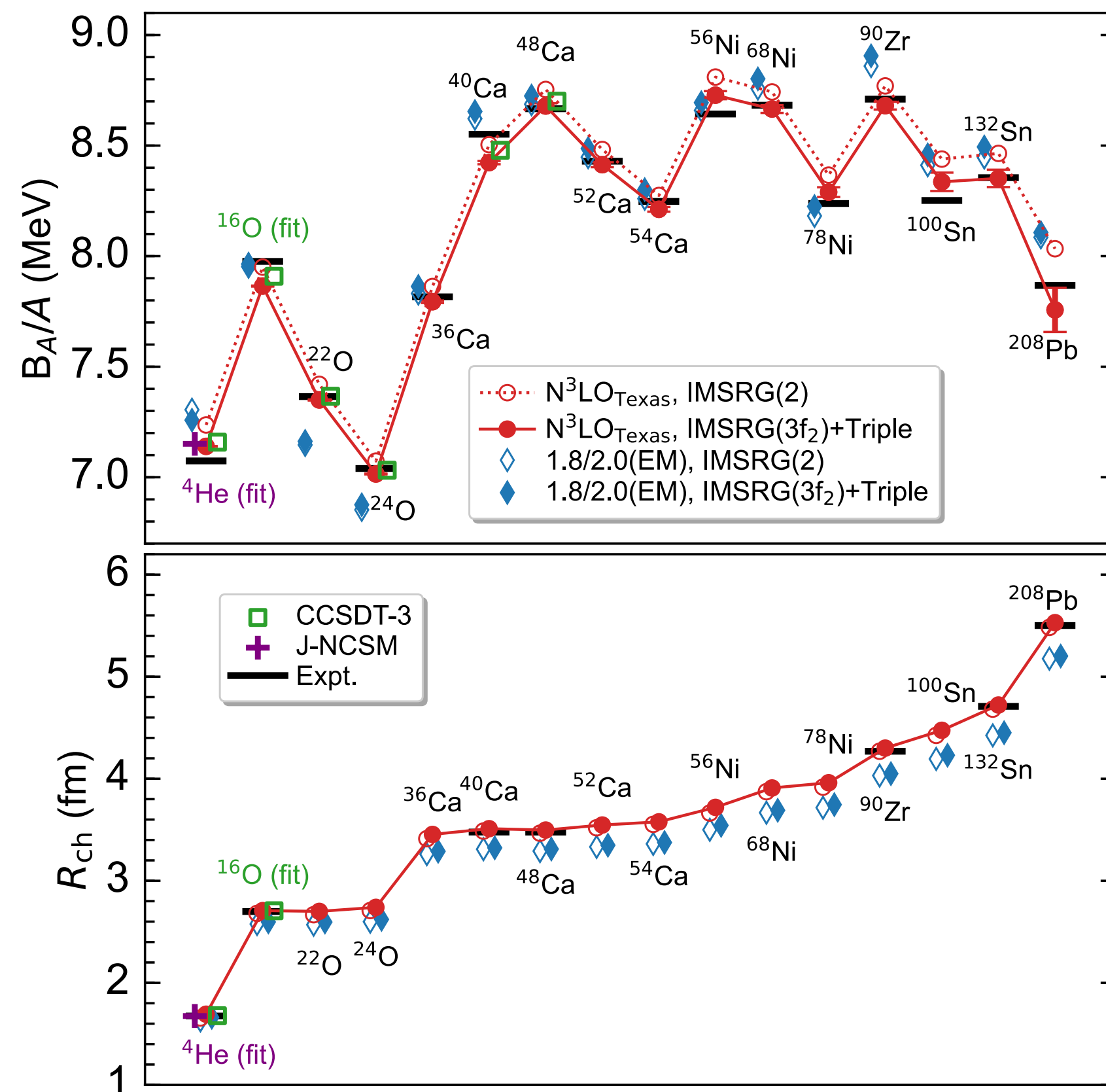
- Adding short-range repulsion appears to increase deformation, probably via reduced pairing.
- Increasing medium-range 2π -exchange increases deformation, presumably by adding attraction in higher partial waves



N3LO_{Texas} : predicting energies, radii, excited states in A=16-208

- towards the *n*-dripline in Ca

More than 30 parameters in this N3LO interaction. A calibration challenge!
Need **informative** experimental data, **powerful** *ab initio* methods, and **emulators**



Where is the pairing in *ab initio*?

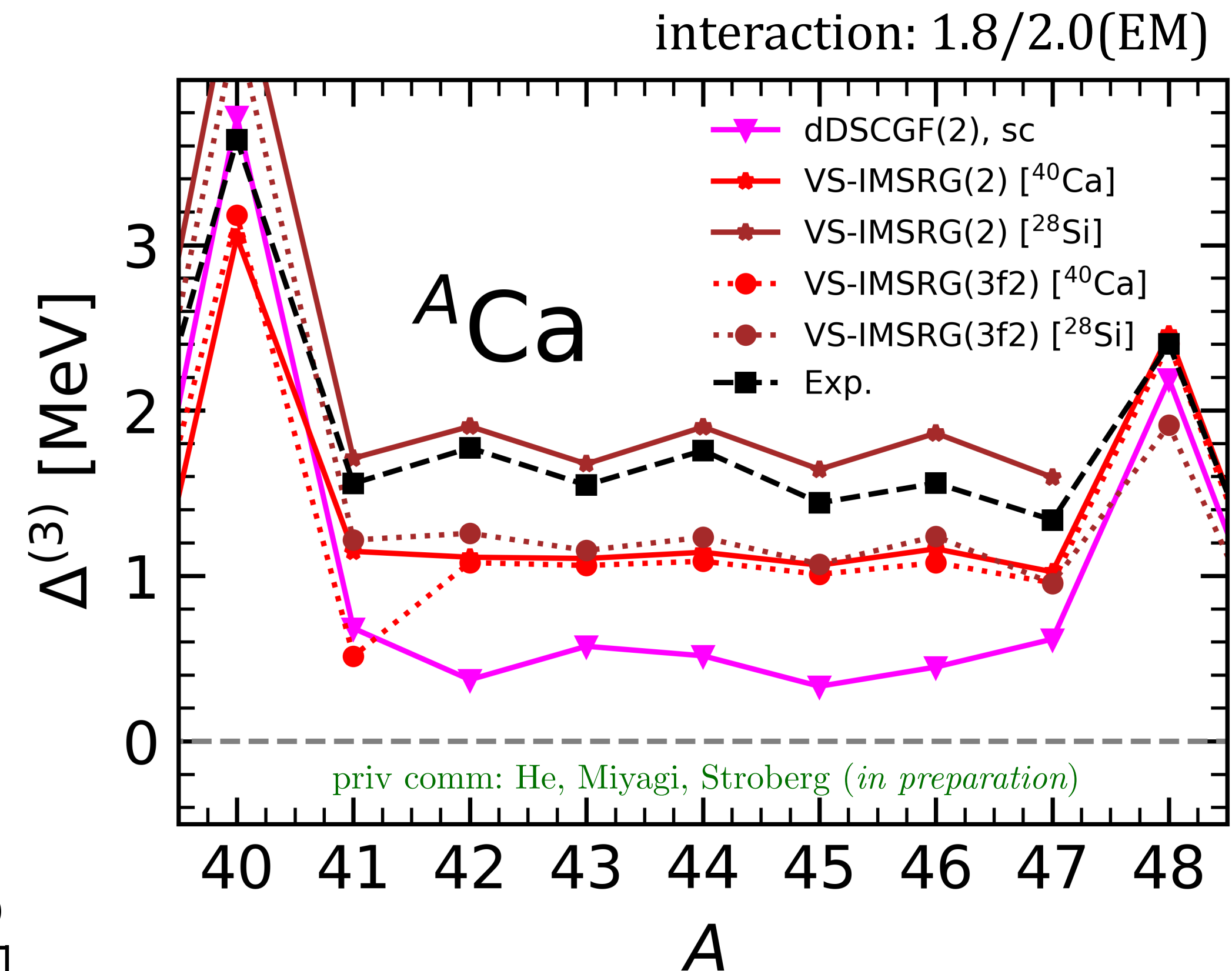
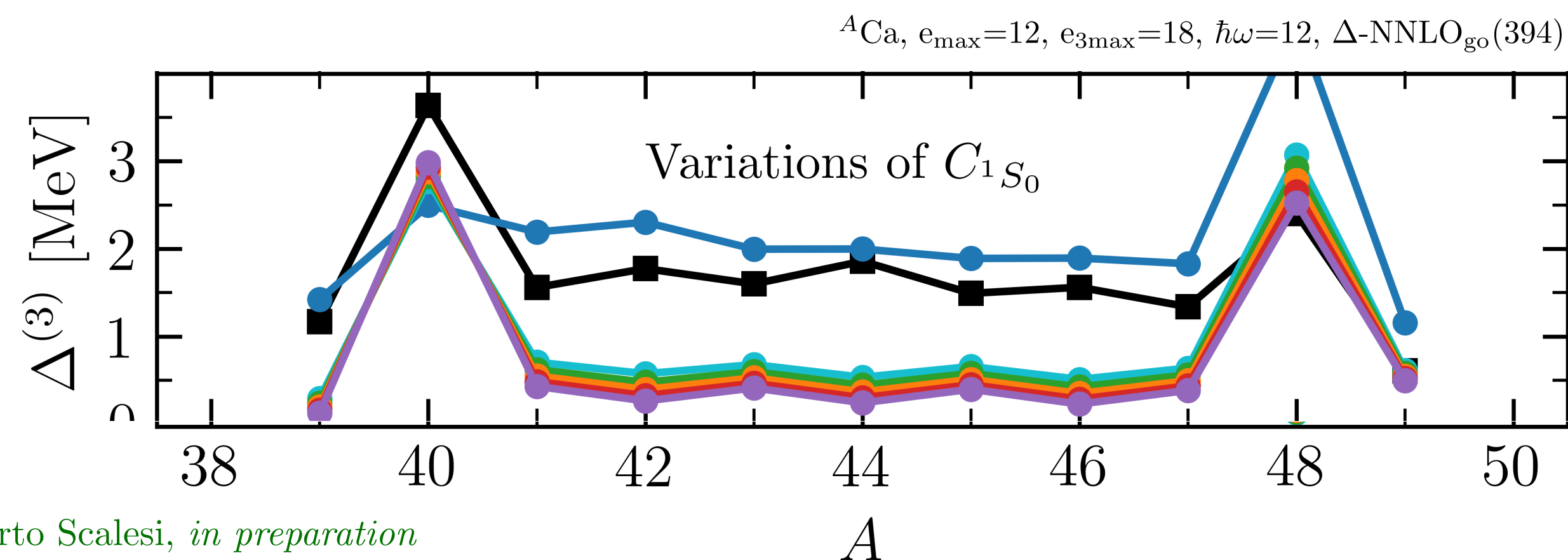
odd-even staggering of masses

$$\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2} [E(N+1) - 2E(N) + E(N-1)],$$

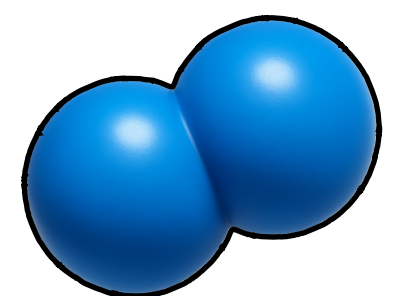
Insufficient $\Delta^{(3)}$ at low-order polynomial cost

Agreement with experiment when opening the ^{40}Ca core (^{28}Si) and VS-IMSRG(2).

Deteriorates with IMSRG(3).

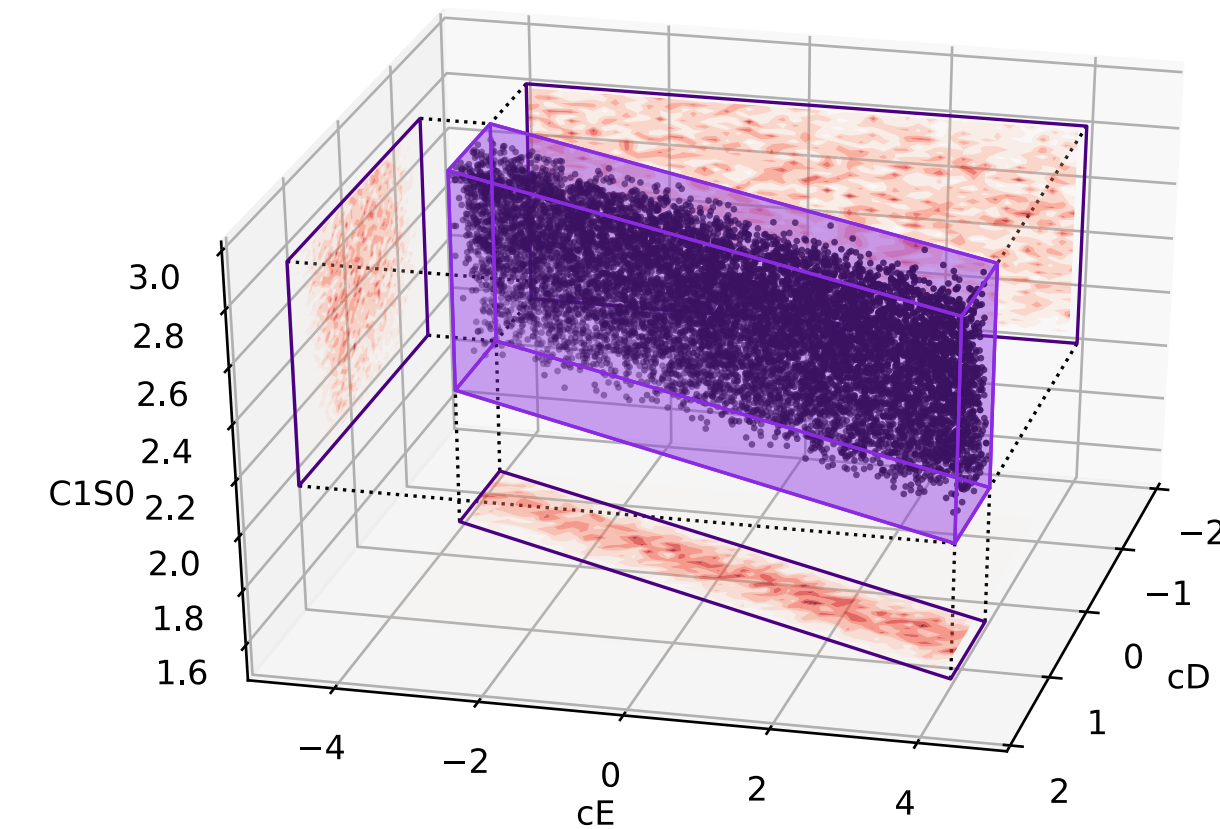
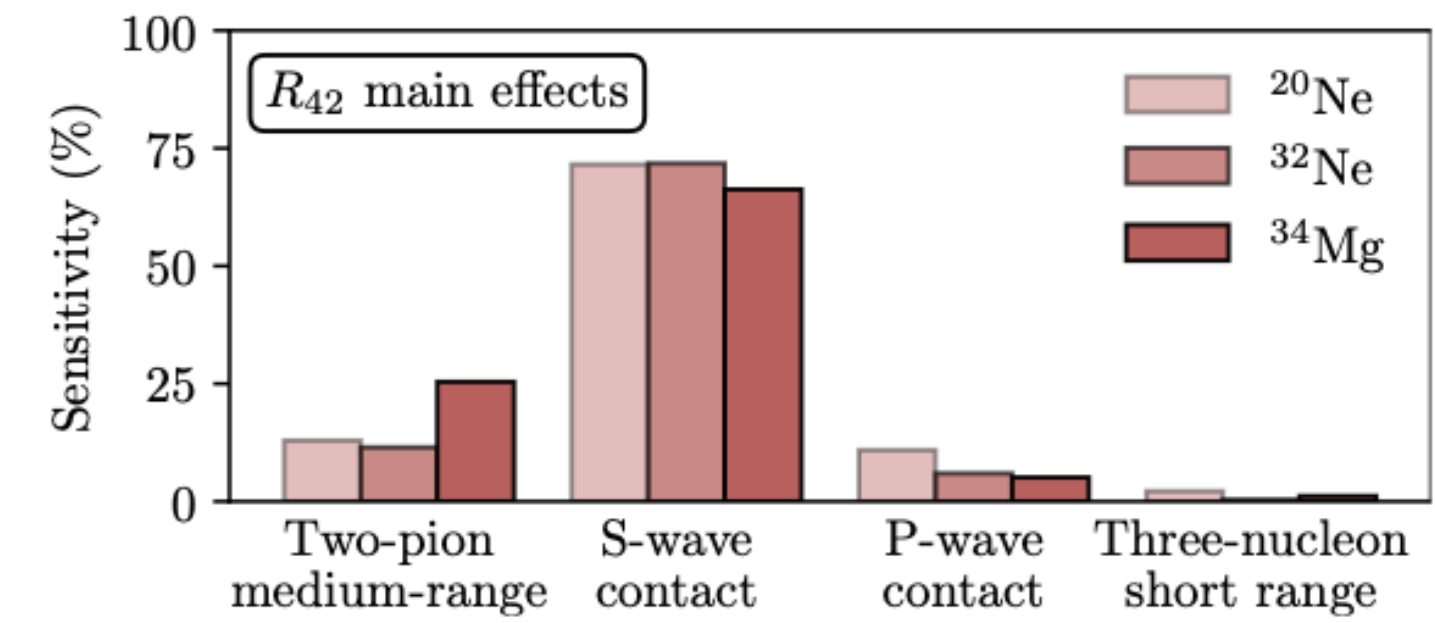
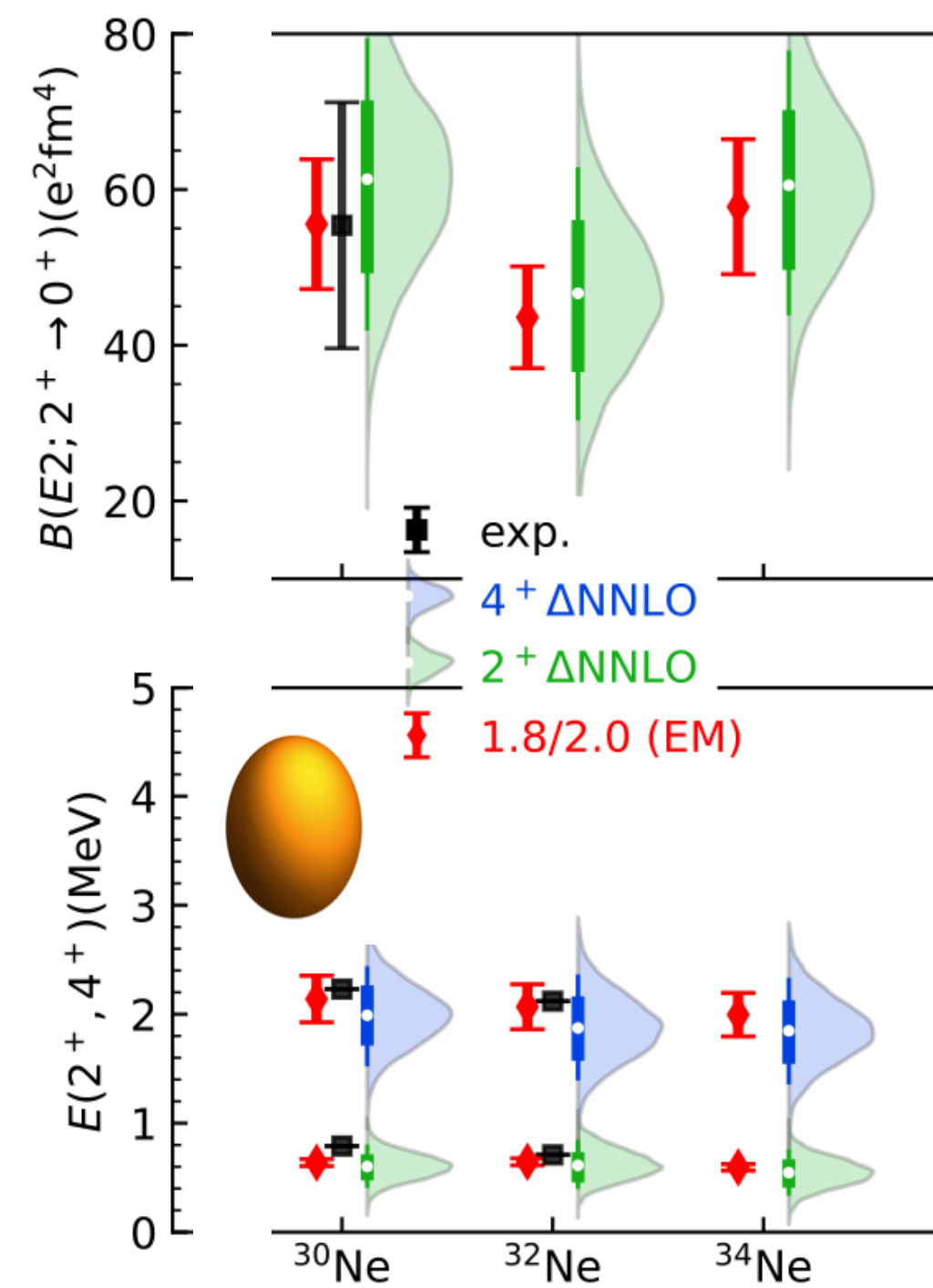
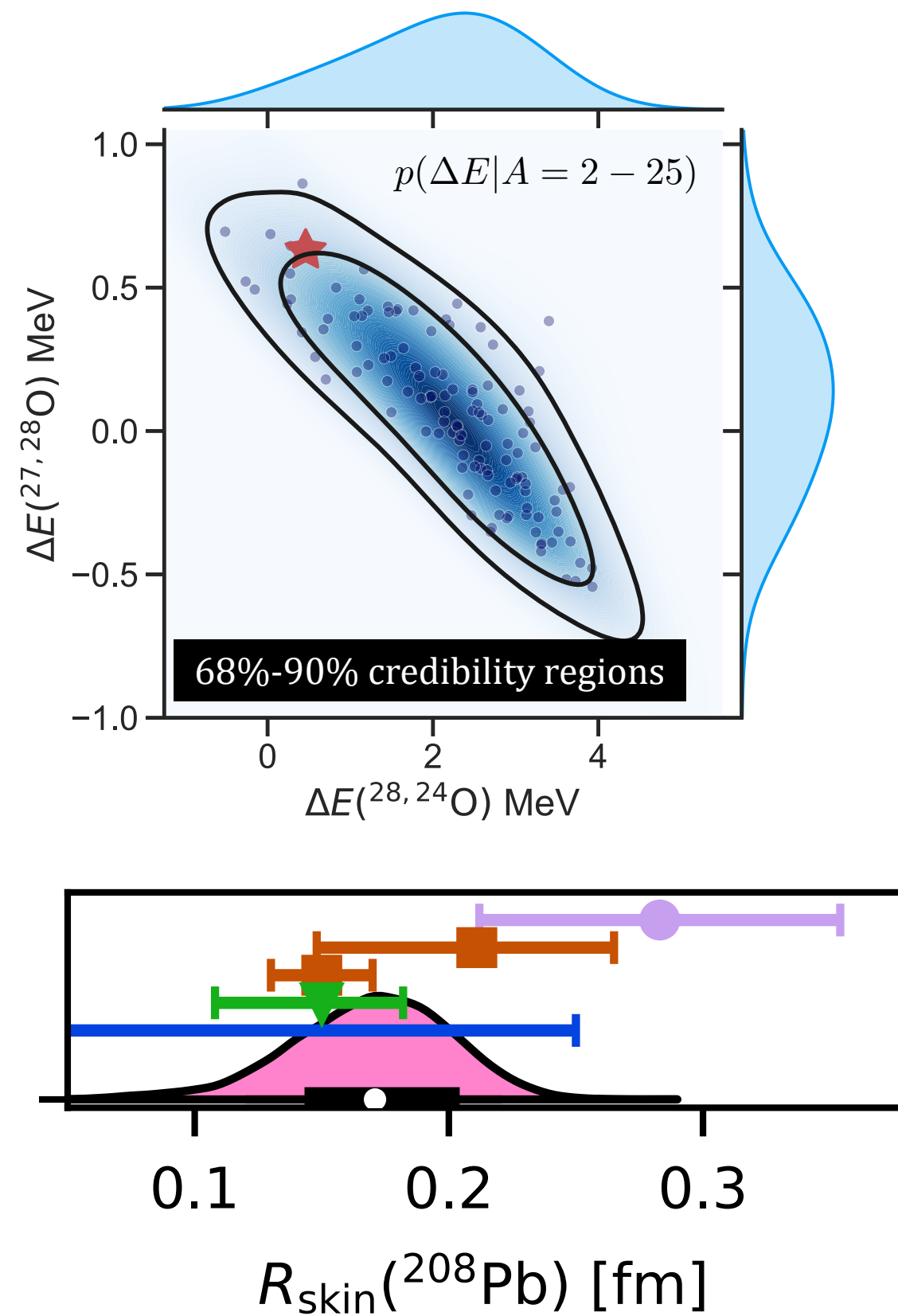


Enhanced S-wave attraction induces pairing
.... and a bound di-neutron.



Outlook

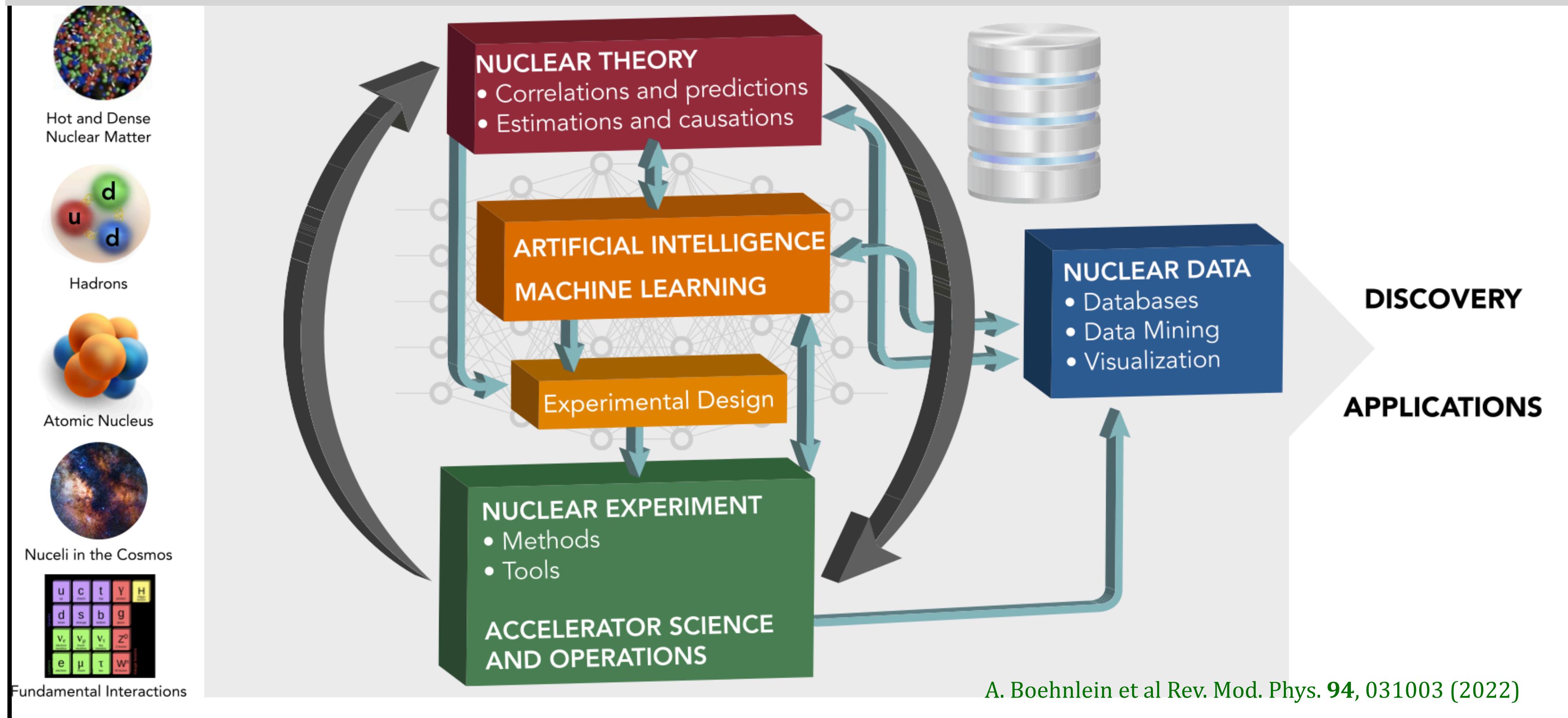
We are quantifying posterior predictive distributions and sensitivities of nuclear observables



Outlook

We are quantifying posterior predictive distributions and sensitivities of nuclear observables

Next, we should try to utilize them in **our decision making process**



Summary

- *Ab initio* nuclear methods are reaching **heavy-mass and deformed nuclei**. High-order and realistic χ EFT is challenging, but we are making progress (N3LO_{Texas}).
- We achieve **multiscale predictions** of binding energies, excitation energies, and transition probabilities, with quantified theory uncertainties, in neutron-rich neon and magnesium isotopes.
- **Emulators** are essential tools for uncertainty quantification, Bayesian inference, and enable us to do experimental design.
- Global sensitivity analysis reveals that **S-wave contacts strongly impact nuclear deformation** in chiral effective field theory.

thanks to all my collaborators!
thank you for your attention!



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