Massachusetts Institute of Technology

Connecting nuclear force parameters to nuclear observables via machine learning emulation

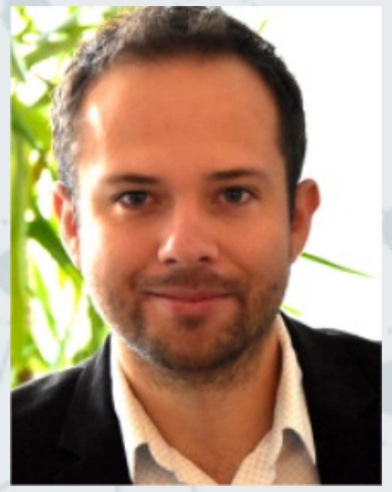
INT26-1: Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond

Antoine Belley

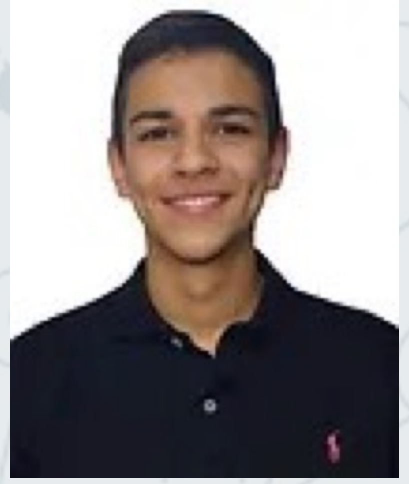
28 April 2026

Acknowledgements

Prof.
Ronald García



Jose Miguel
Muñoz Arias



EMA lab

G. Mondeel

A. Brinson

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Shortcomings of the Standard Model

Shortcomings of the Standard Model

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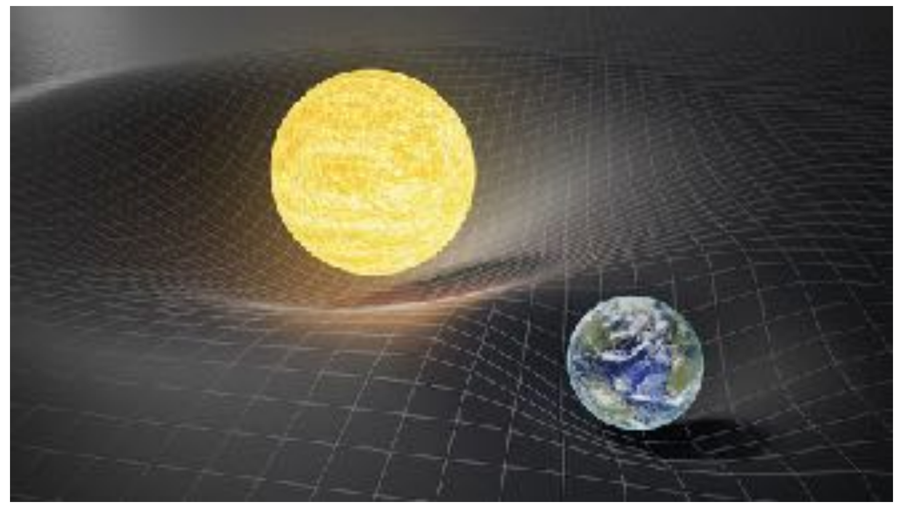

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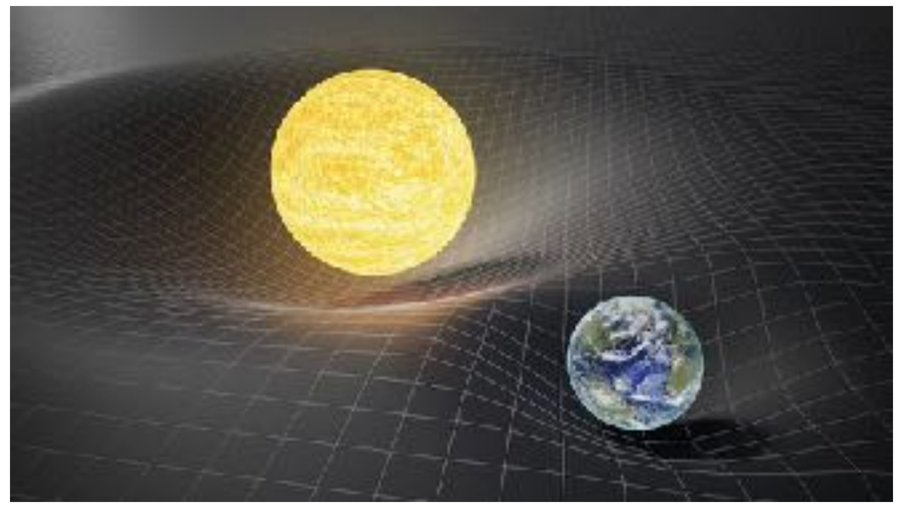

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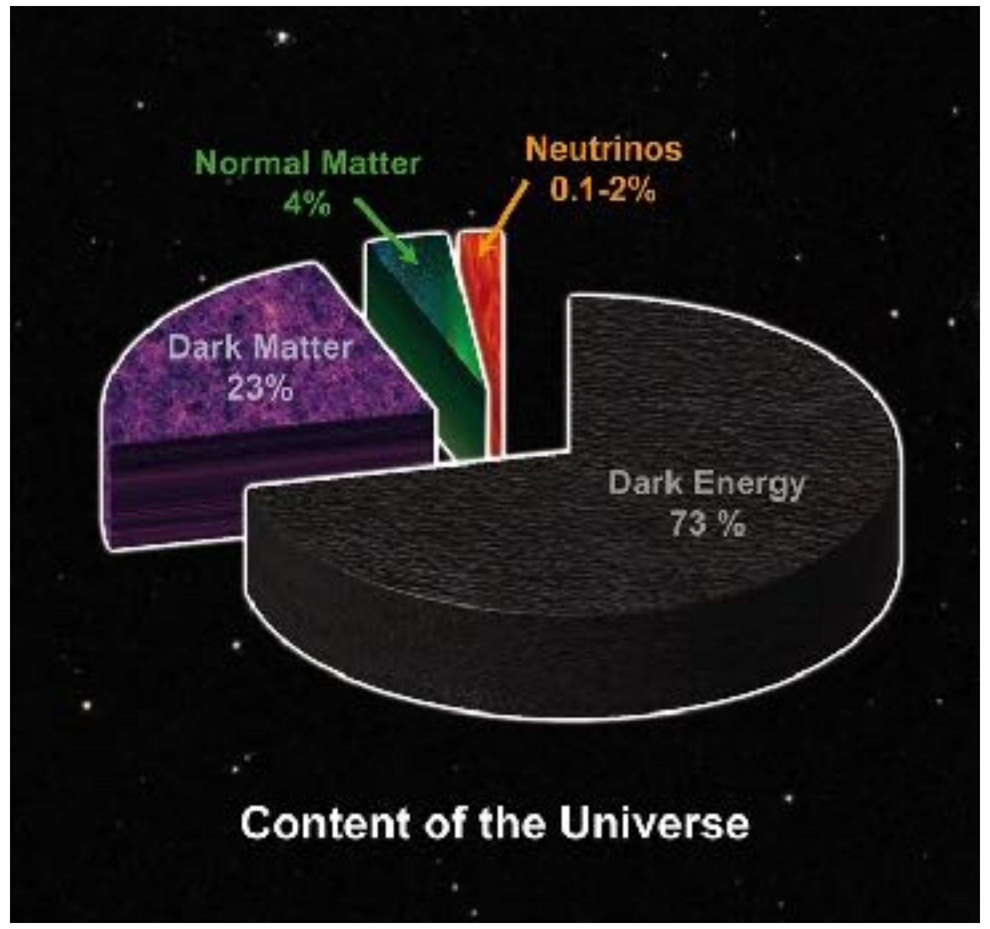
- Fails to explain most of the mass and energy of the universe



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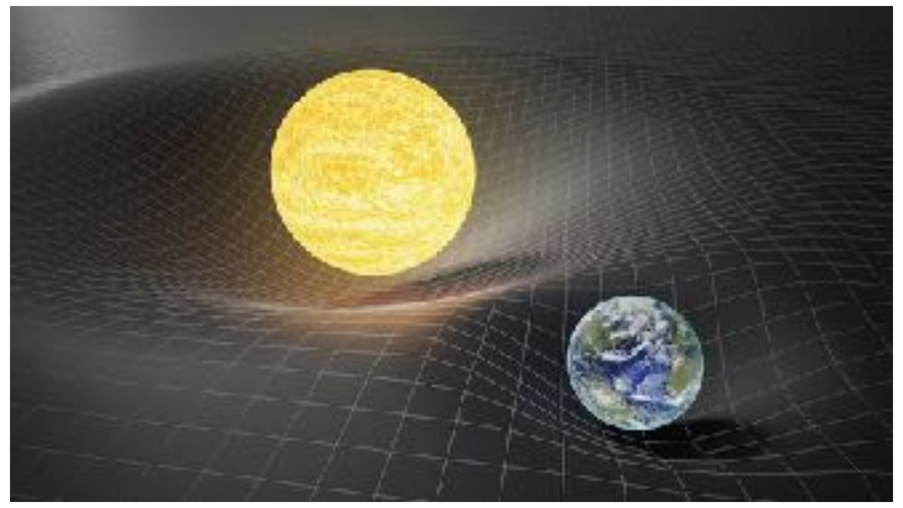

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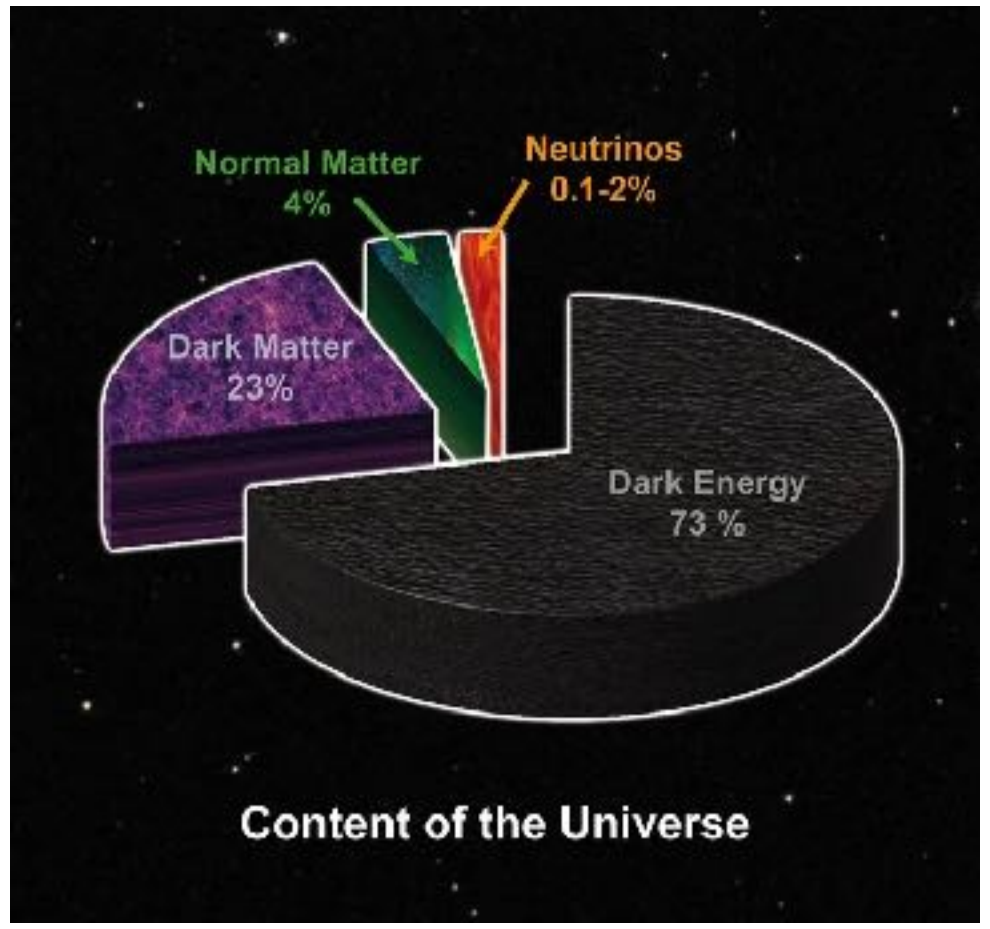

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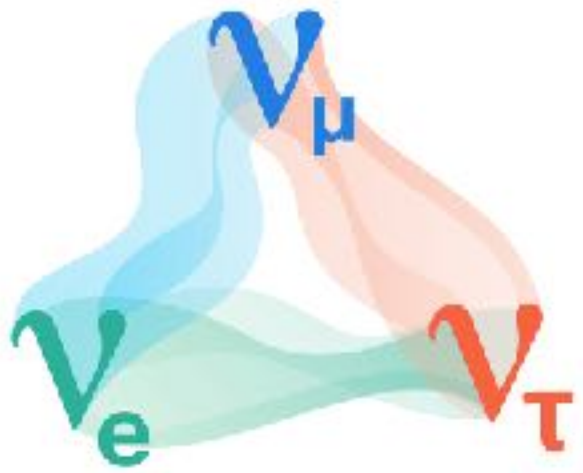

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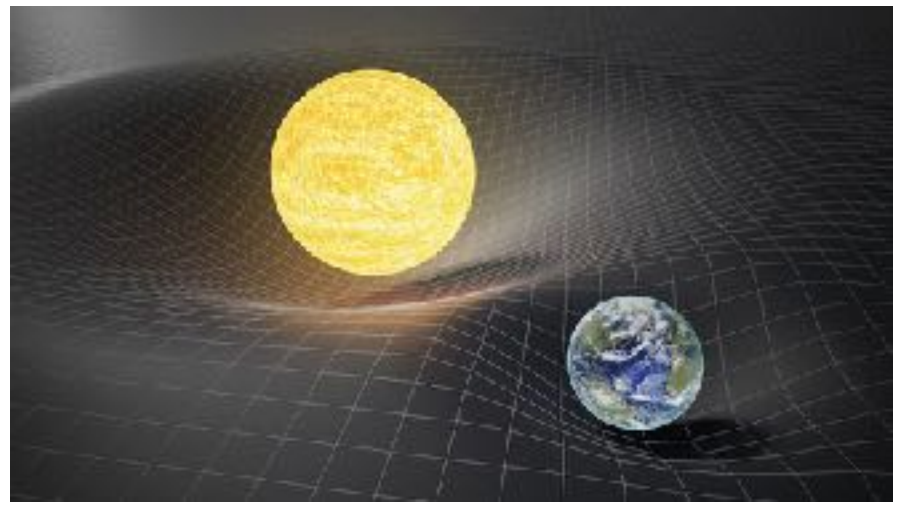

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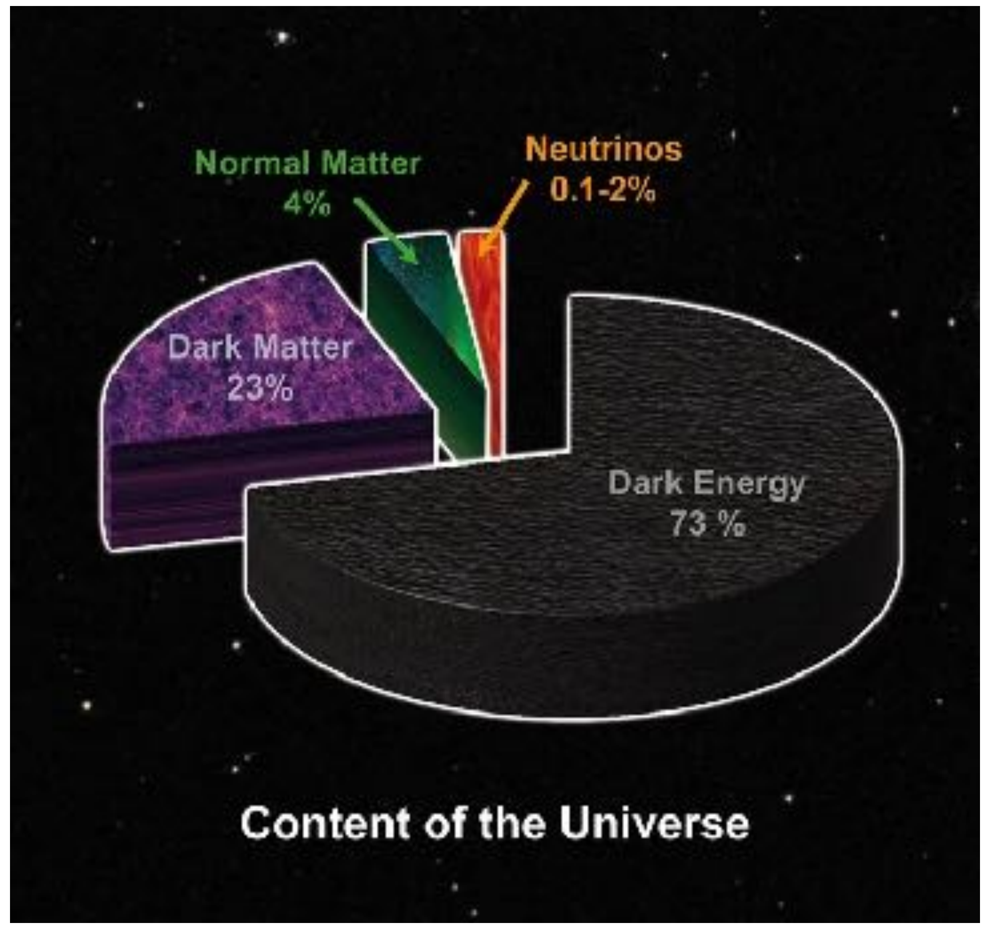

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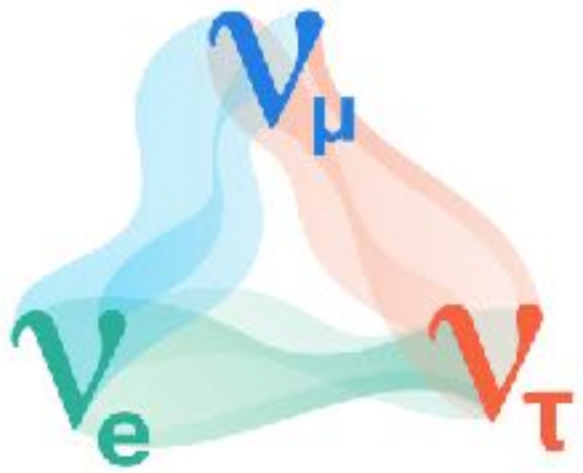

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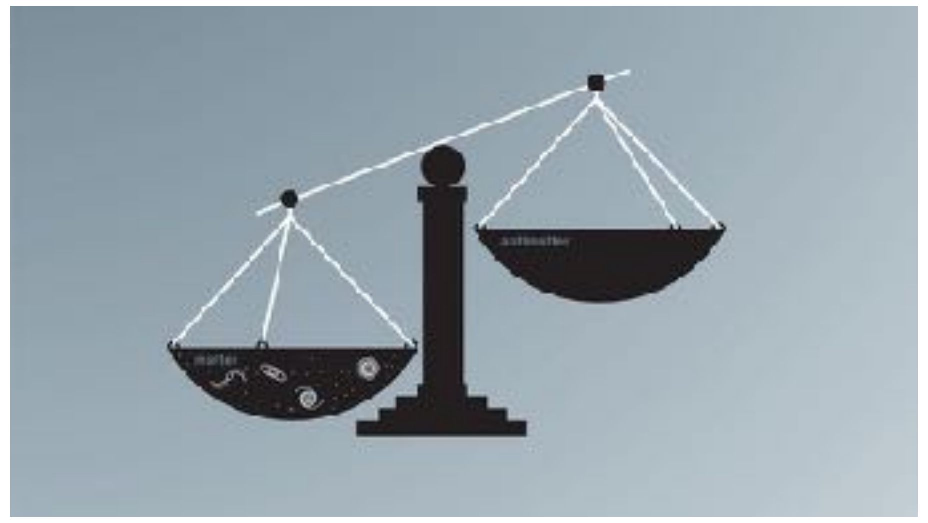

Credit: Symmetry Magazine / Sandbox Studio, Chicago

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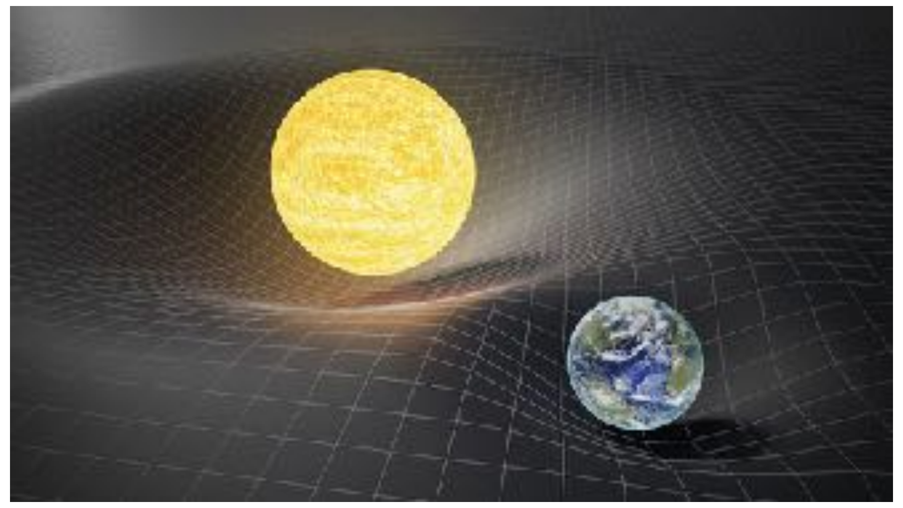

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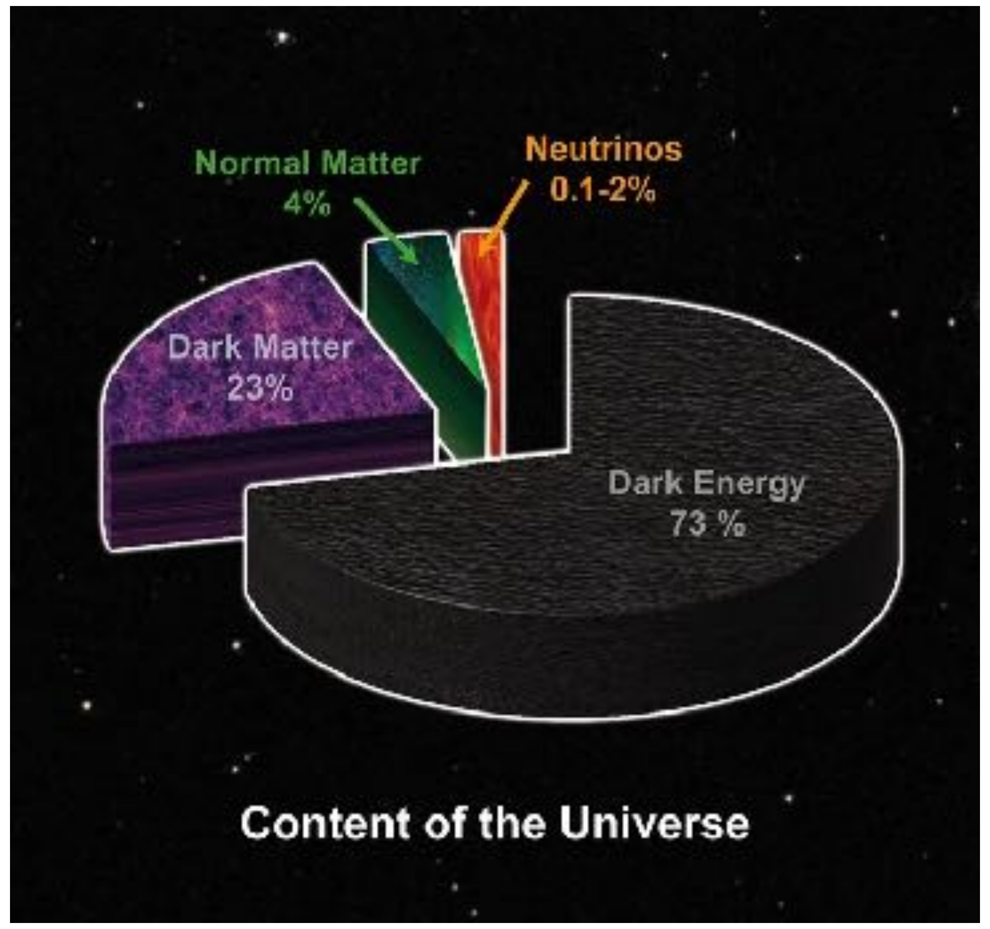

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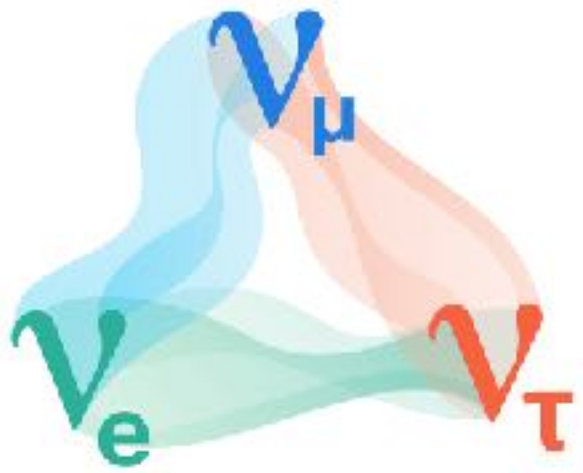

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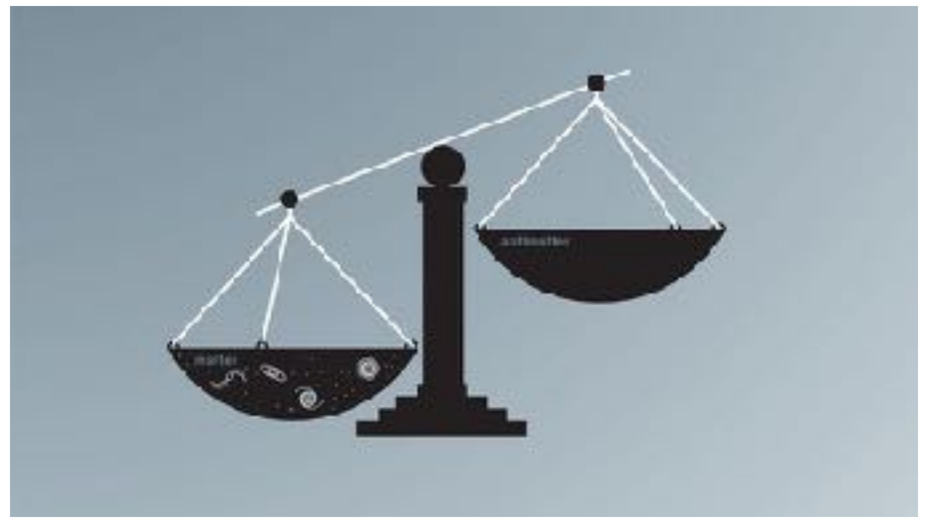

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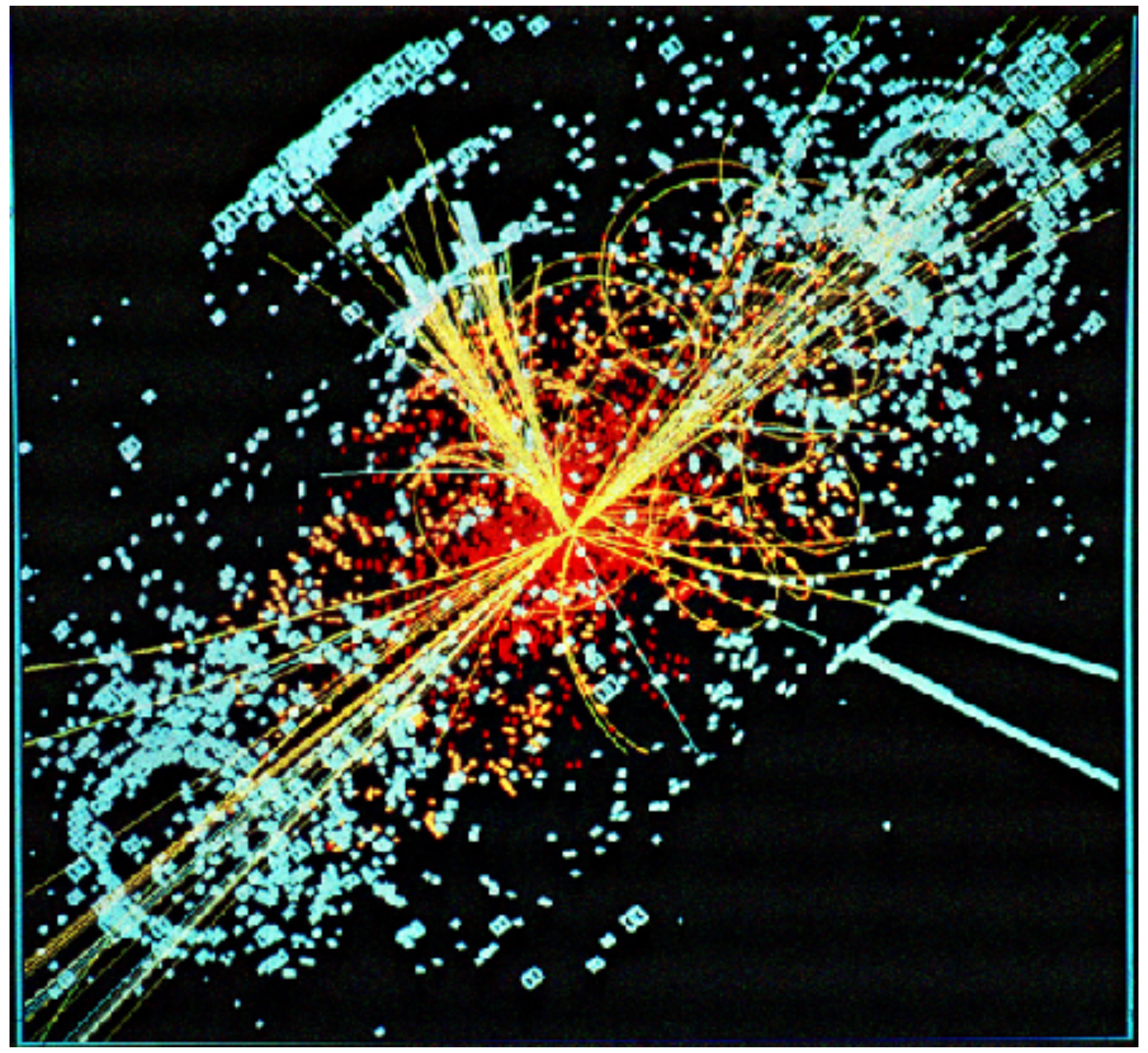
How should we search beyond the Standard Model to explain these shortcomings?

Going Beyond

TeV Scale ⟷ < MeV Scale

1. High energy Frontier



Lucas Taylor / CERN - http://cdsweb.cern.ch/record/628469

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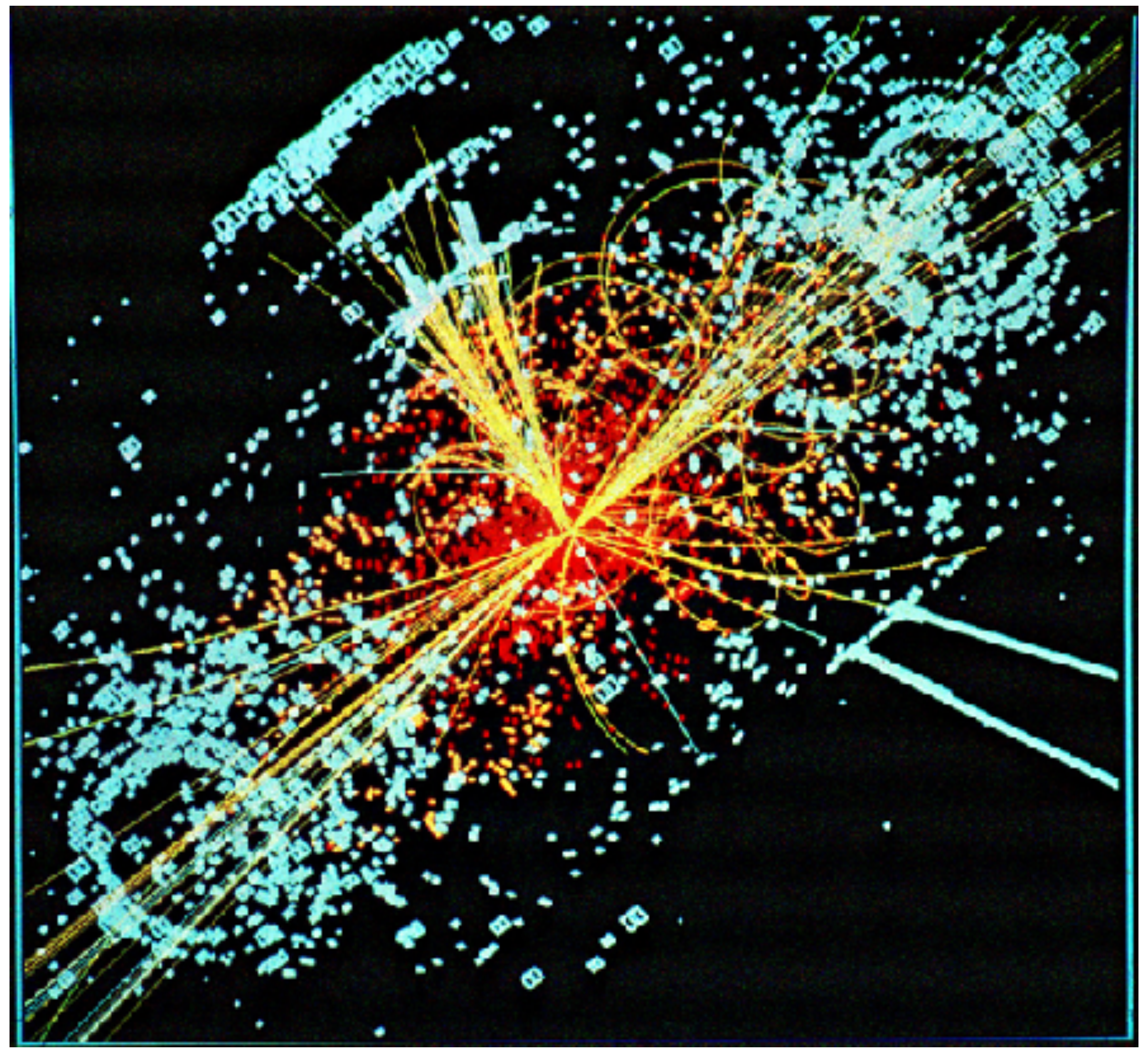

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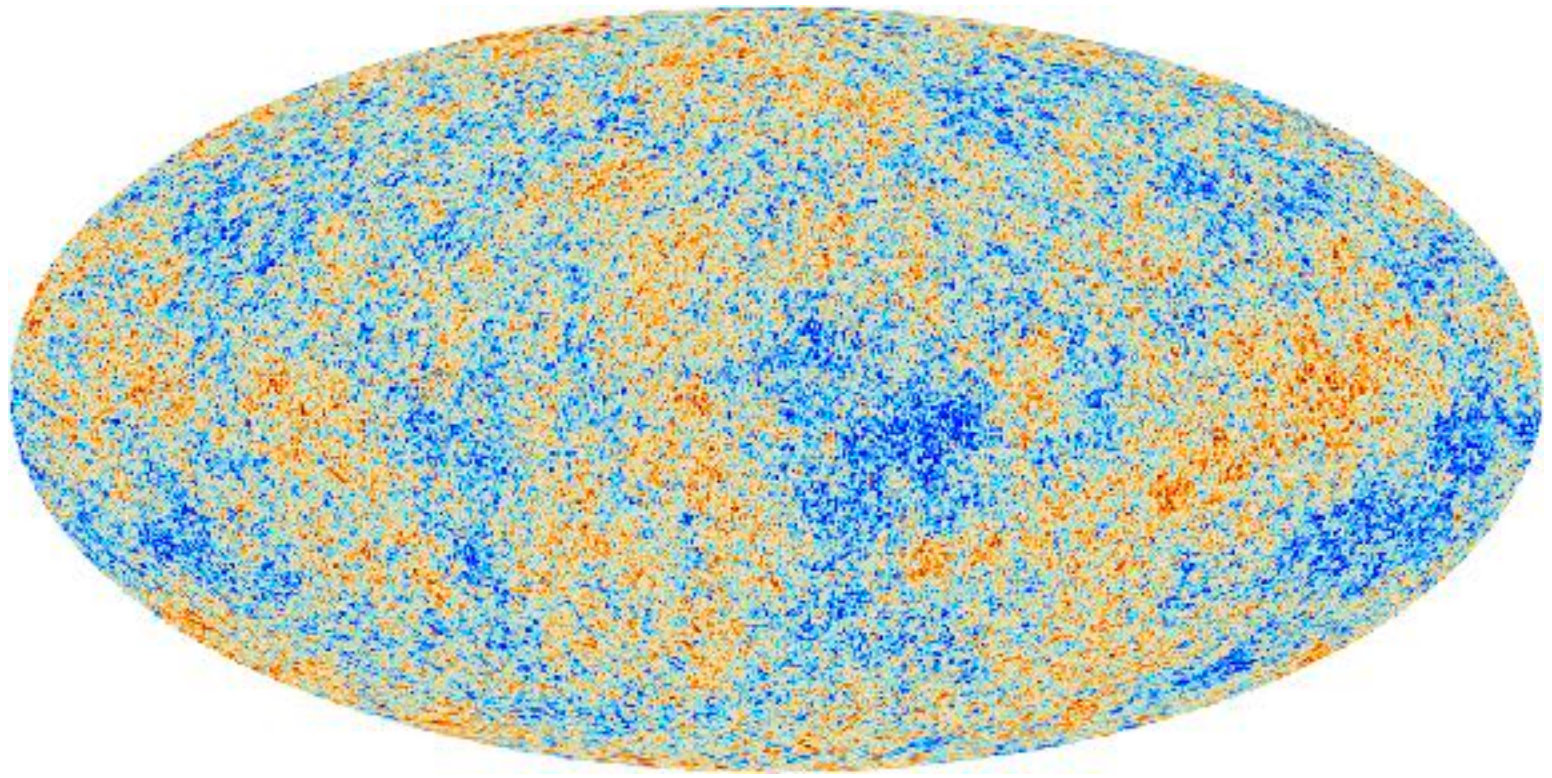
2. Cosmo+Astro Frontier



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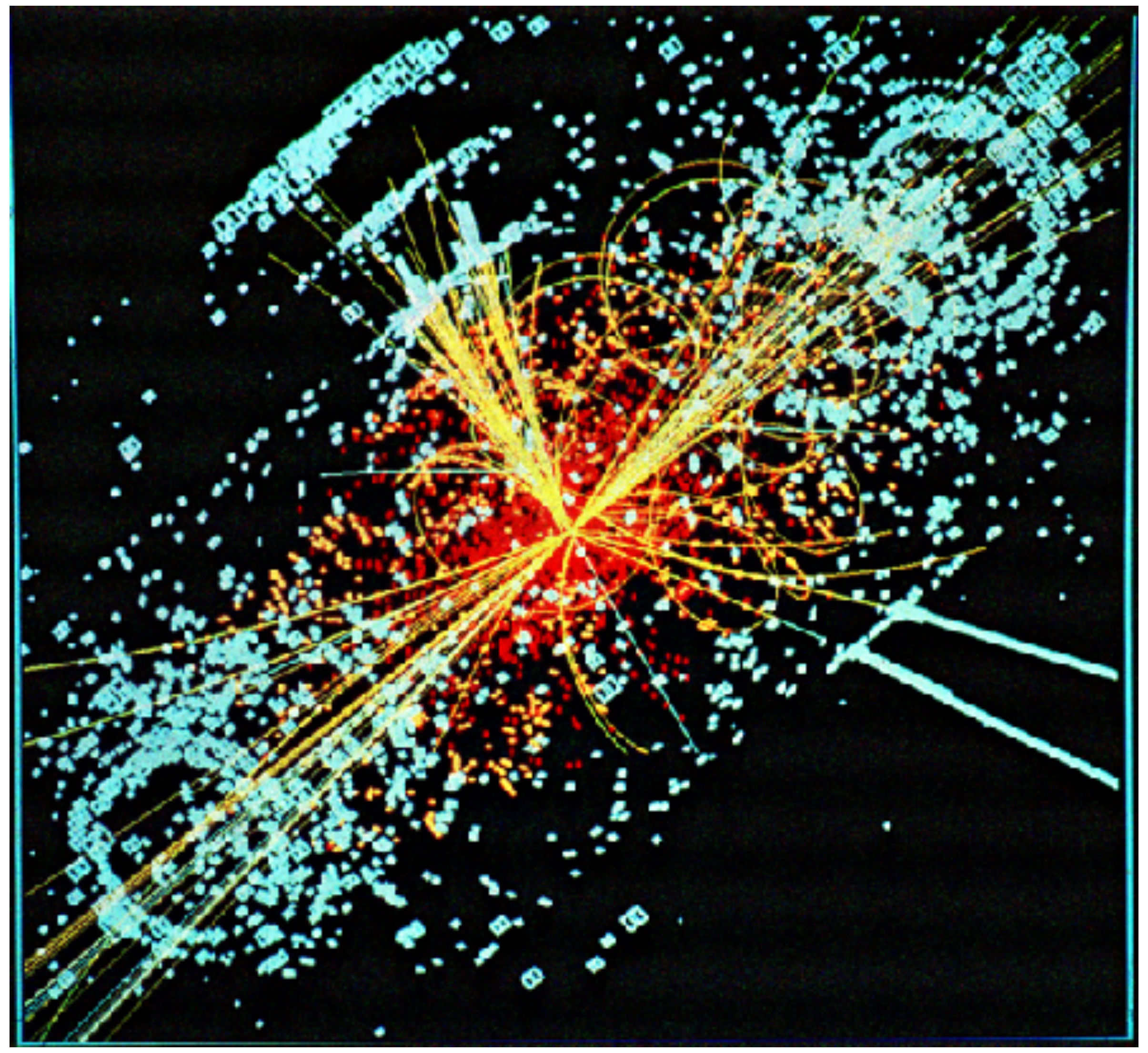

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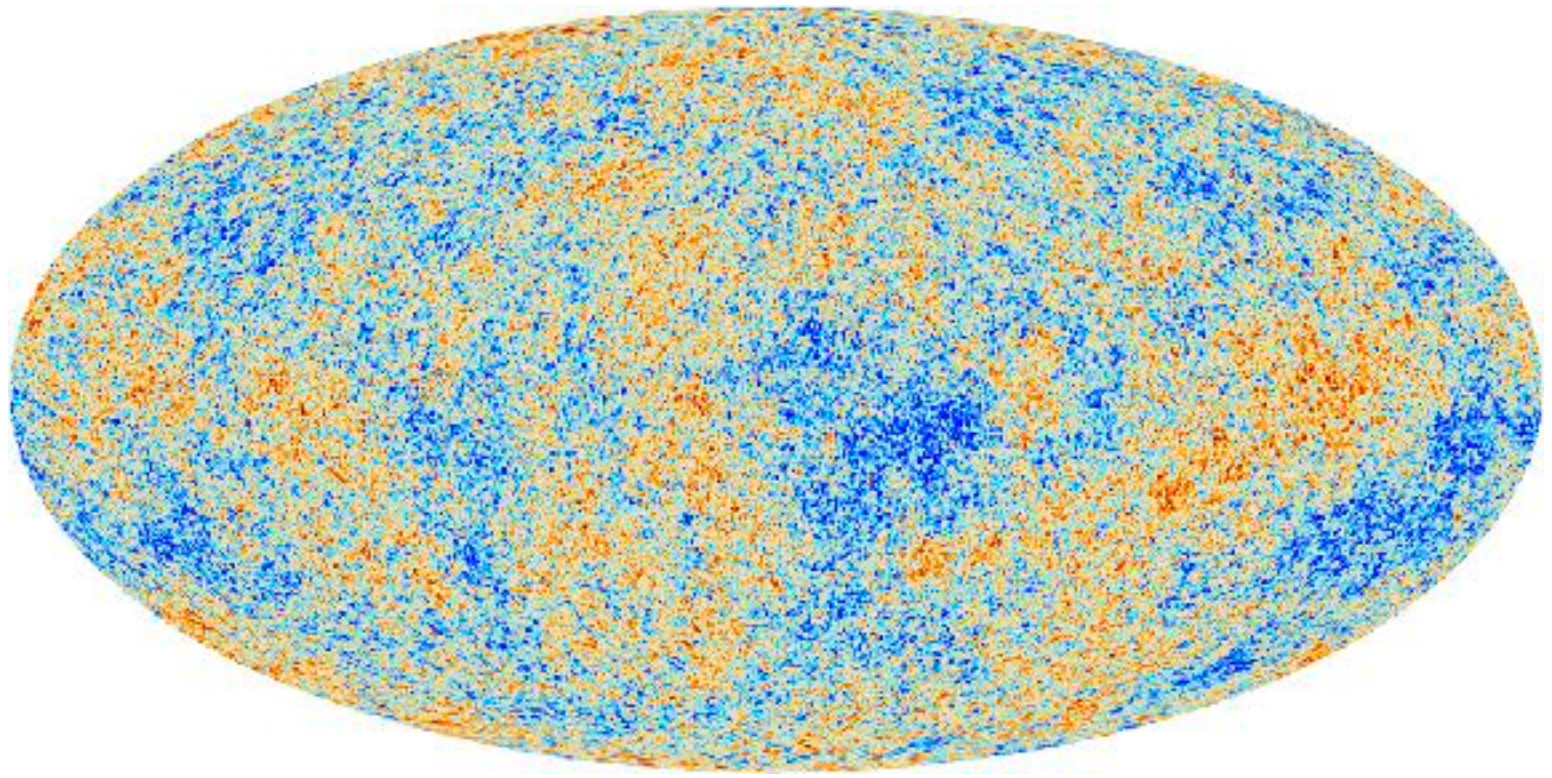
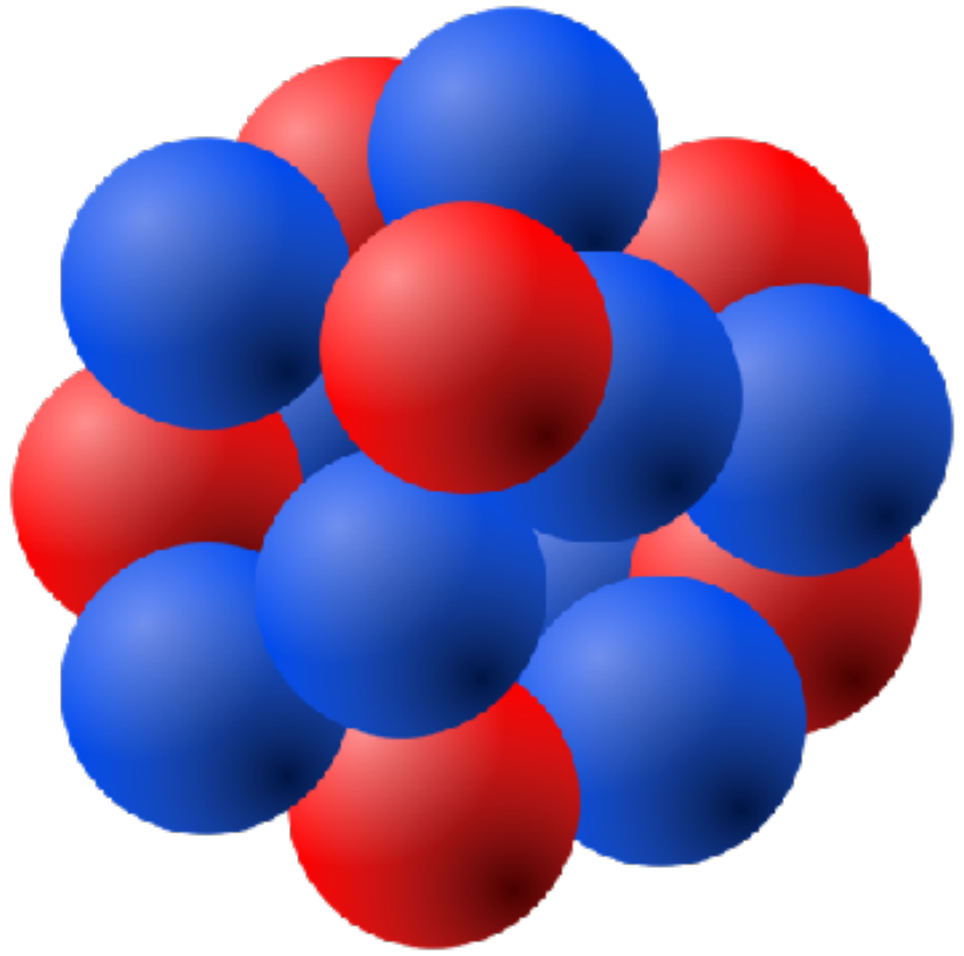


3. Precision frontier



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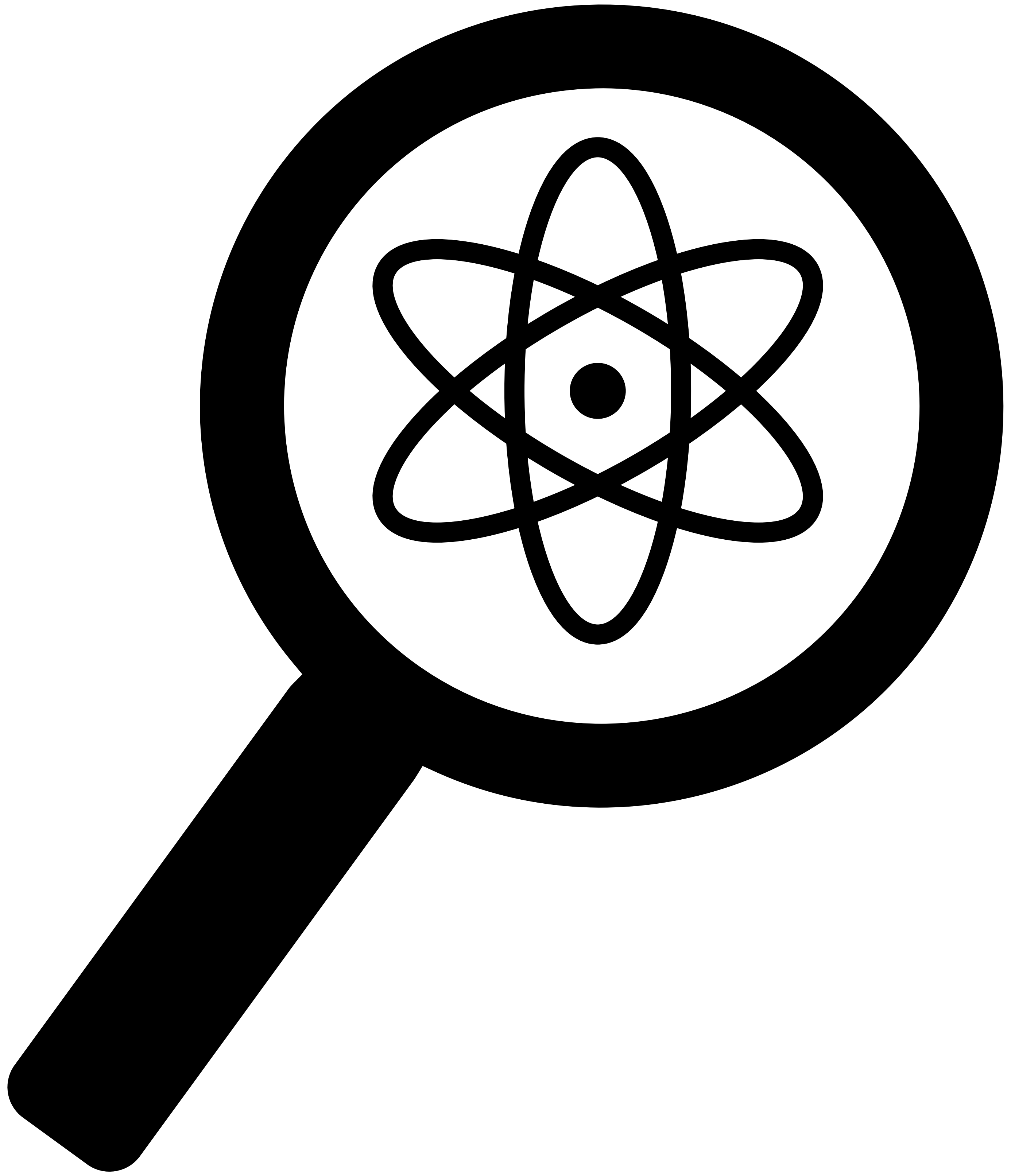
Atomic Nucleus as a Probe



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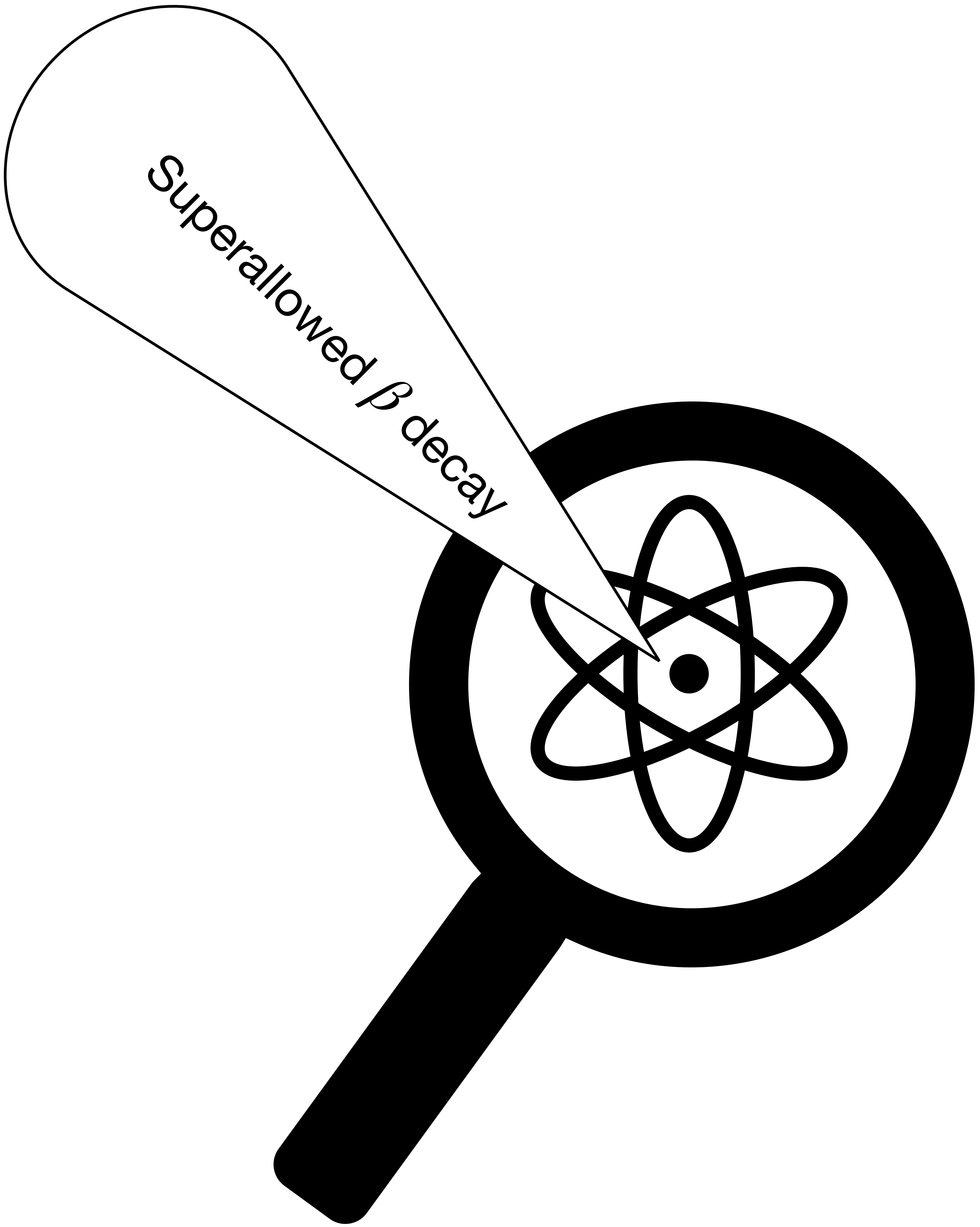

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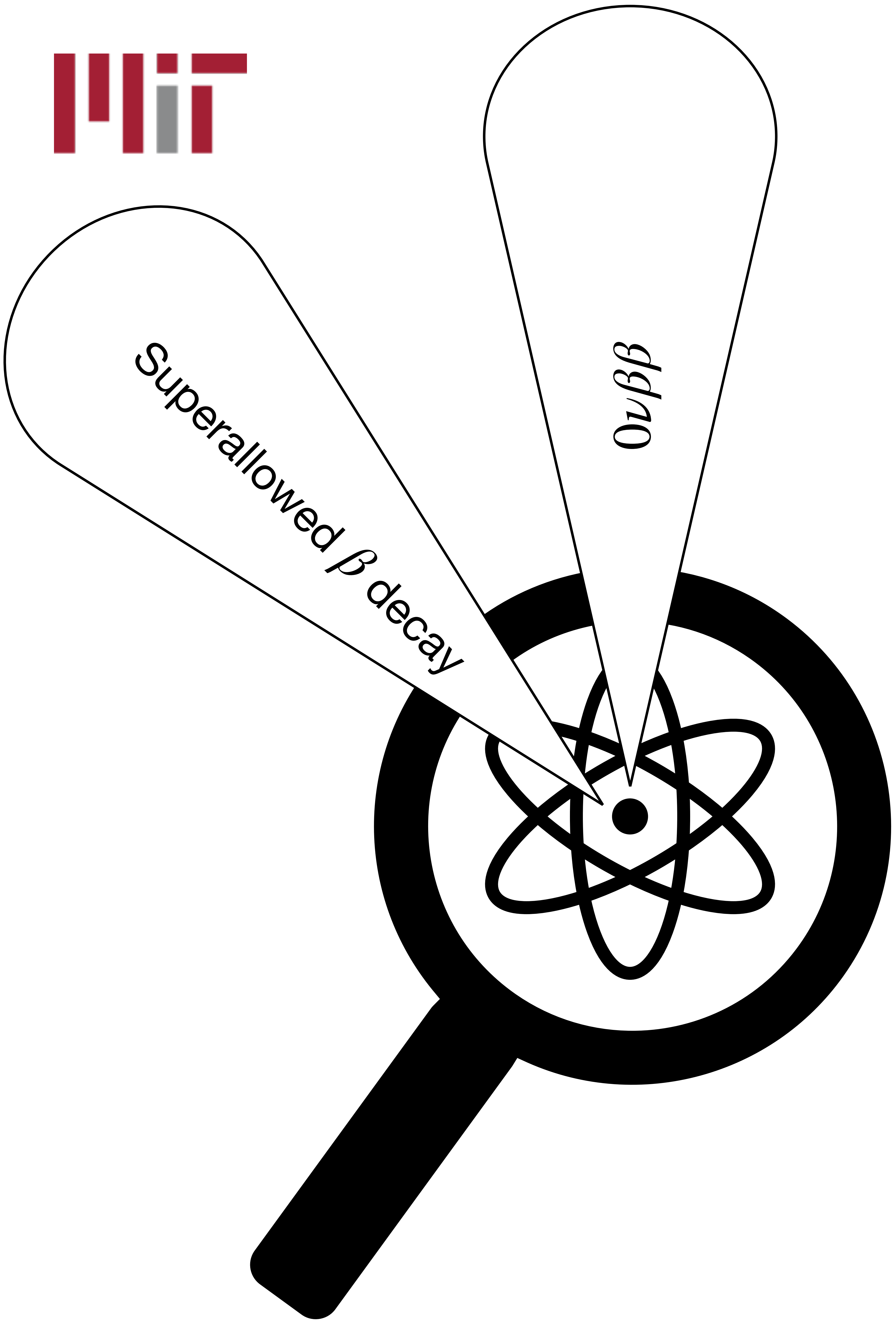

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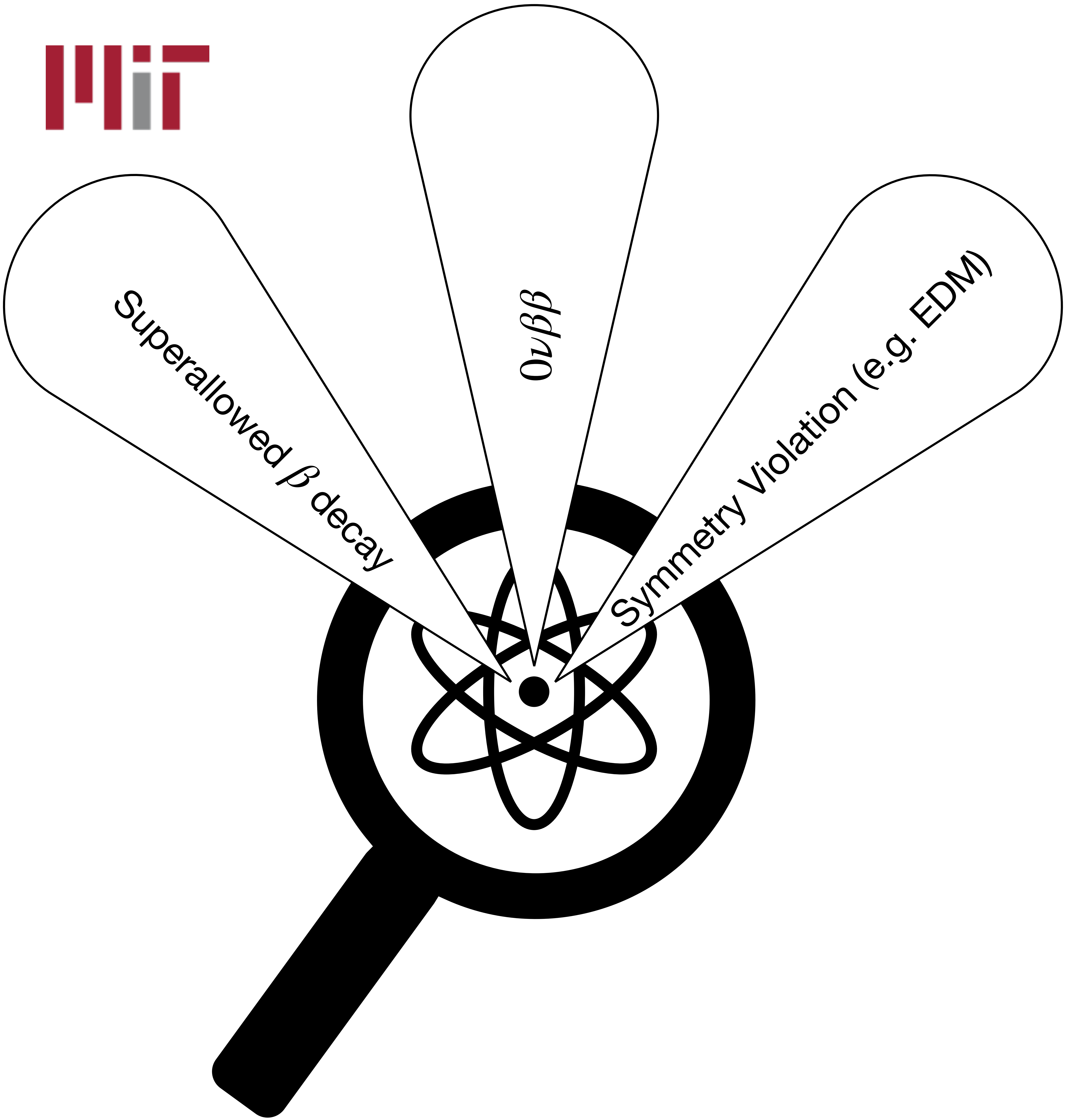

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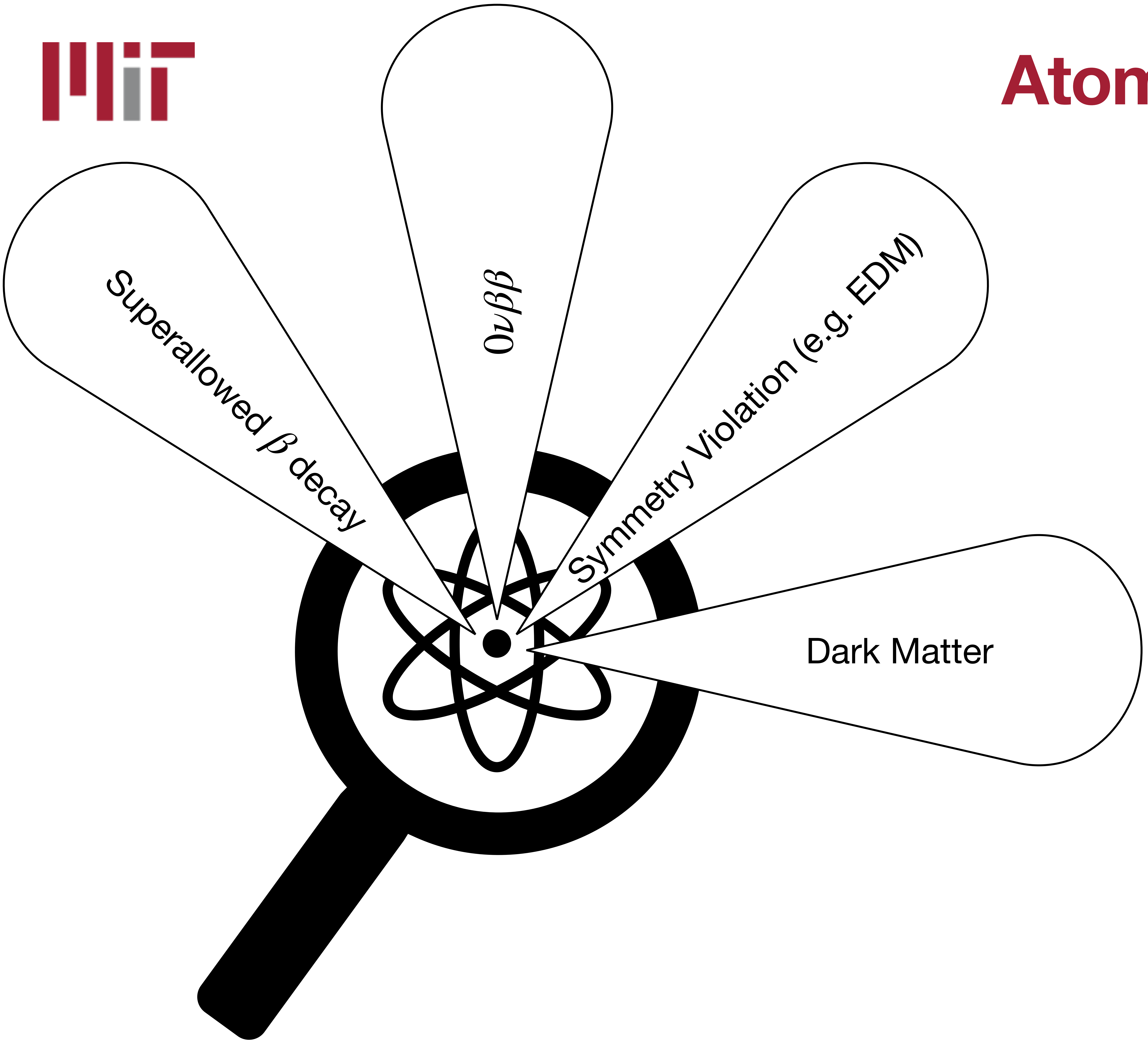

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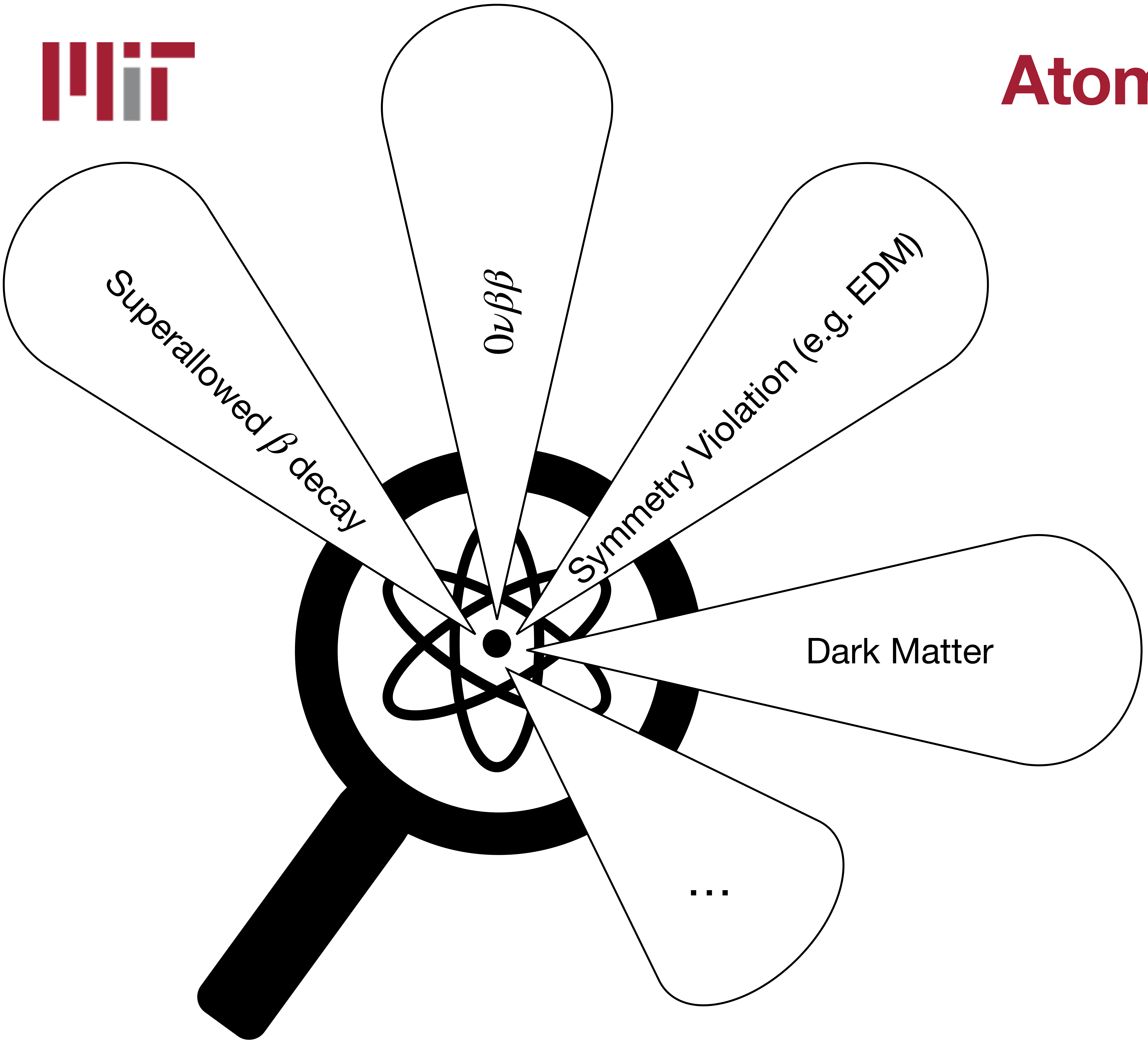

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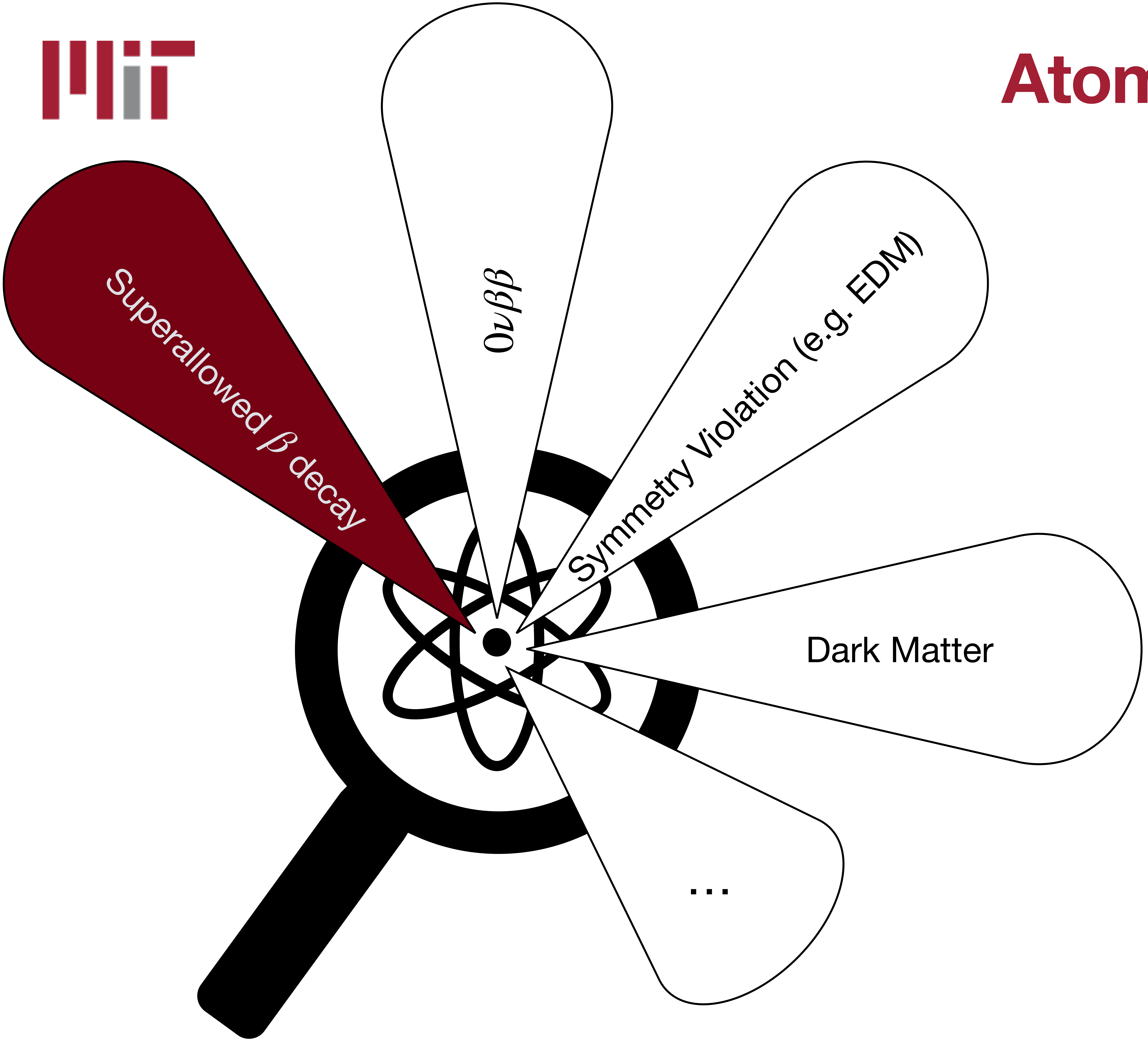

1. Looking at deviation from Standard Model prediction.

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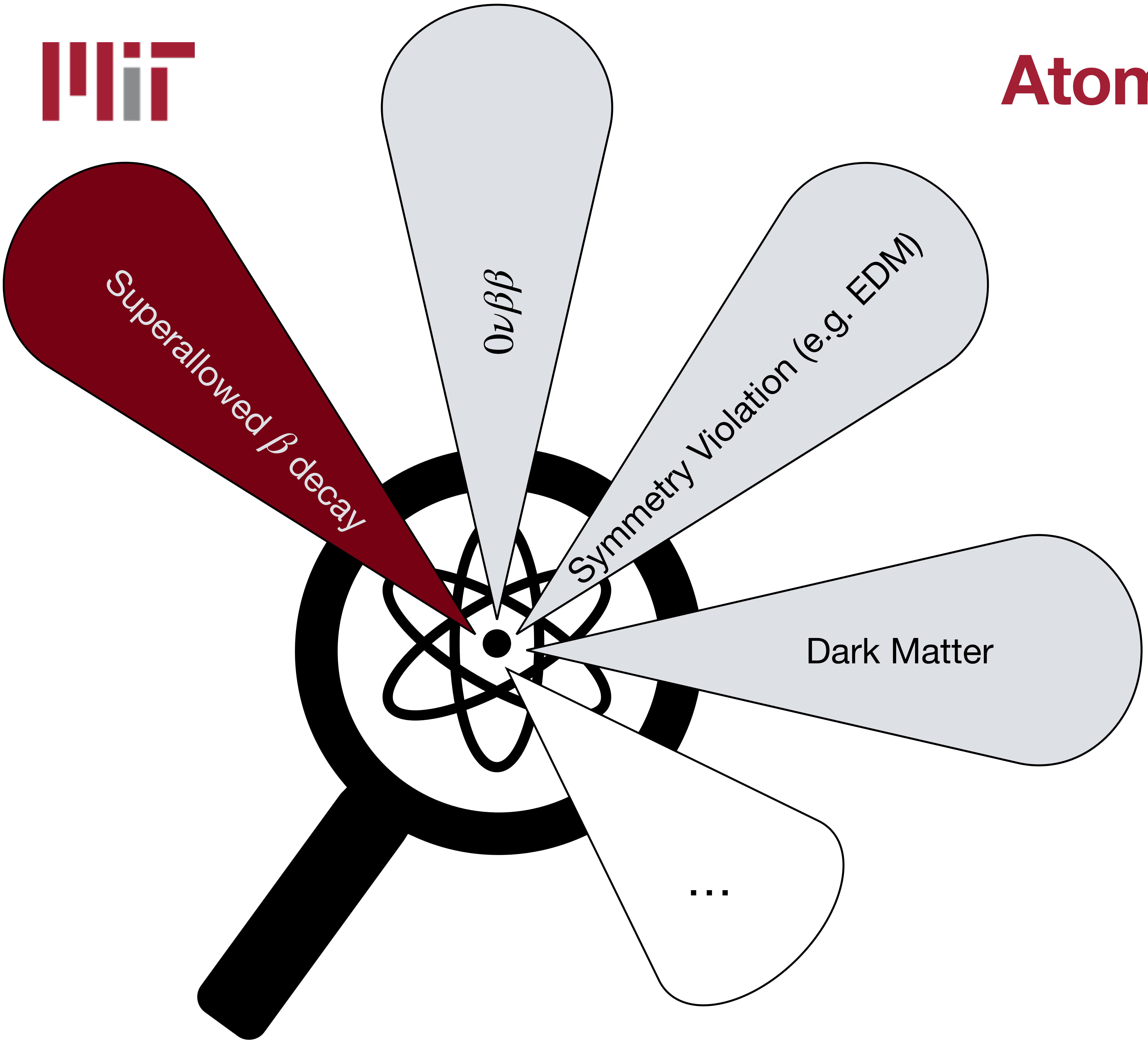

1. Looking at deviation from Standard Model prediction.

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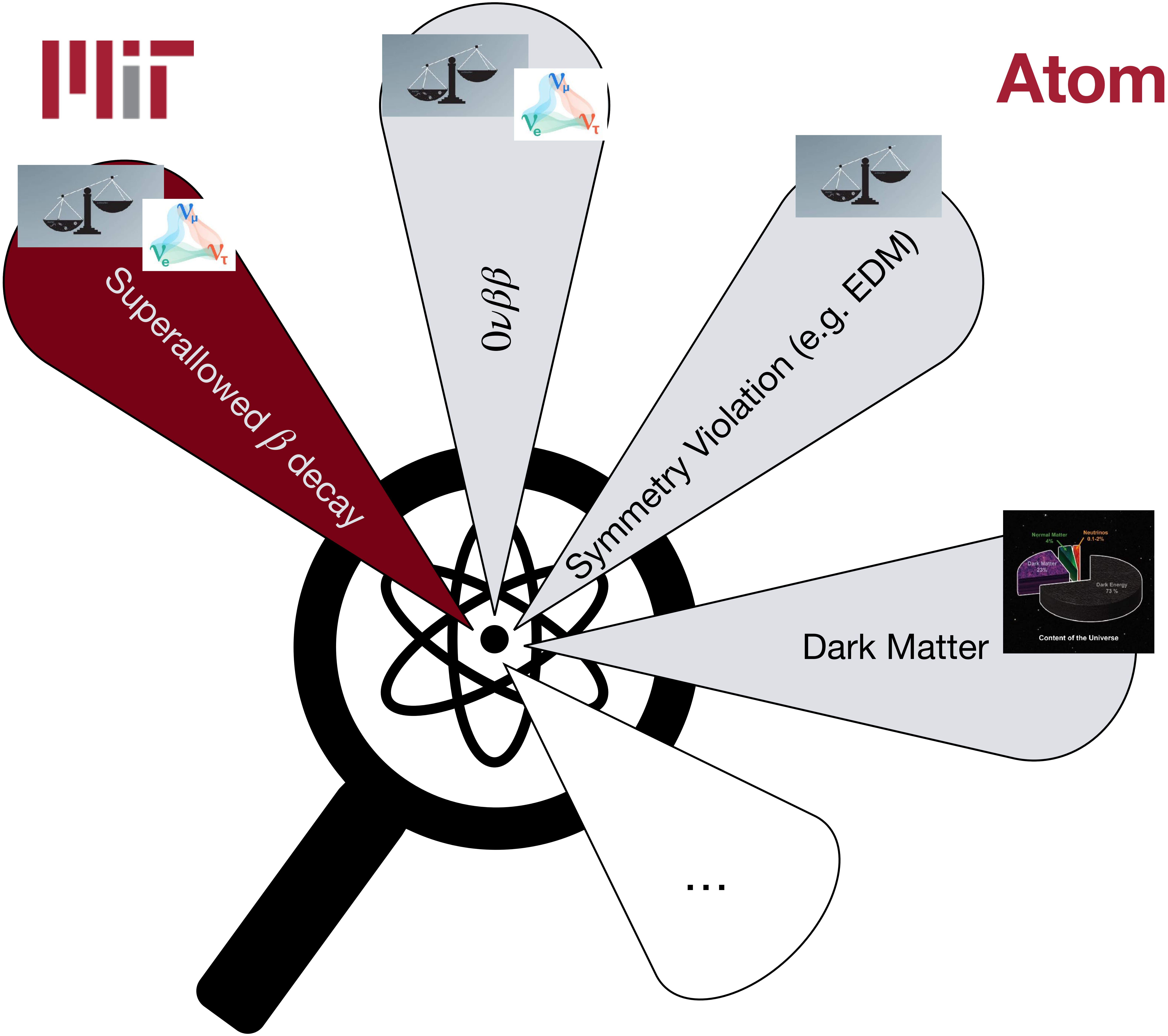

1. Looking at deviation from Standard Model prediction.
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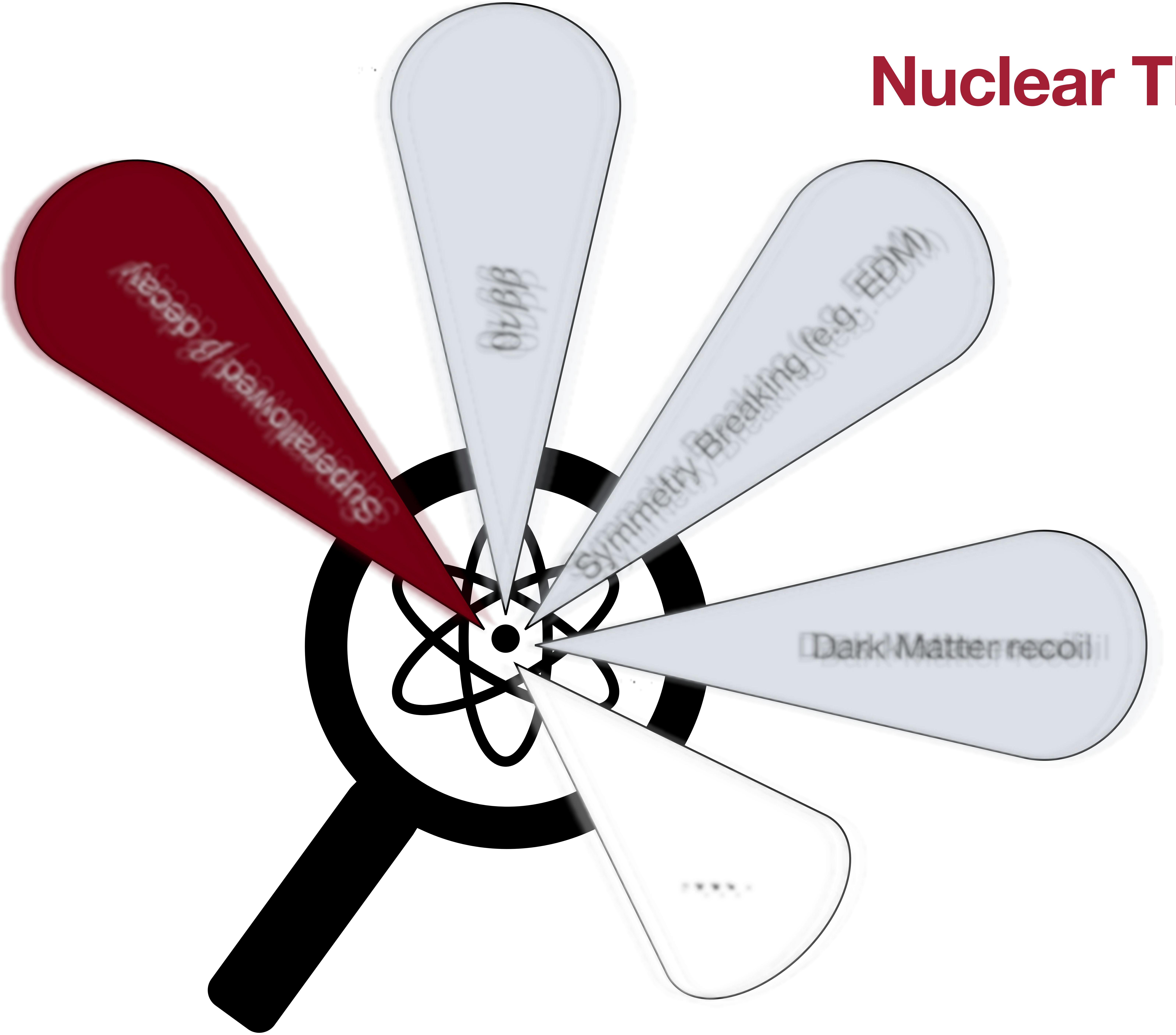
The Need for Nuclear Theory

In all cases, nuclear theory inputs are required in order to interpret experimental results:

- **Superallowed β decay:** Corrections from Standard Model δ_{NS} and δ_C.
- $\boldsymbol{0\nu\beta\beta}$**:** Nuclear matrix elements $M^{0\nu}$.
- **Electric Dipole Moment:** The nuclear Schiff Moment.
- **Dark Matter Scattering:** WIMP Scattering structure factor S_A.
- …

Nuclear Theory Blur



Nuclear Theory Challenges

Understanding nuclear structure from microscopic physics

Figures courtesy of J. Muñoz

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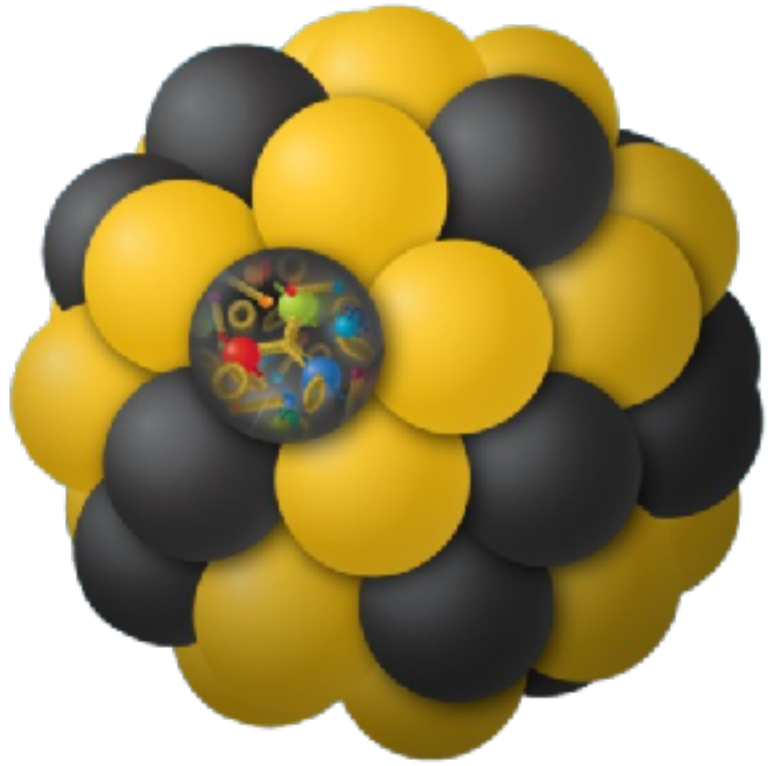
Nuclear Interactions



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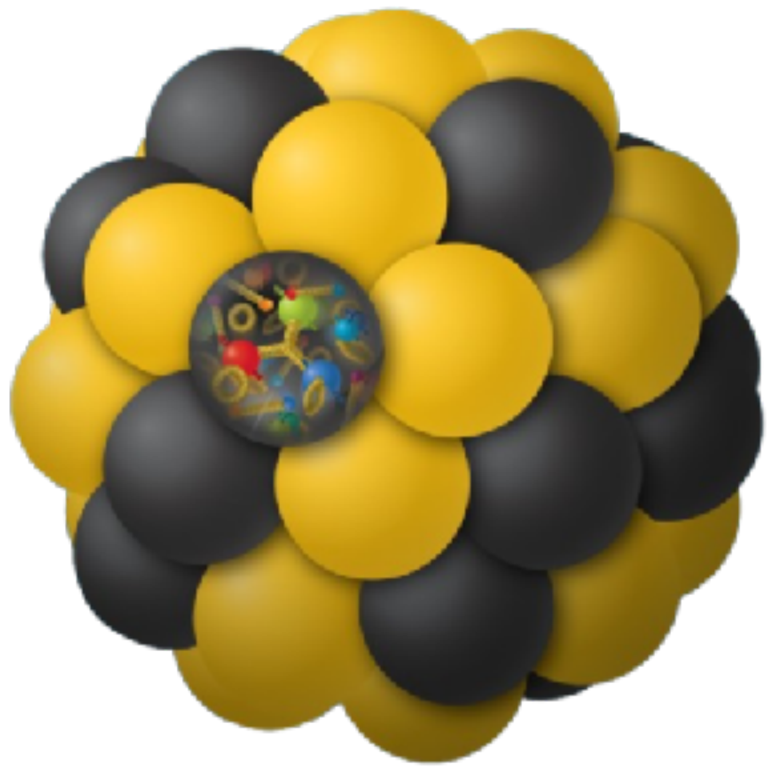

Nucleon-Nucleon force
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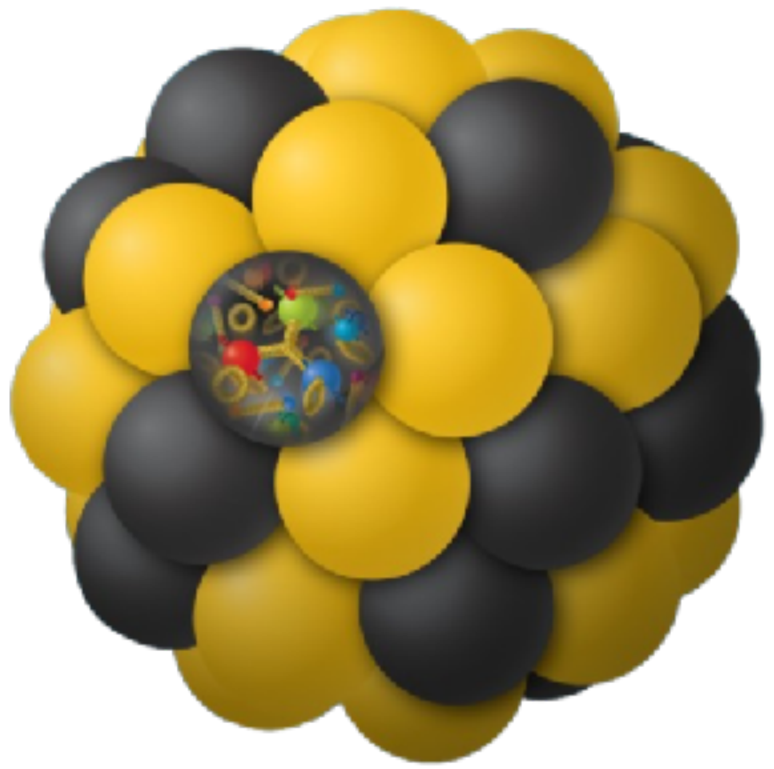

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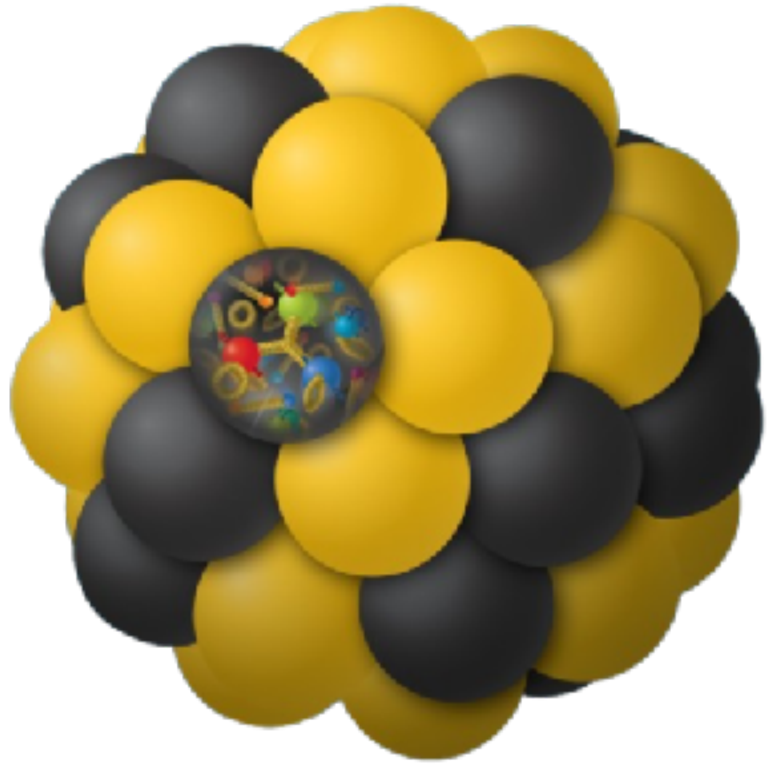
Wave functions



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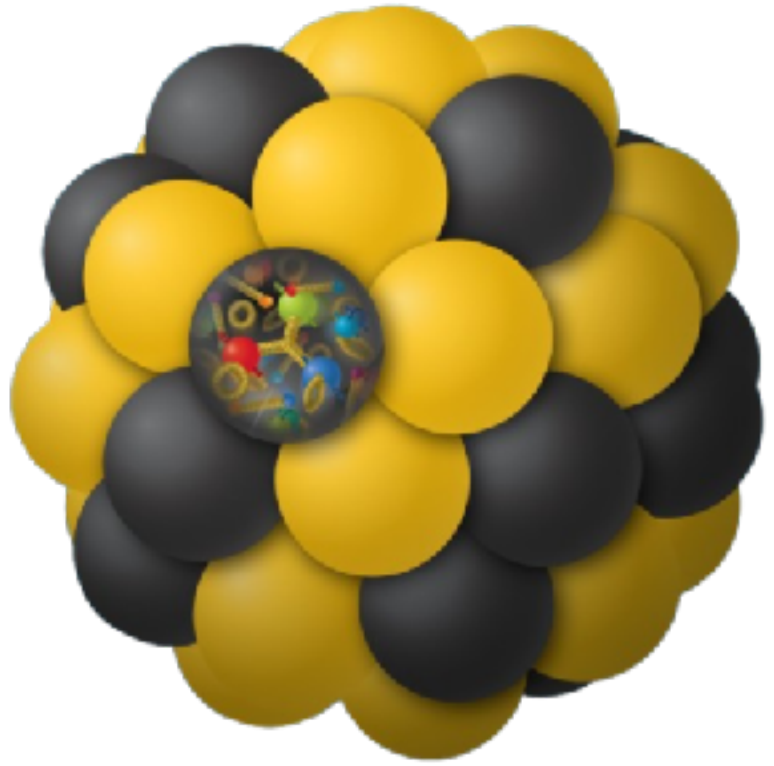

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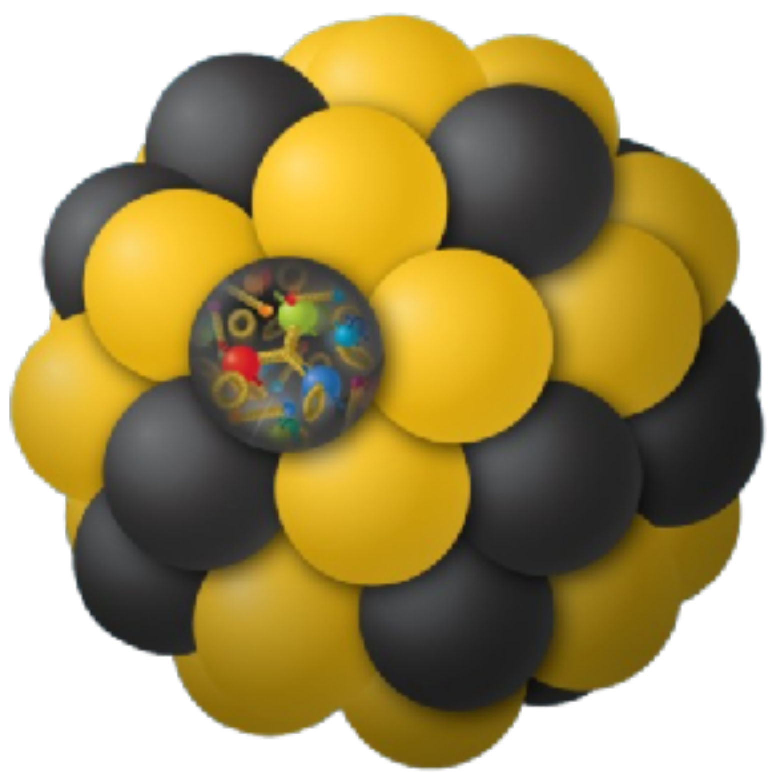

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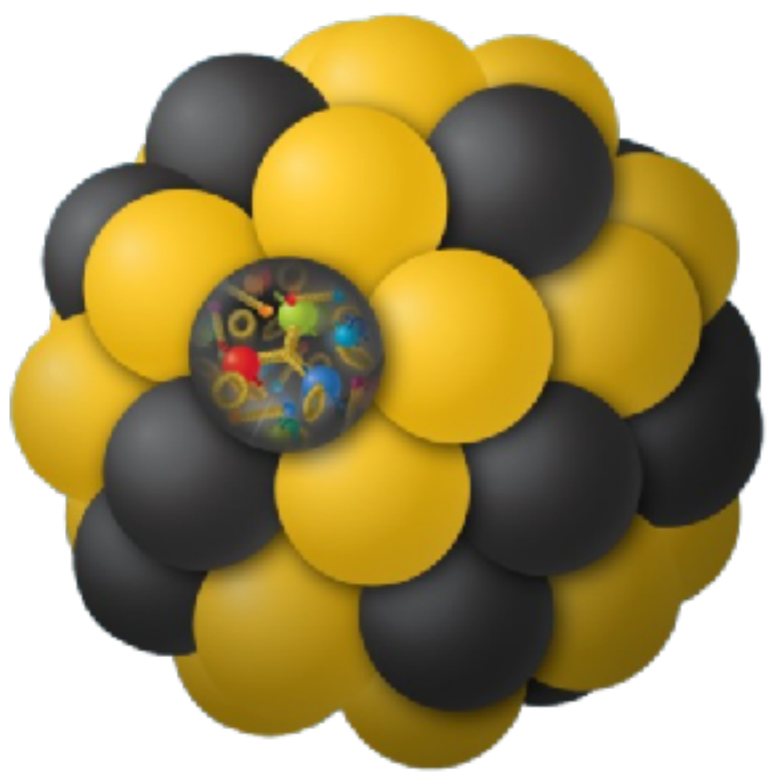
Nuclear Interactions	Wave functions	Observables



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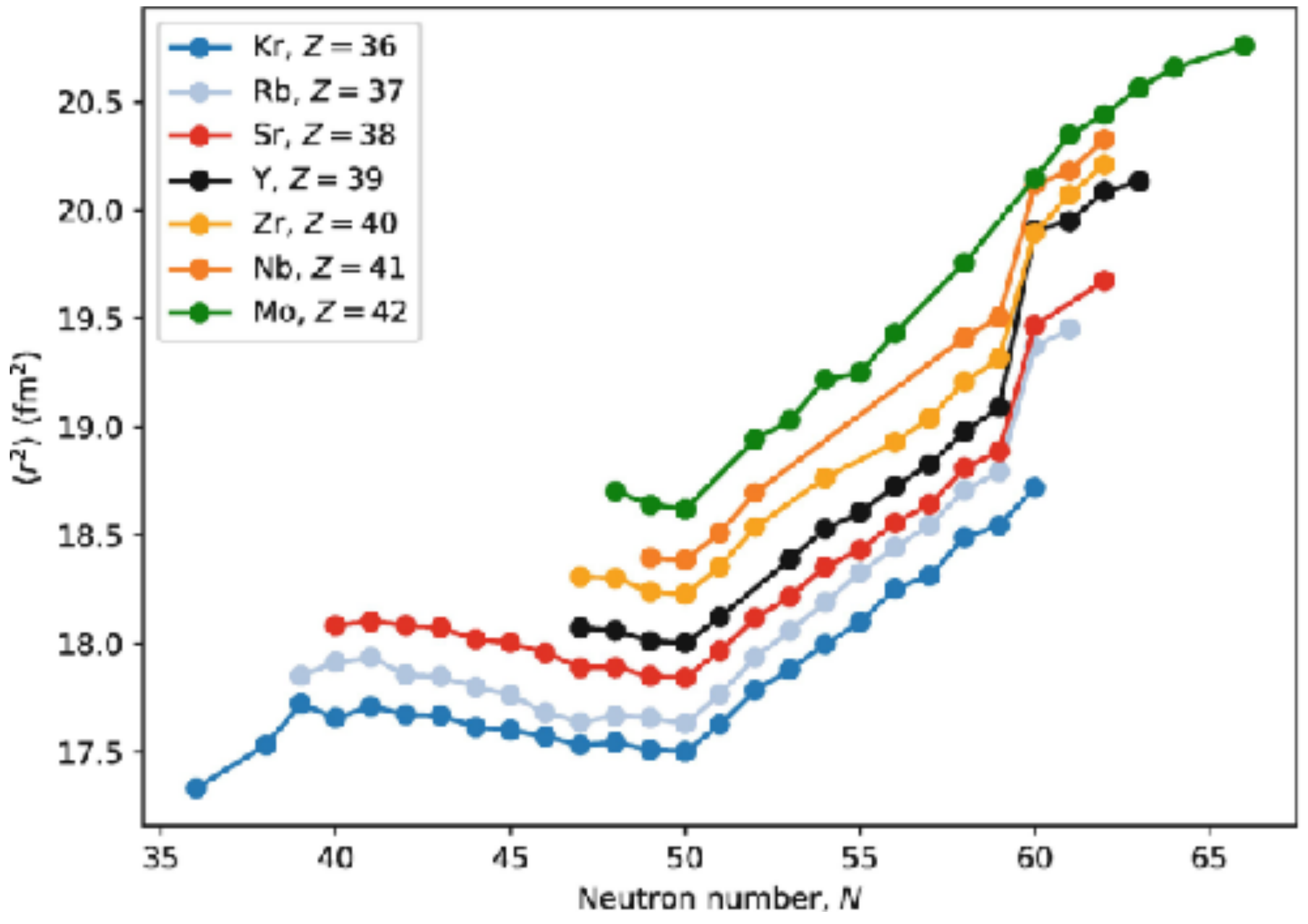

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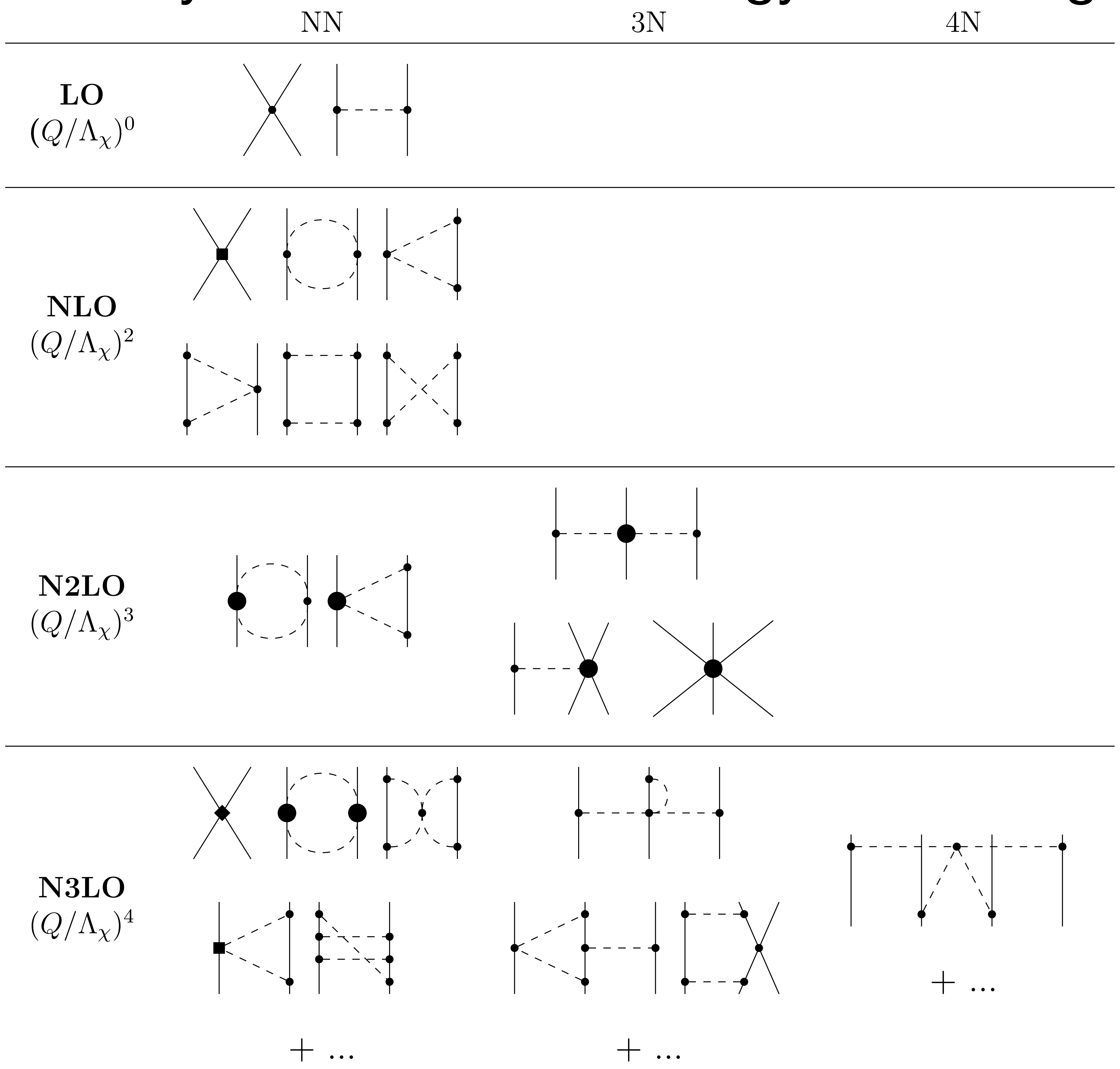
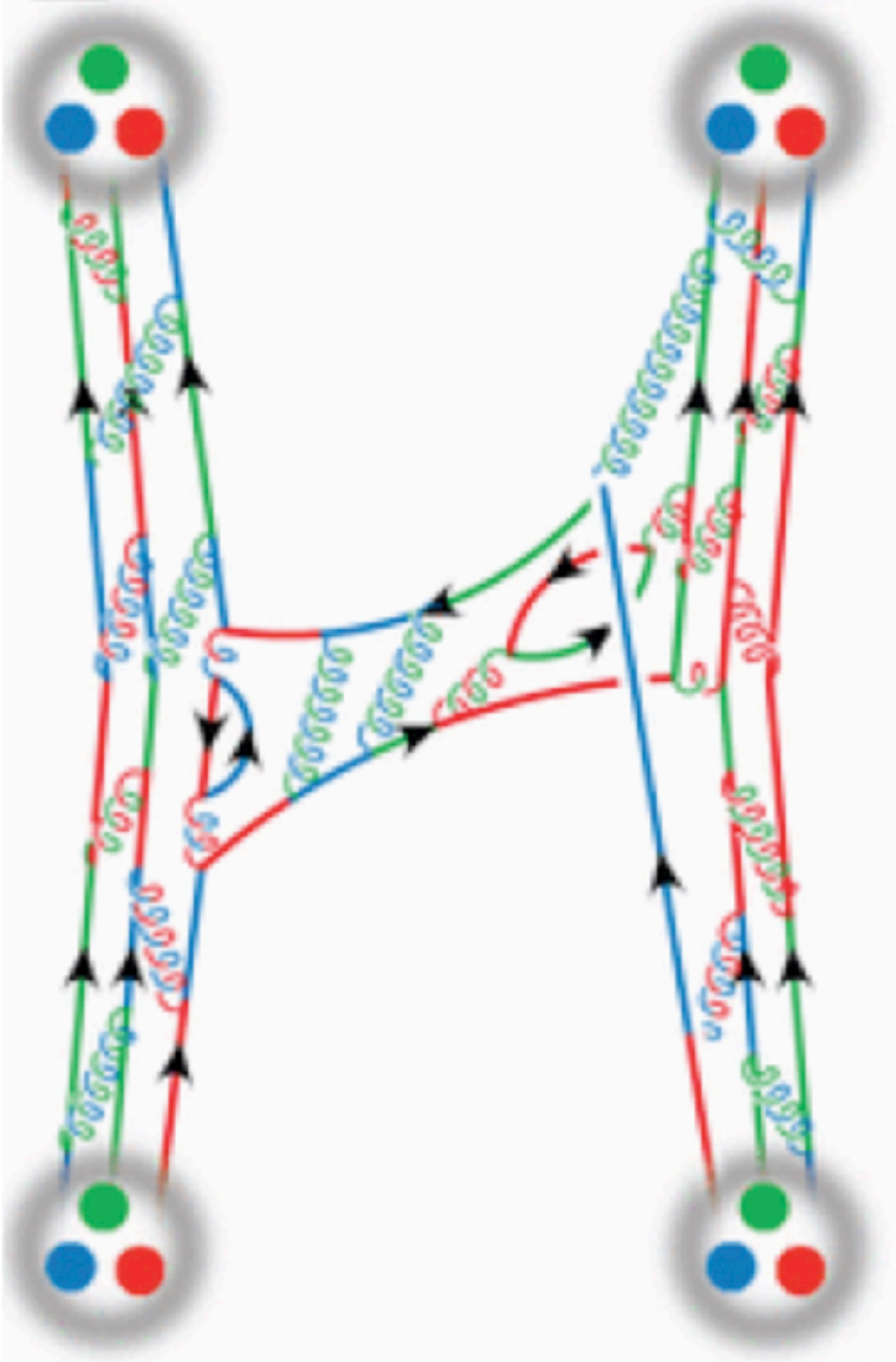
χ-EFT

Expansion order by order of the nuclear forces

Reproduces symmetries of low-energy QCD using nucleons as fields and pions as force carriers.





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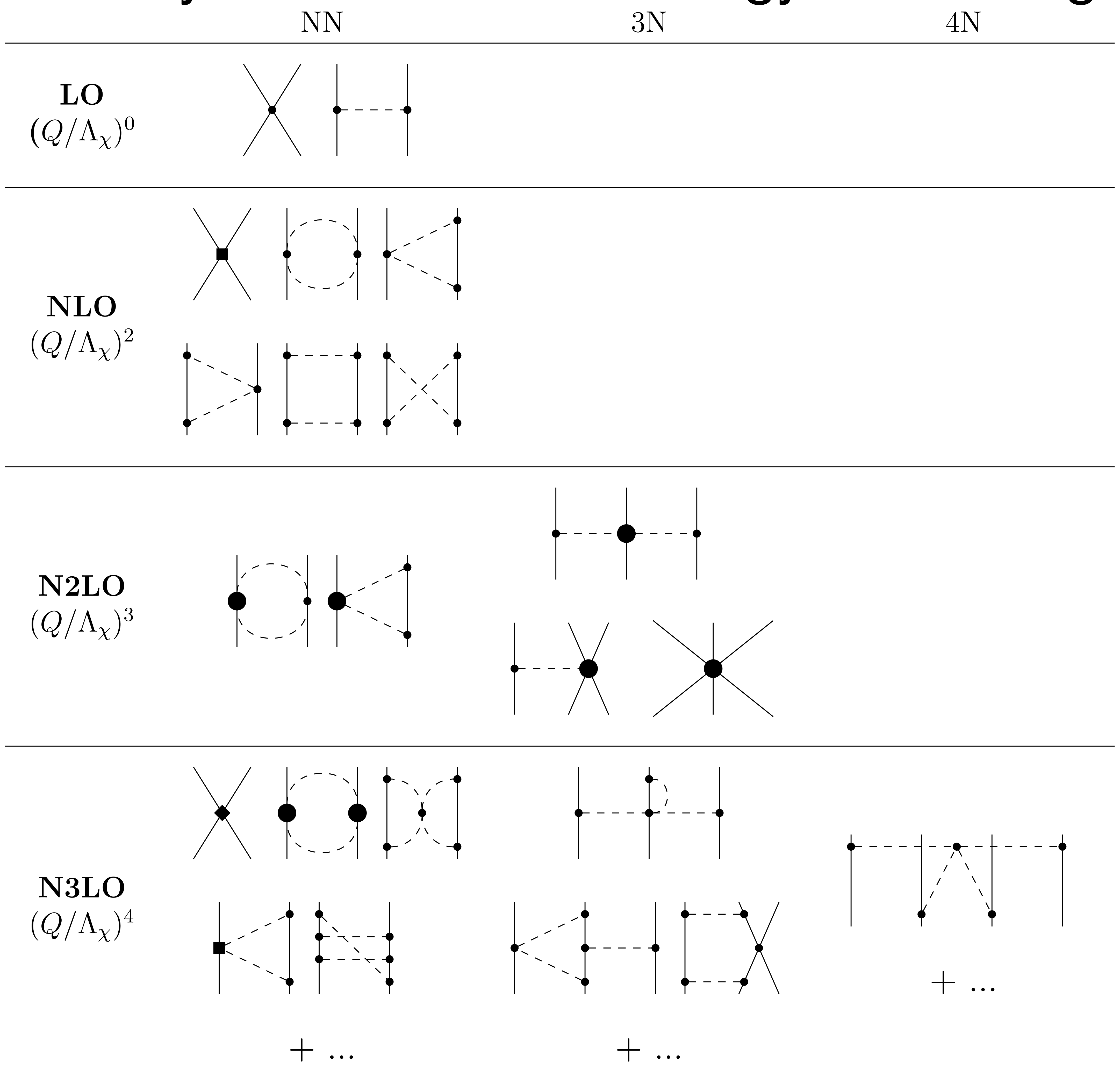

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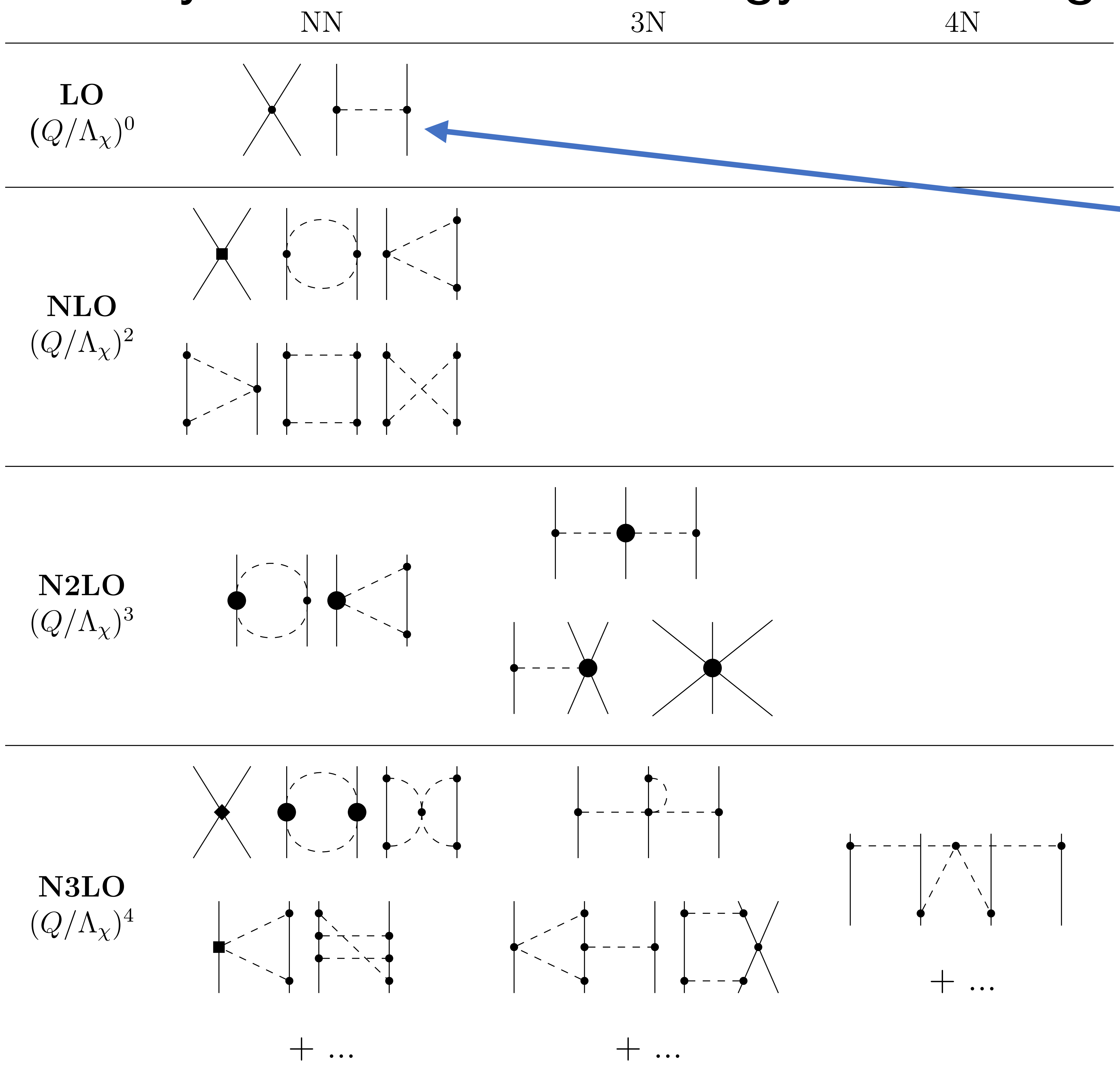

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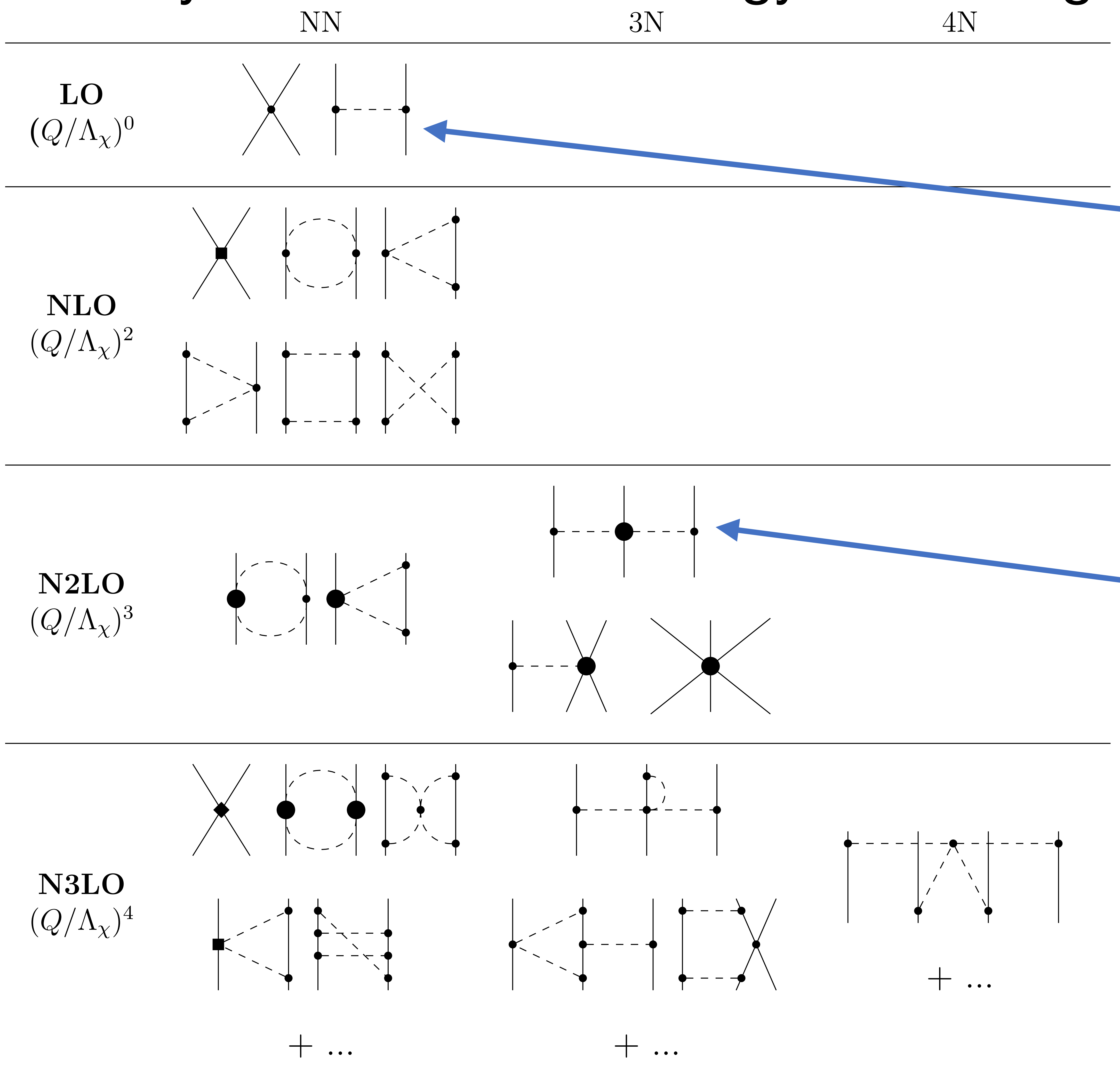

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Three- (and higher-)body forces needed

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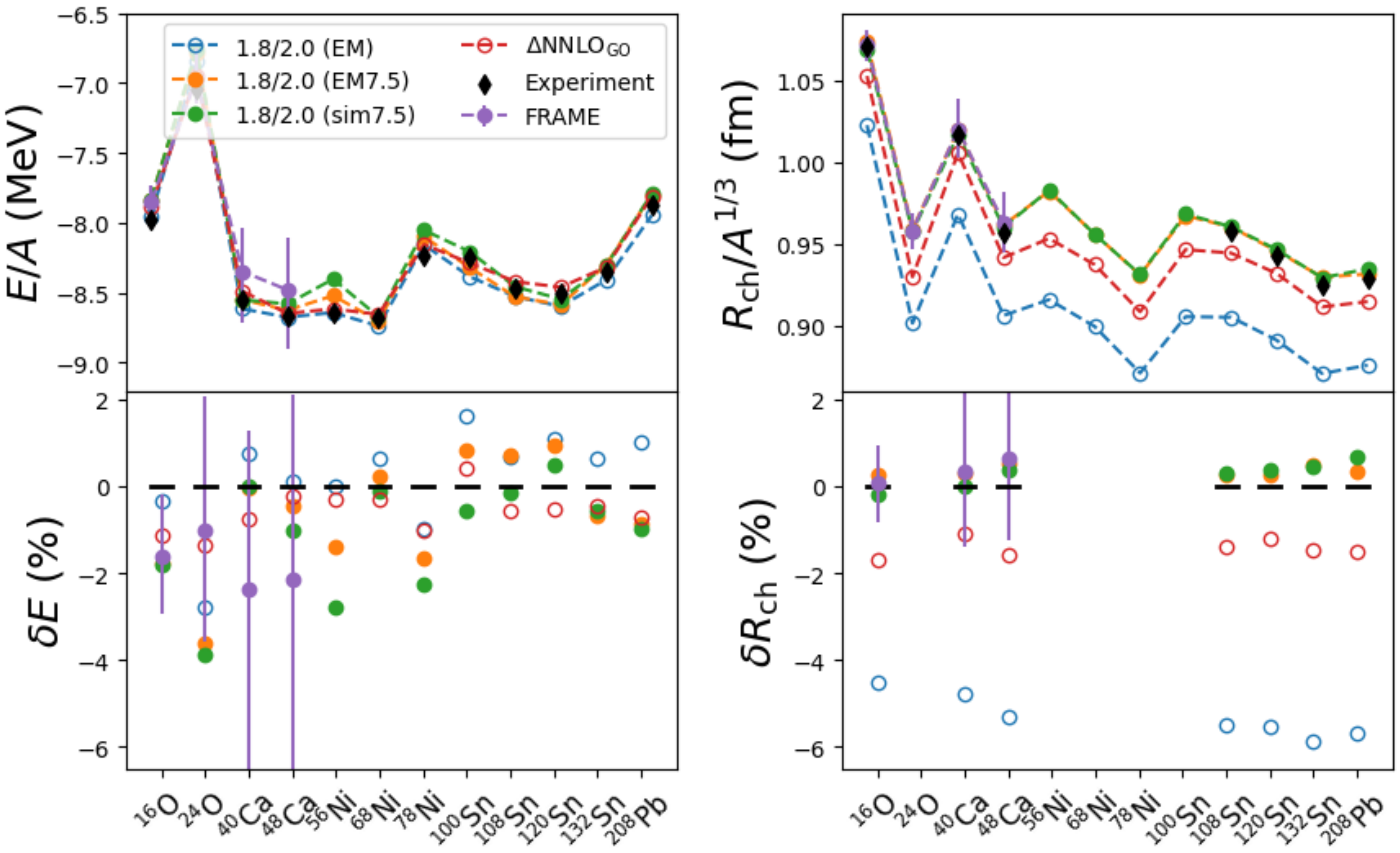

Arthuis, et al., arXiv:2401.06675 (2024)

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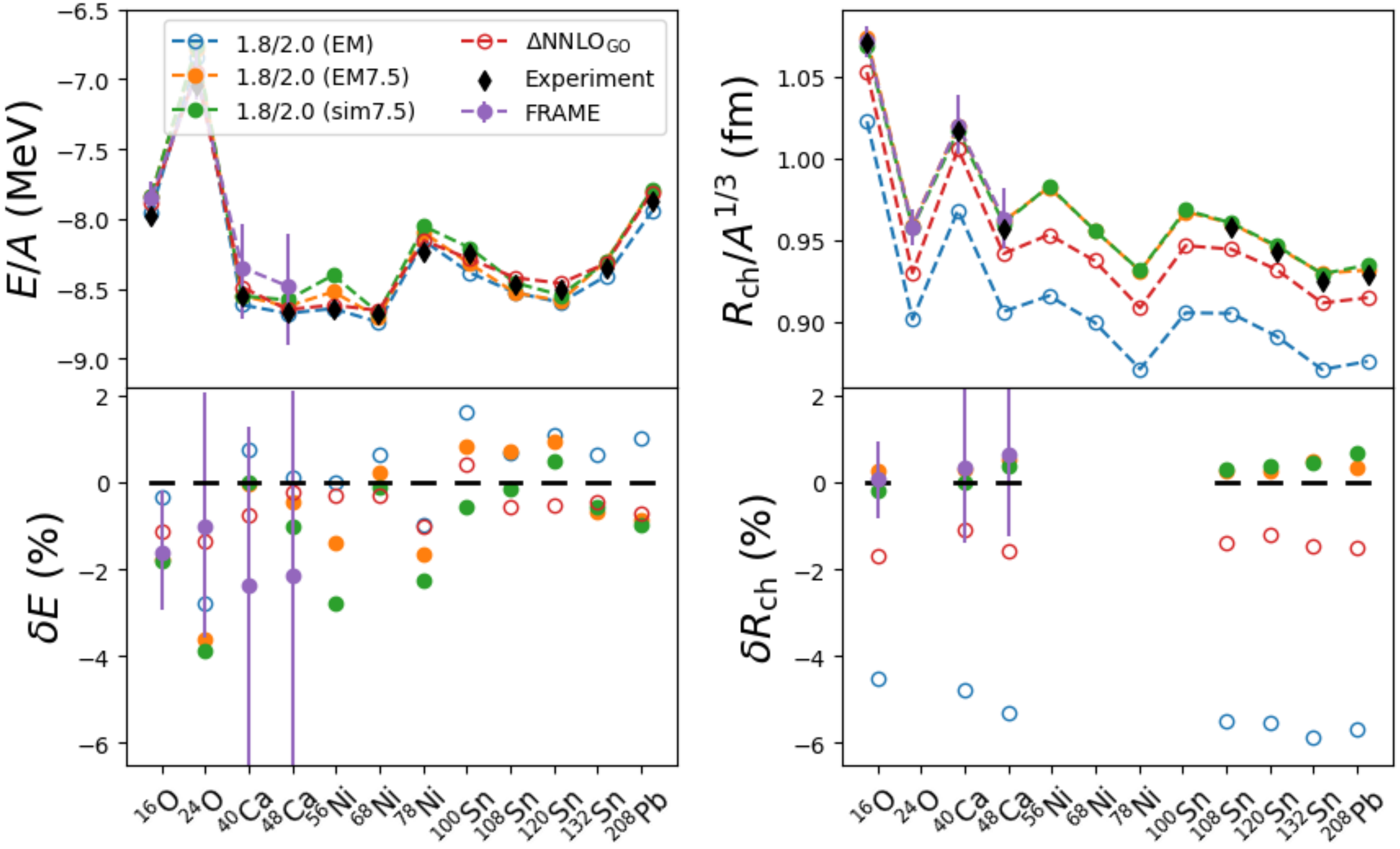

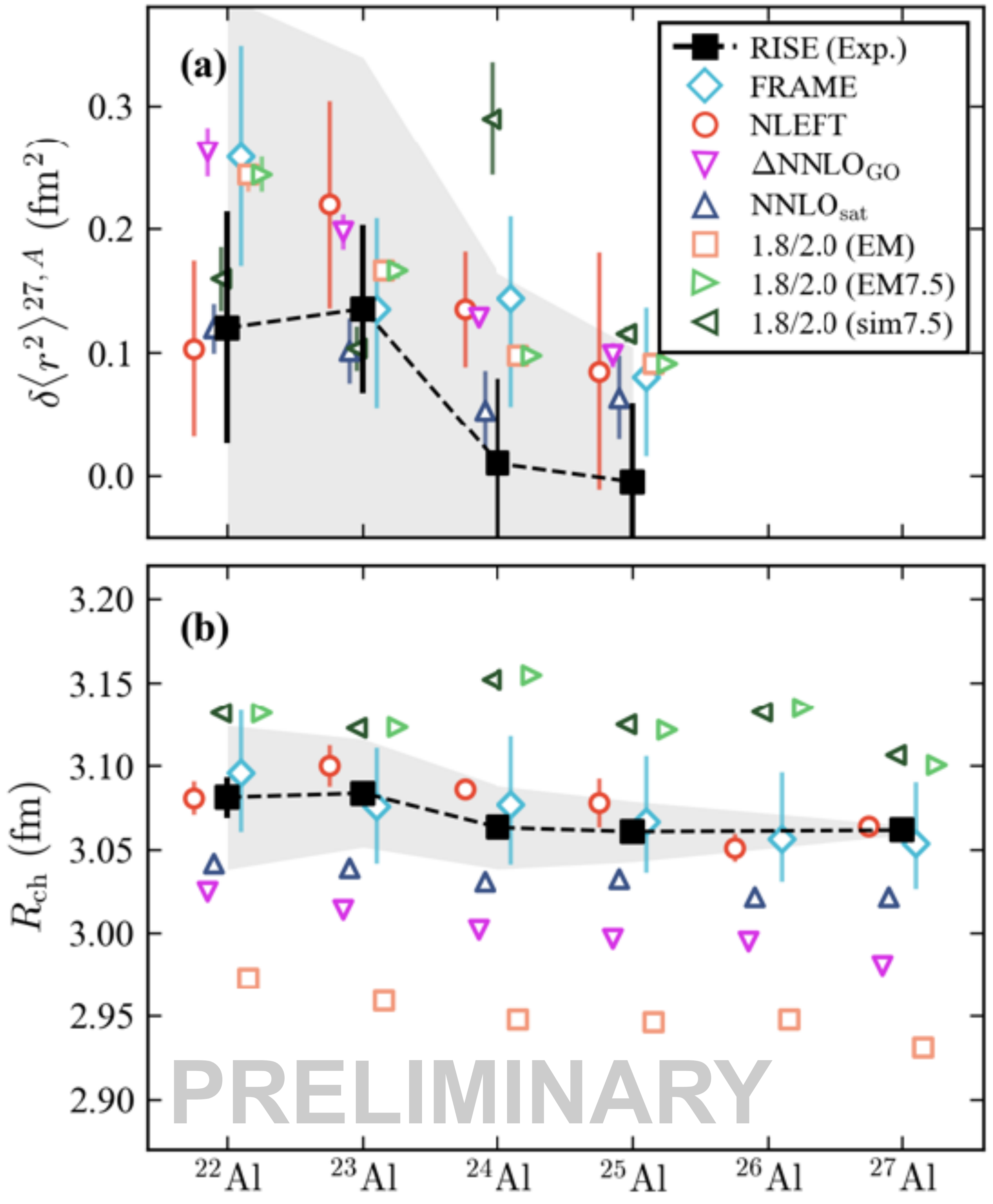

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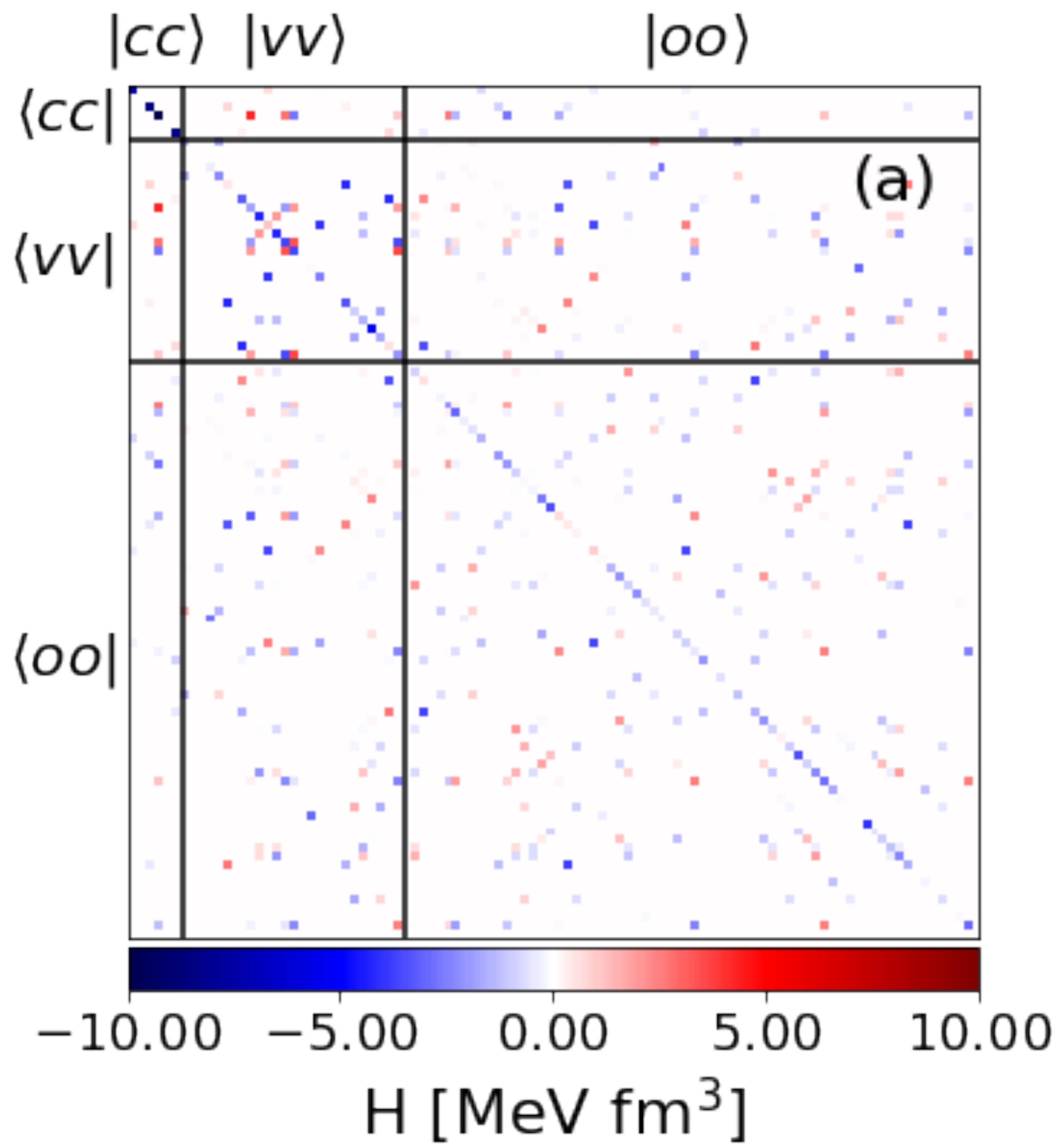
Hard/impossible to consider all interactions together to assign a robust uncertainty

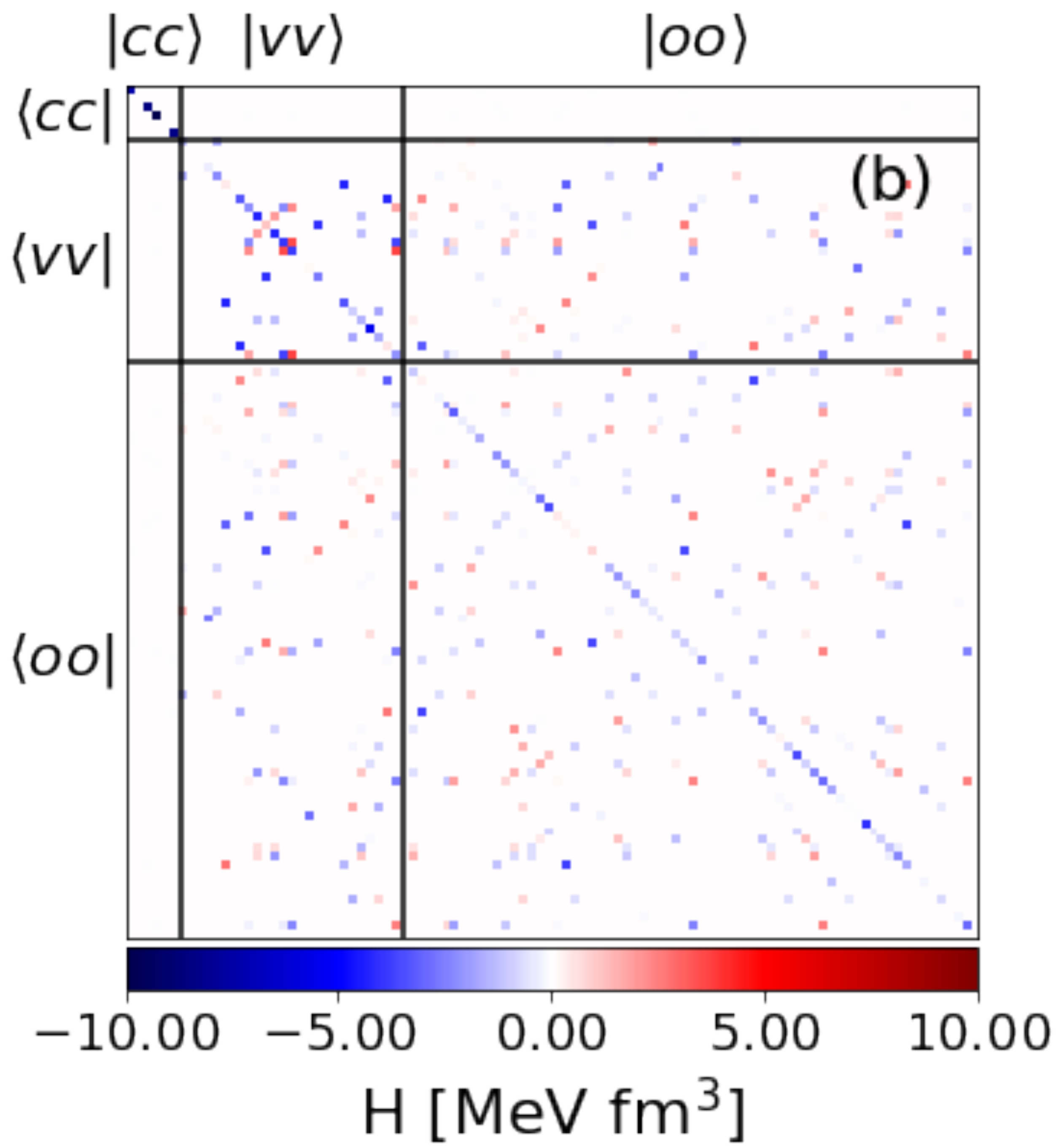
The VS-IMSRG

Valence-Space In Medium Similarity Renormalization Group



Bare Hamiltonian

$$\hat{H}(0)$$



Core is decoupled

$$\hat{H}(s) = e^{\Omega_c(s)}\hat{H}(0)e^{-\Omega_c(s)}$$

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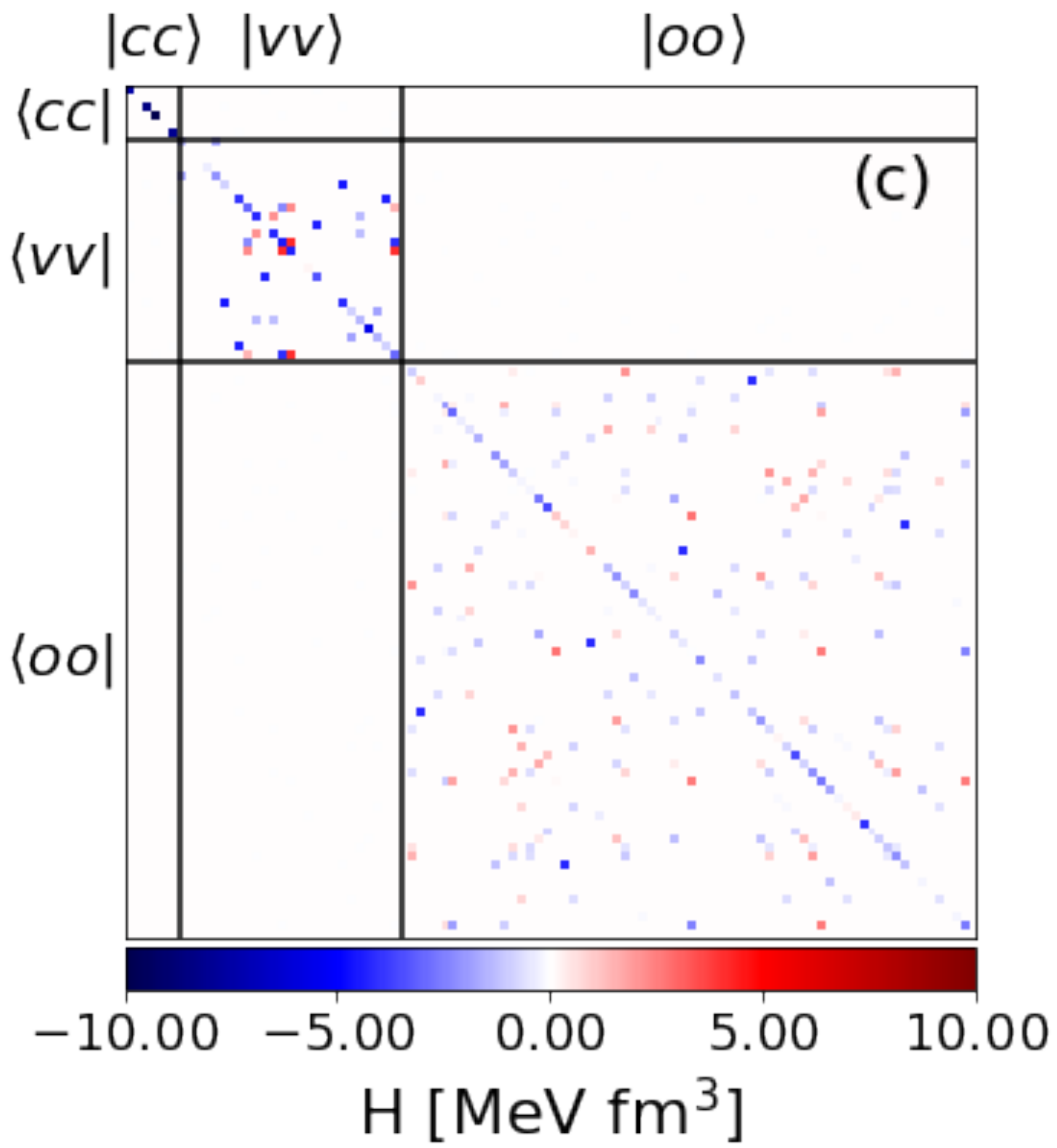

Valence-space is decoupled

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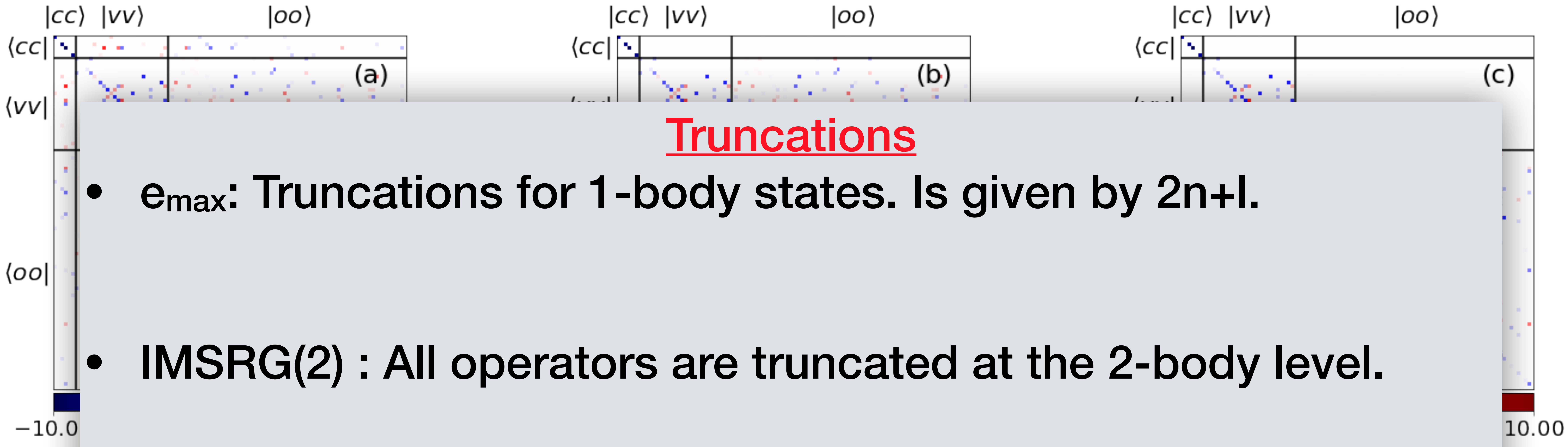

Truncations

- e_{max}: Truncations for 1-body states. Is given by 2n+l.
- IMSRG(2) : All operators are truncated at the 2-body level.

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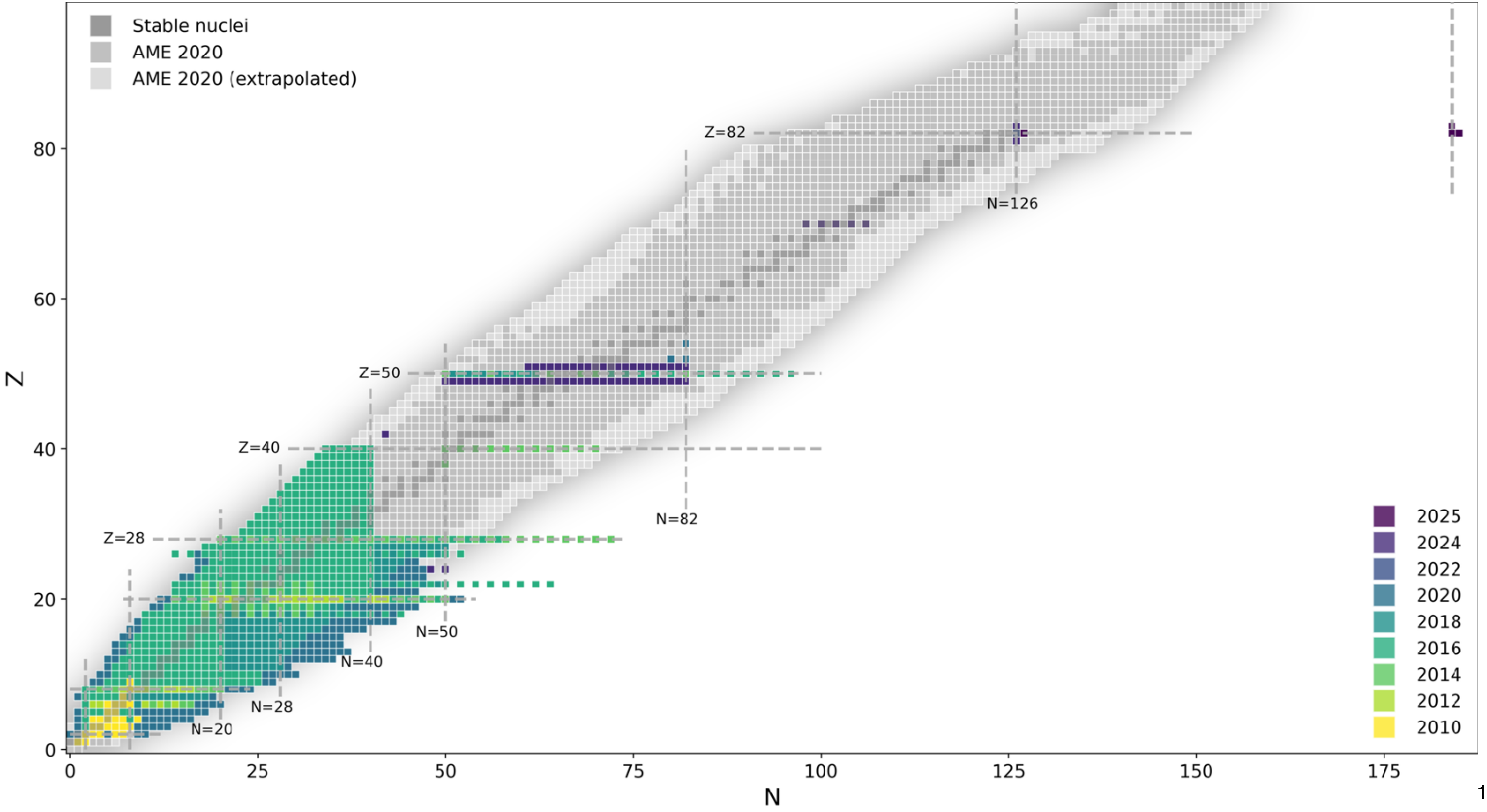
$$\hat{H}_c = e^{\Omega_c(\infty)}\hat{H}(0)e^{-\Omega_c(\infty)}$$

Valence-space is decoupled

$$\hat{H}(s) = e^{\Omega_v(s)}\hat{H}_c e^{-\Omega_v(s)}$$

Ab initio Revolution



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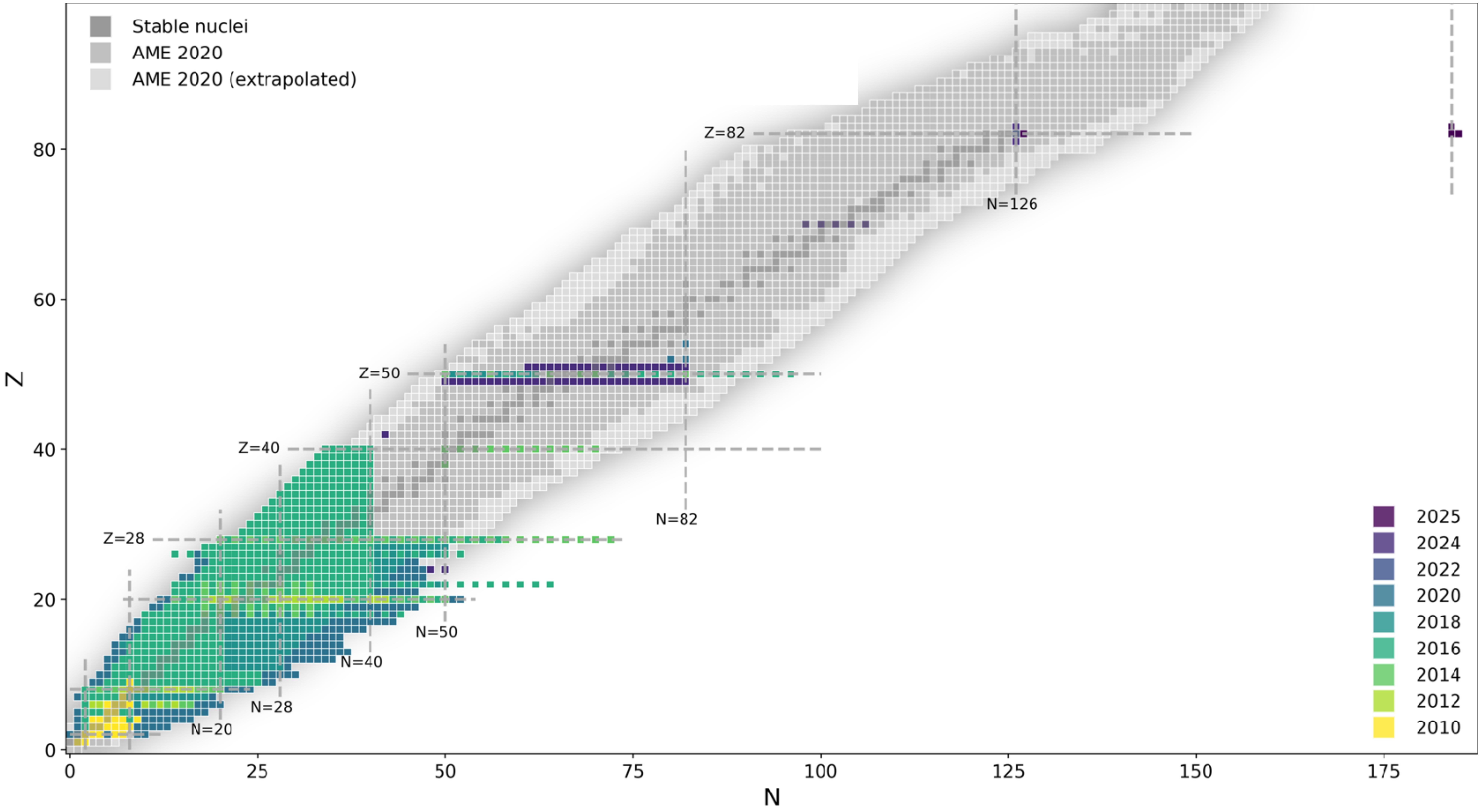
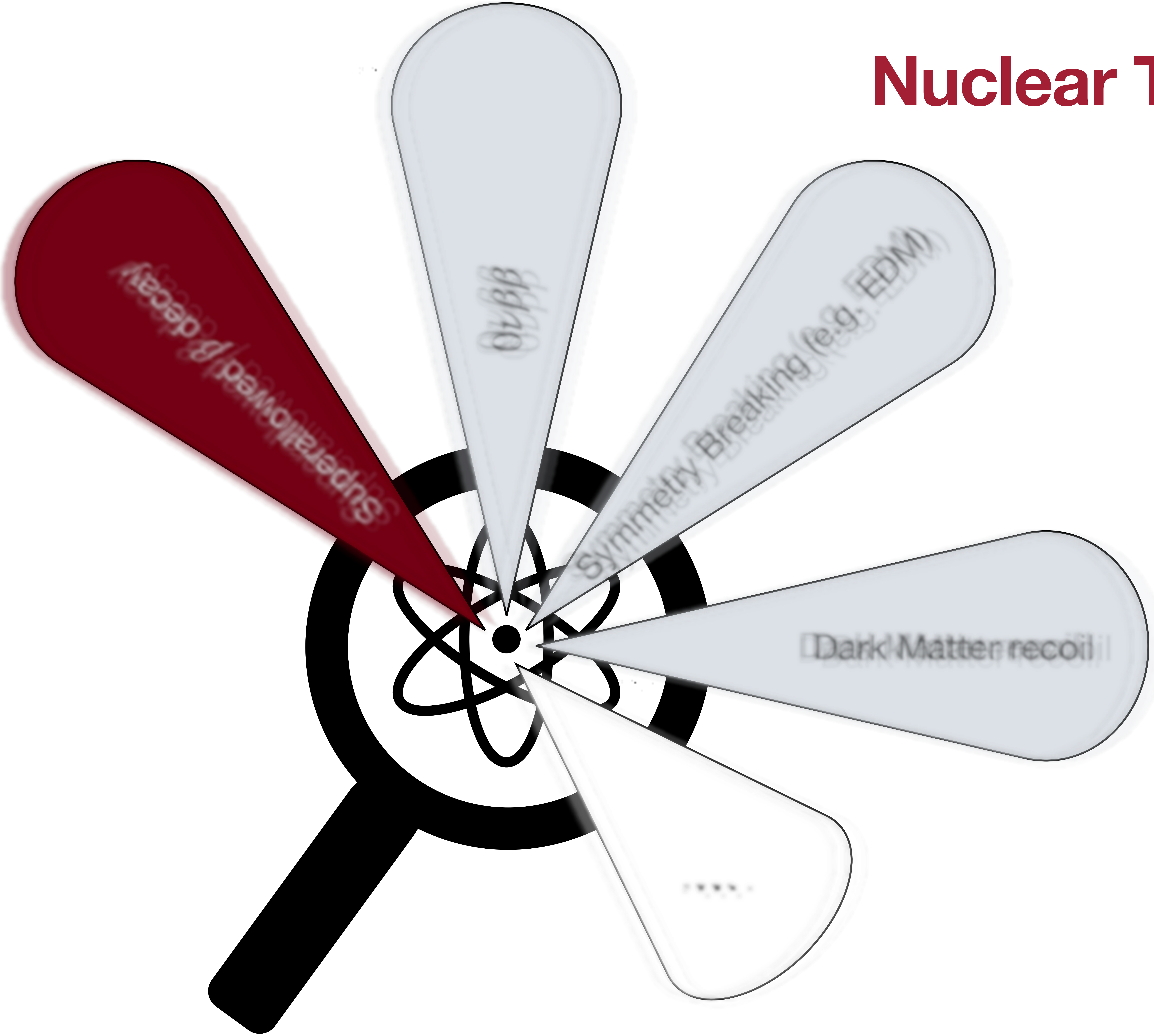
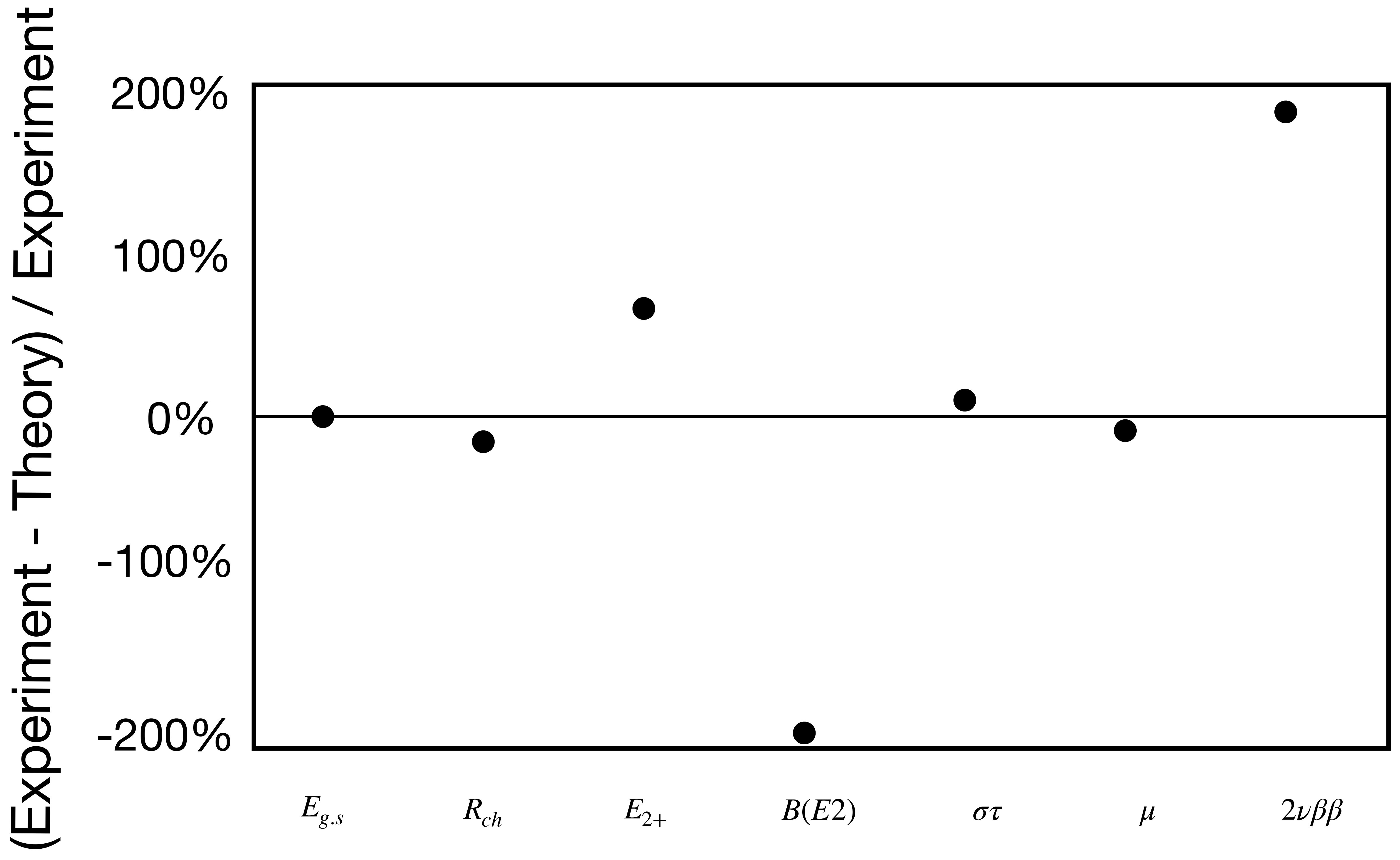


Python version on github!

Nuclear Theory Blur



Using other observables



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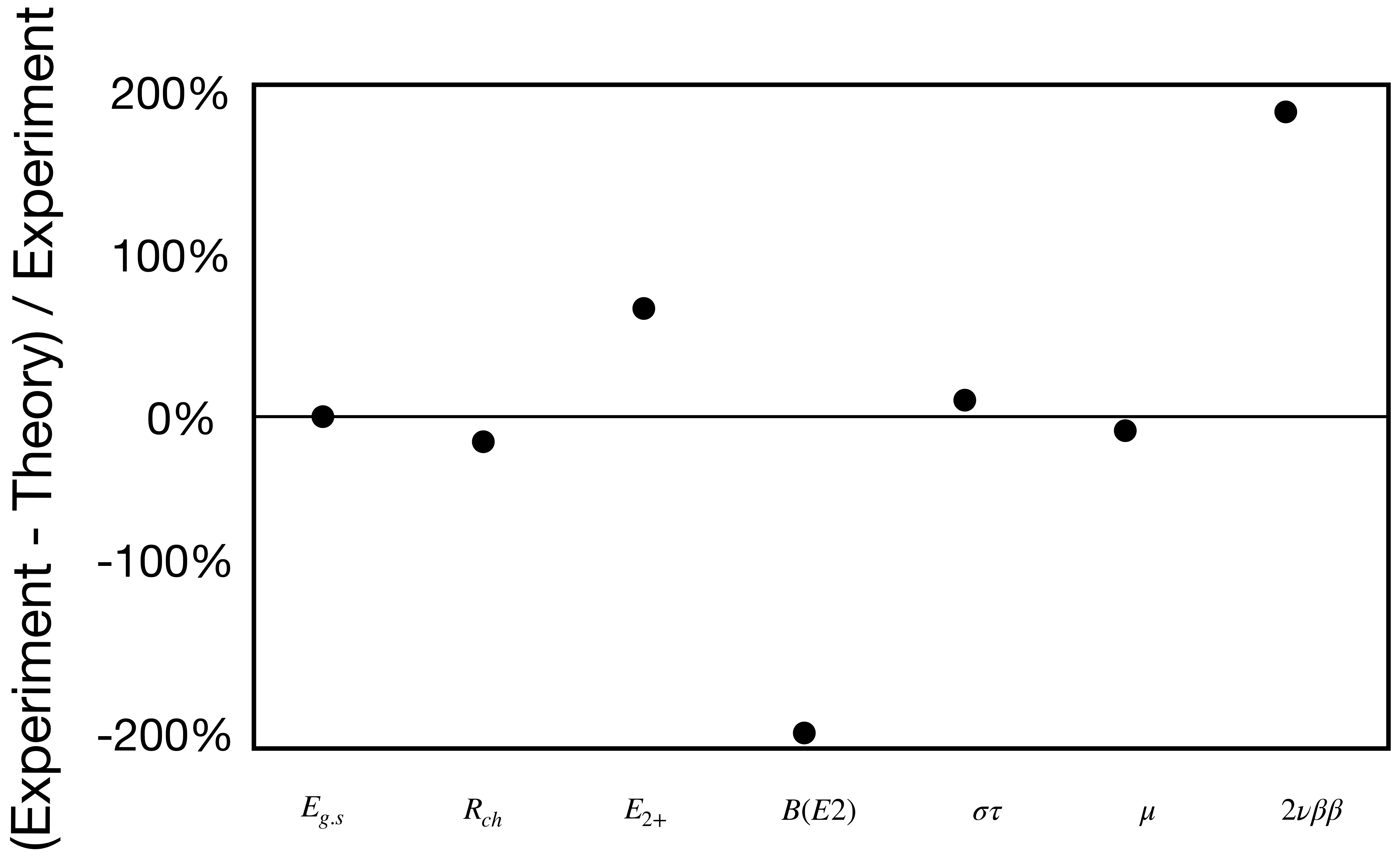

Should I trust this model for $0\nu\beta\beta$?

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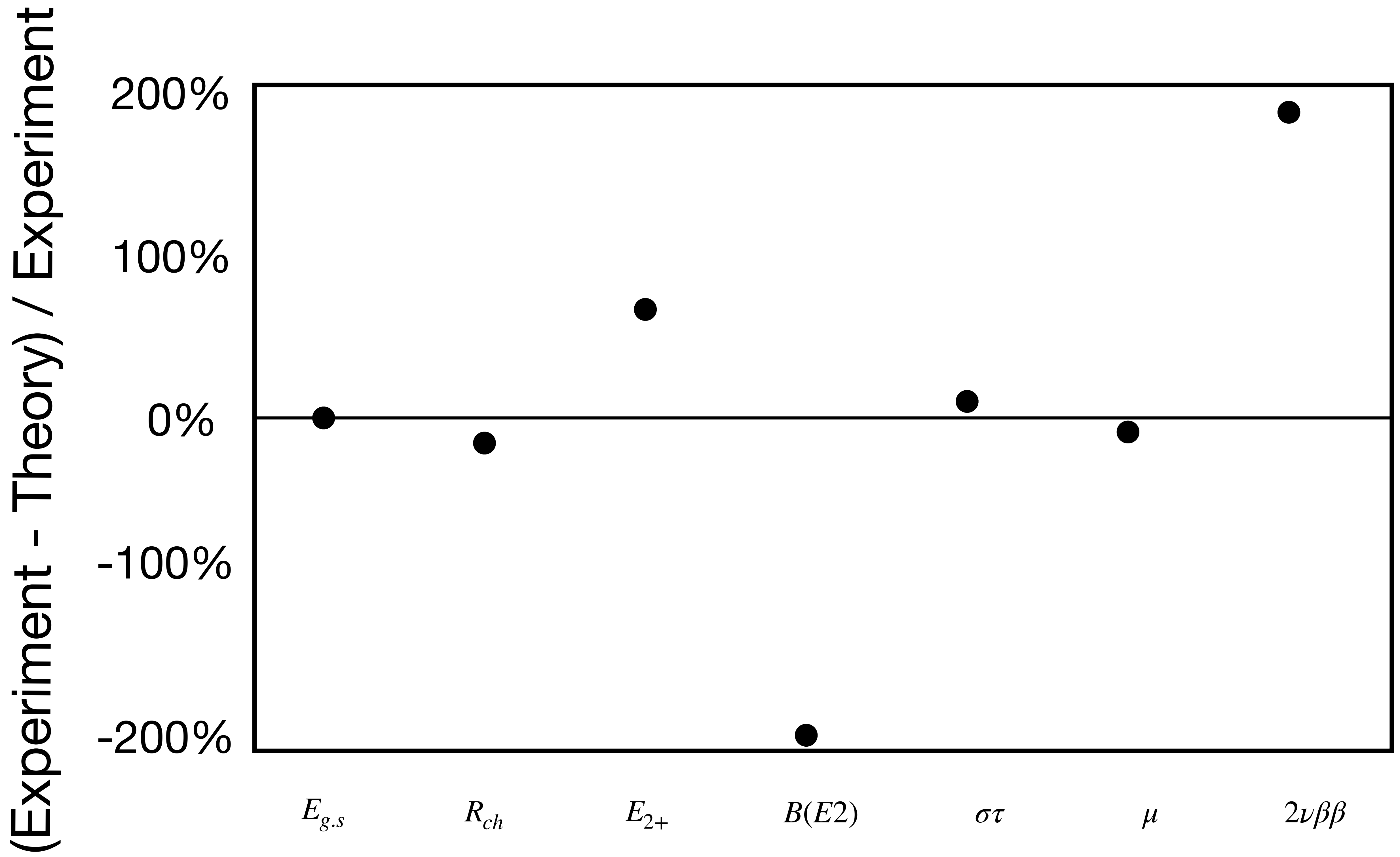

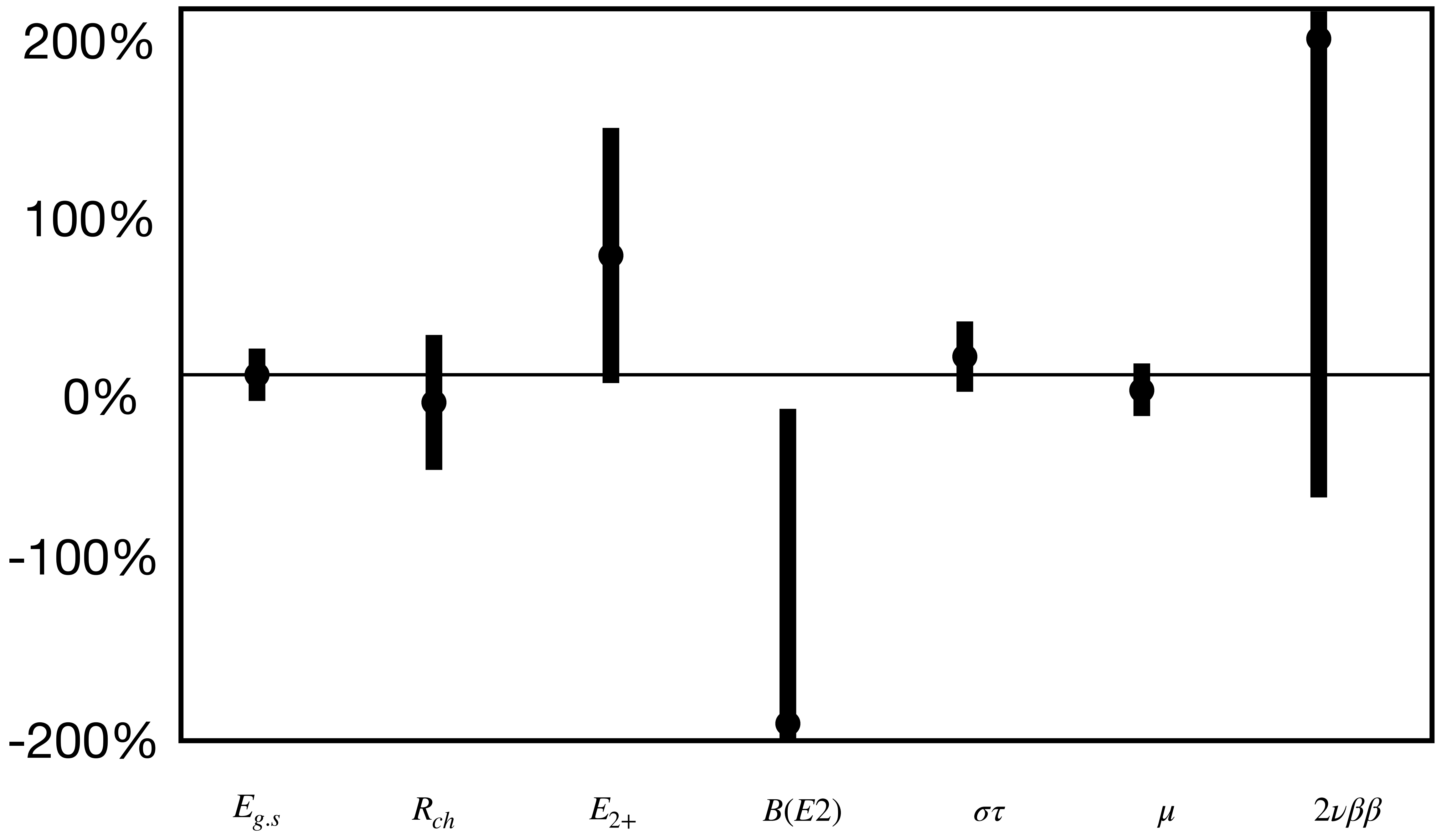

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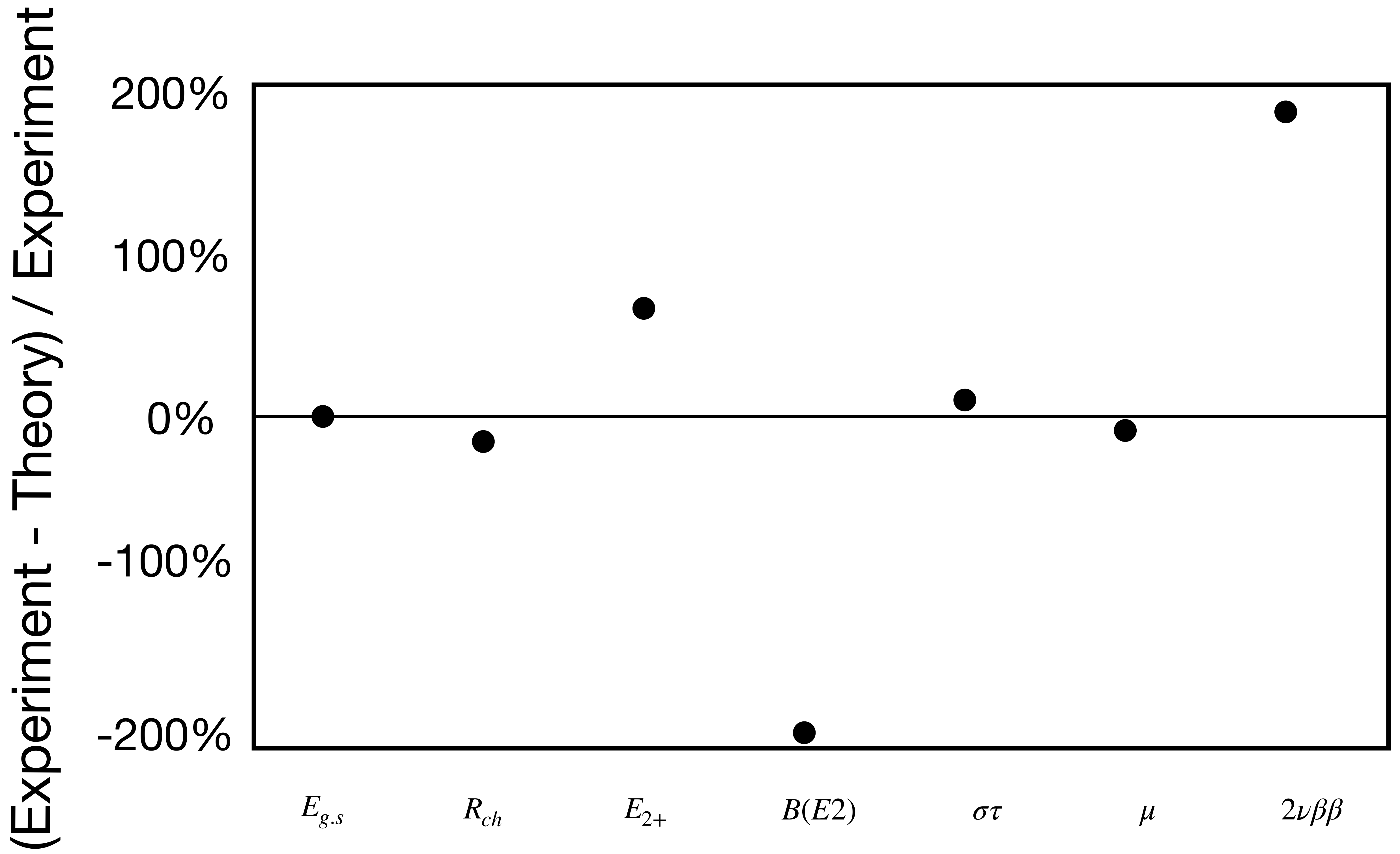
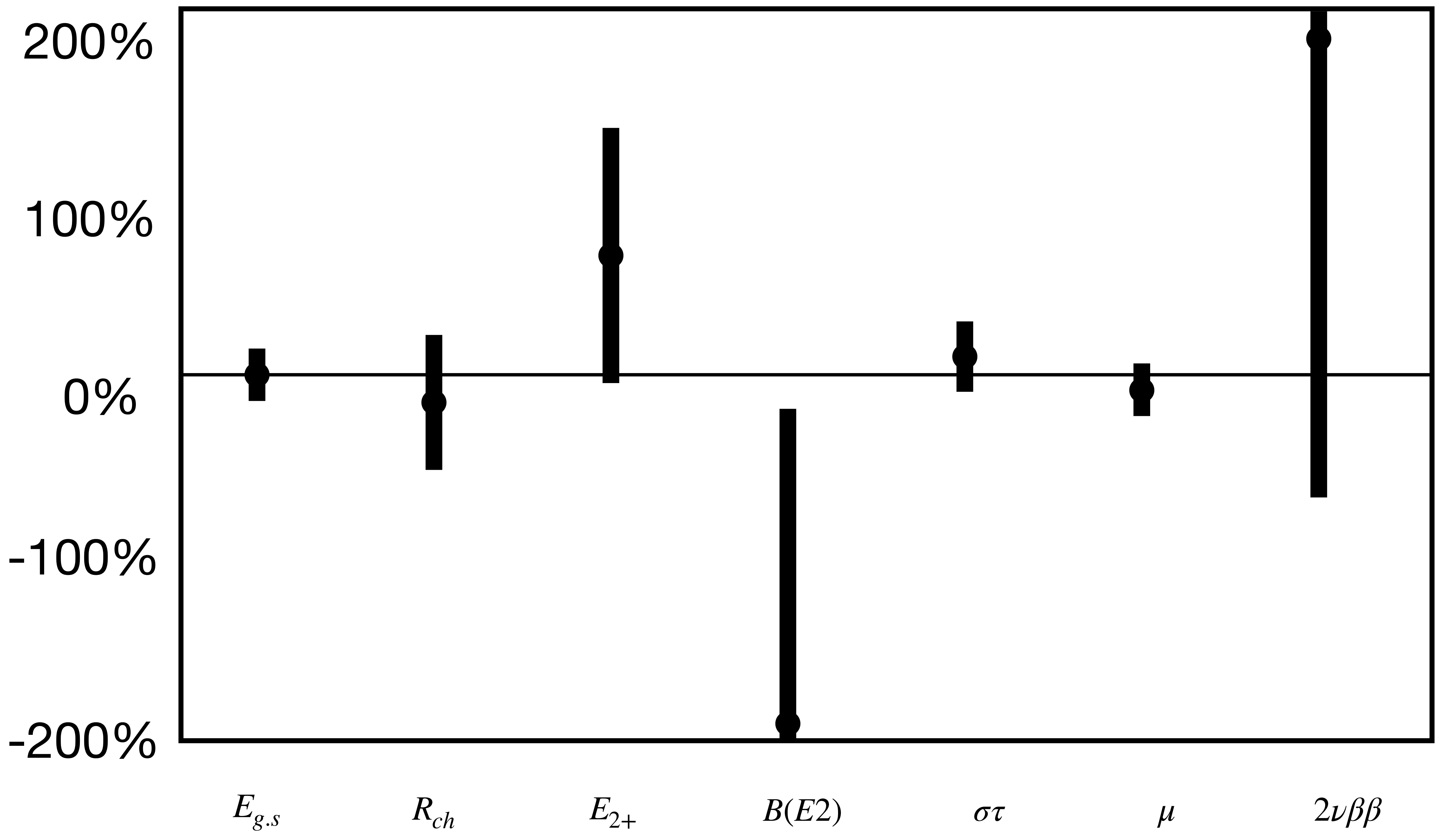


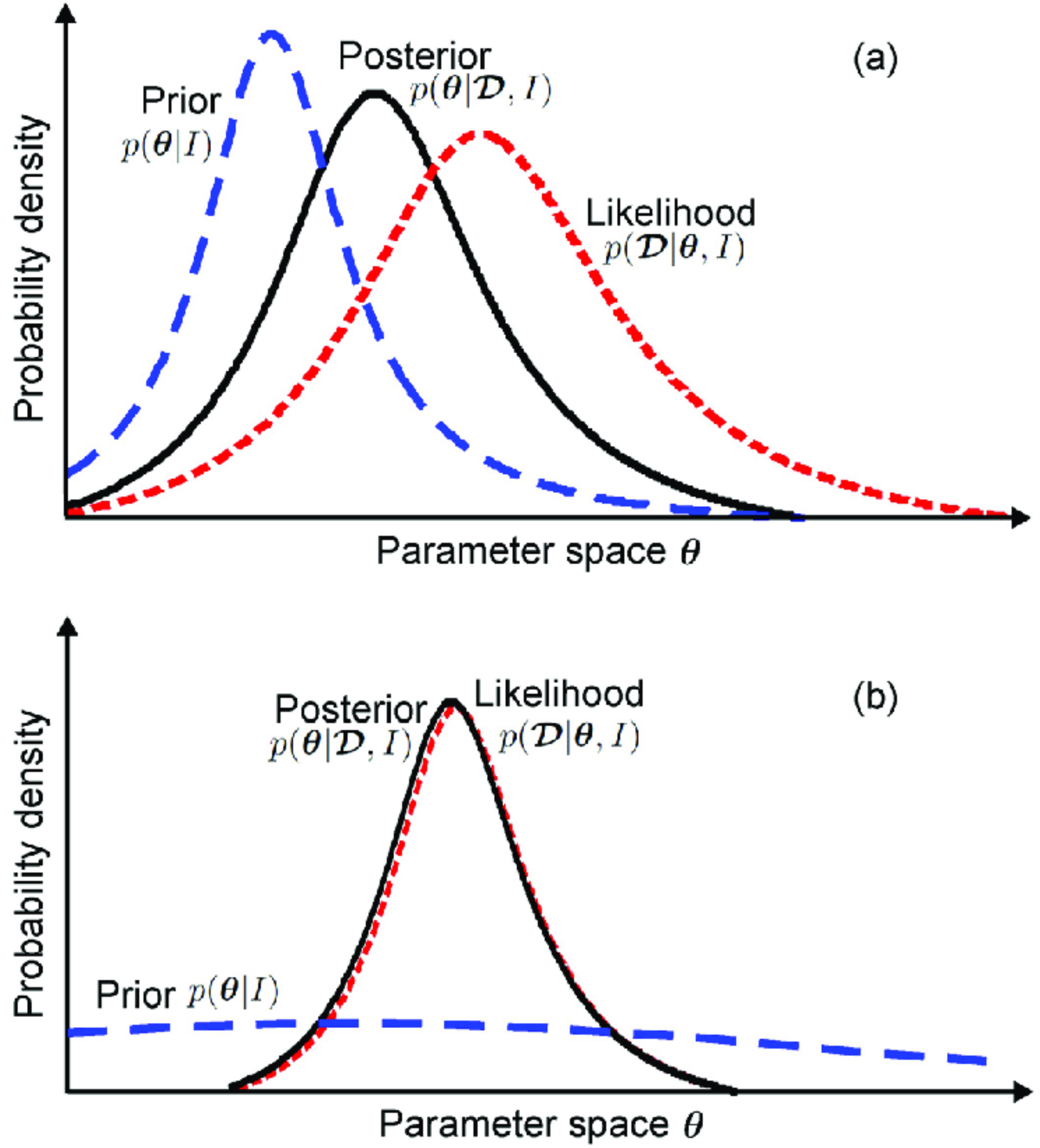


Should I trust this model for $0\nu\beta\beta$?

Should I trust this prediction and uncertainties for $0\nu\beta\beta$?

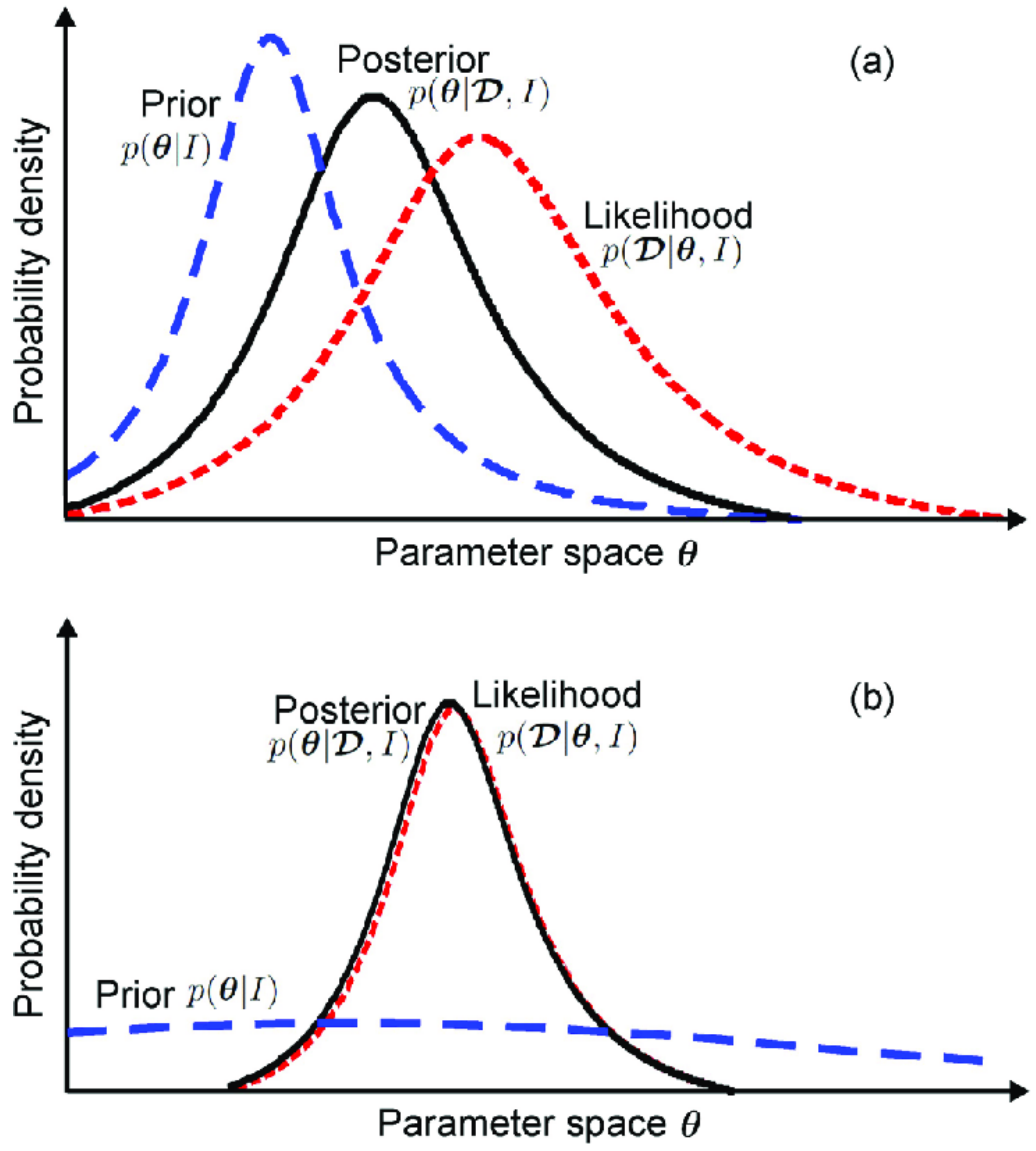
Uncertainty quantification

Procedure for UQ in the Bayesian Approach



Ning Xiang - https://doi.org/10.1121/10.0001731

Procedure for UQ in the Bayesian Approach



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The catch

Need many samples.

Due to the large cost of many-body methods, for 1 isotope:

- Take ~**1 year** to compute all samples on HPC cluster.
- Cost > **$2 million!**
- Huge environmental impact (**220 tree-years** calculated using green-algorithms.org v3.0)

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Emulators for Many-Body Methods

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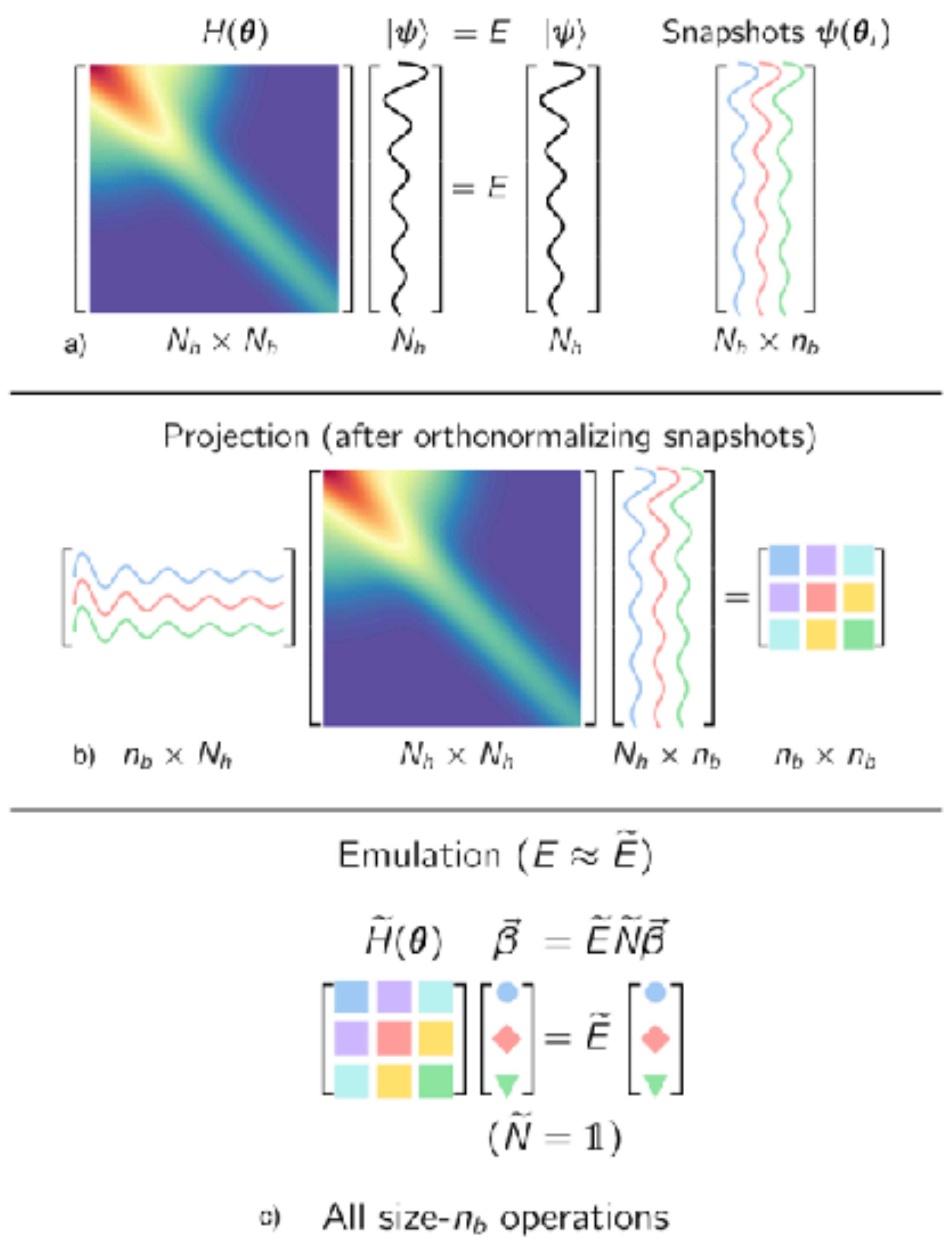

Duguet, et al., Rev. Mod. Phys. **96**, 031002 (2024)

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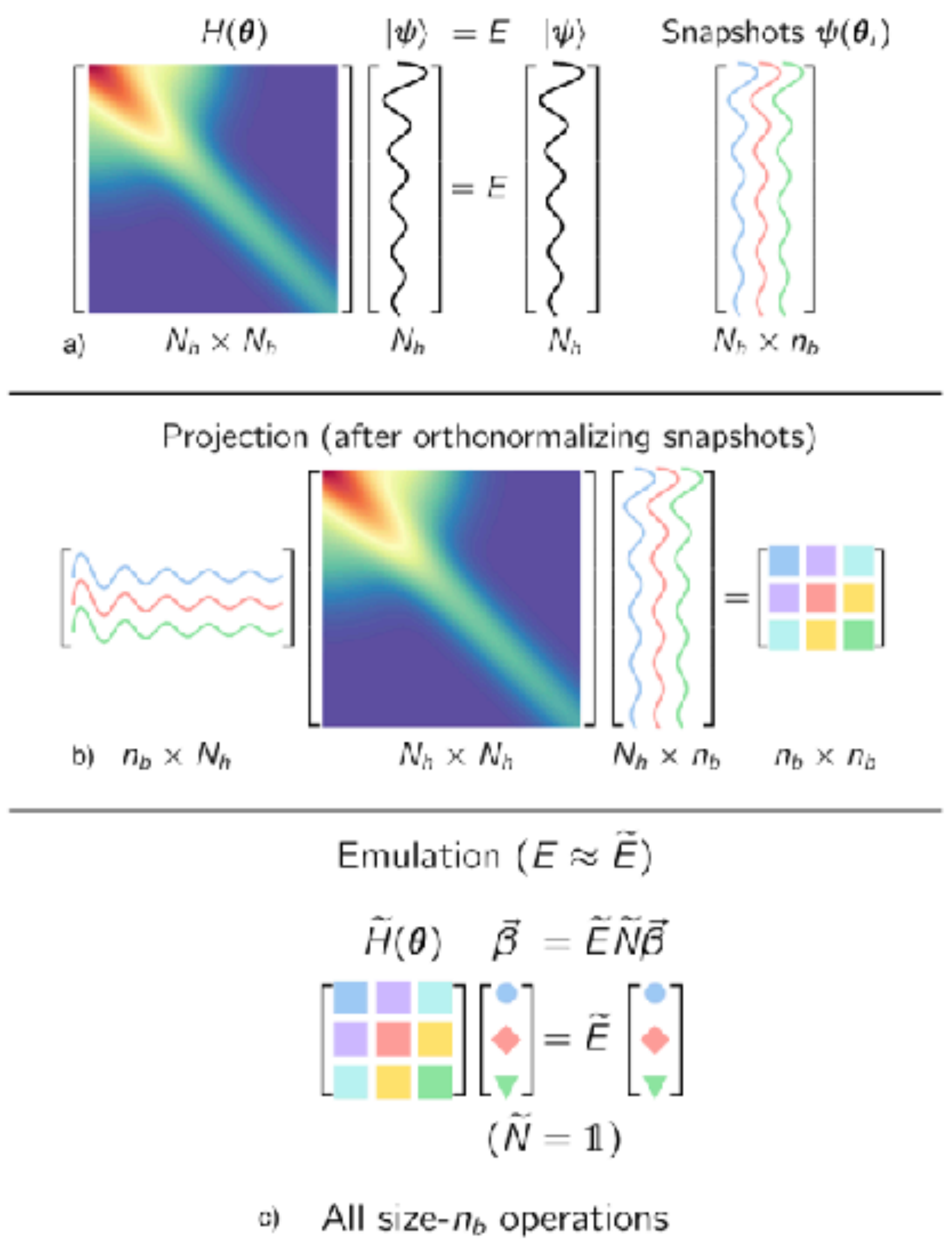
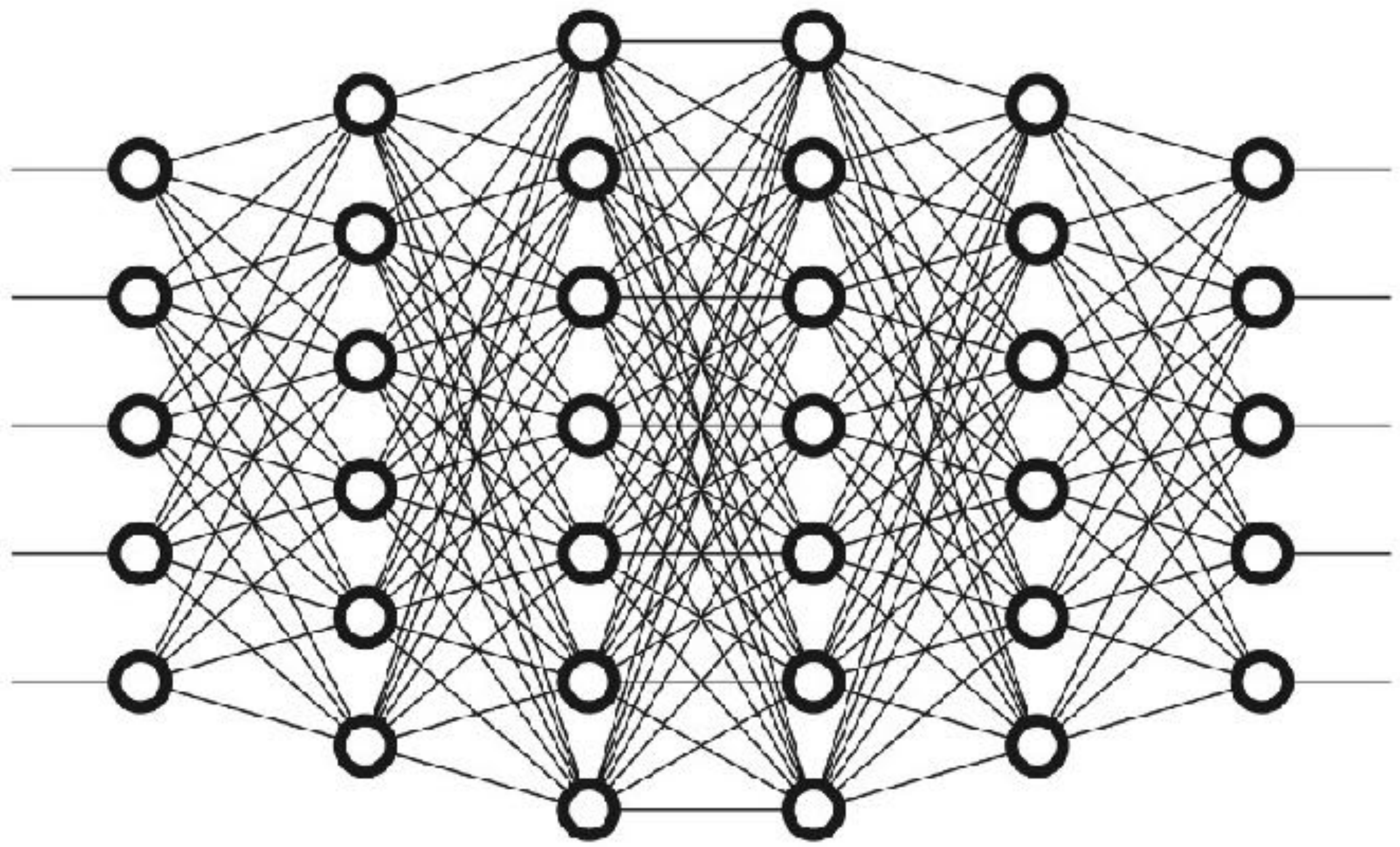
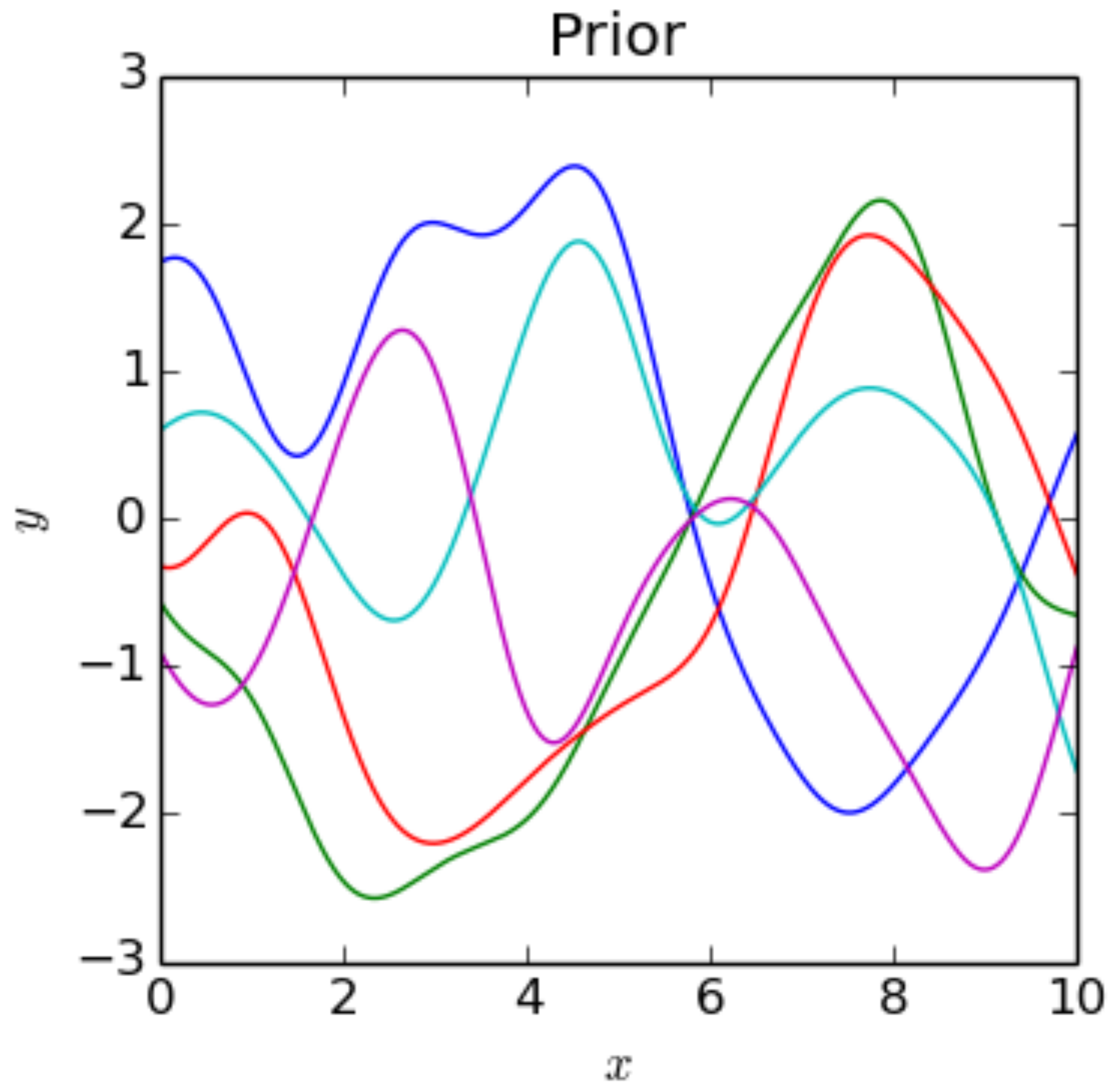


Duguet, et al., Rev. Mod. Phys. **96**, 031002 (2024)

2. Data driven



Using Gaussian Process as an Emulator



$$f(\mathbf{x}) = \mathcal{N}(\mu, K(\mathbf{x}, \mathbf{x}))$$

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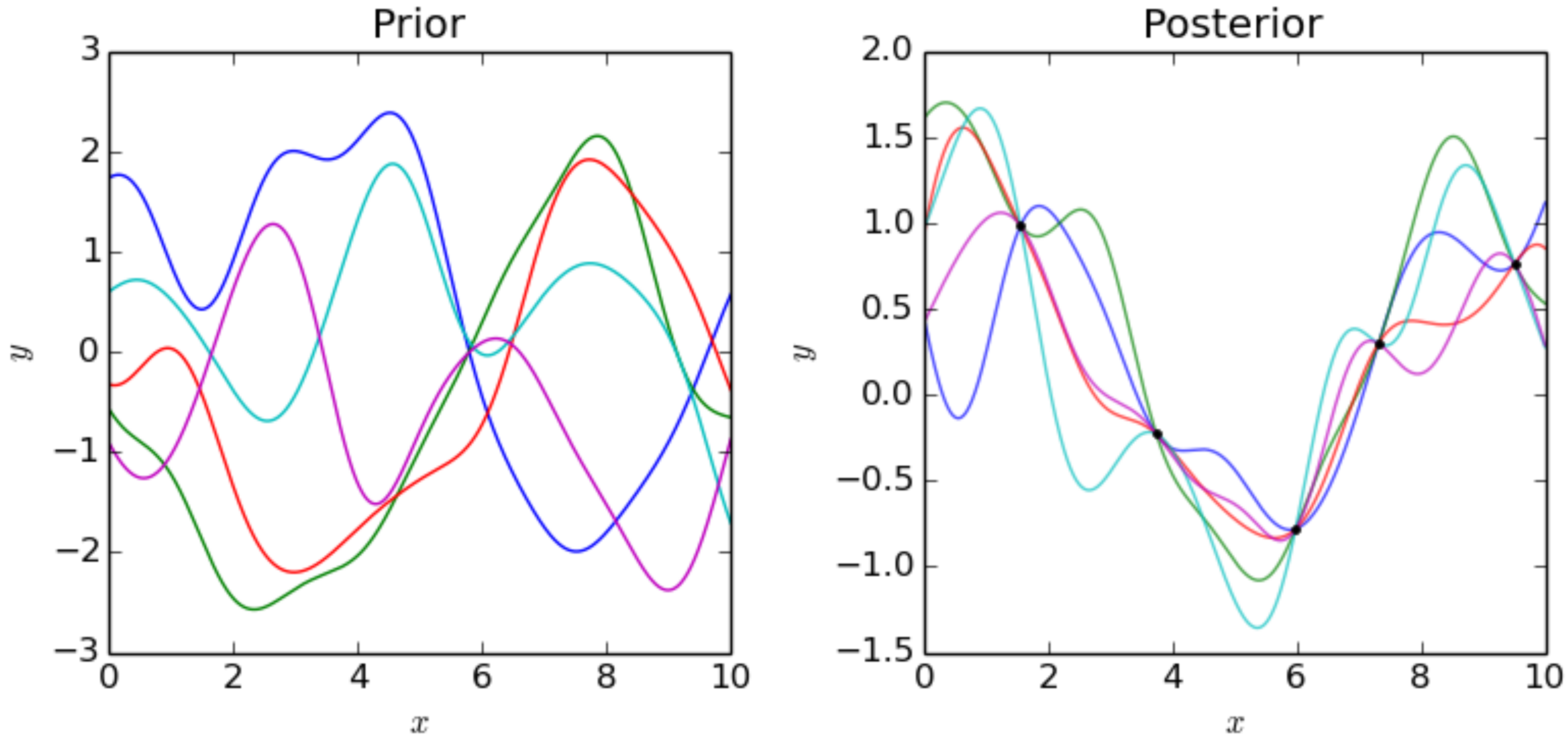

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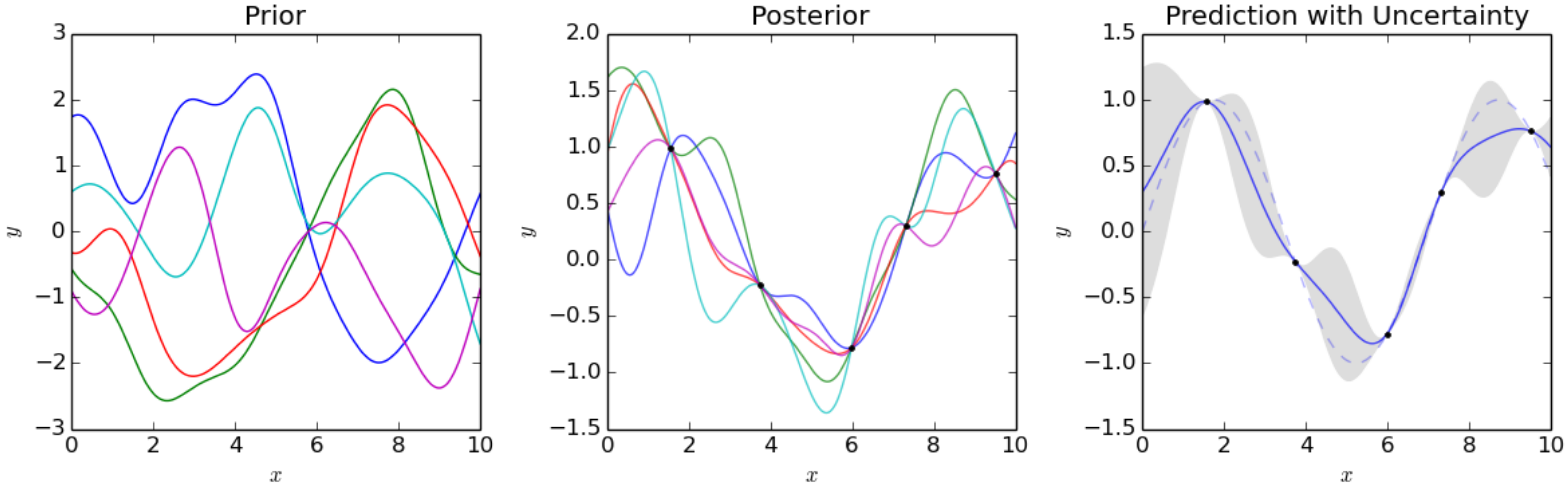

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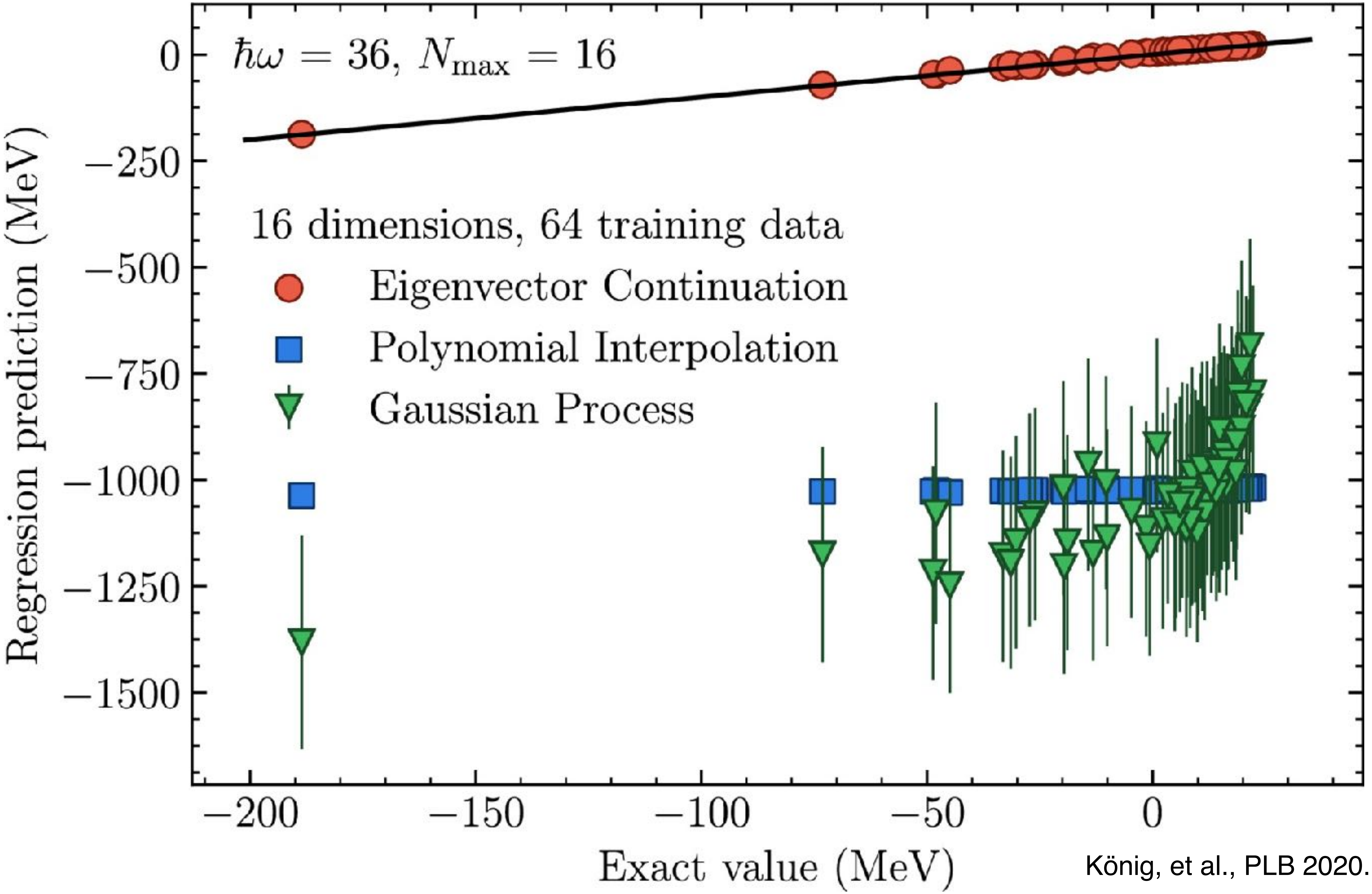

König, et al., PLB 2020.135814

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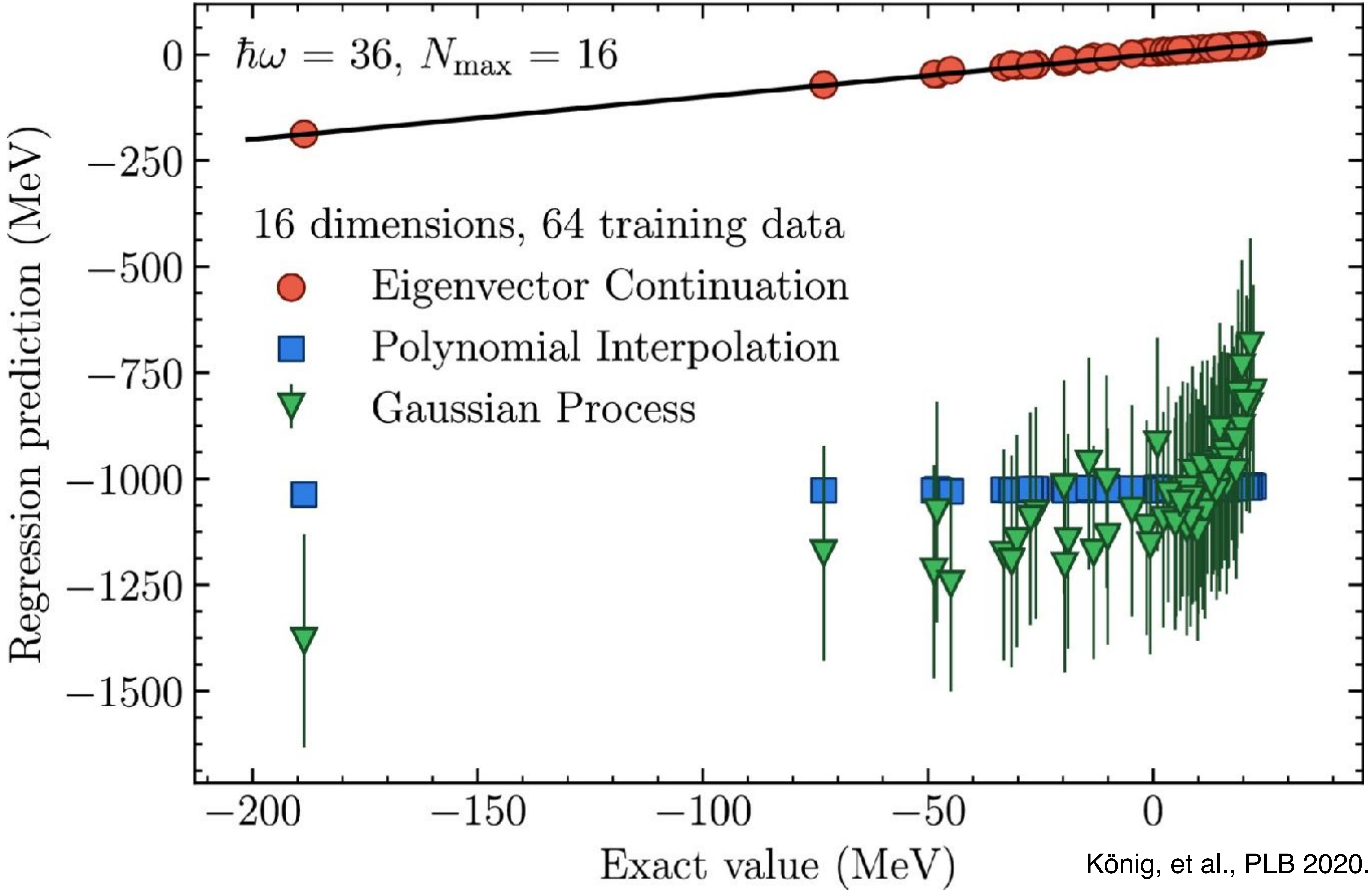

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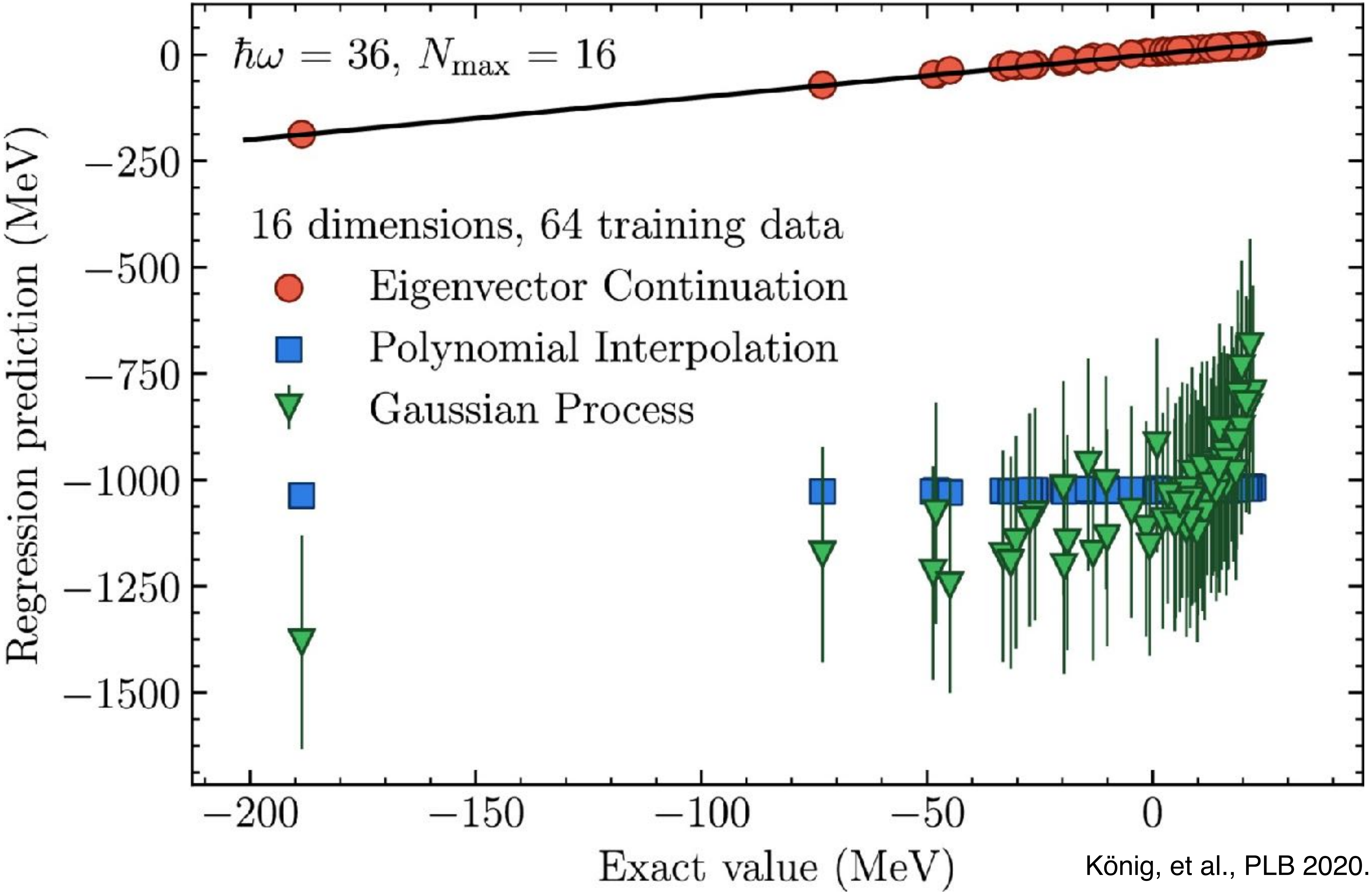


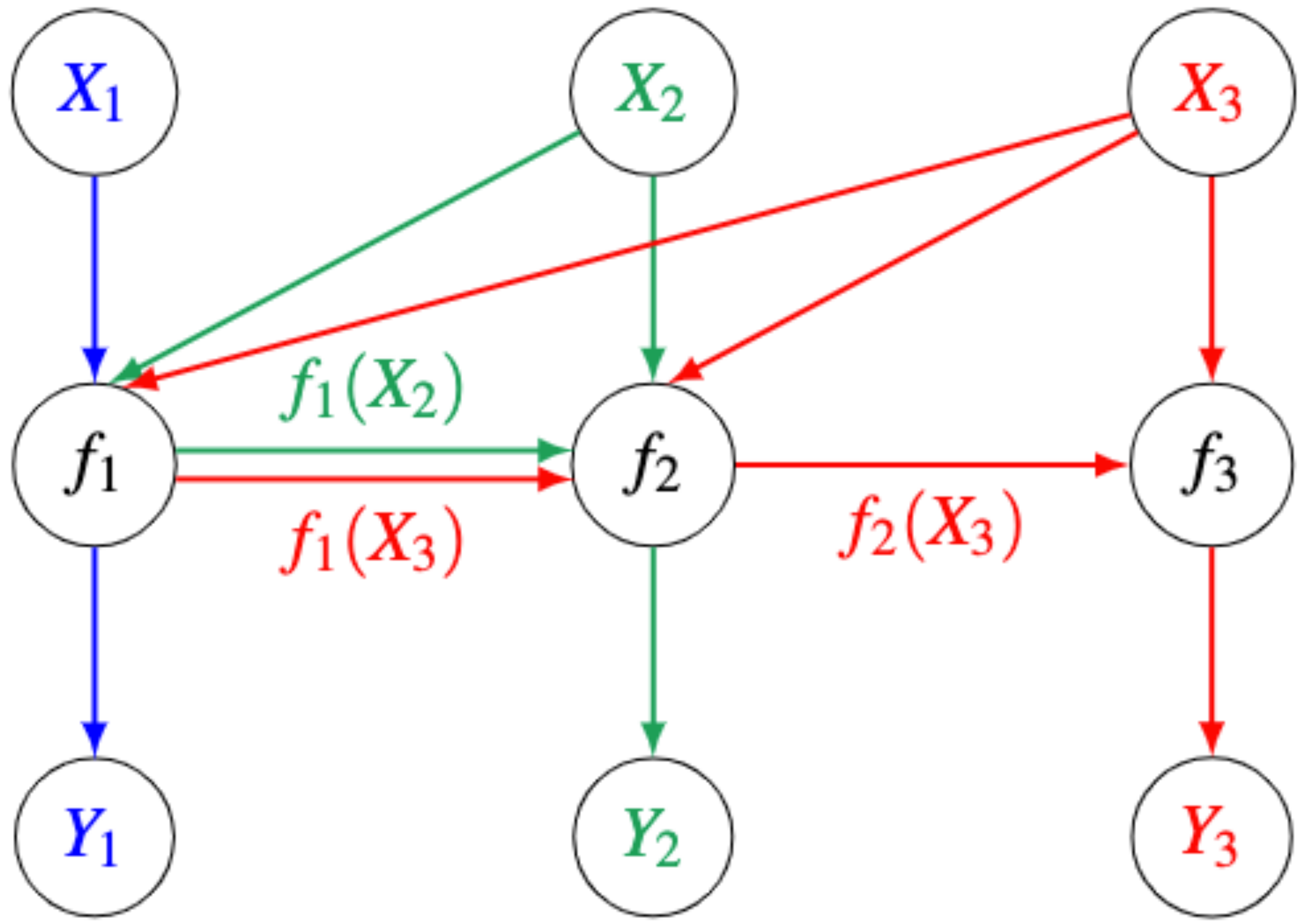
König, et al., PLB 2020.135814

The MM-DGP Algorithm

- **Deep Gaussian Processes [1]**: Stack multiple GPs in a neural network-like architecture for improved hierarchical learning.

- **Multi-Fidelity Modelling**: Model low-to-high fidelity differences by passing outputs from one fidelity as inputs to the next.

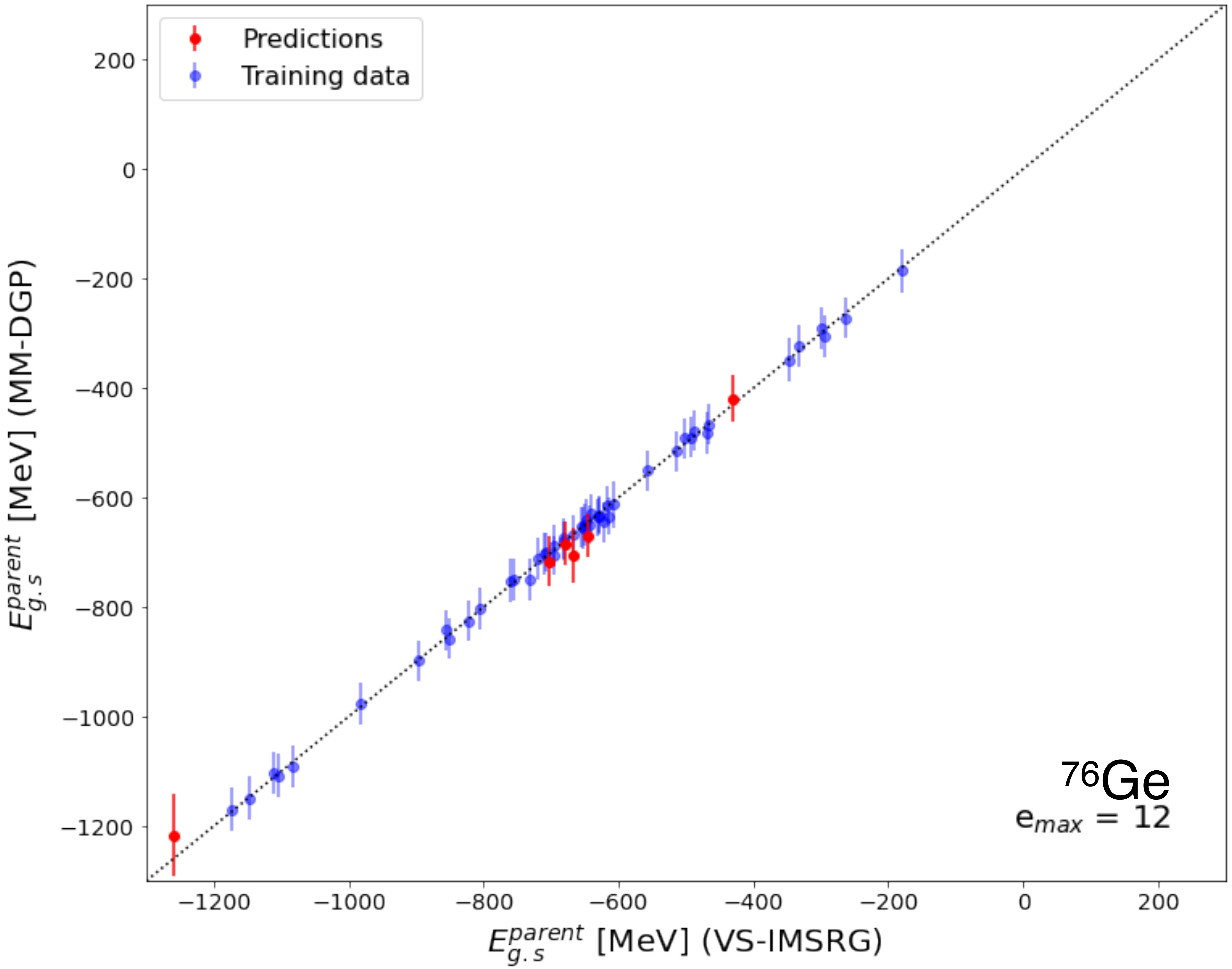
- **MM-DGP Extension**: Adapted to handle multiple outputs across fidelity levels, creating the Multi-output Multi-fidelity Deep Gaussian Process (MM-DGP).



[1] Kurt Cutajar, Mark Pullin, Andreas Damianou, Neil Lawrence, Javier González arXiv:1903.07320 (2021).

The MM-DGP Algorithm: Energies

e_{max}	# of training points
4	250
6	100
8	90
10	50
12	50



Root Mean Square Error = 11 MeV

Getting Posterior Distributions

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Prior: 8188 “non-implausible” samples (Phys. Rev. C **109**, 064314)

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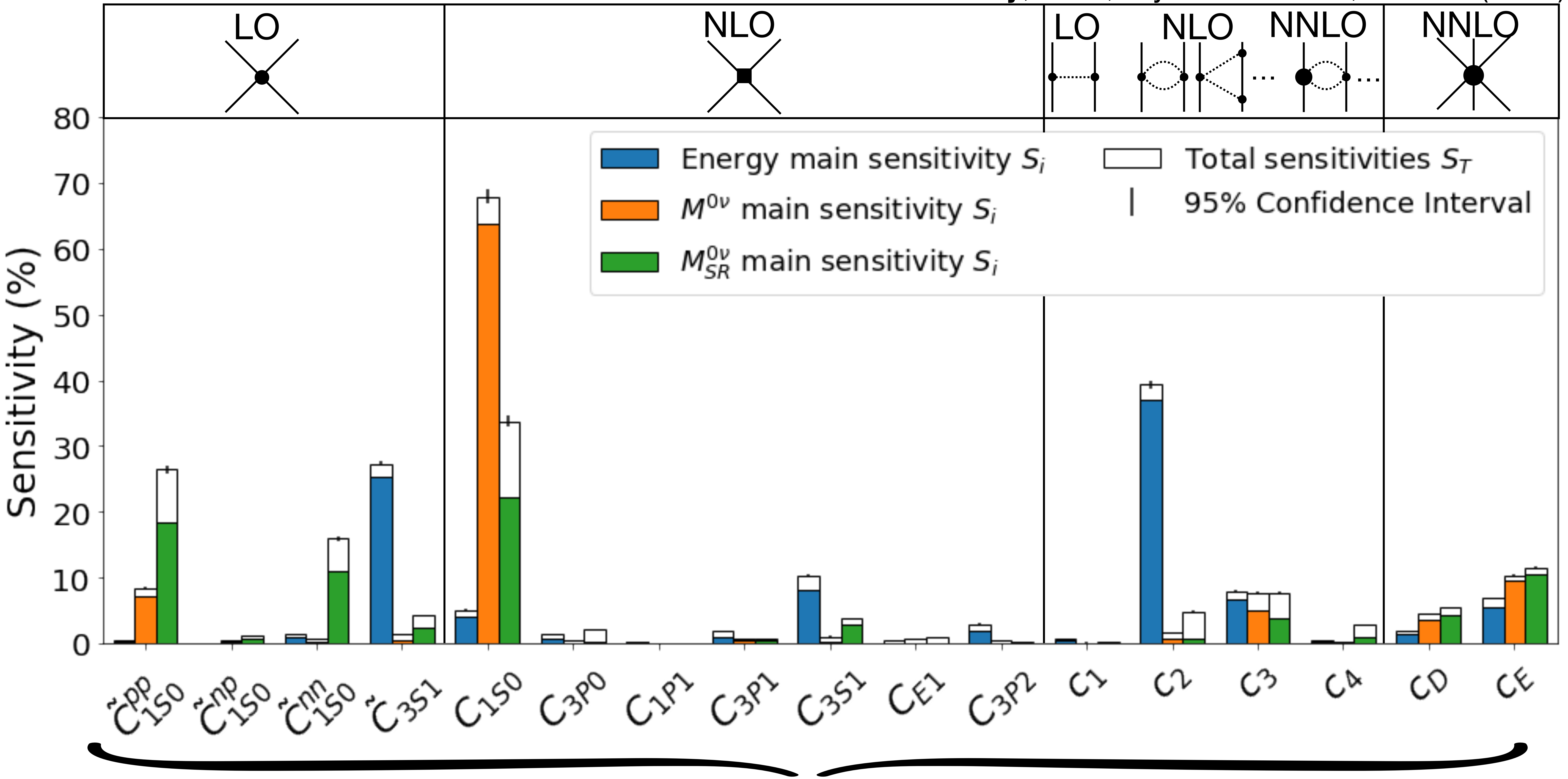
The different sources of errors ϵ are assumed to be normally distributed and independent

The MM-DGP Algorithm: GSA

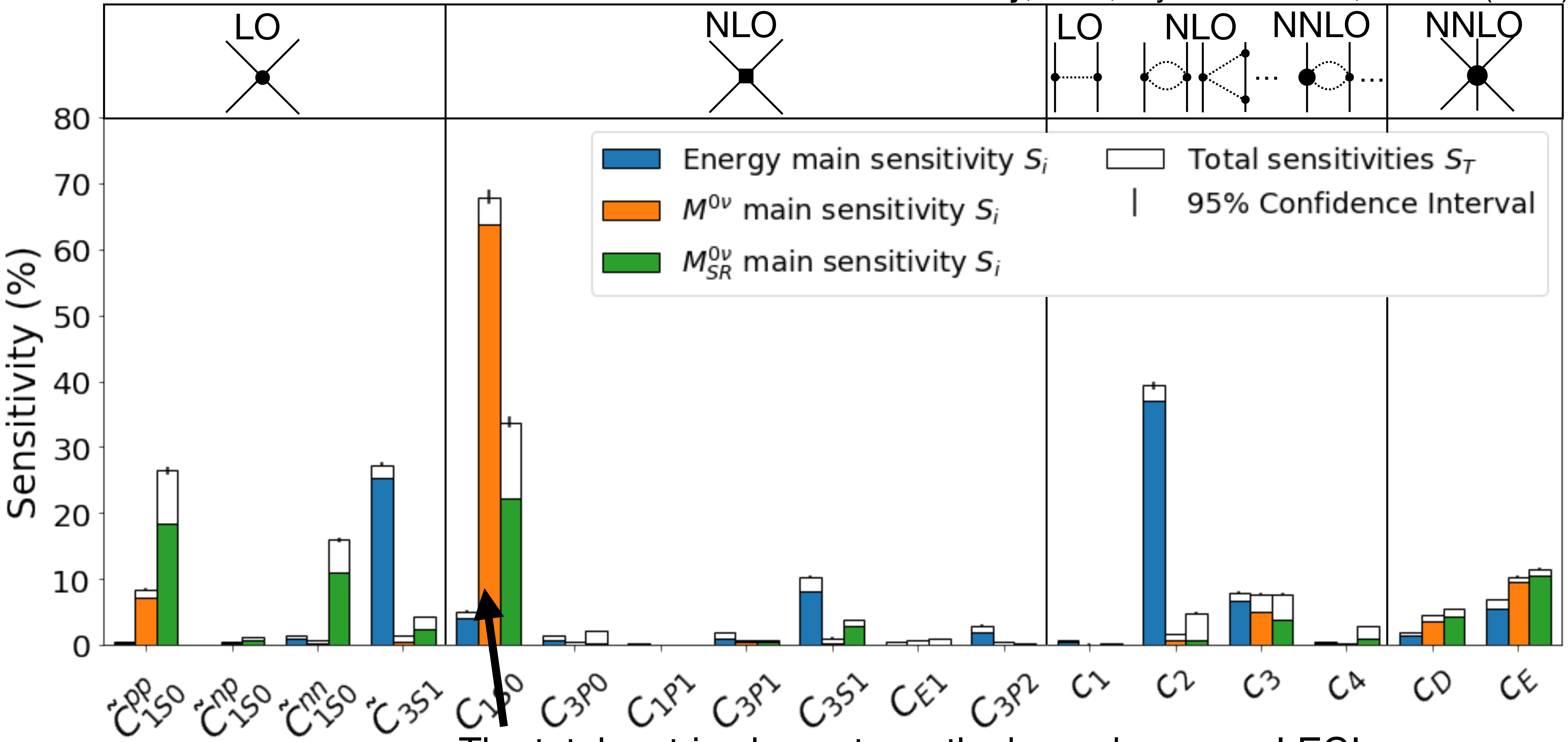
Belley, et al.,Phys. Rev. C **113**, 014319 (2026)



Low-energy constants, i.e. parameters of the nuclear

The MM-DGP Algorithm: GSA

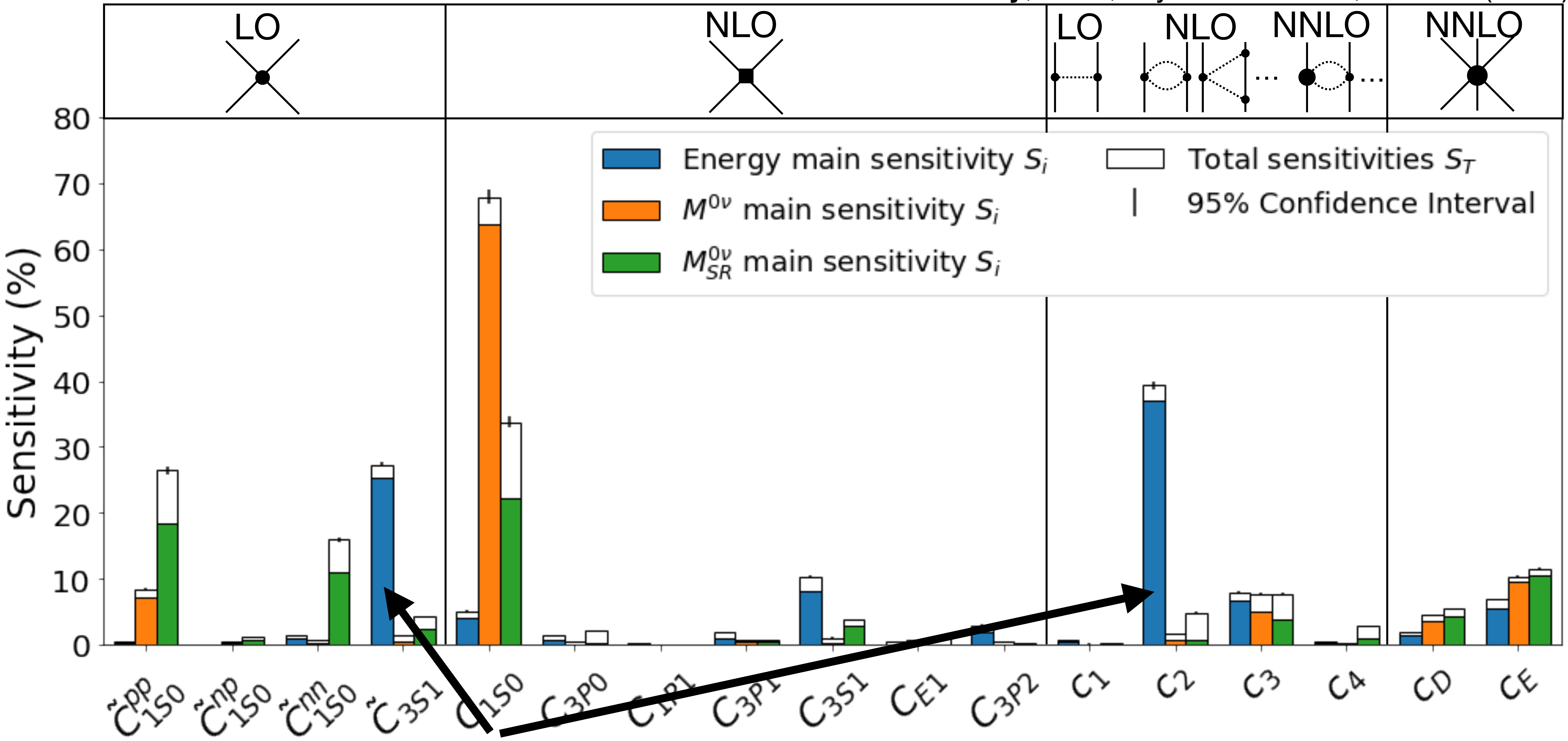
Belley, et al.,Phys. Rev. C **113**, 014319 (2026)



The total matrix element mostly depends on one LEC!

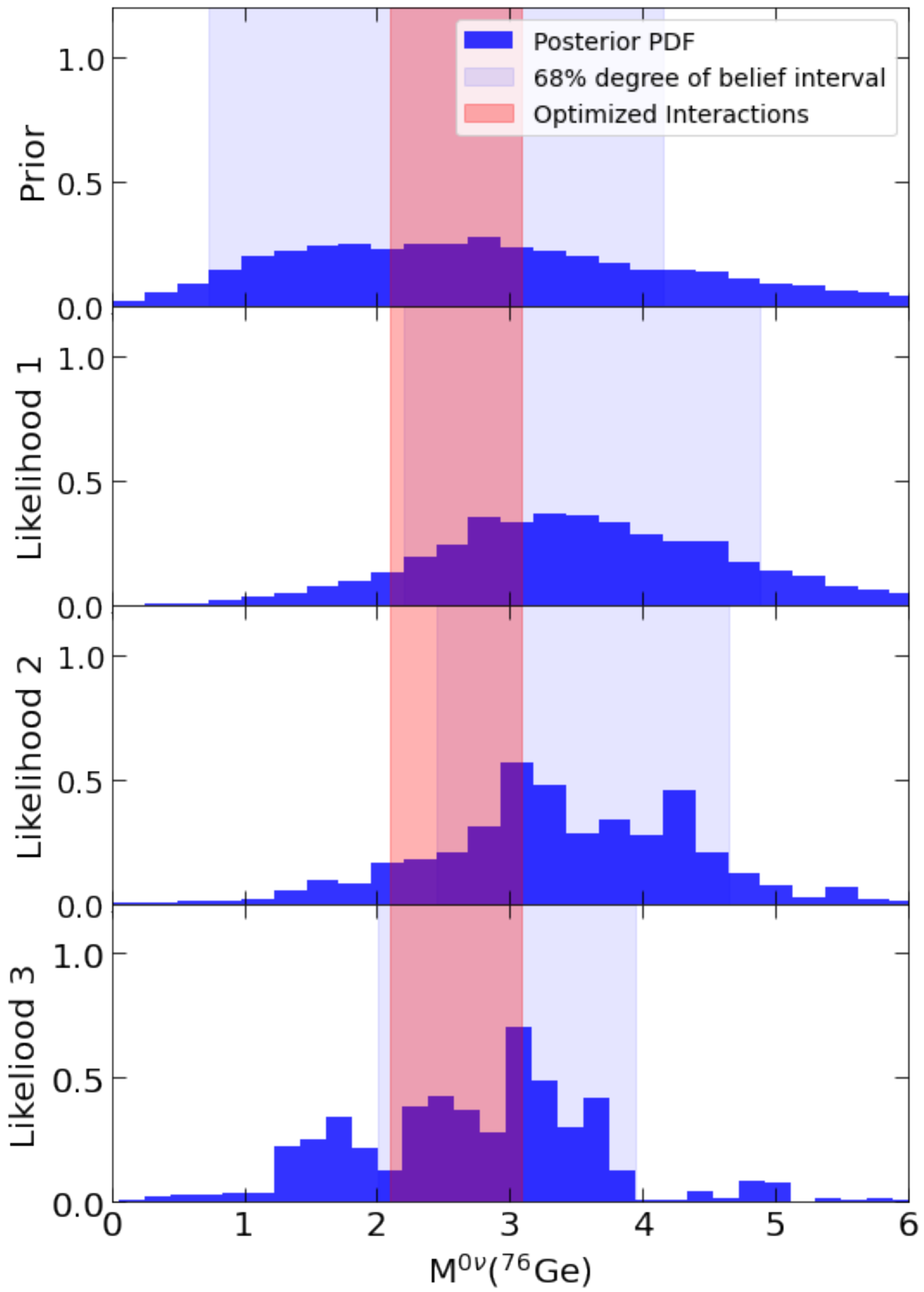
The MM-DGP Algorithm: GSA

Belley, et al.,Phys. Rev. C **113**, 014319 (2026)



Results for energies are consistent with results of physics-based emulators of the coupled cluster method.

Choosing a Likelihood: Example $0\nu\beta\beta$



Likelihood 1: Only contains $^1S_0$ neutron-proton phase shifts at 50 MeV.

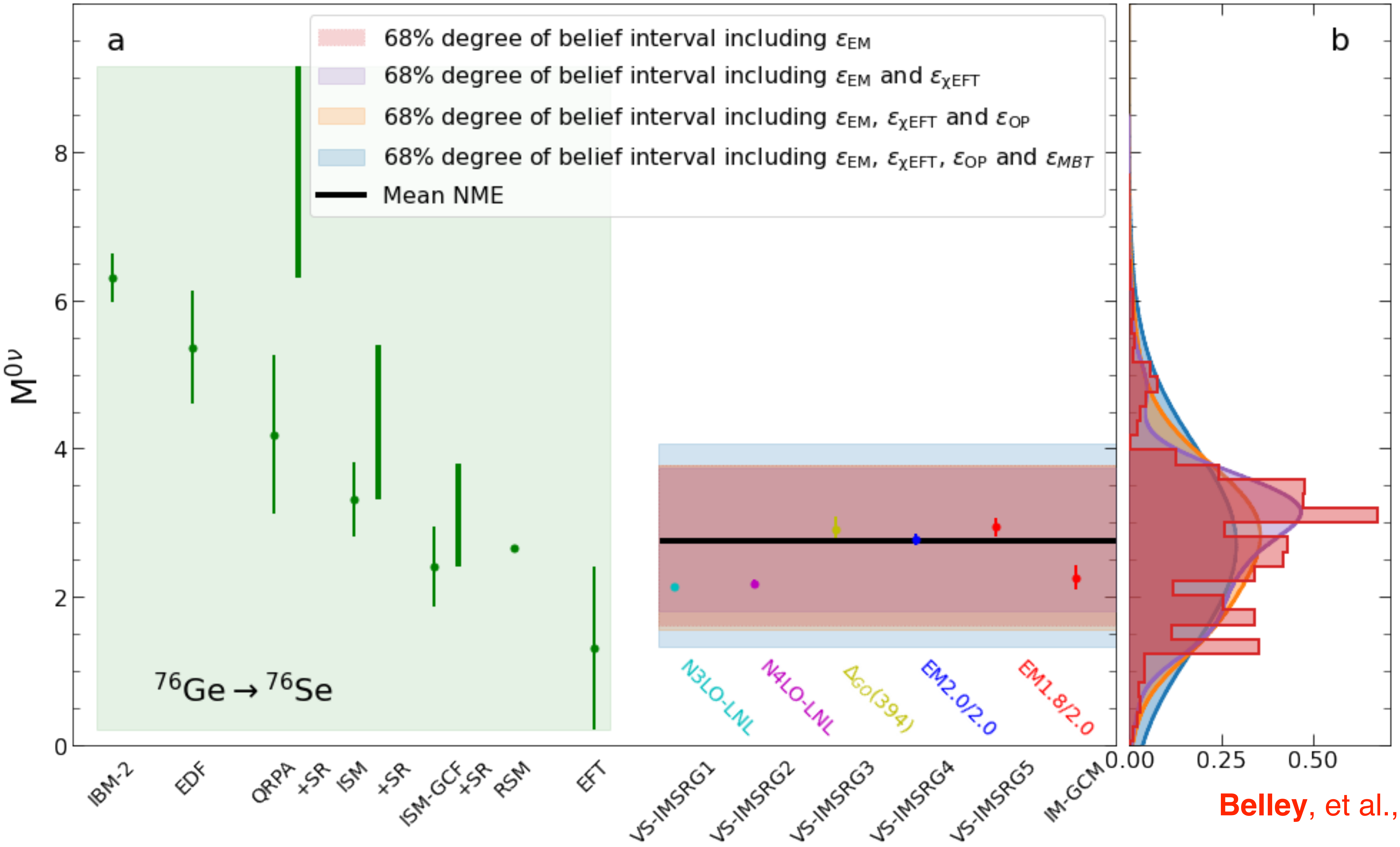
Likelihood 2: Contains $^1S_0$ neutron-proton phase shifts at 50 MeV and observables for A=2-4.

Likelihood 3: Contains $^1S_0$ neutron-proton phase shifts at 50 MeV and observables for A=2-4,16.

A2-4: $E(^2H)$, $r_p(^2H)$, $Q(^2H)$, $E(^3H)$, $E(^4He)$, $r_p(^4He)$

A16: $E(^{16}O)$, $r_p(^{16}O)$

Combining All Sources of Uncertainty



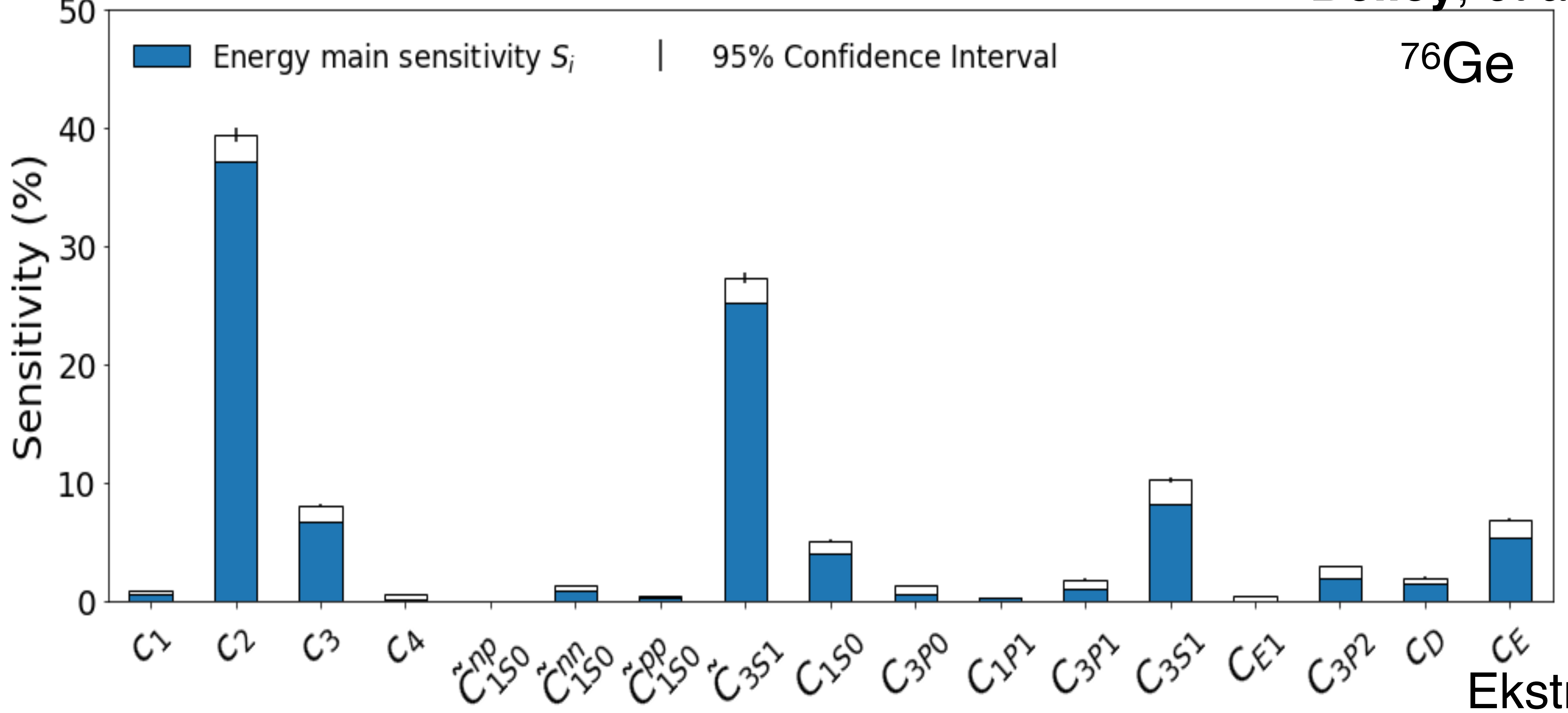
$$M^{0\nu\beta\beta} = 2.60^{+1.28}_{-1.36}$$

Belley, et al., Phys. Rev. Lett. 132, 182502

The MM-DGP Algorithm: GSA

Belley, et al.,Phys. Rev. C **113**, 014319 (2026)

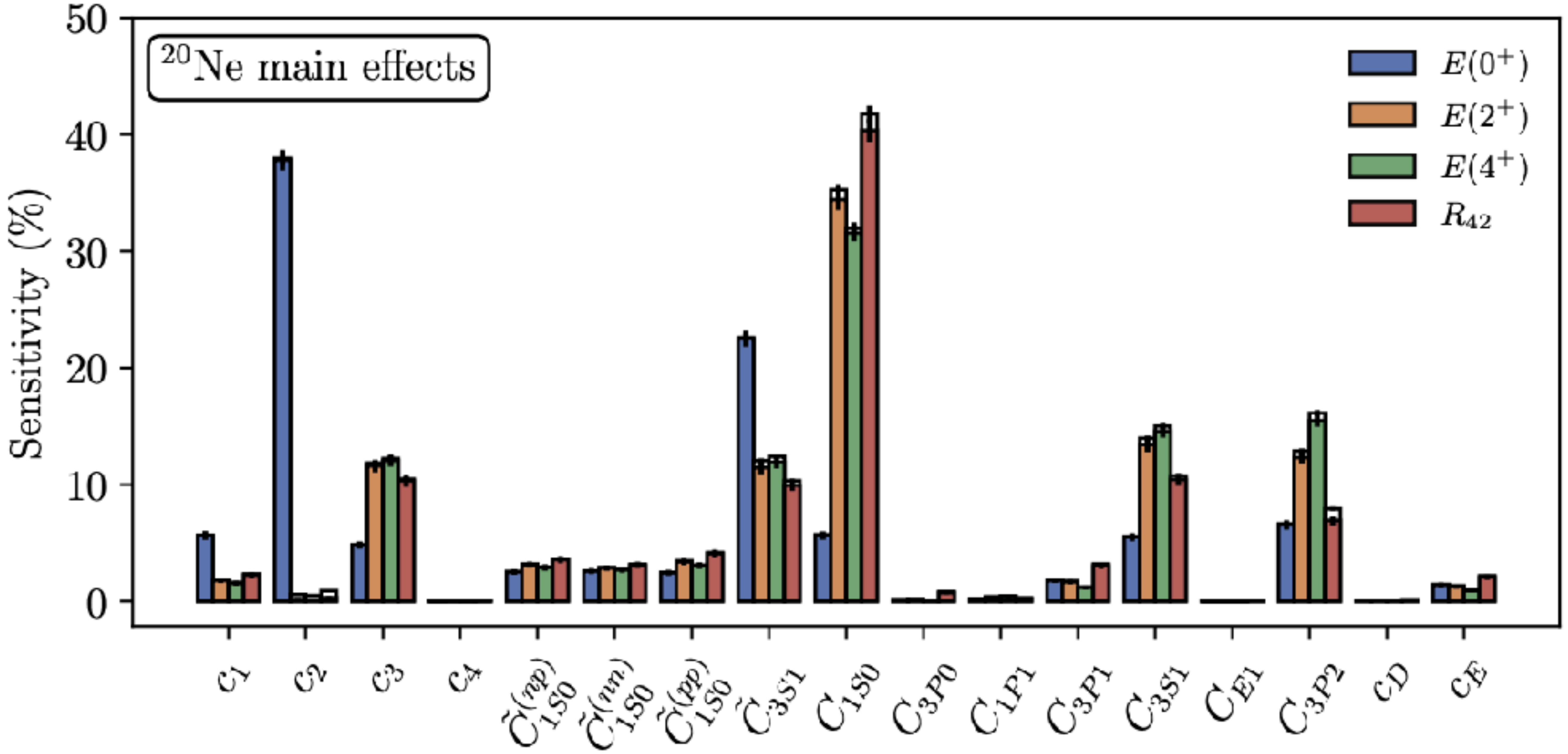
Data driven MM-DGP



Ekström, et al., arXiv:2305.06955 (2023)

vs

Physics Driven

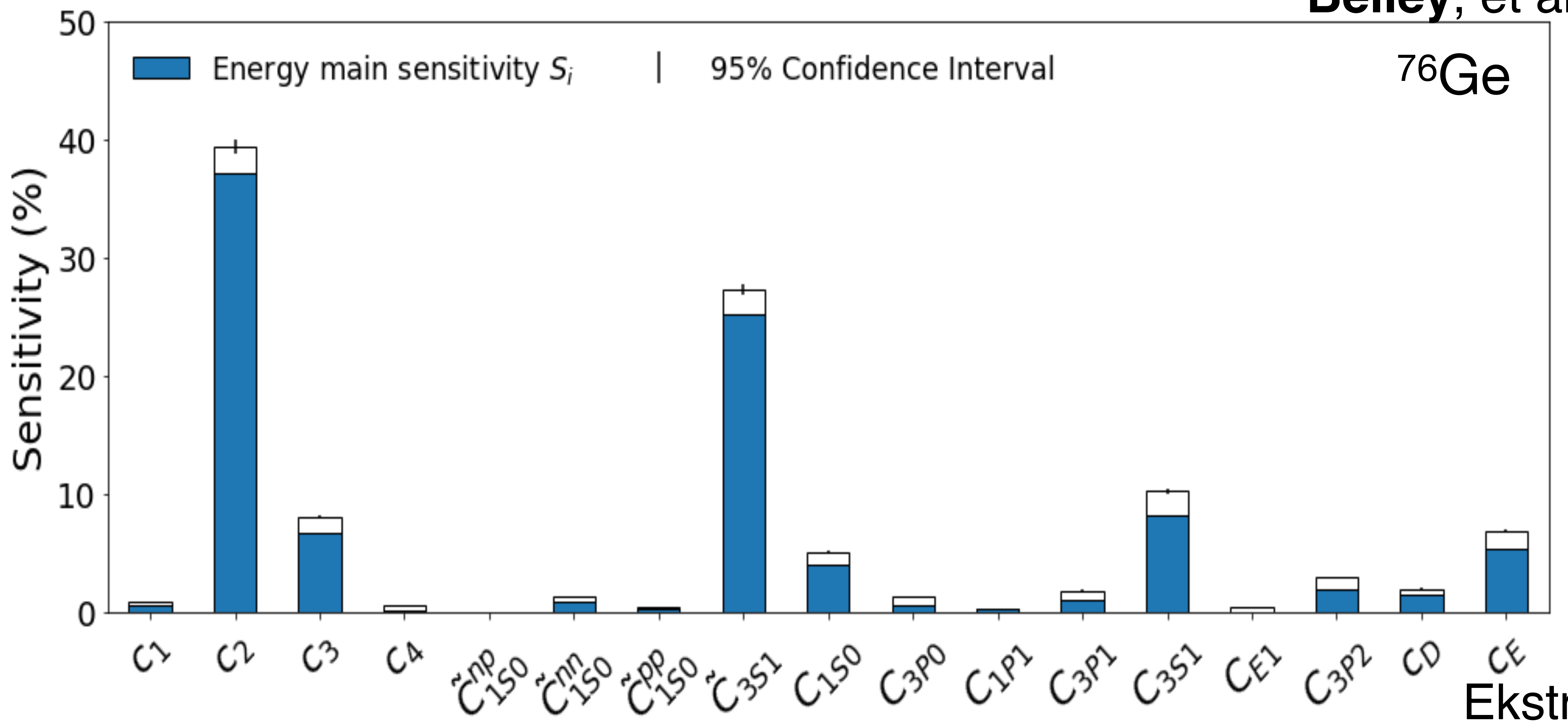


Global emulation

The MM-DGP Algorithm: GSA

Belley, et al.,Phys. Rev. C **113**, 014319 (2026)

Data driven MM-DGP



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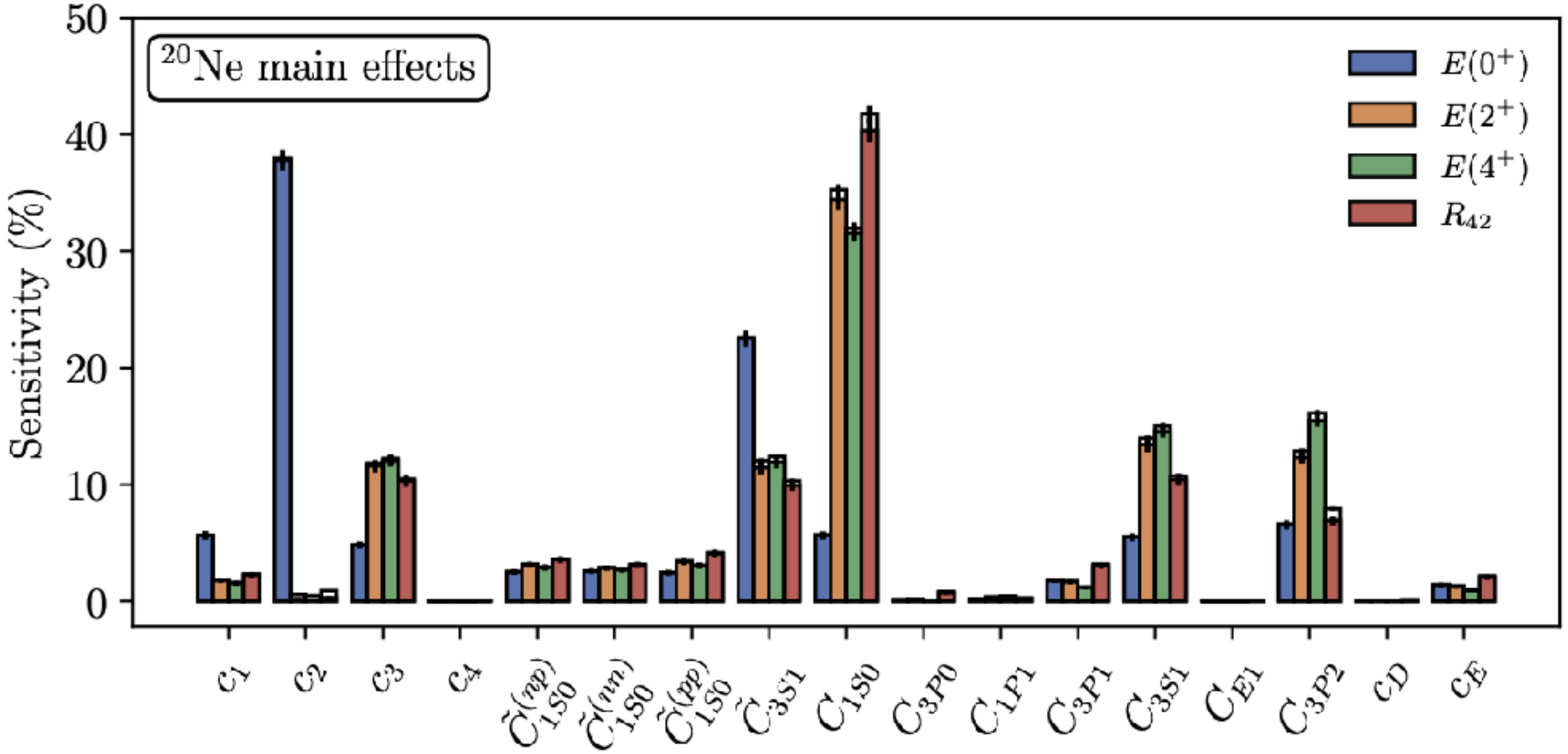
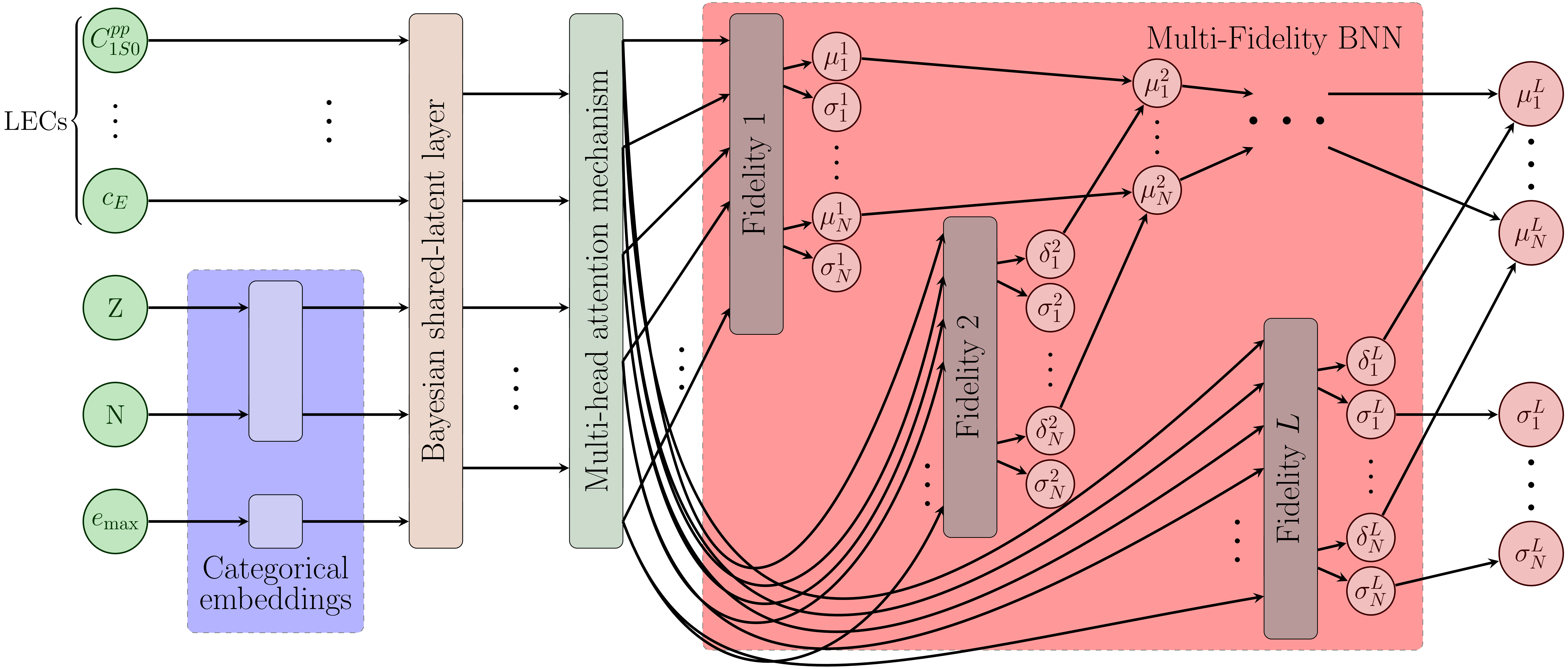


Jose Miguel Muñoz Arias

BANNANE

BAyesian Neural Network for Atomic Nuclei Emulation



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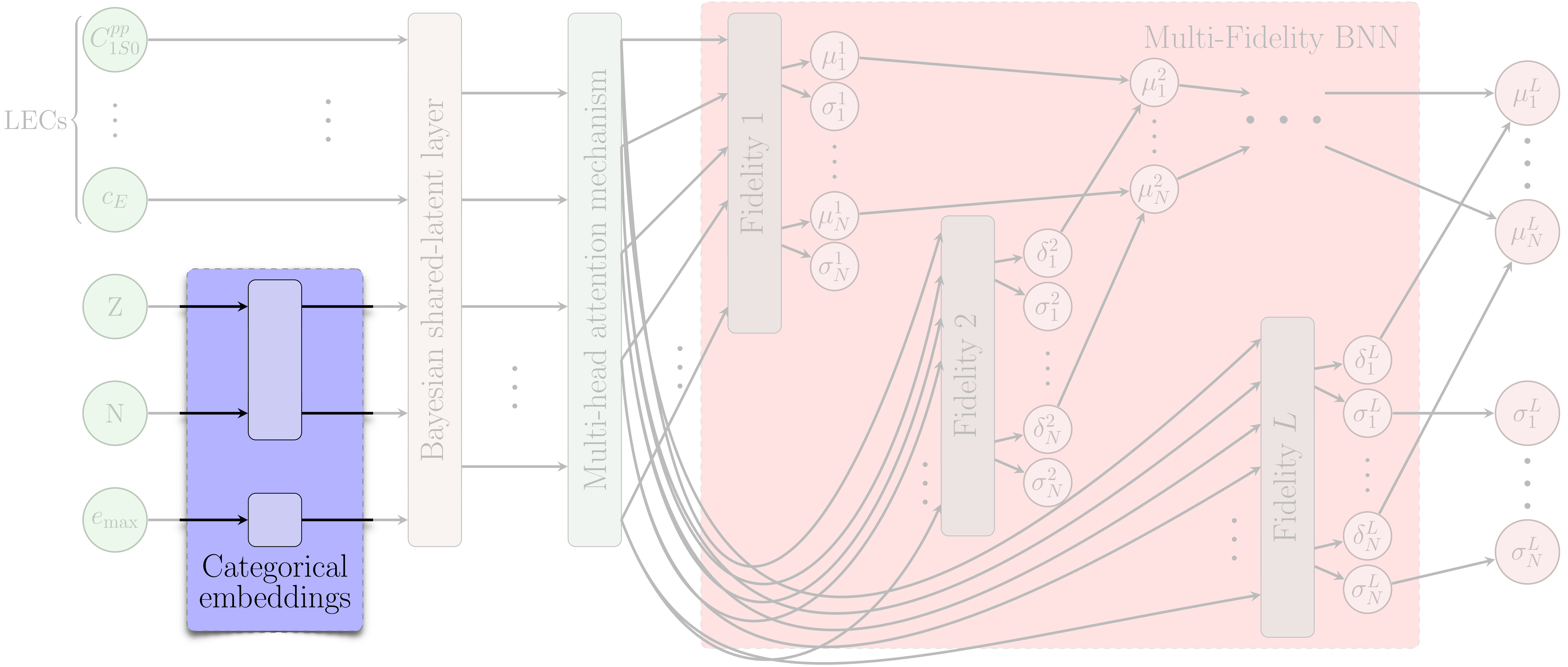
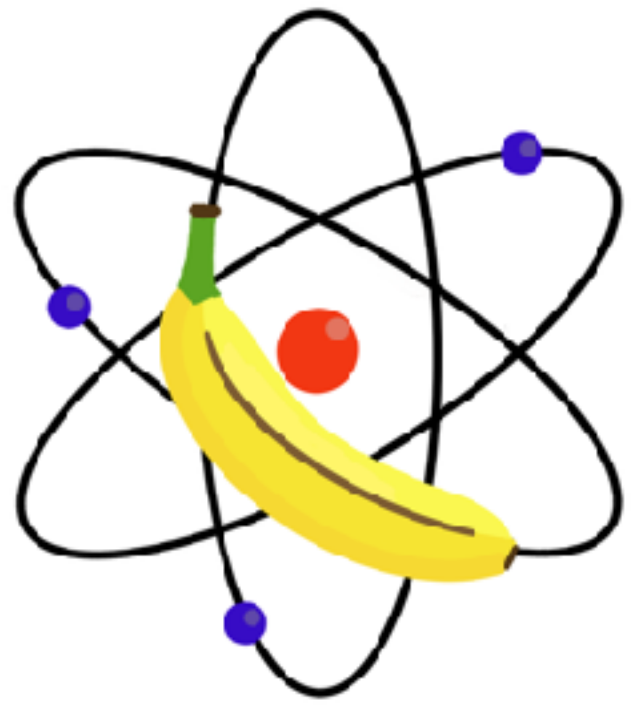


Embeddings



Embeddings

Encodes discrete data into a vector space, while learning their relative positions, e.g.

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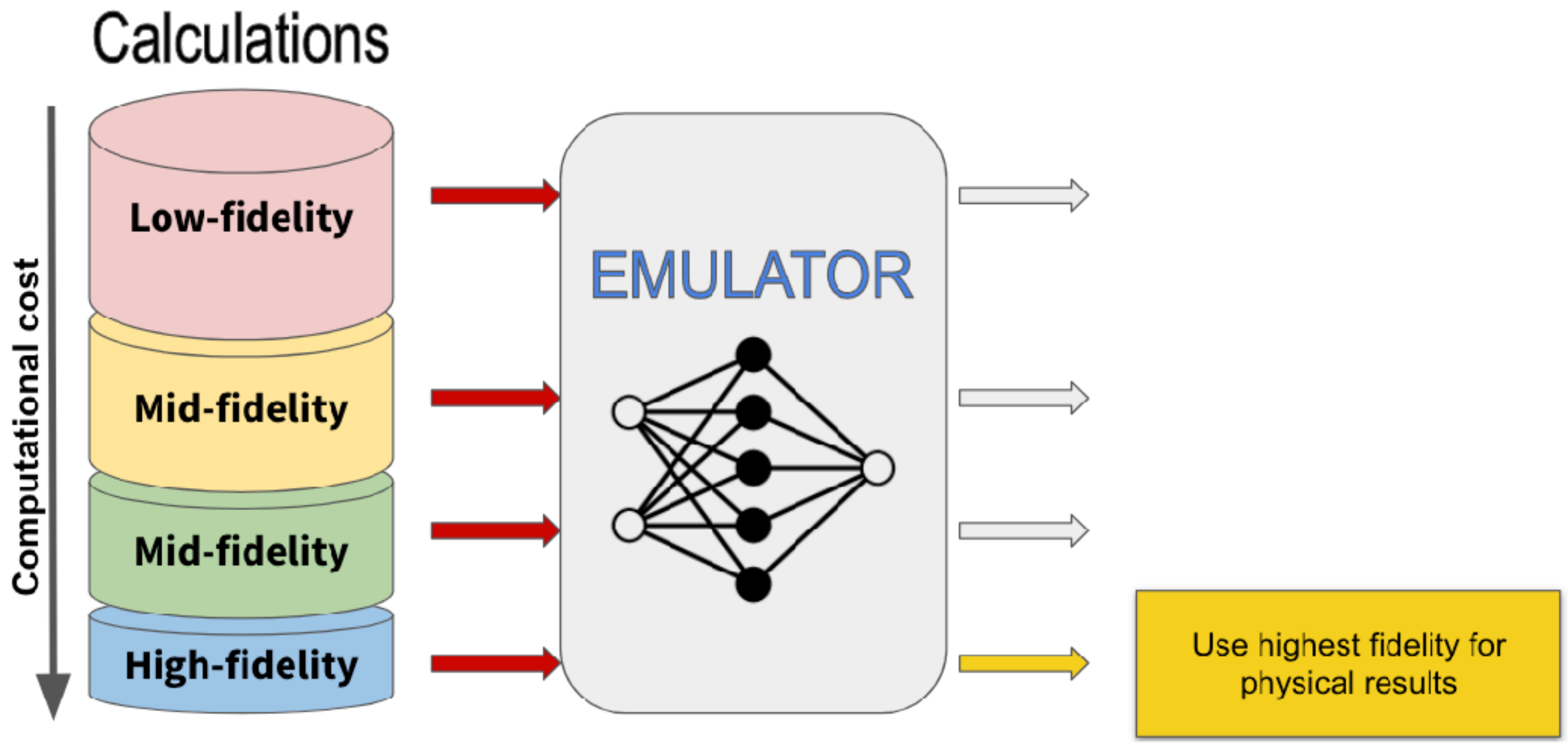

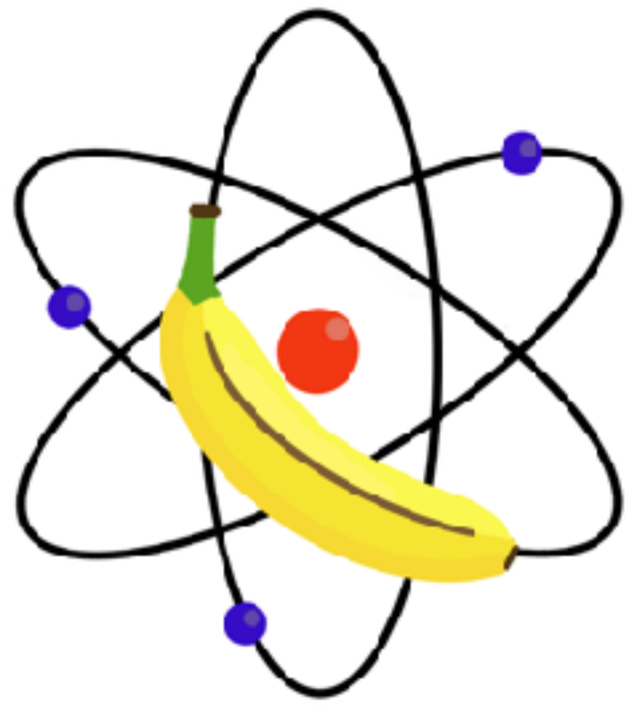

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- **Positions in the nuclear chart: ordering of N and Z**

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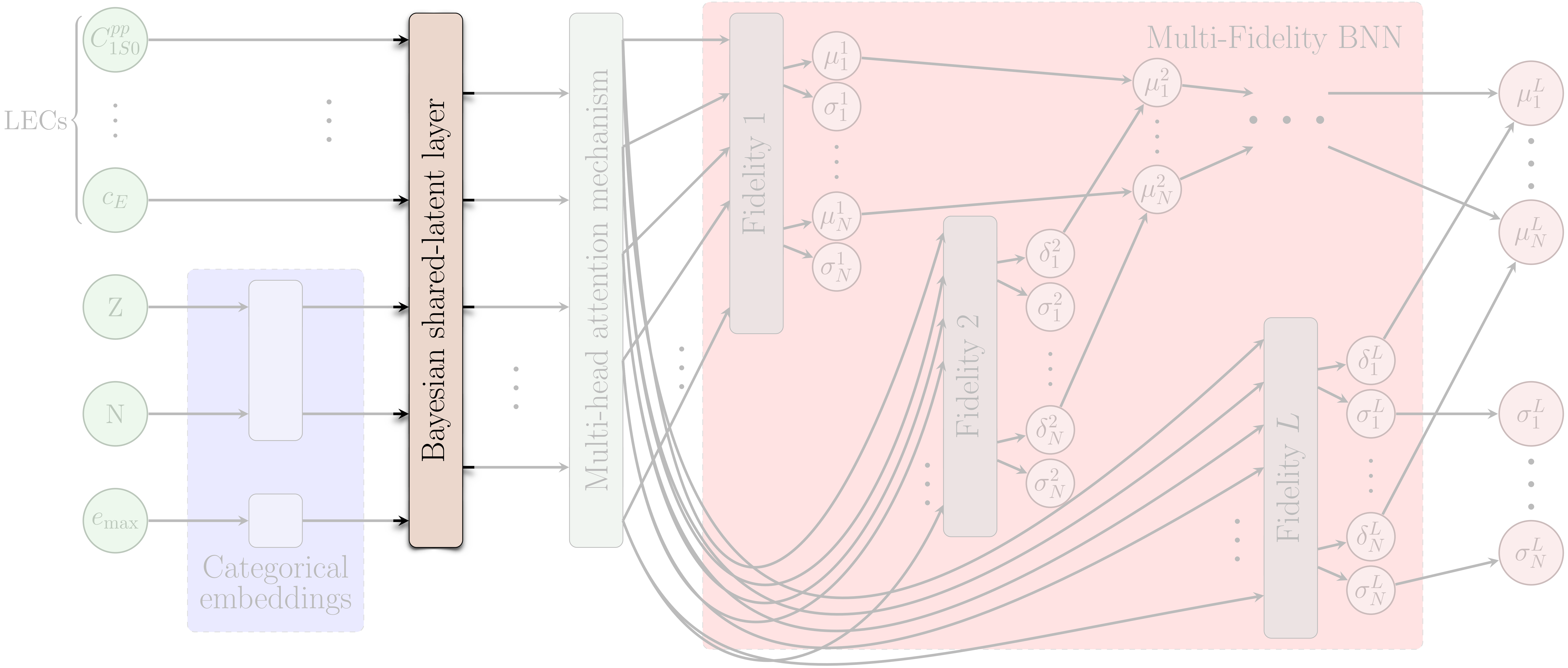

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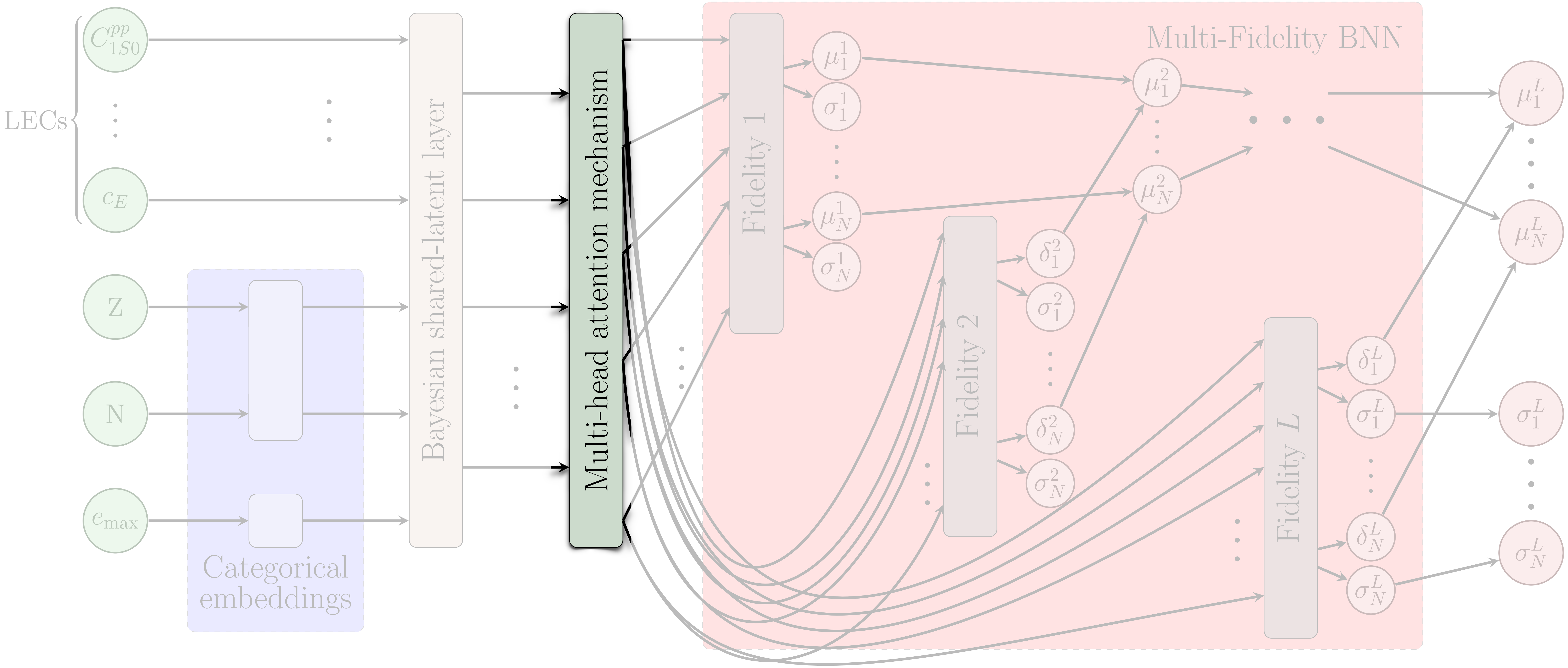
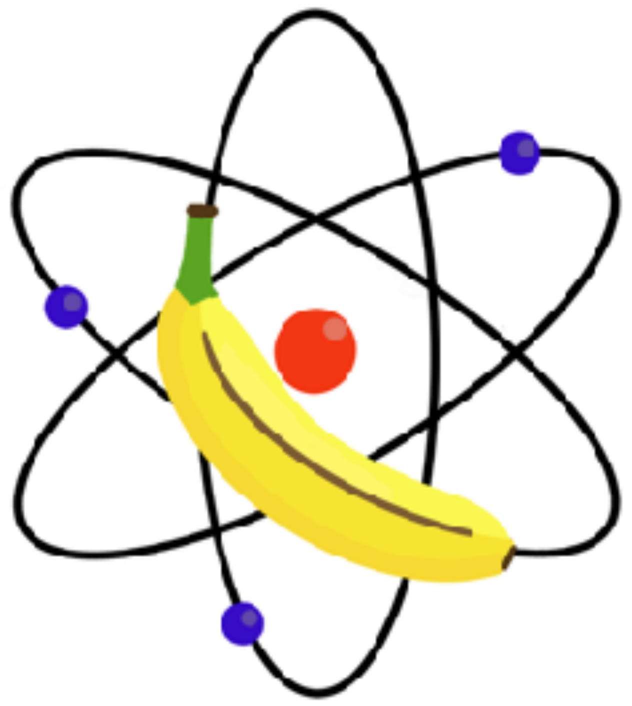
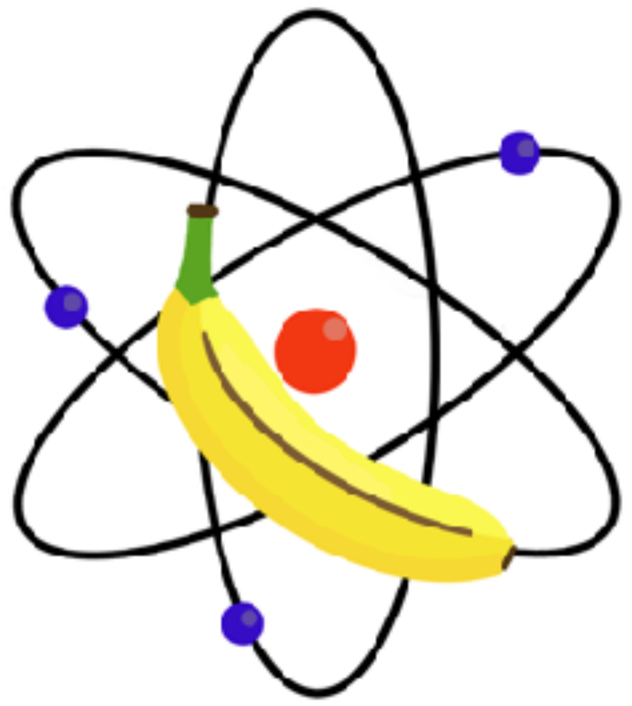




Attention!

- **Attention Mechanisms learns how the embeddings need to be adapted due to other inputs**
- **Responsible to for the improvements of large language models in recent years!**



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Attention Is All You Need

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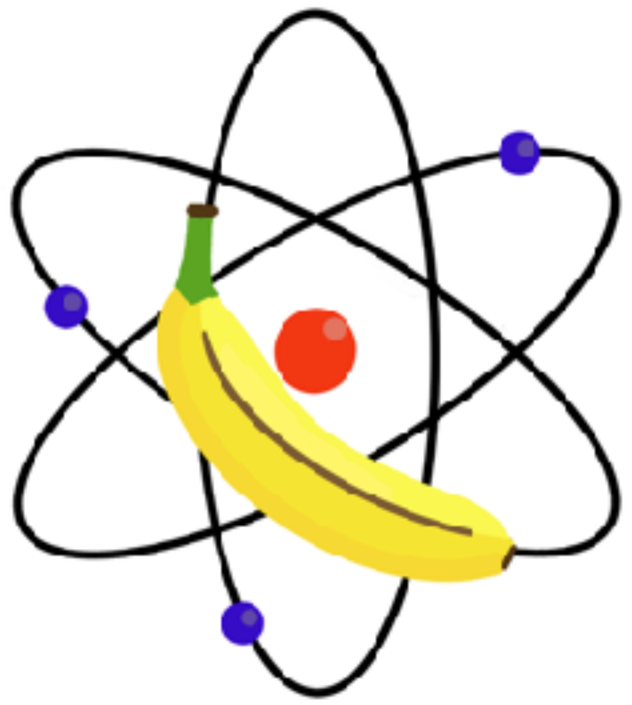
Illia Polosukhin* ‡ illia.polosukhin@gmail.com

244, 184 citations



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Illia Polosukhin* ‡ illia.polosukhin@gmail.com

244, 184 citations

Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, ... Demis Hassabis + Show authors

48, 990 citations

Attention!

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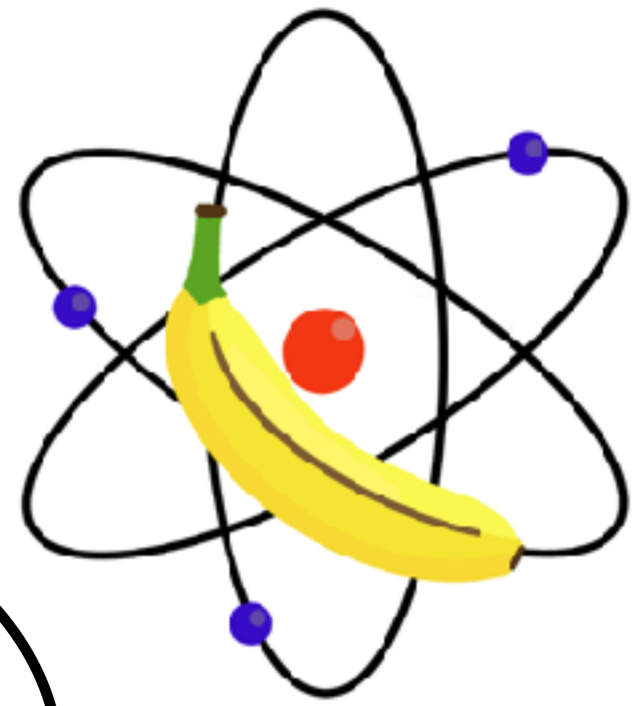

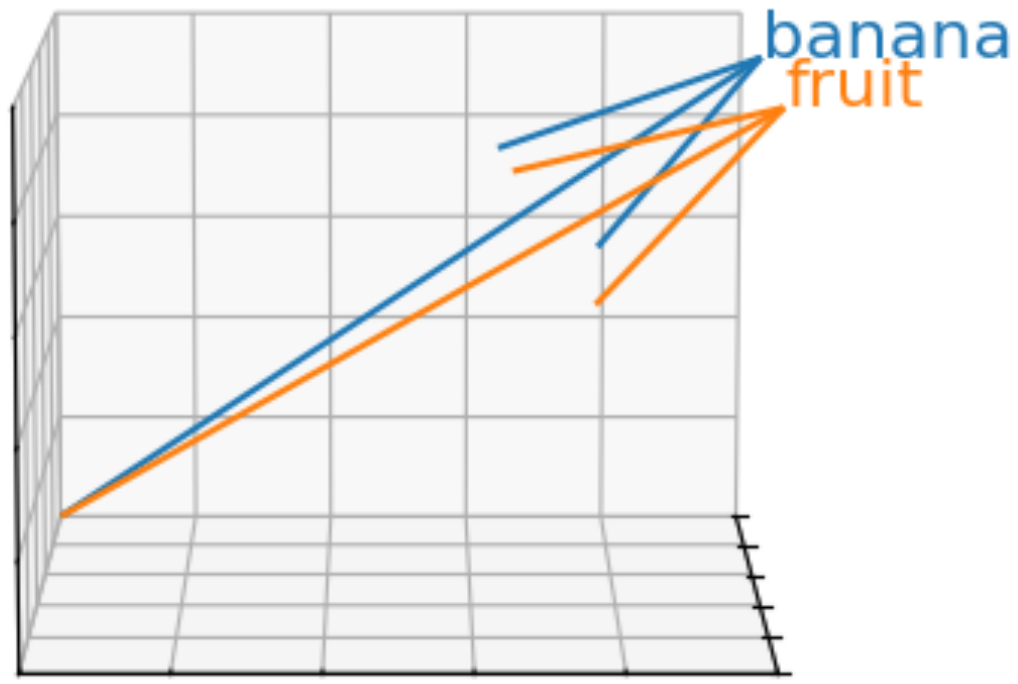

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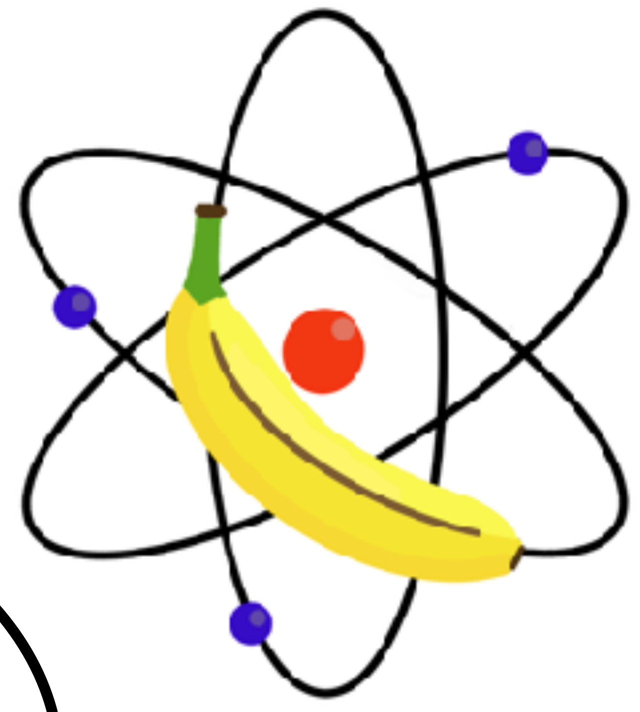
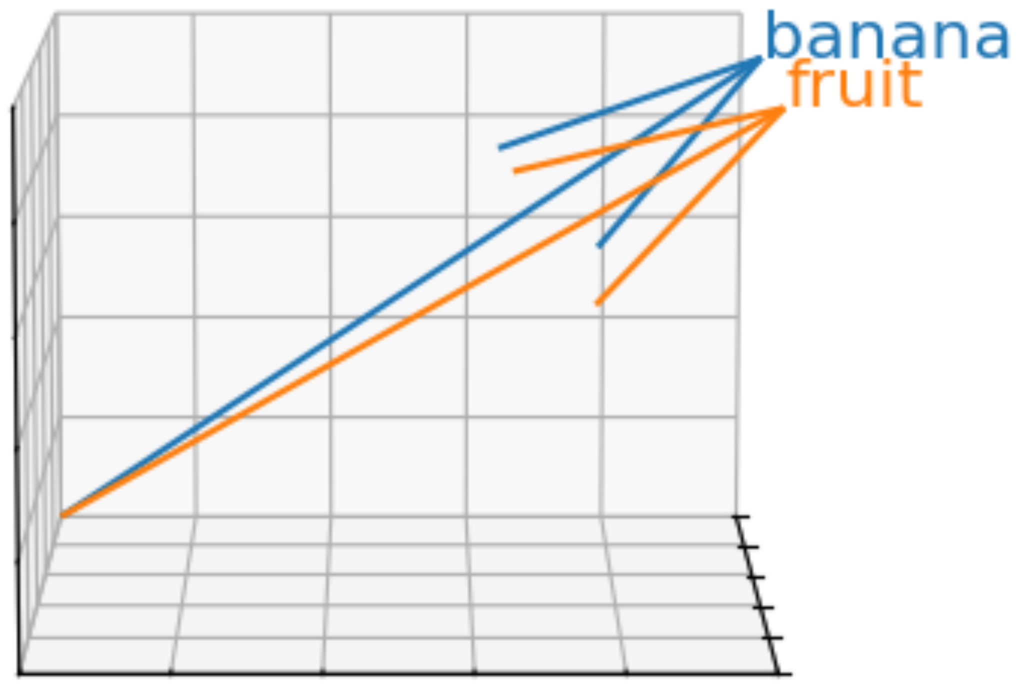


ChatGPT:



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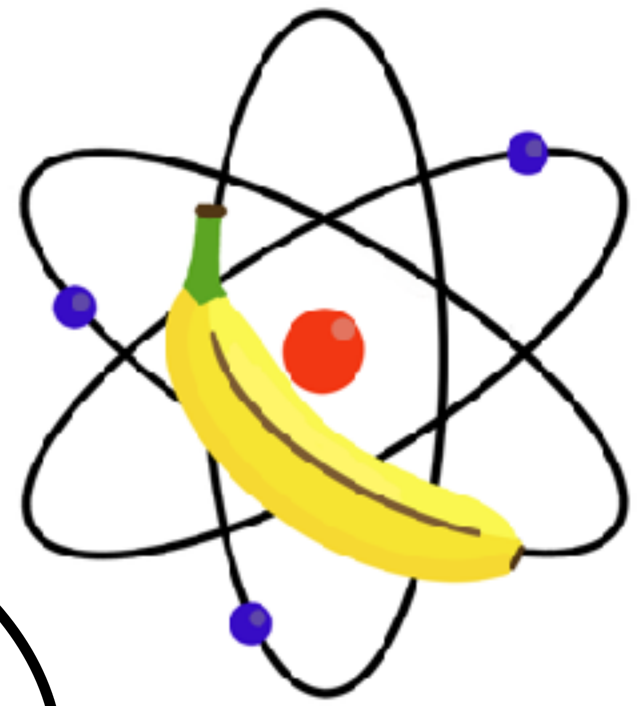

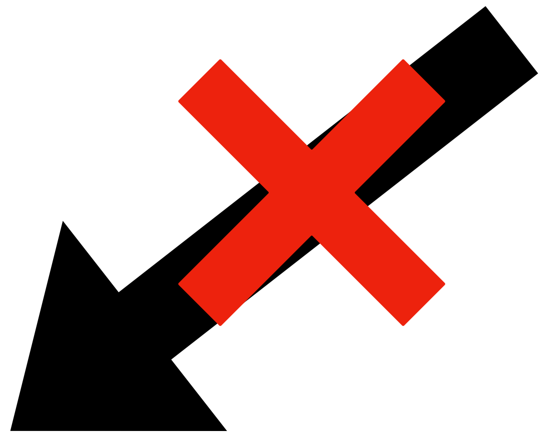

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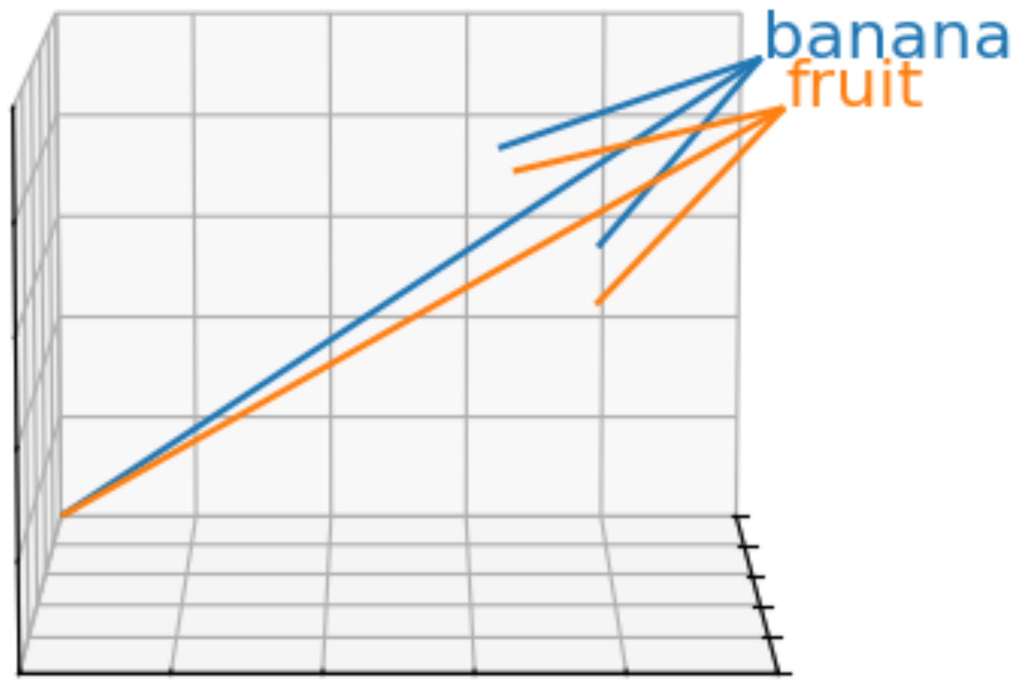

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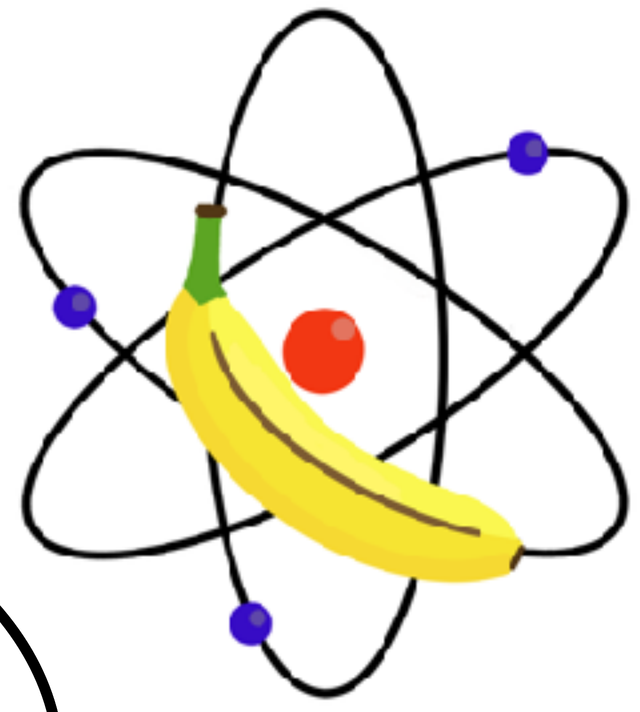
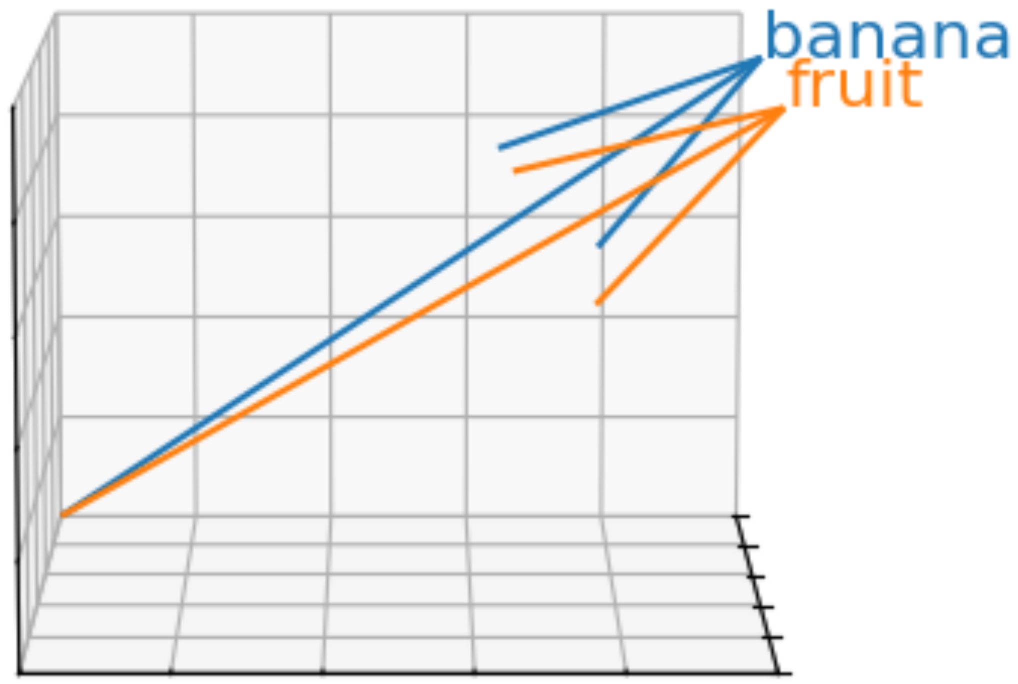
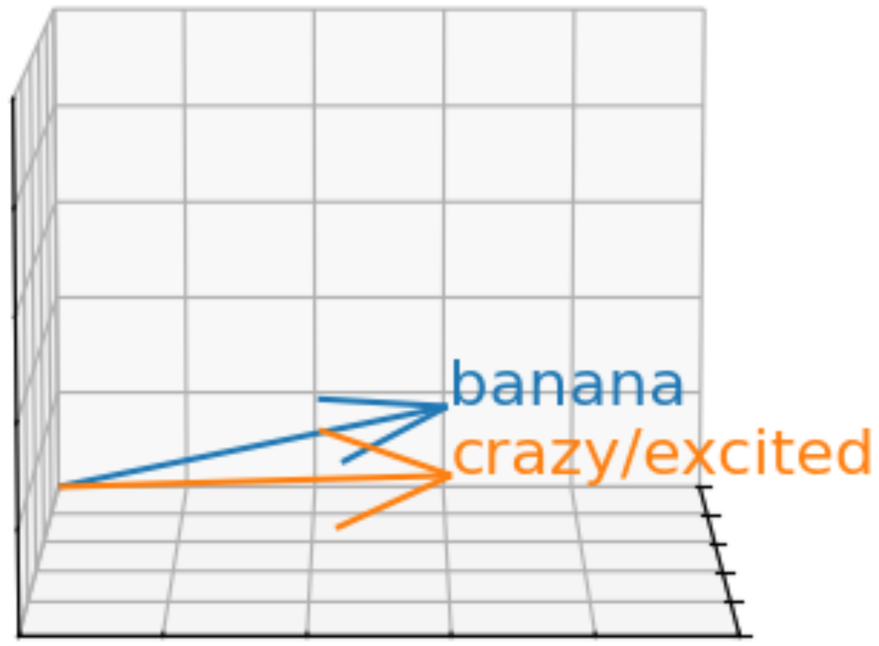
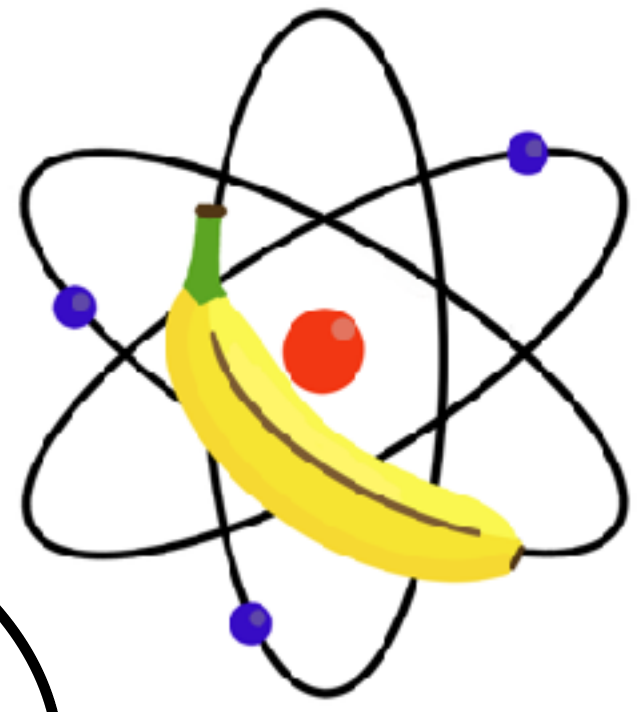


ChatGPT:





Attention!



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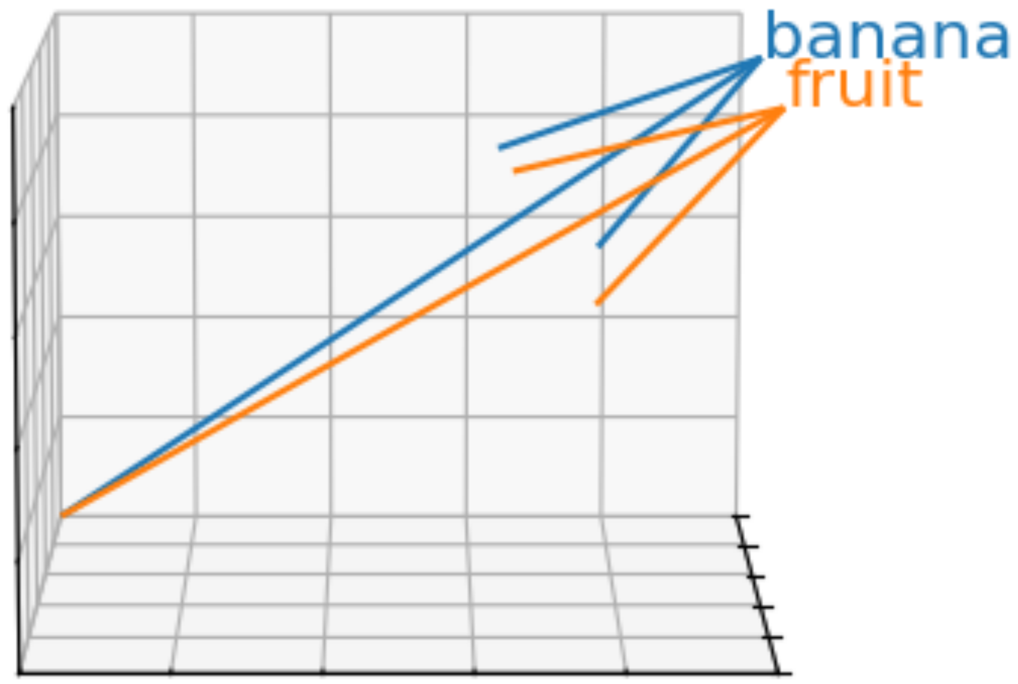

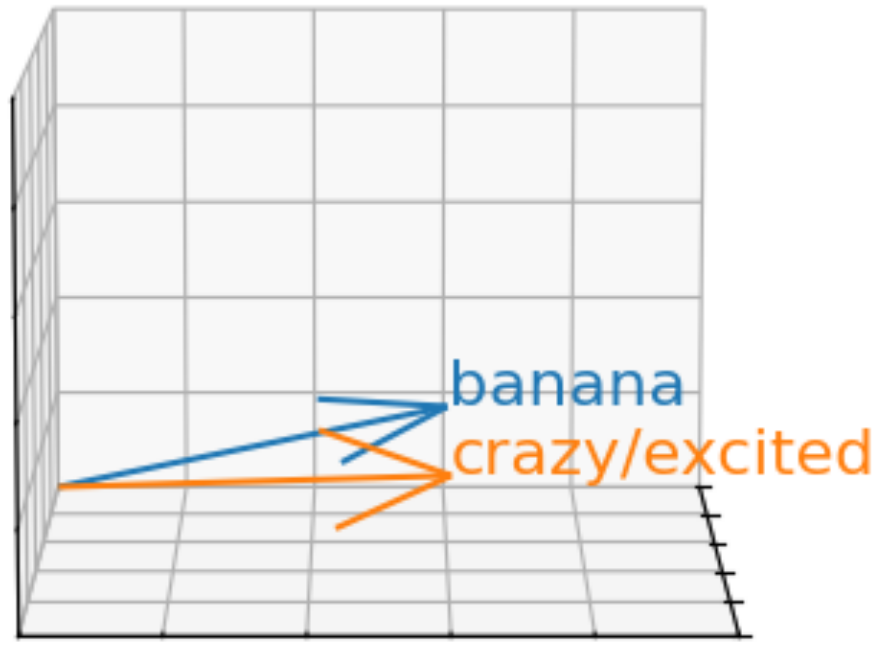

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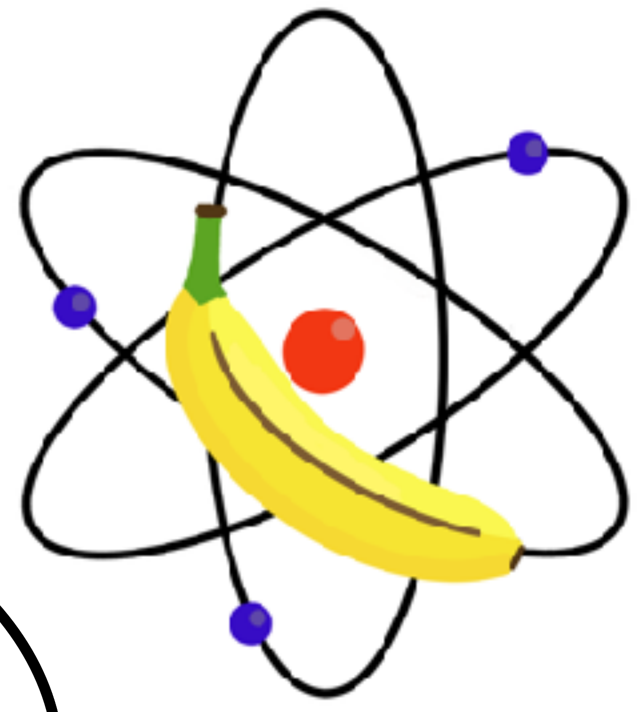

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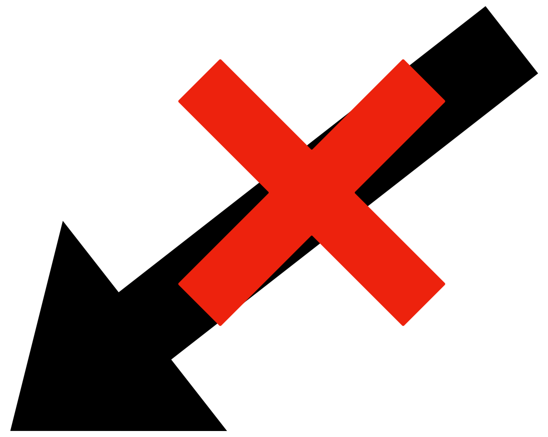
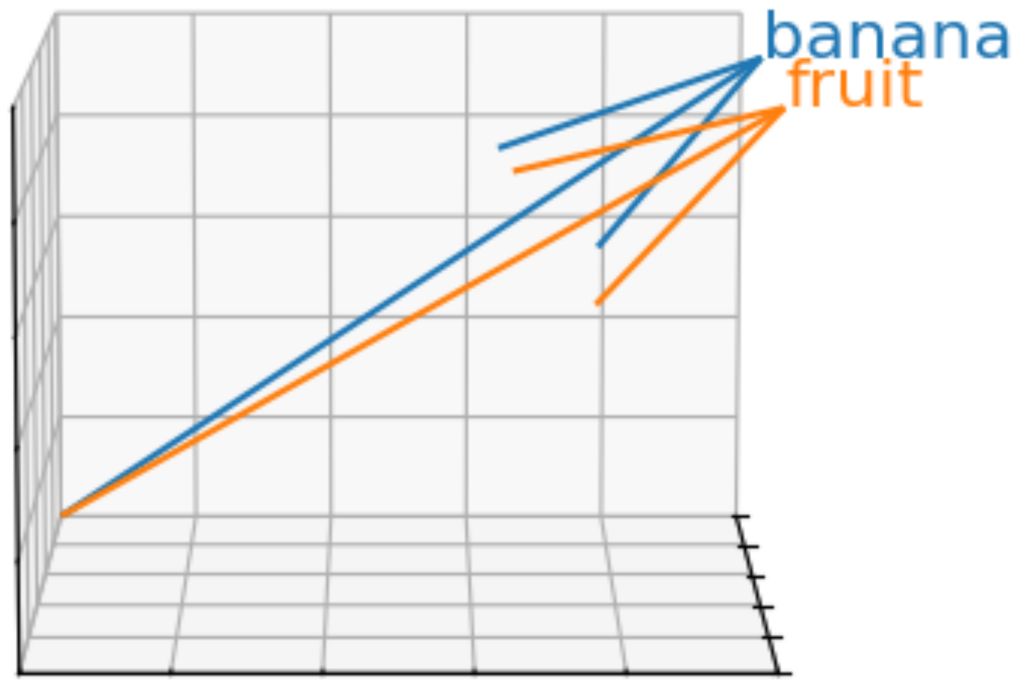
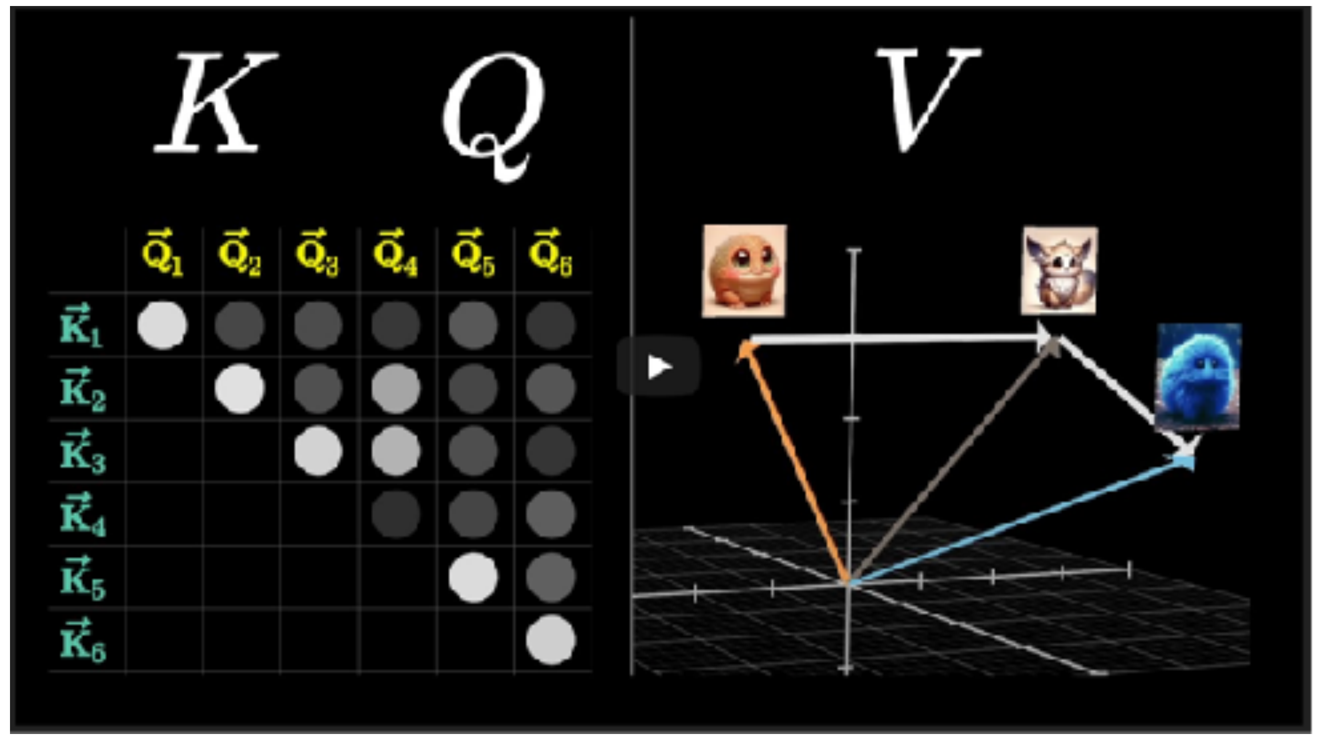
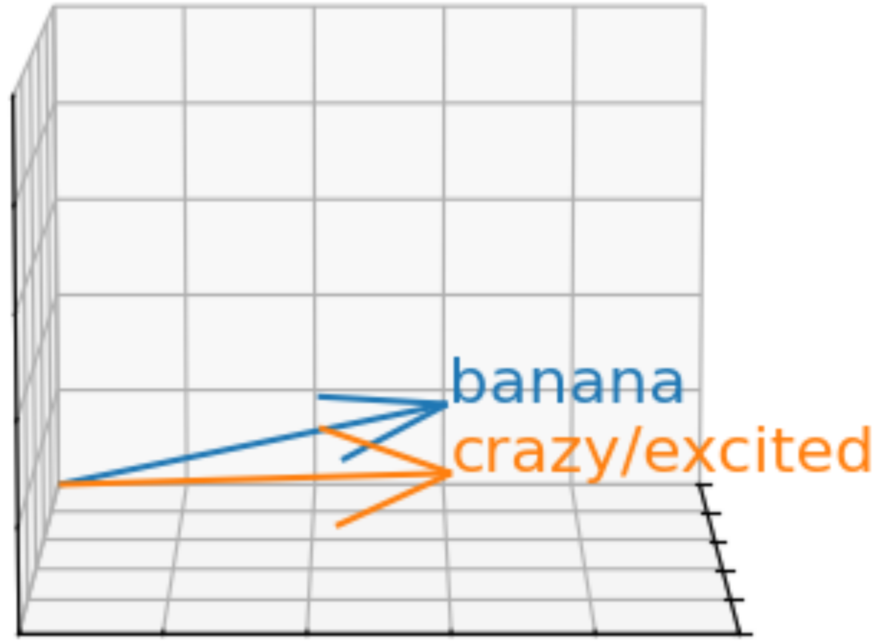


3Blue1Brown:

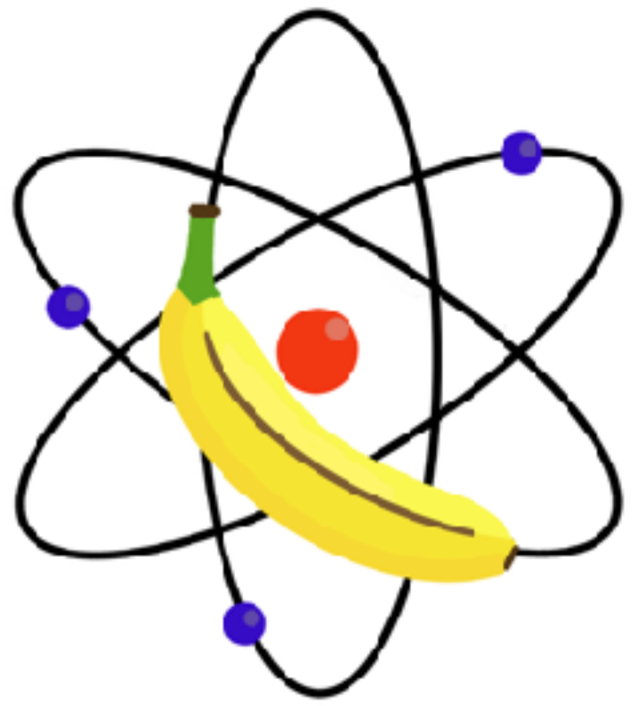




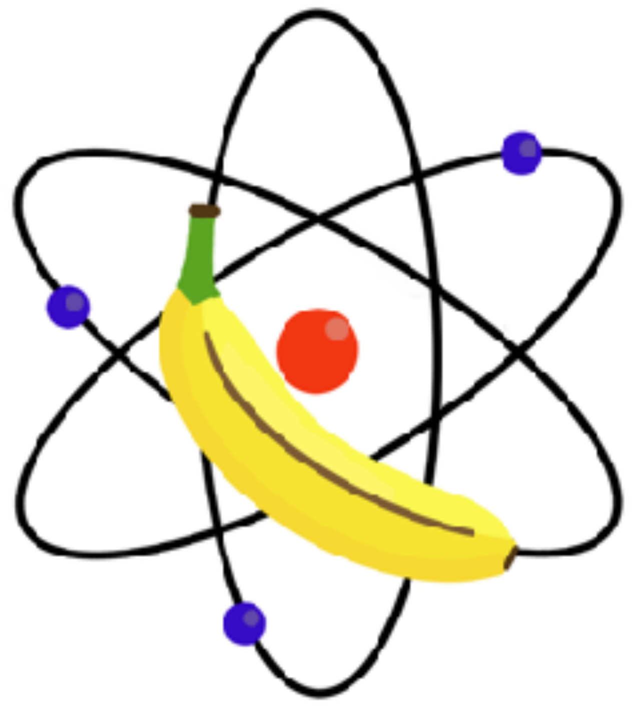


Attention

Embeddings: $\vec{x}_i$'s



Embeddings: $\vec{x}_i$'s $\longleftarrow$ N input of dimension M   i.e. X -> NxM



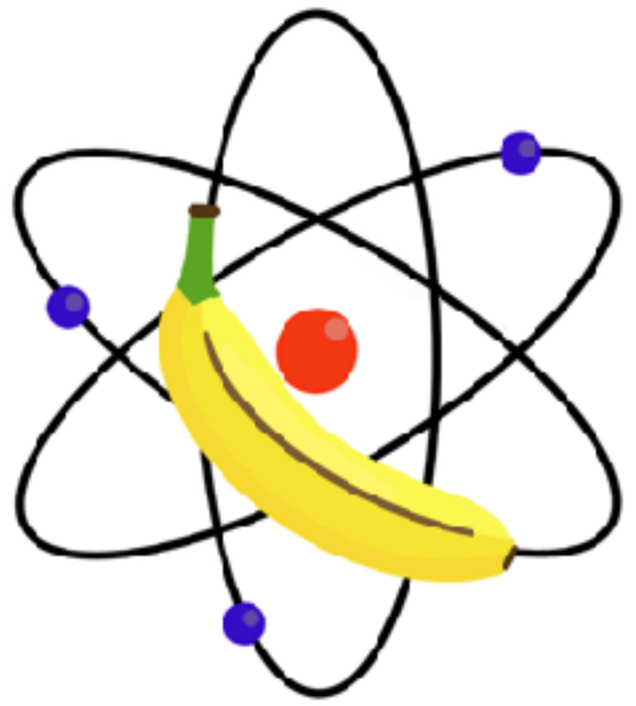
Attention

Embeddings: $\vec{x}_i$'s ⟵ N input of dimension M   i.e. X -> NxM

Query matrix: $W_Q \rightarrow Q = W_Q X$

Key matrix: $W_K \rightarrow K = W_K X$

Value matrix: $W_V \rightarrow V = W_V X$



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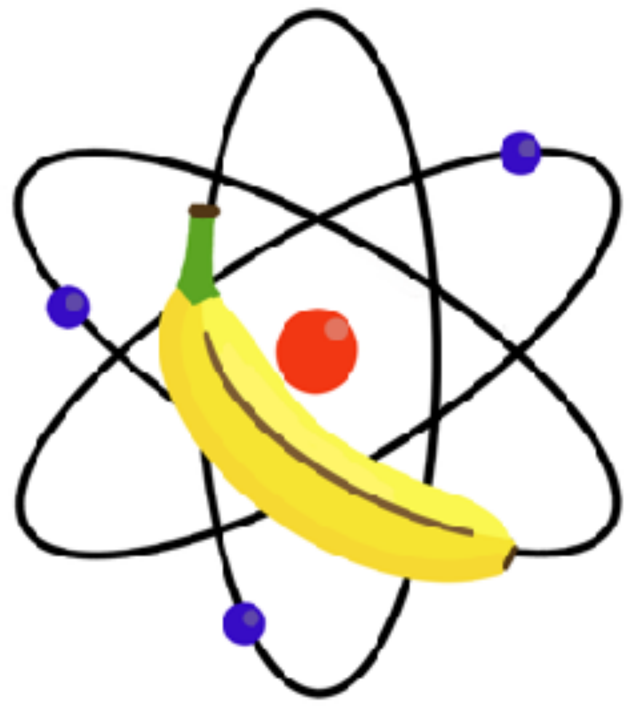
All matrix elements of these matrices are tunable parameters.



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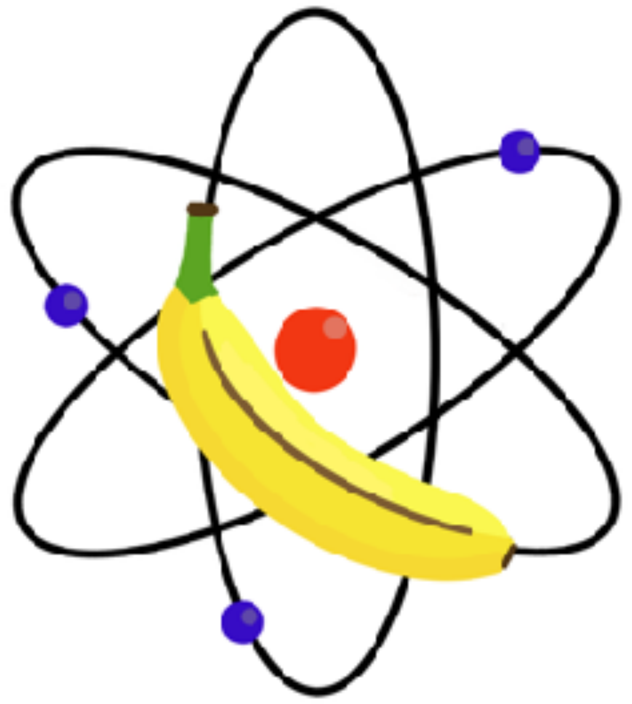
All matrix elements of these matrices are tunable parameters.

$$\boxed{Attention(Q, K, V) = softmax\left(\frac{QK^T}{\sqrt{d}}\right)V}$$



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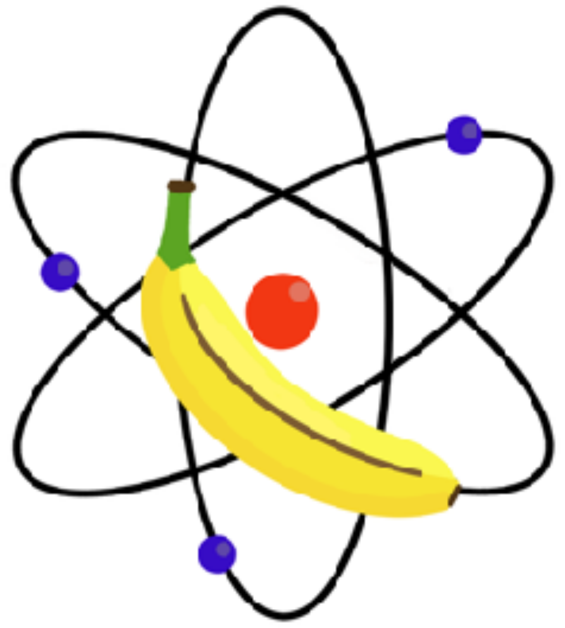
All matrix elements of these matrices are tunable parameters.

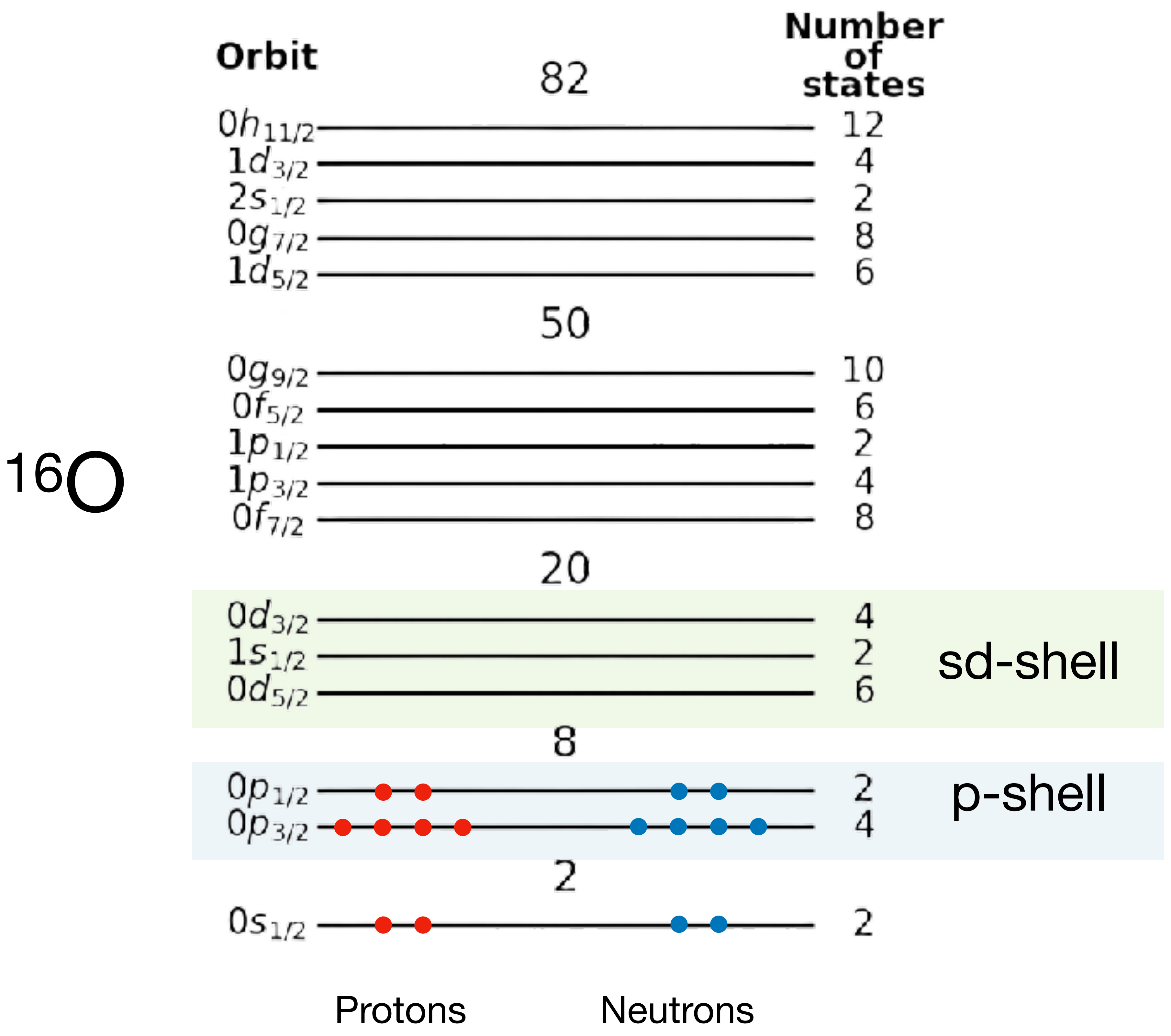
$$\boxed{Attention(Q, K, V) = softmax\left(\frac{QK^T}{\sqrt{d}}\right)V}$$

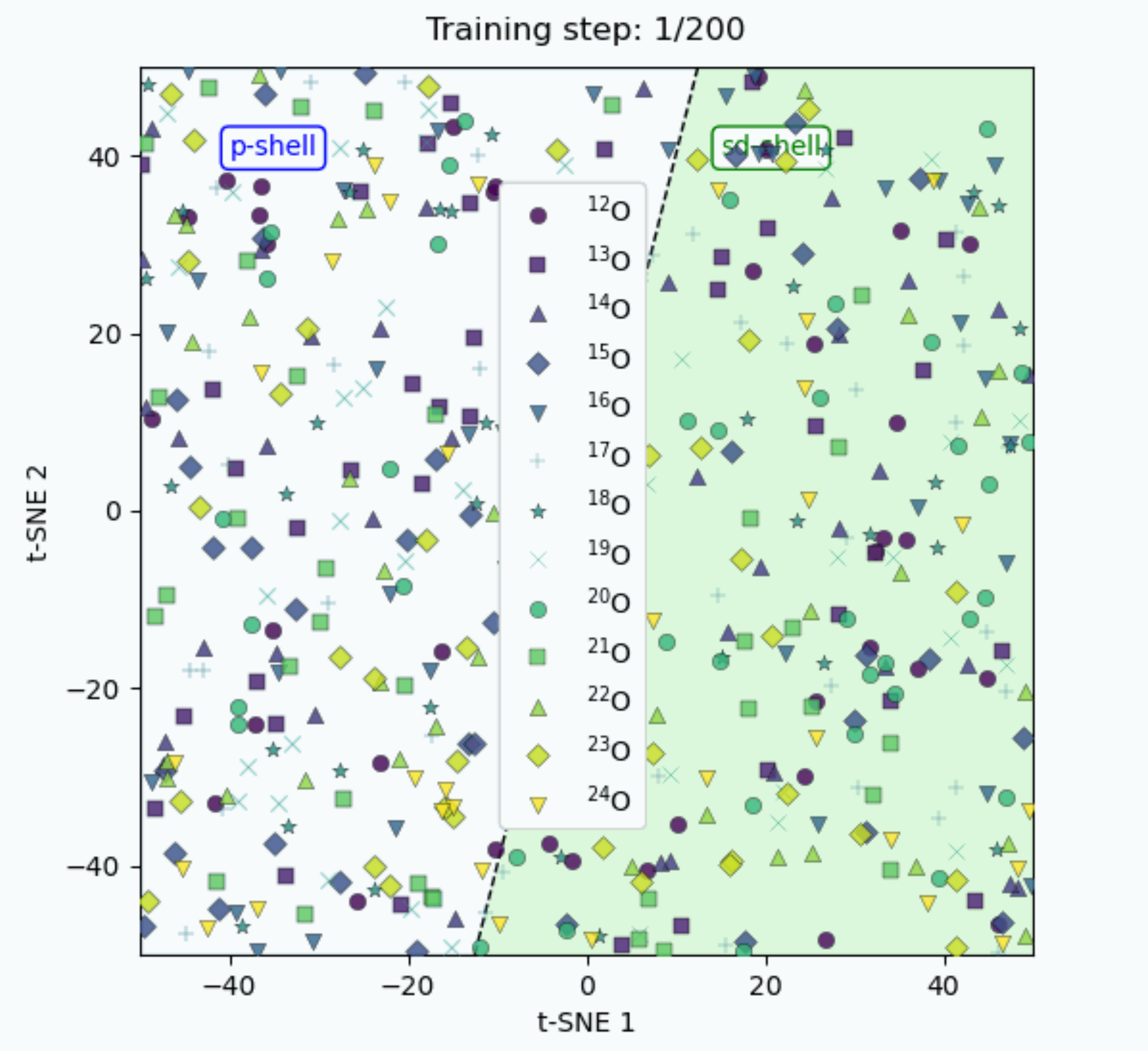
Finally $X \rightarrow X + Attention(Q, K, V)$

Visualizing the Embeddings



- Projection of embeddings from the attention mechanism.
- Model is learning nuclear shells!





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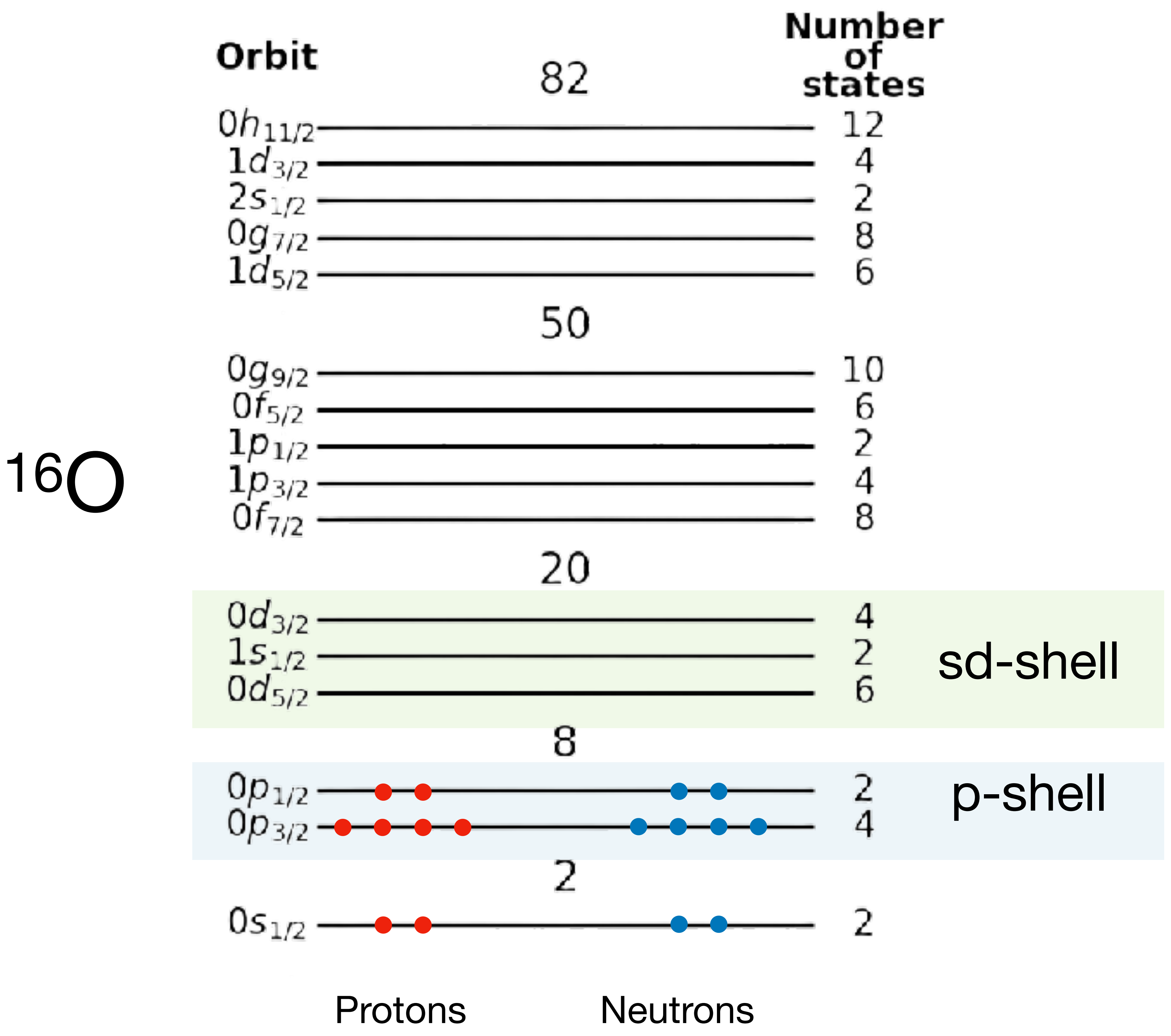

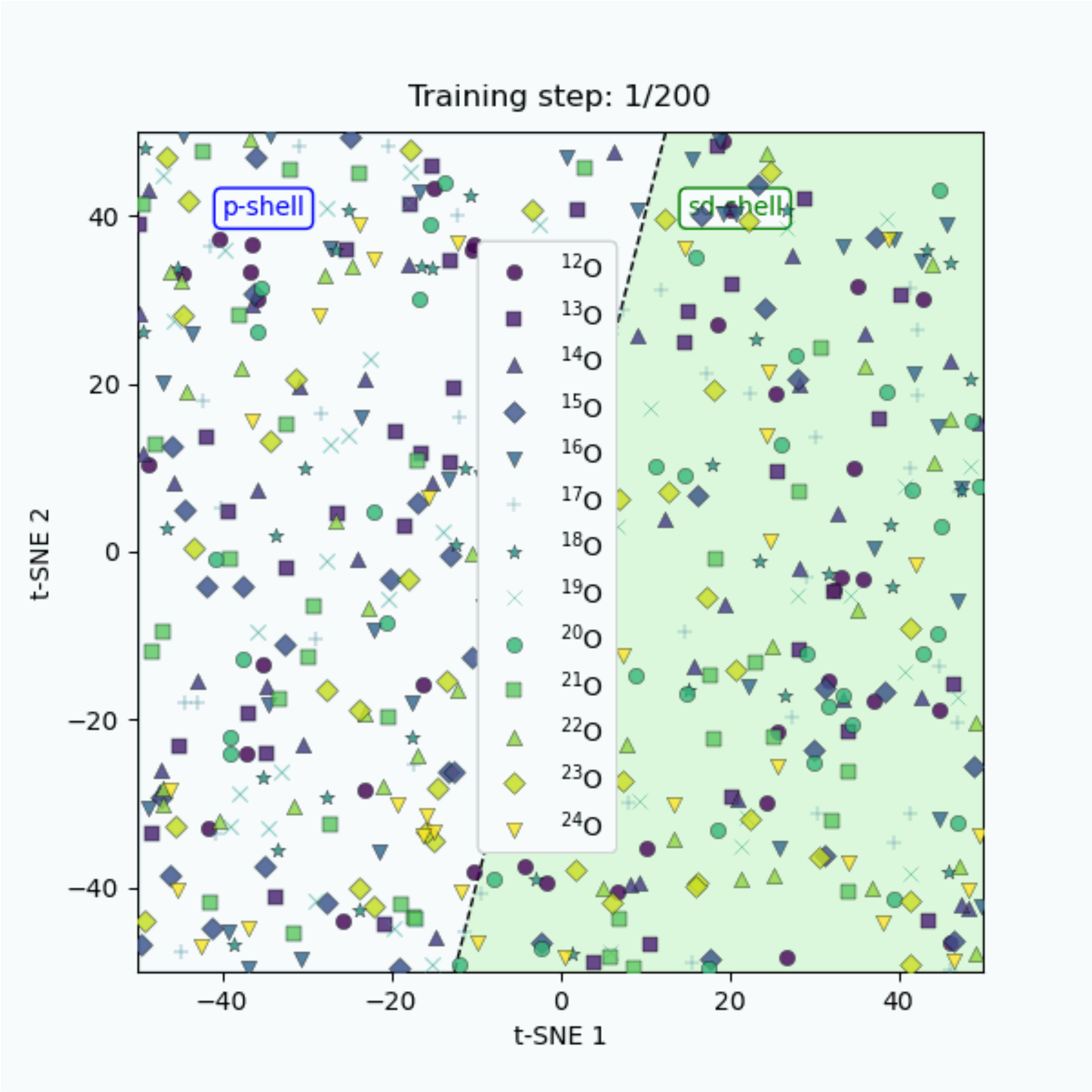

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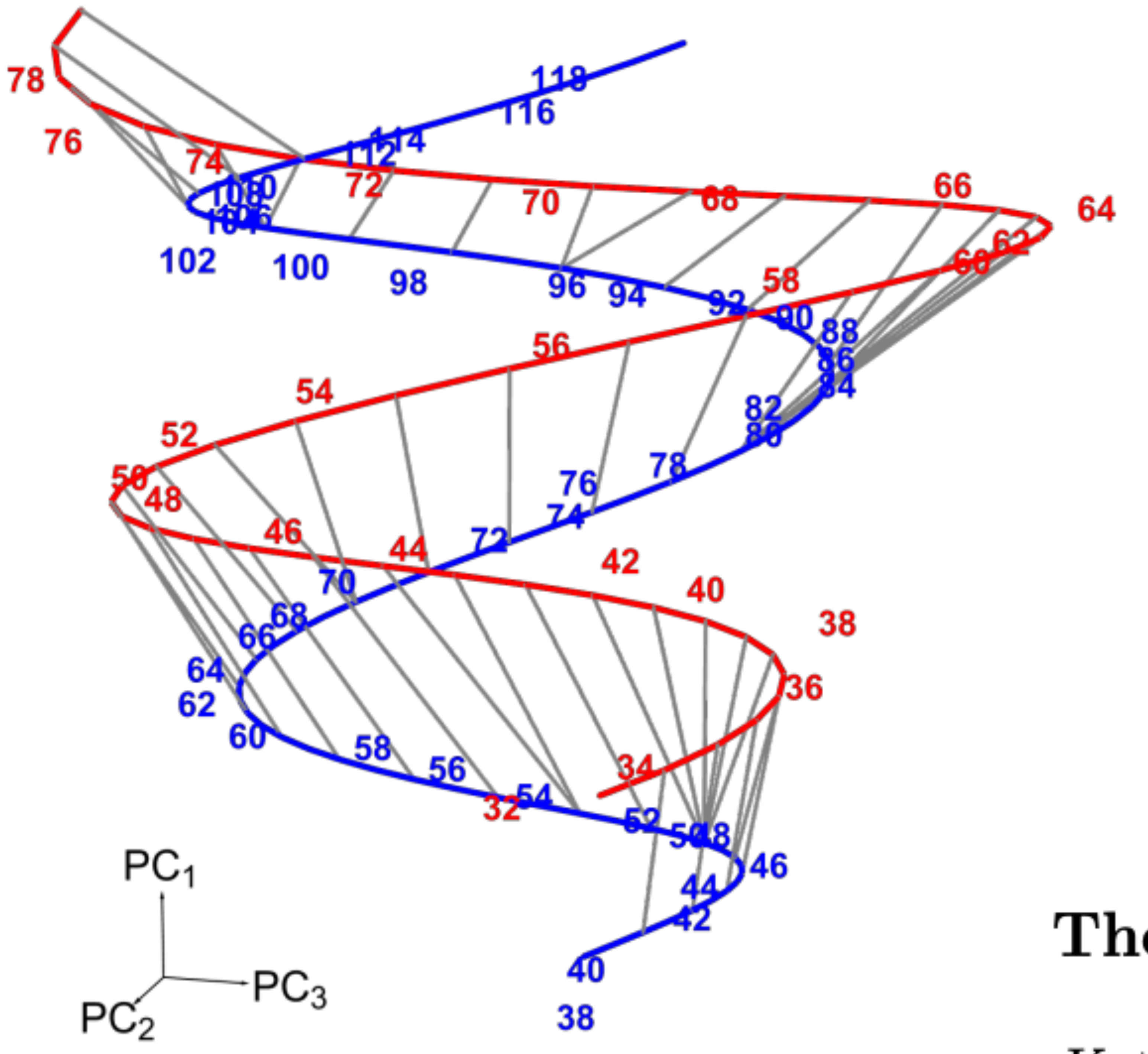
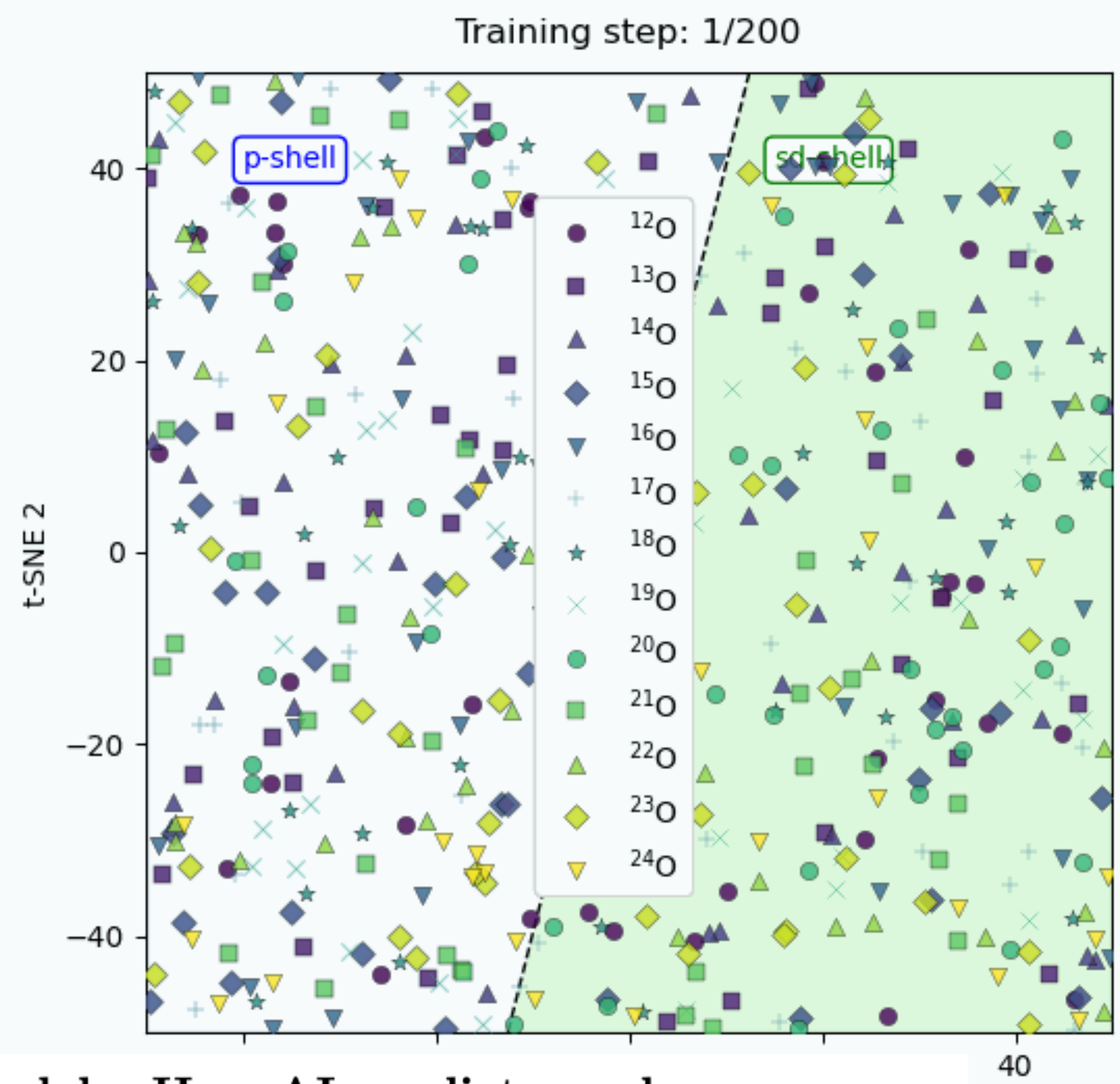
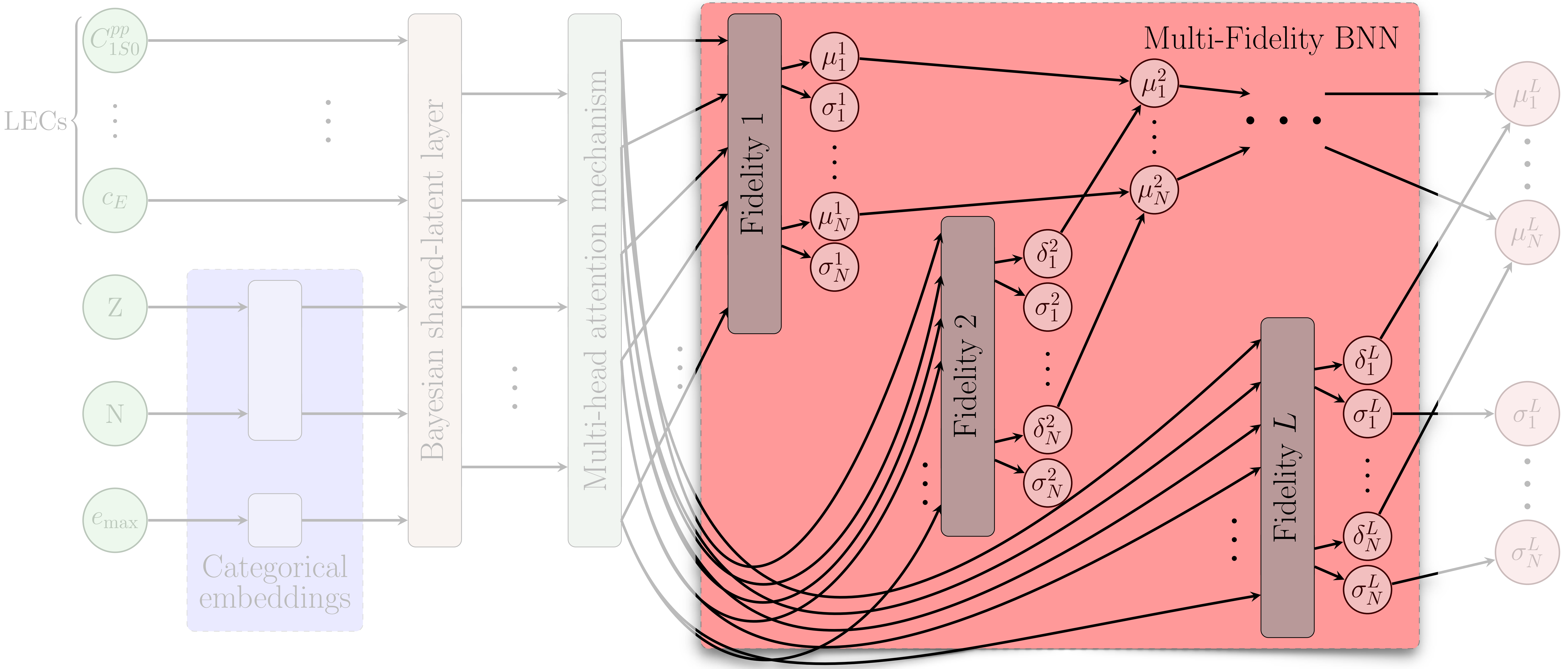




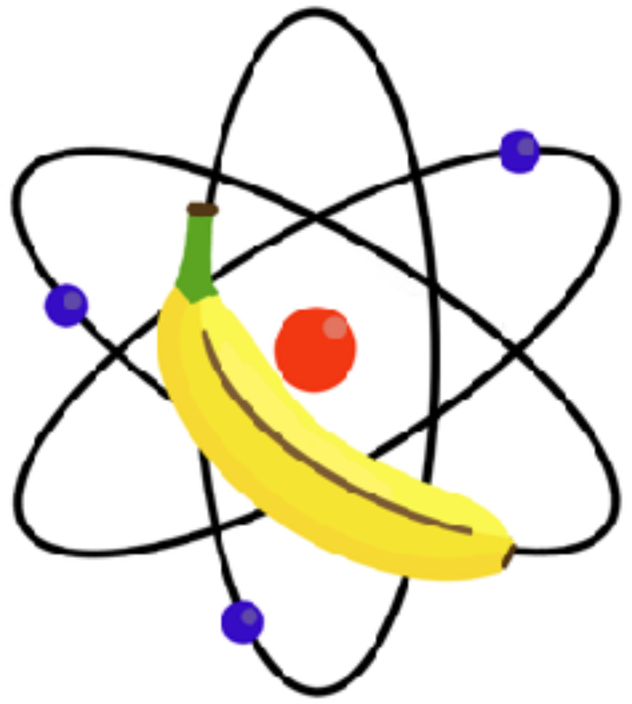
The DNA of nuclear models: How AI predicts nuclear masses

Kate A. Richardson,[1,2,*] Sokratis Trifinopoulos,[1,2,3,4,†] and Mike Williams[1,2,‡]

BAyesian Neural Network for Atomic Nuclei Emulation

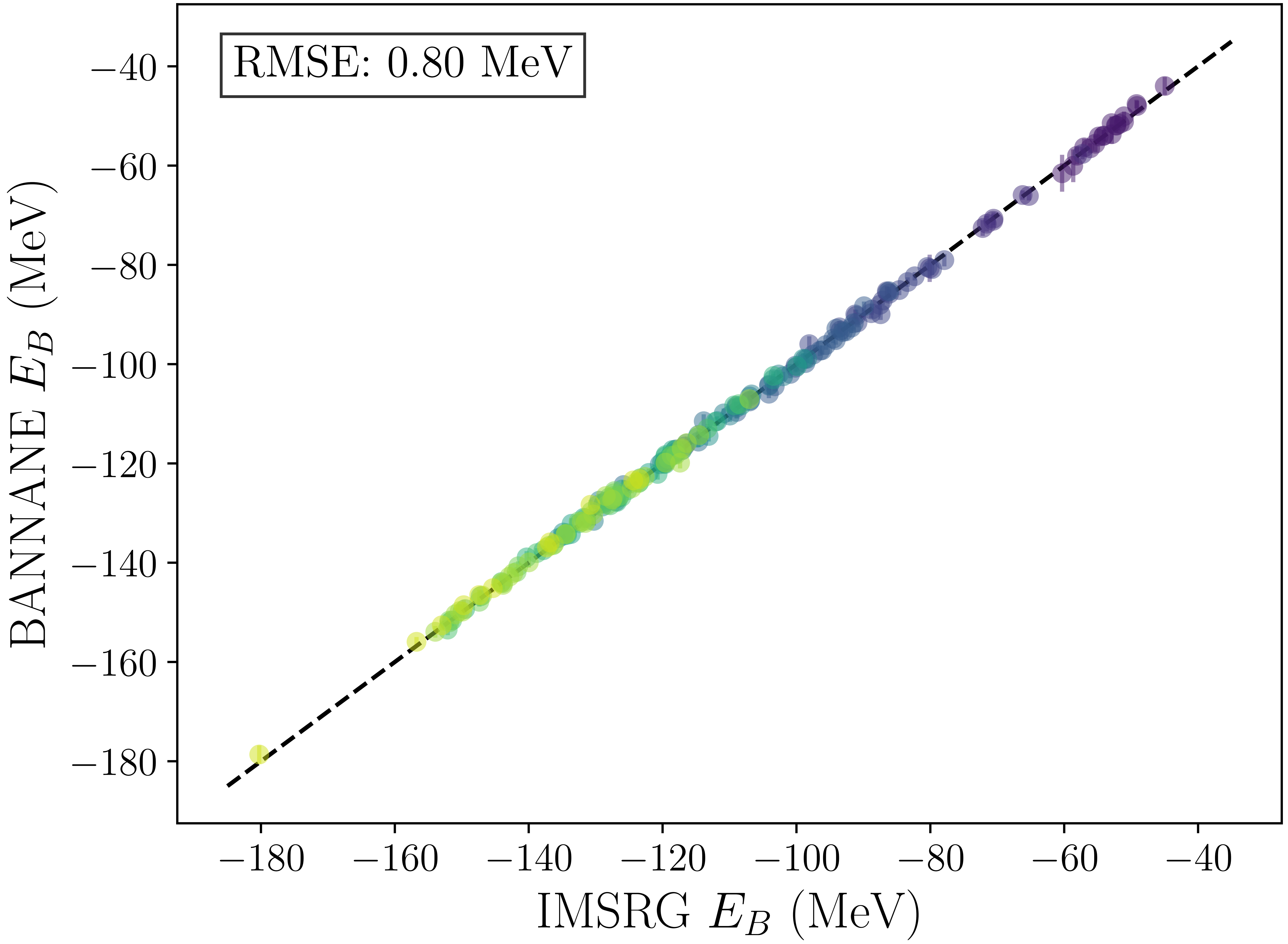


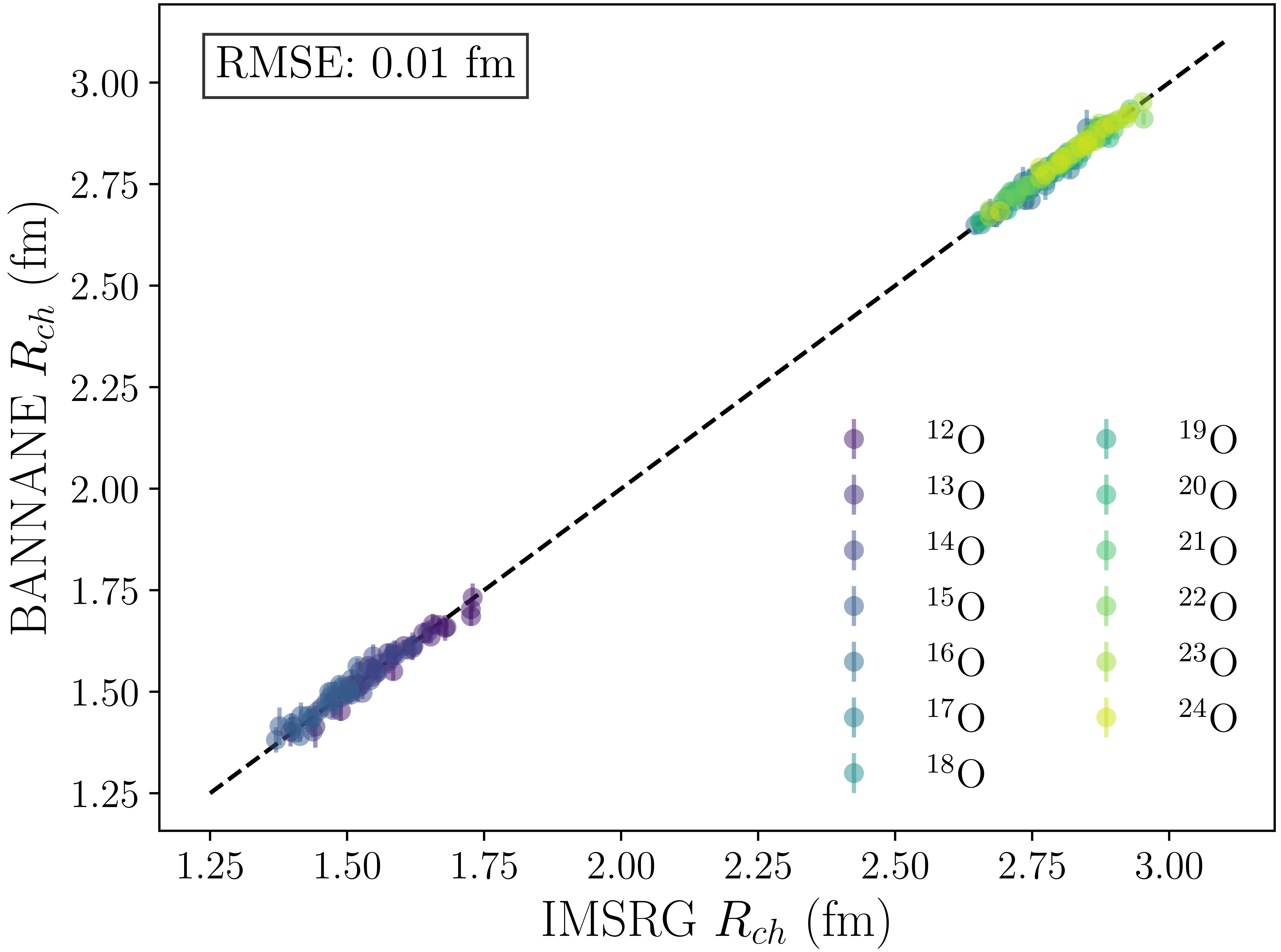
Results



Emulating Multiple Isotopes

Belley, et al.,Phys. Rev. Lett. **136**, 082501 (2026)

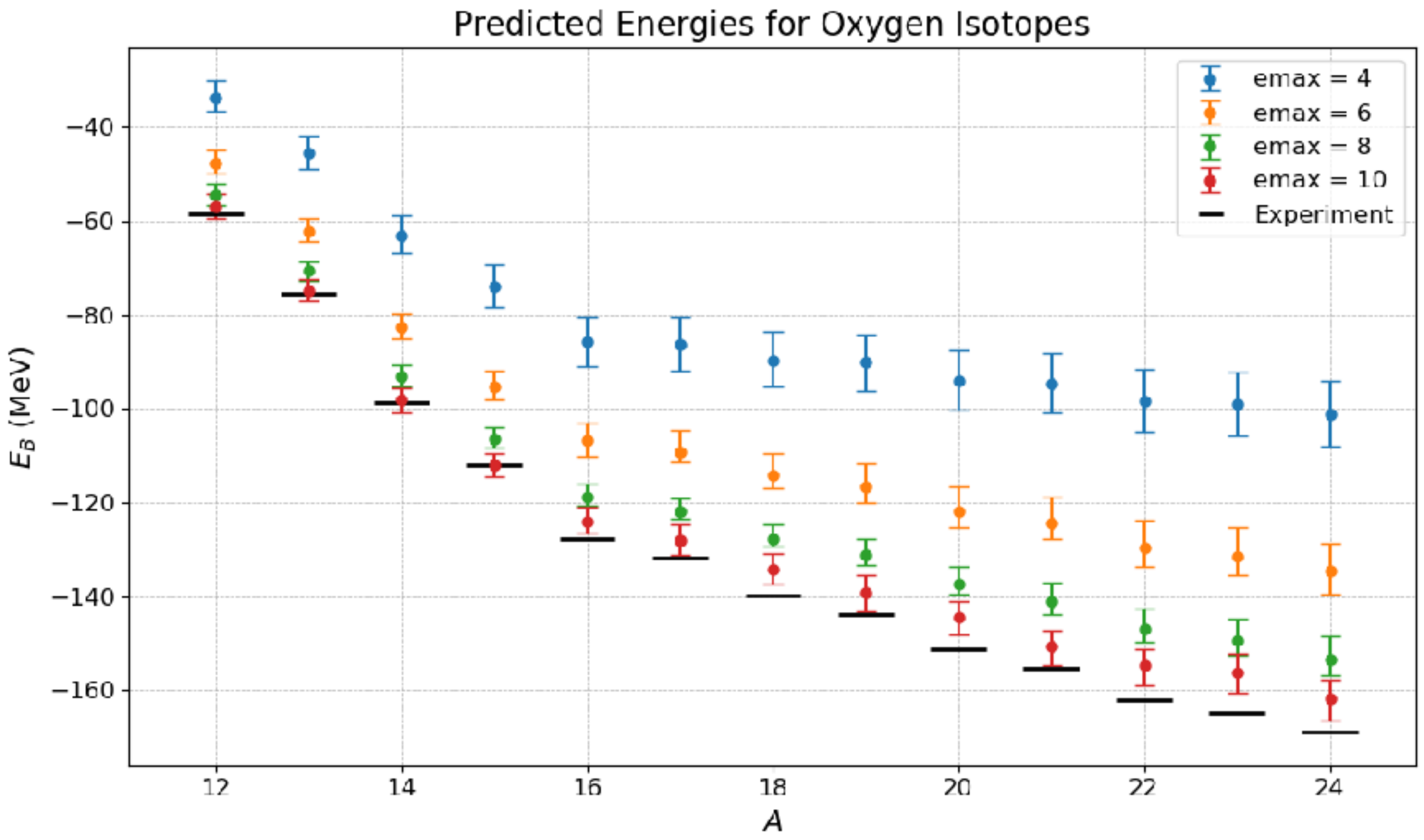


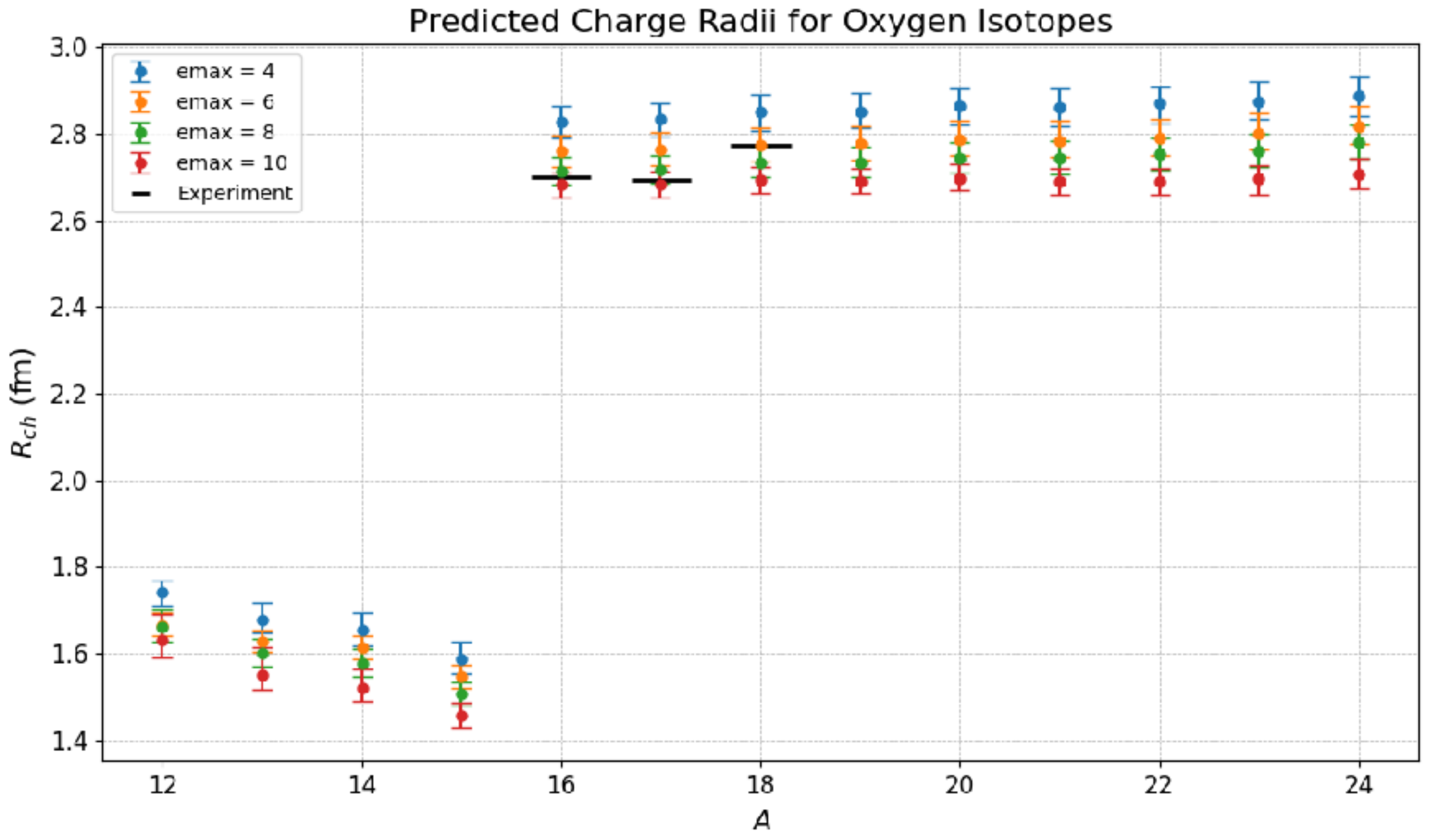


BANNANE achieves state-of-the-art emulation, with smaller errors than other emulators while emulating over a full isotopic chain.

Emulating Multiple Isotopes

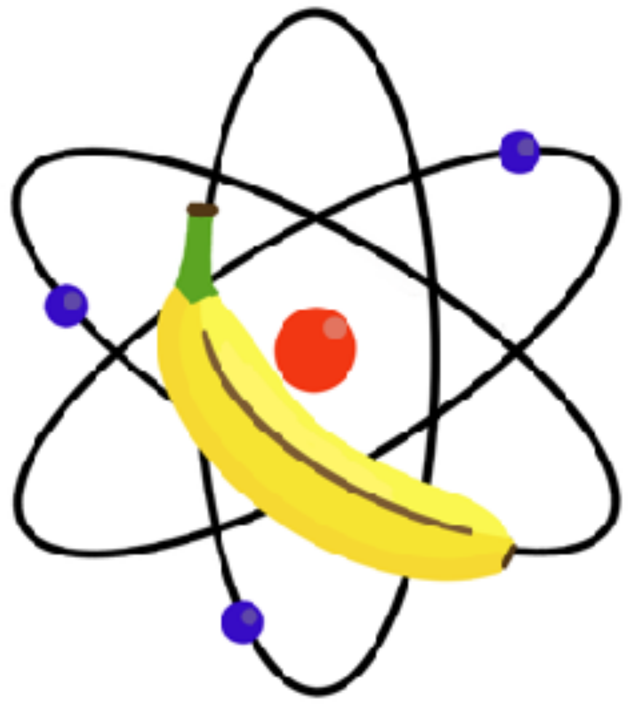
Belley, et al.,Phys. Rev. Lett. **136**, 082501 (2026)

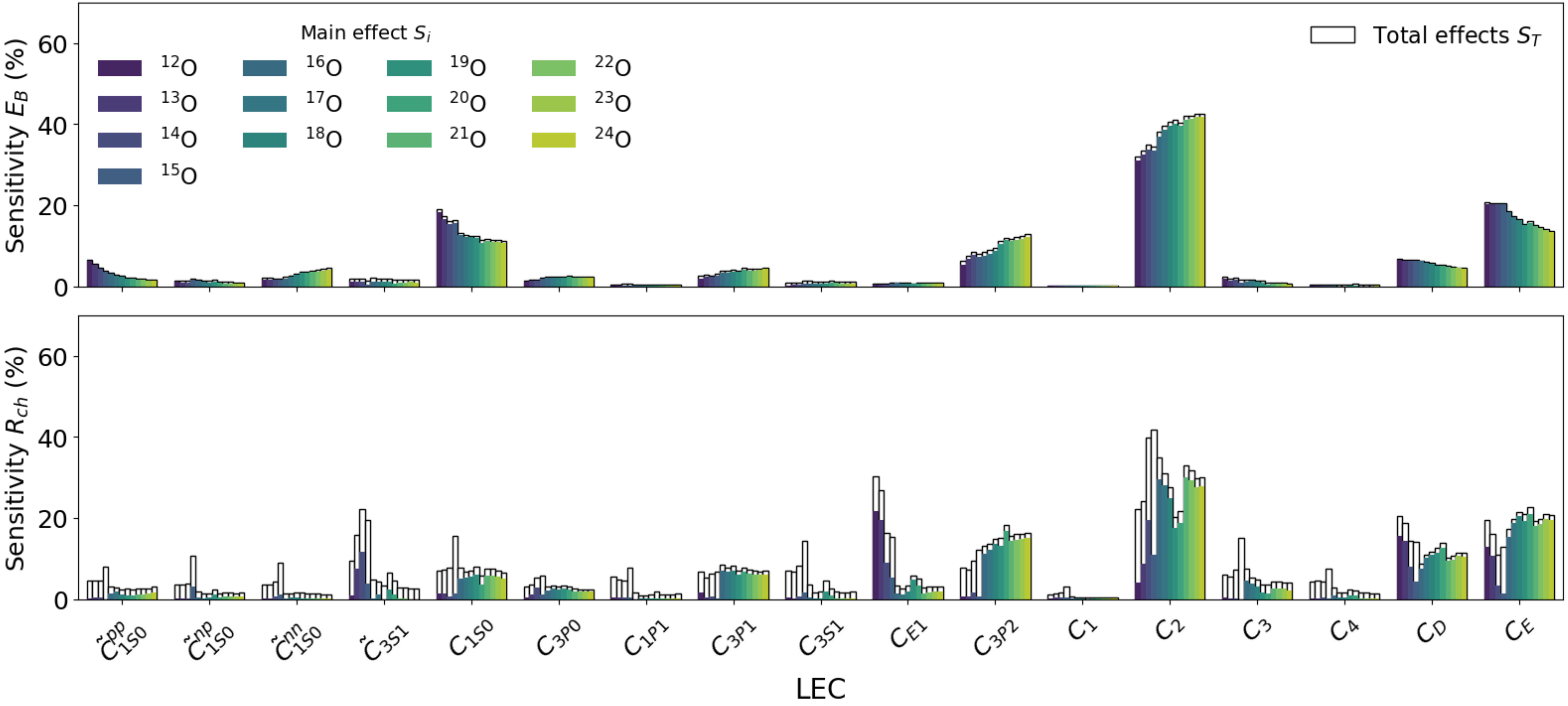




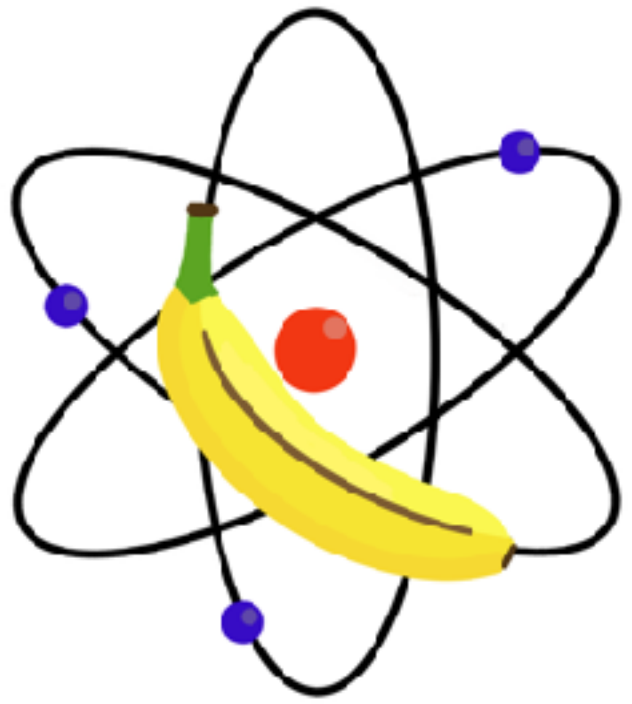
Combining this with UQ technique, we can predict observables with associated uncertainties over the full isotopic chains in a few minutes.

Emulating Multiple Isotopes

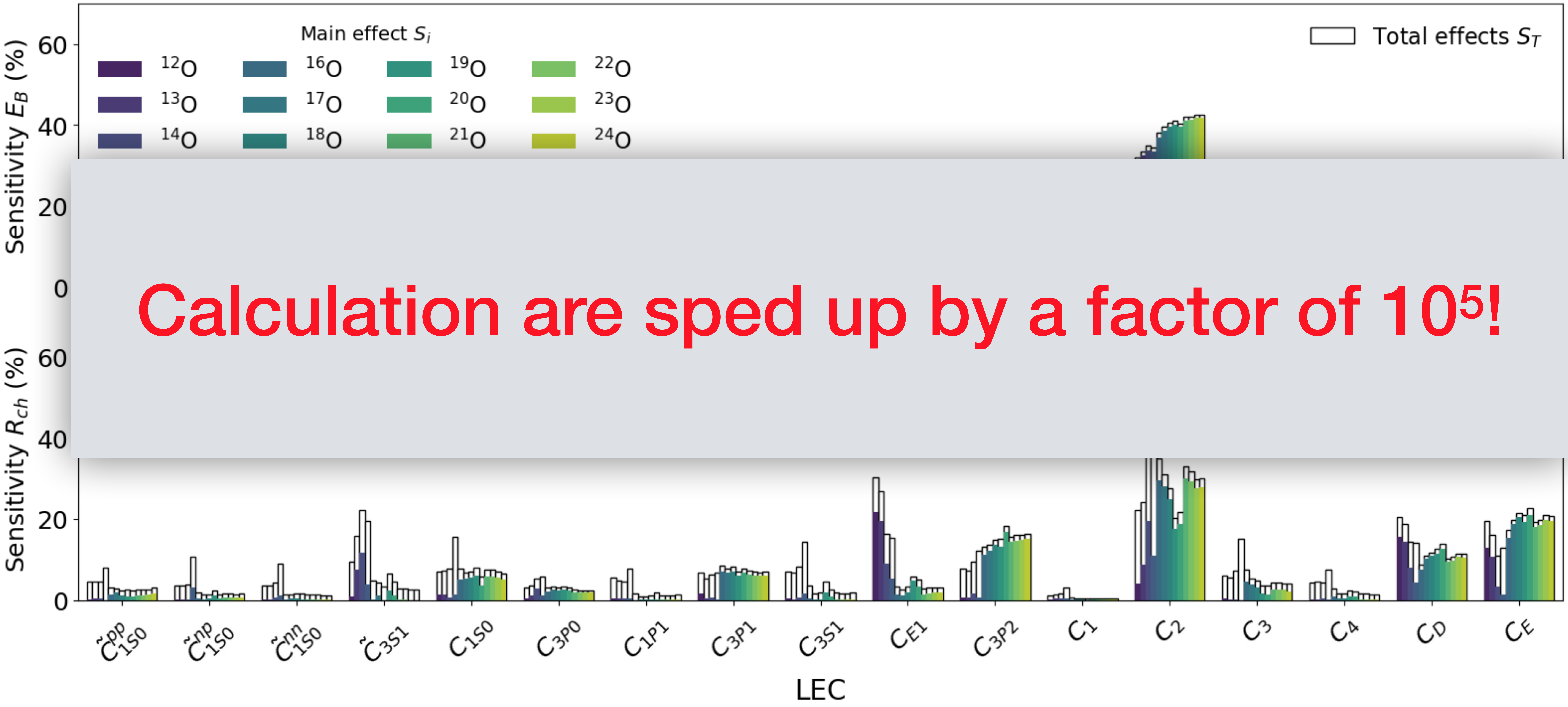




Global sensitivity analysis is consistent with other emulators!



Emulating Multiple Isotopes

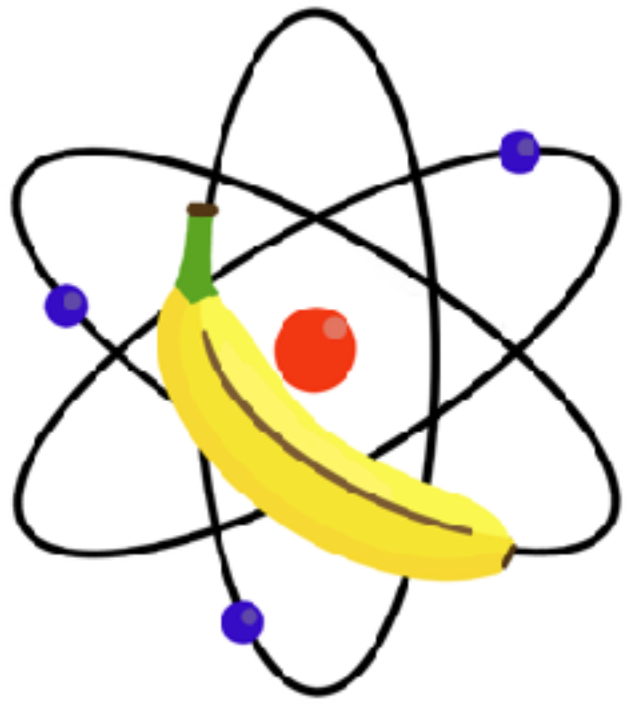


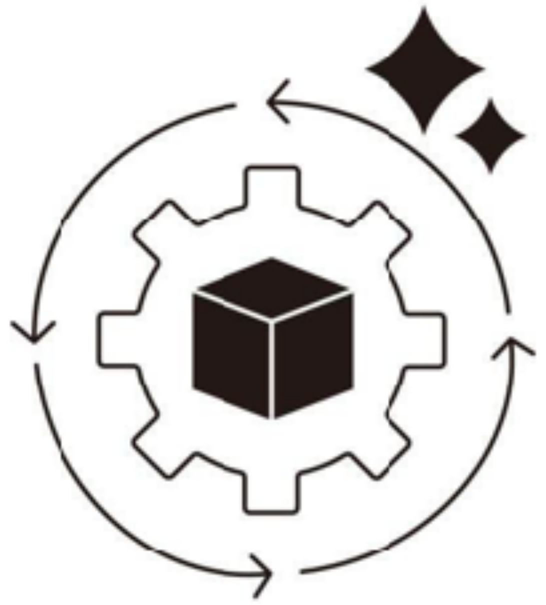
Calculation are sped up by a factor of 10^5!

Global sensitivity analysis is consistent with other emulators!

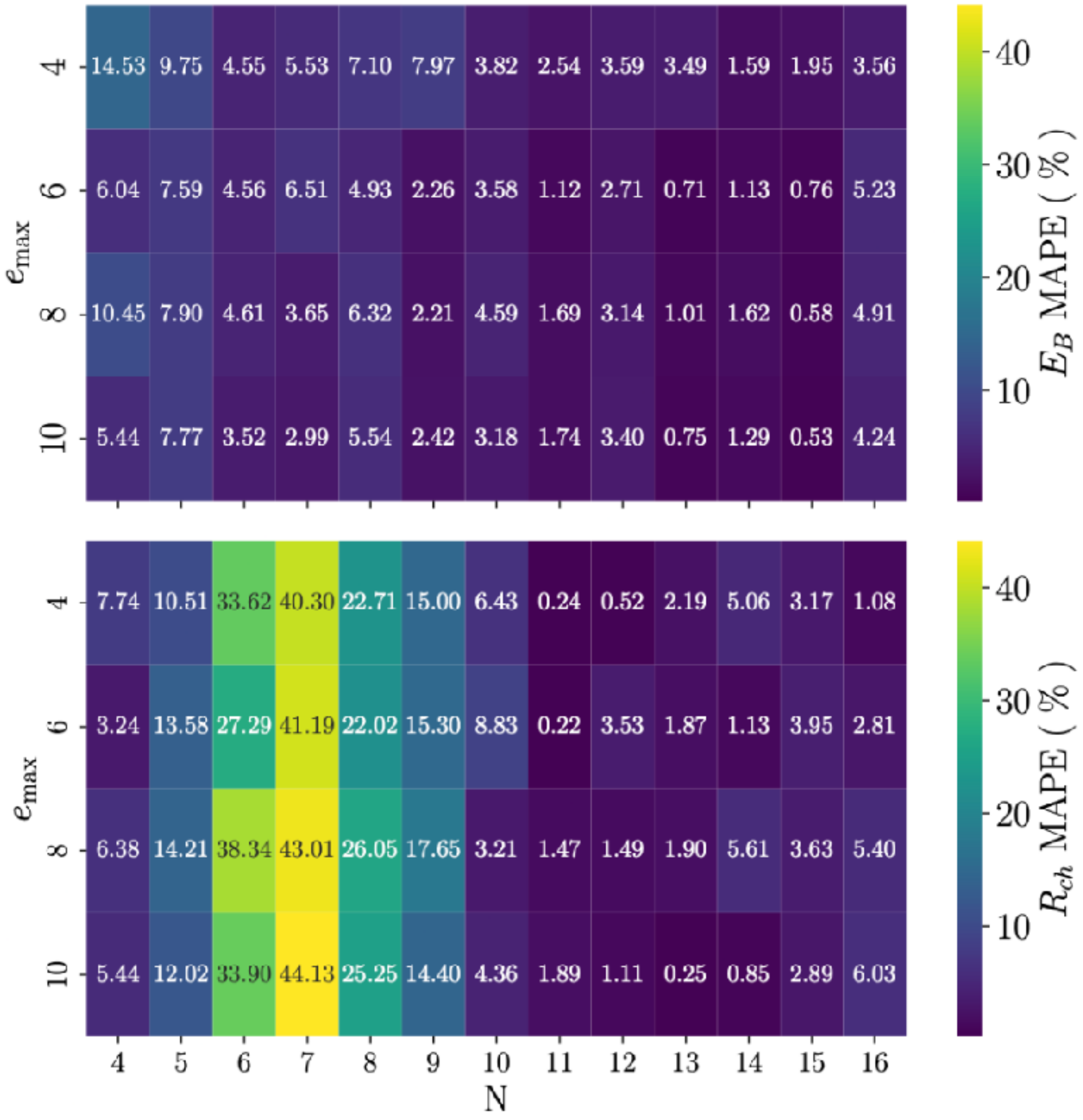
Challenges

Emulating To Unseen Data





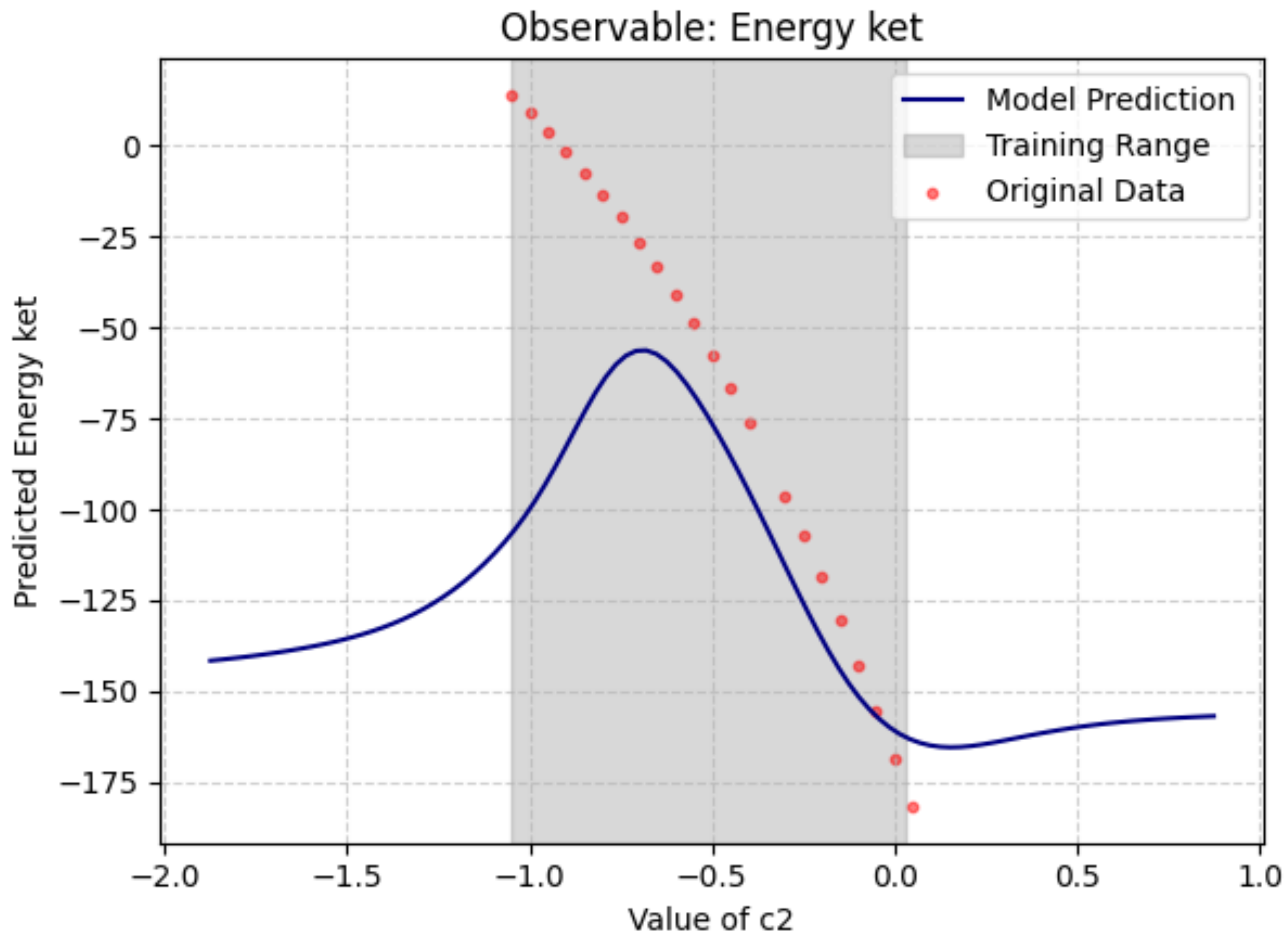
Zero-shot Learning

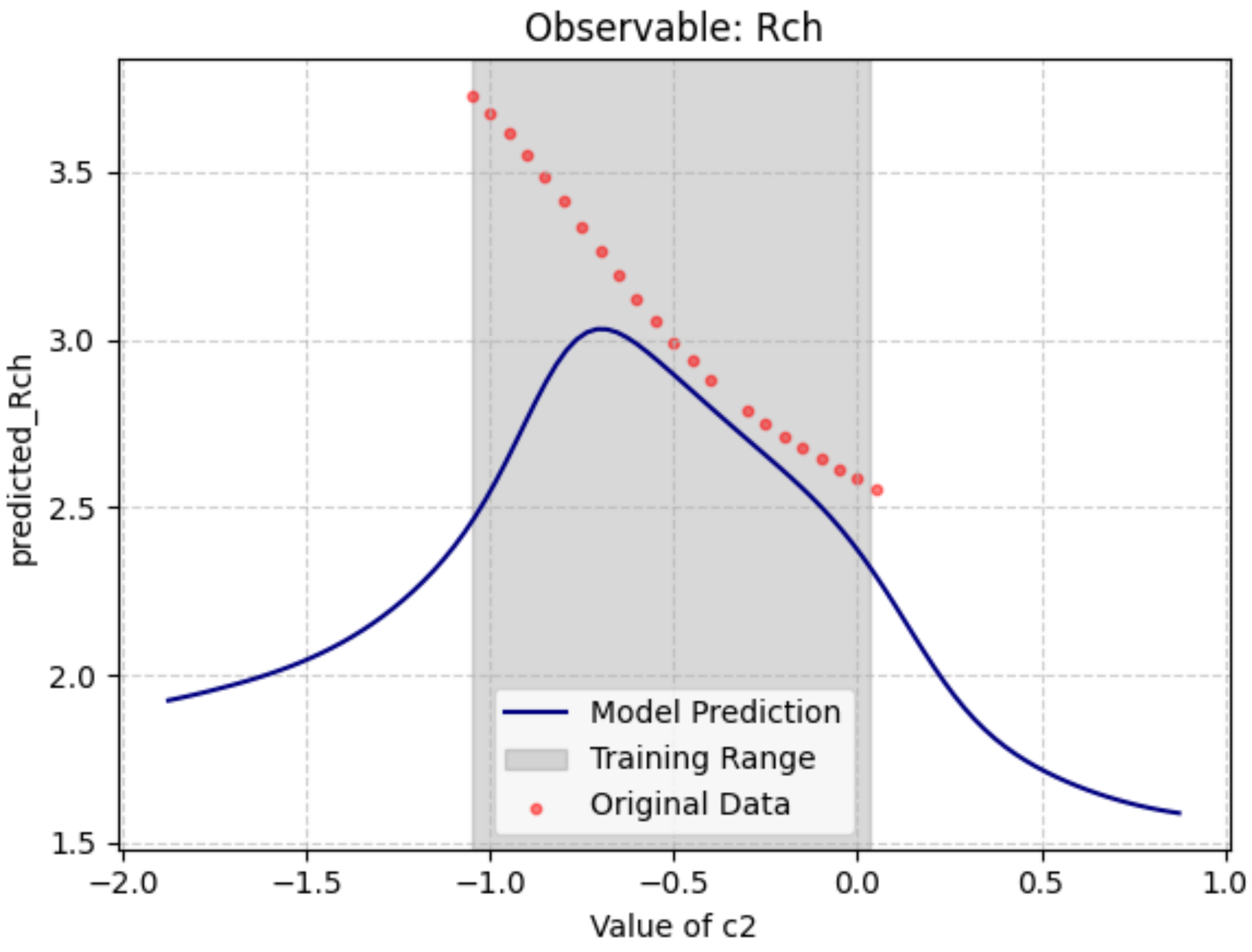


Difference with model and IMSRG when no data is used to train in a specific isotope.

Emulating Outside the Physical Range

Model Extrapolation vs. Low-Energy Constants (LECs)





Emulators for Many-Body Methods

There are two? ways to build an emulator for nuclear physics:

Physics driven **Data driven**

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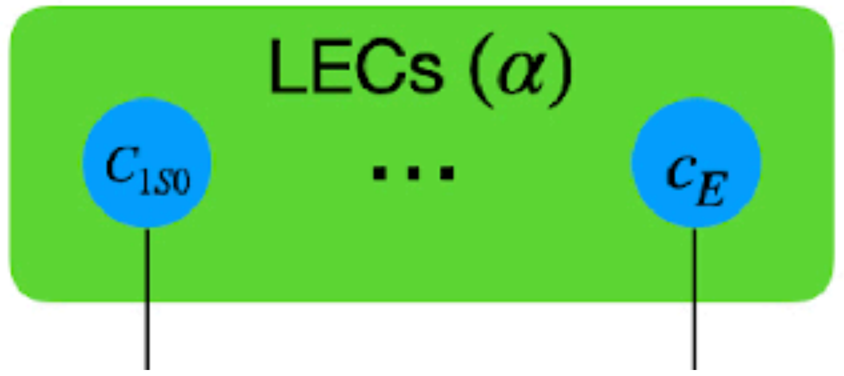
PMMs

PINNs

NN, GPs

Physics Driven BANNANE?

Jose Miguel Muñoz Arias



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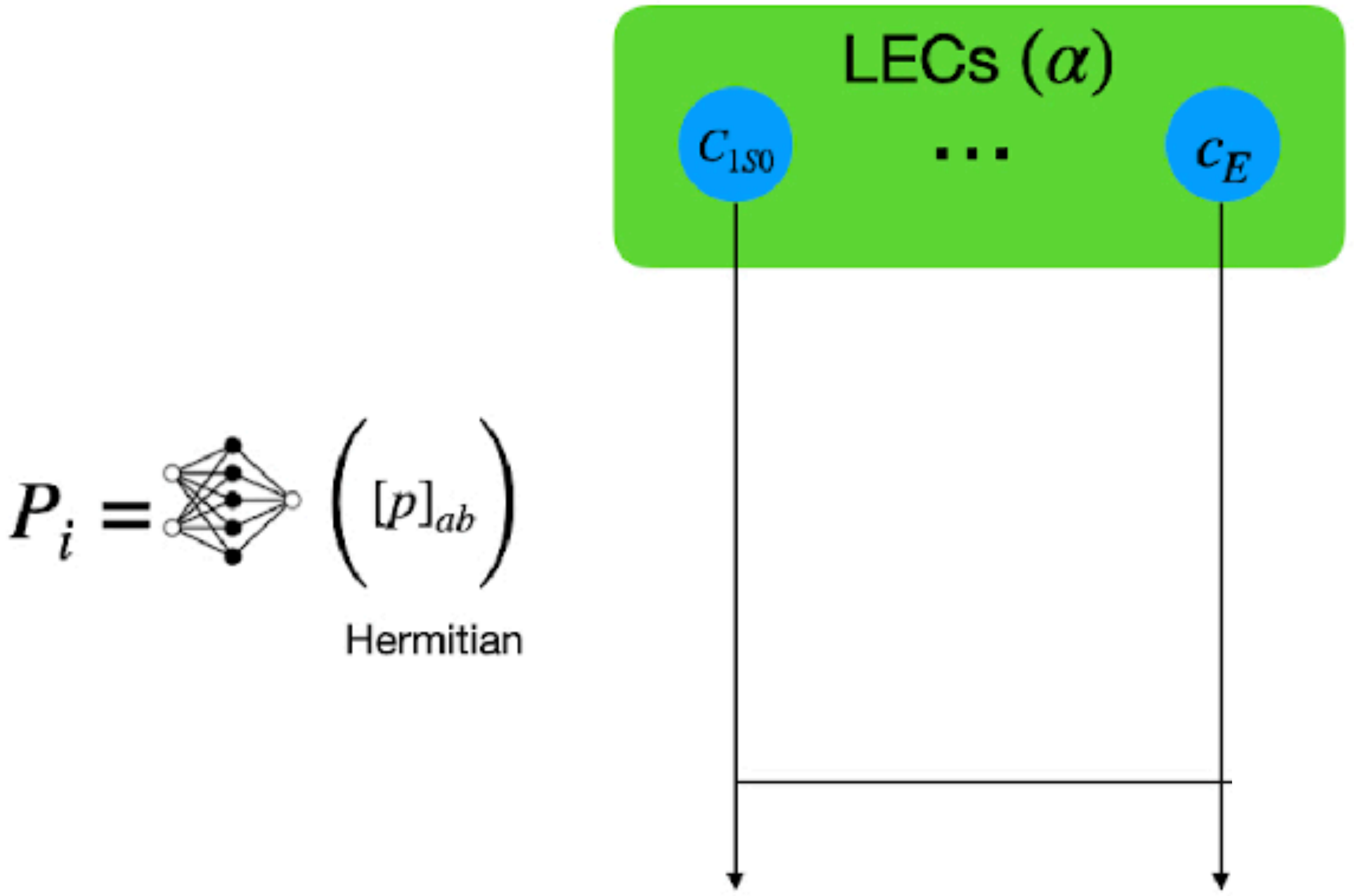

$$M_k(\alpha, N, Z, f) = P_0 + C_{1S0}P_{1S0} + \ldots + c_E P_E$$

Physics Driven BANNANE?

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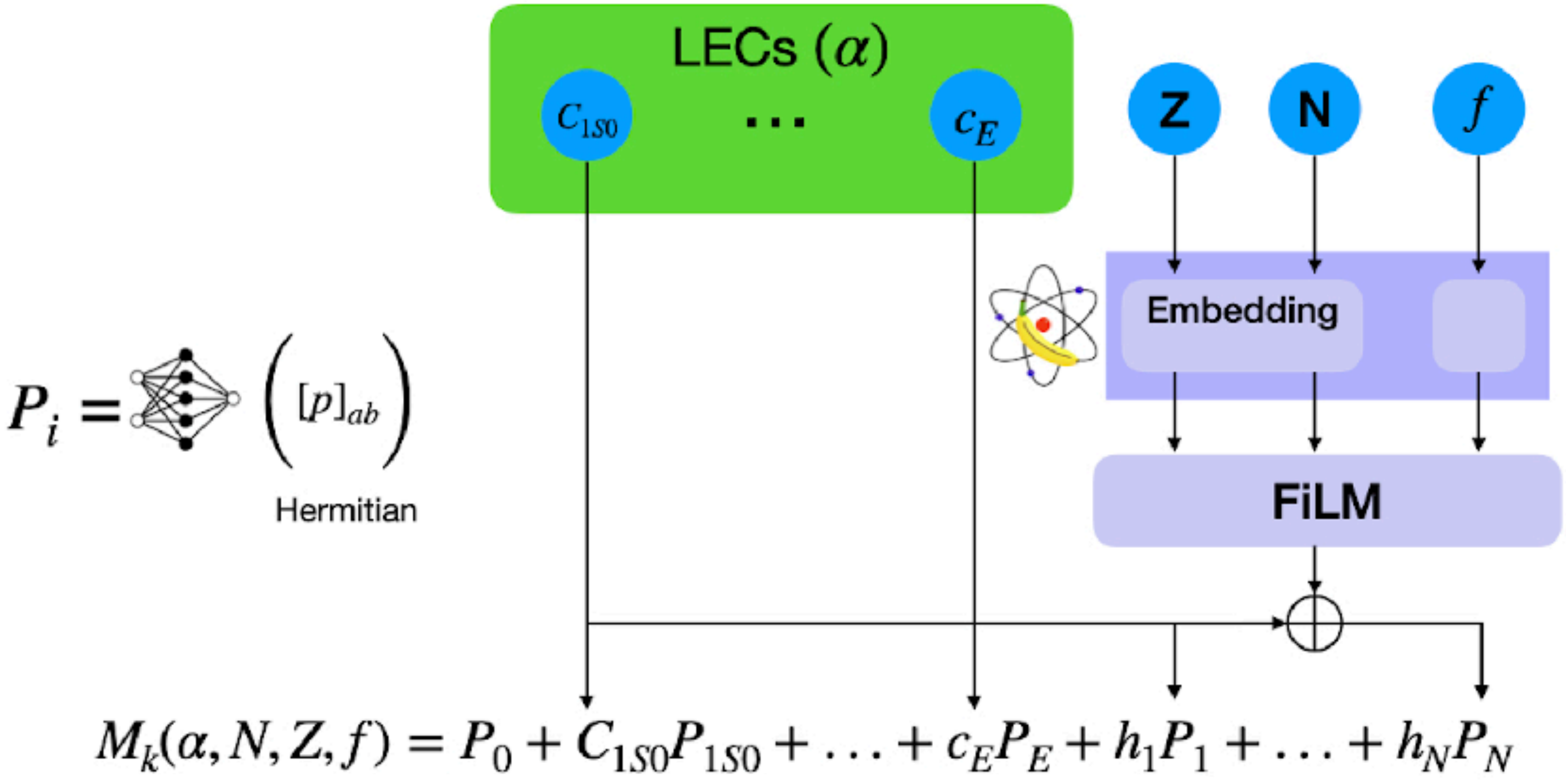

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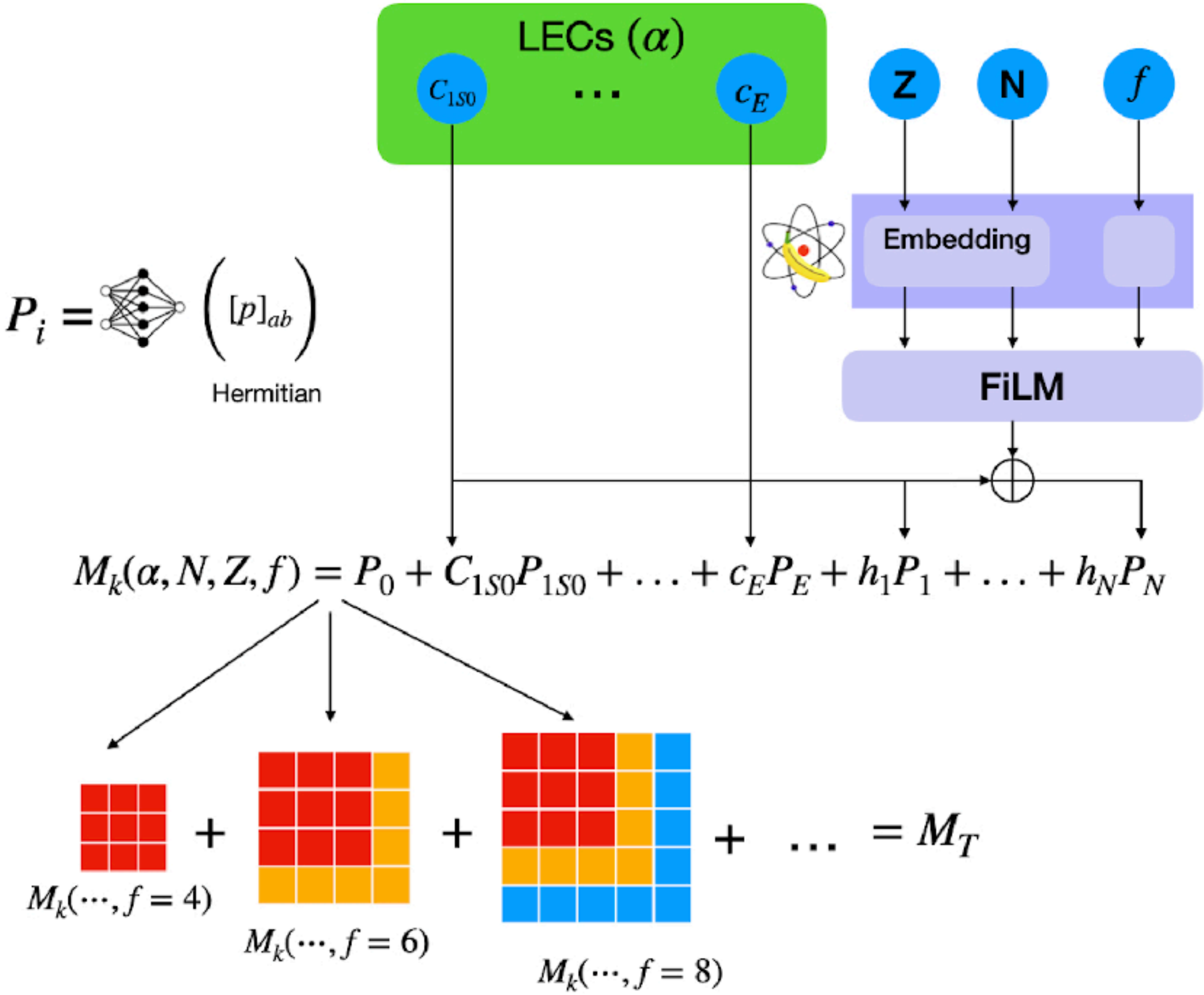

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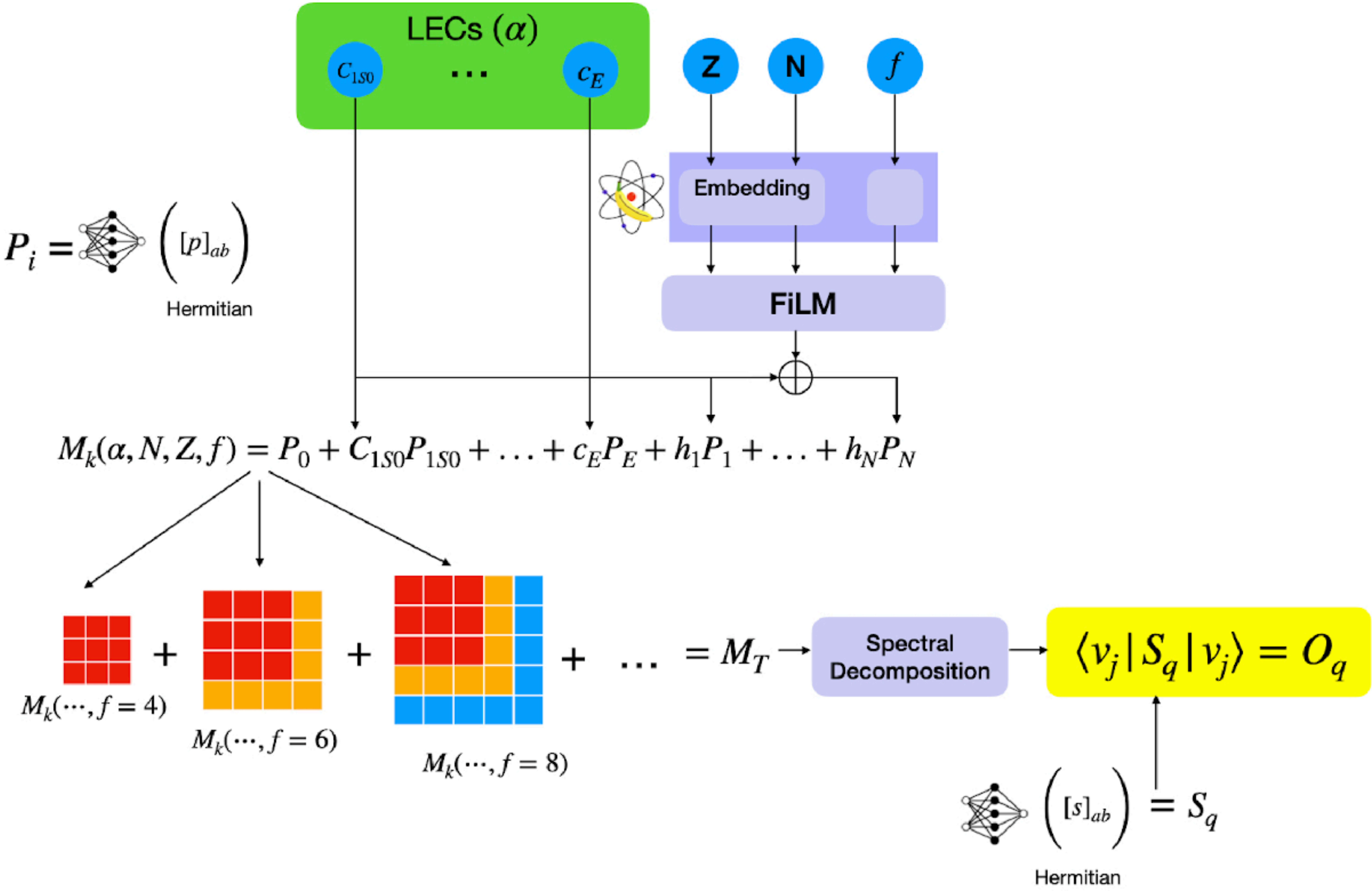

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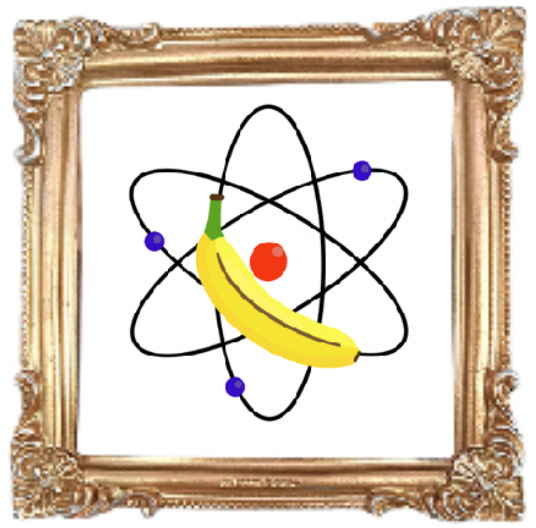
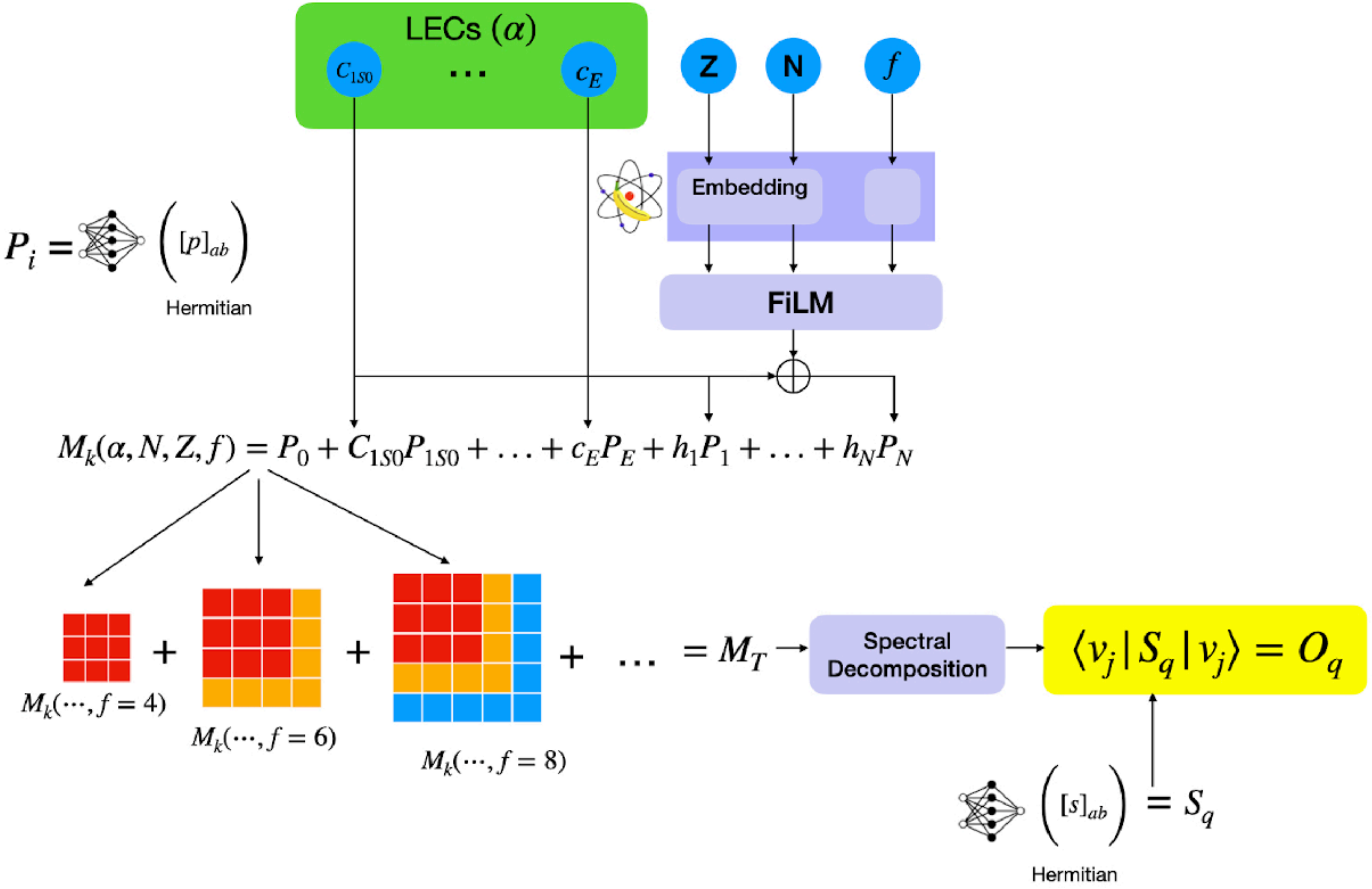
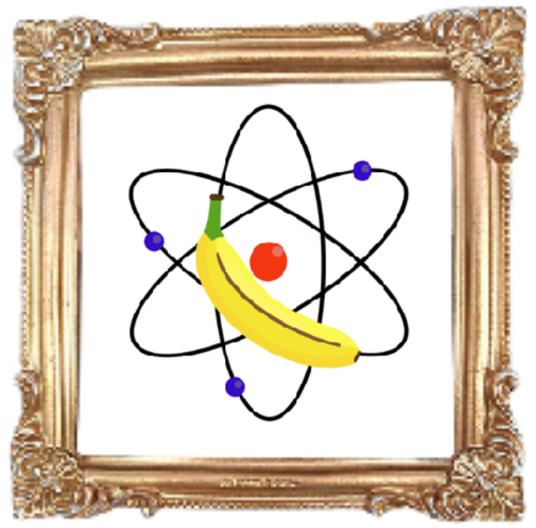


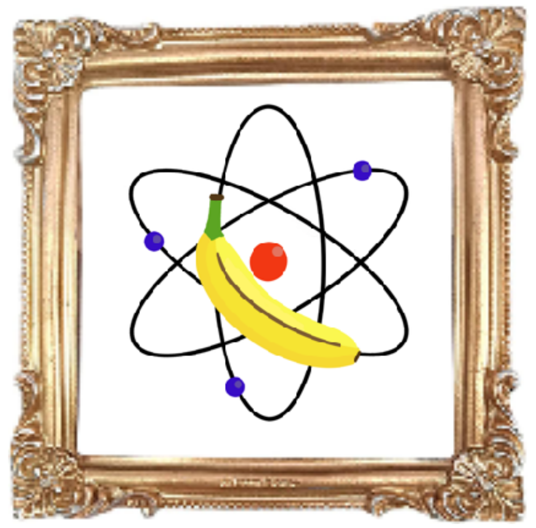
Physics Driven BANNANE?

Feature Resolved Affine Matrix Emulator (FRAME)



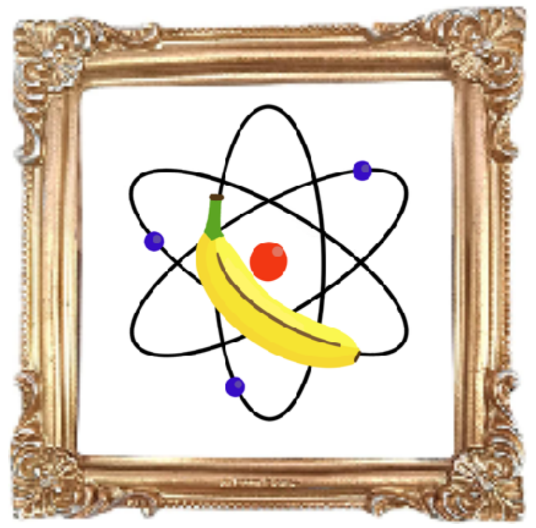


Anchor and Refinement



Anchor and Refinement

$$M(N,Z,f,\alpha) = [M_{f_{min}} + \sum_{p=1}^{f} \xi(f;N,Z,\alpha)\Delta M_p]$$



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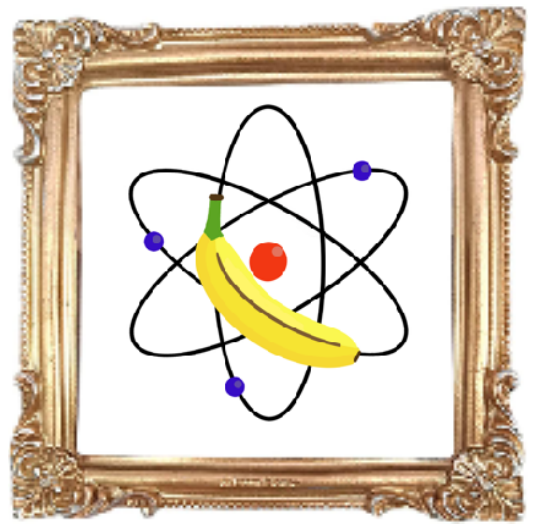
Anchor: Matrix at the lowest fidelity



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Refinement: Corrections from higher fidelities

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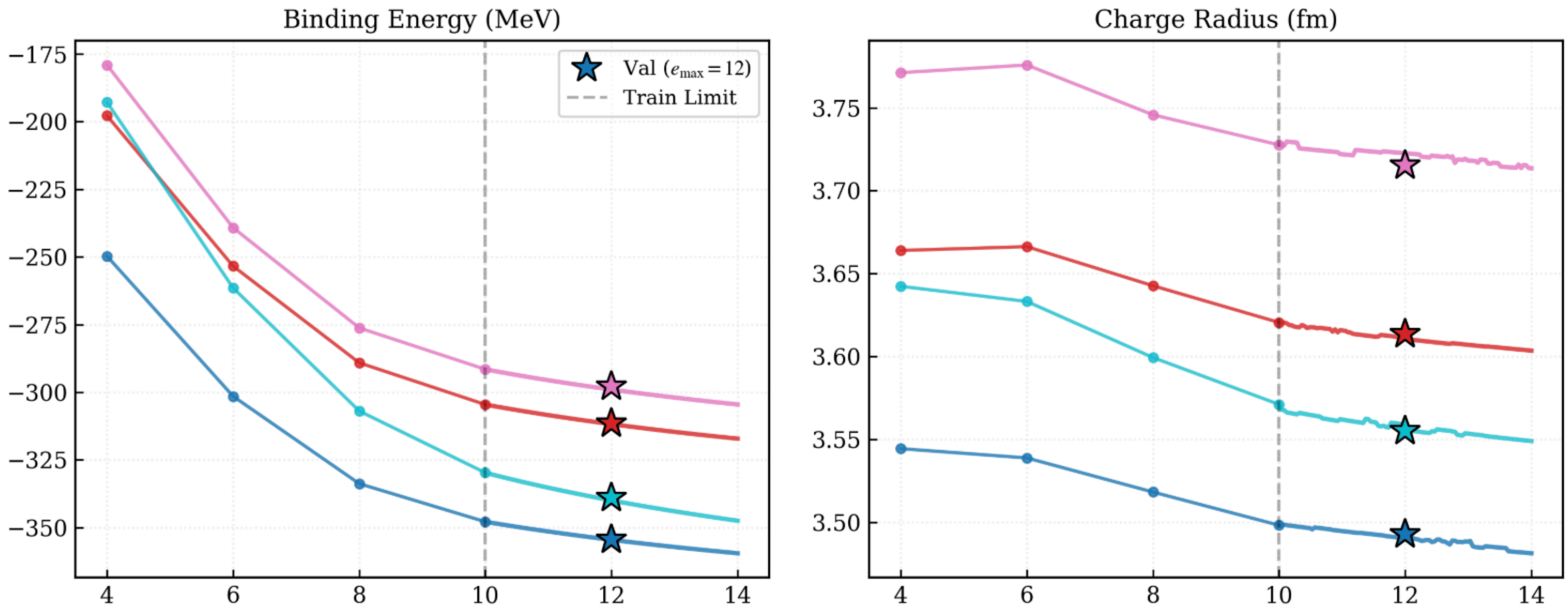
Anchor: Matrix at the lowest fidelity

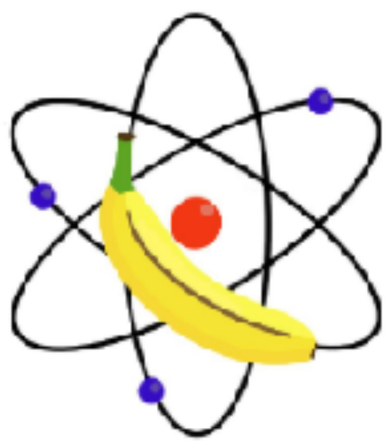
Refinement: Corrections from higher fidelities

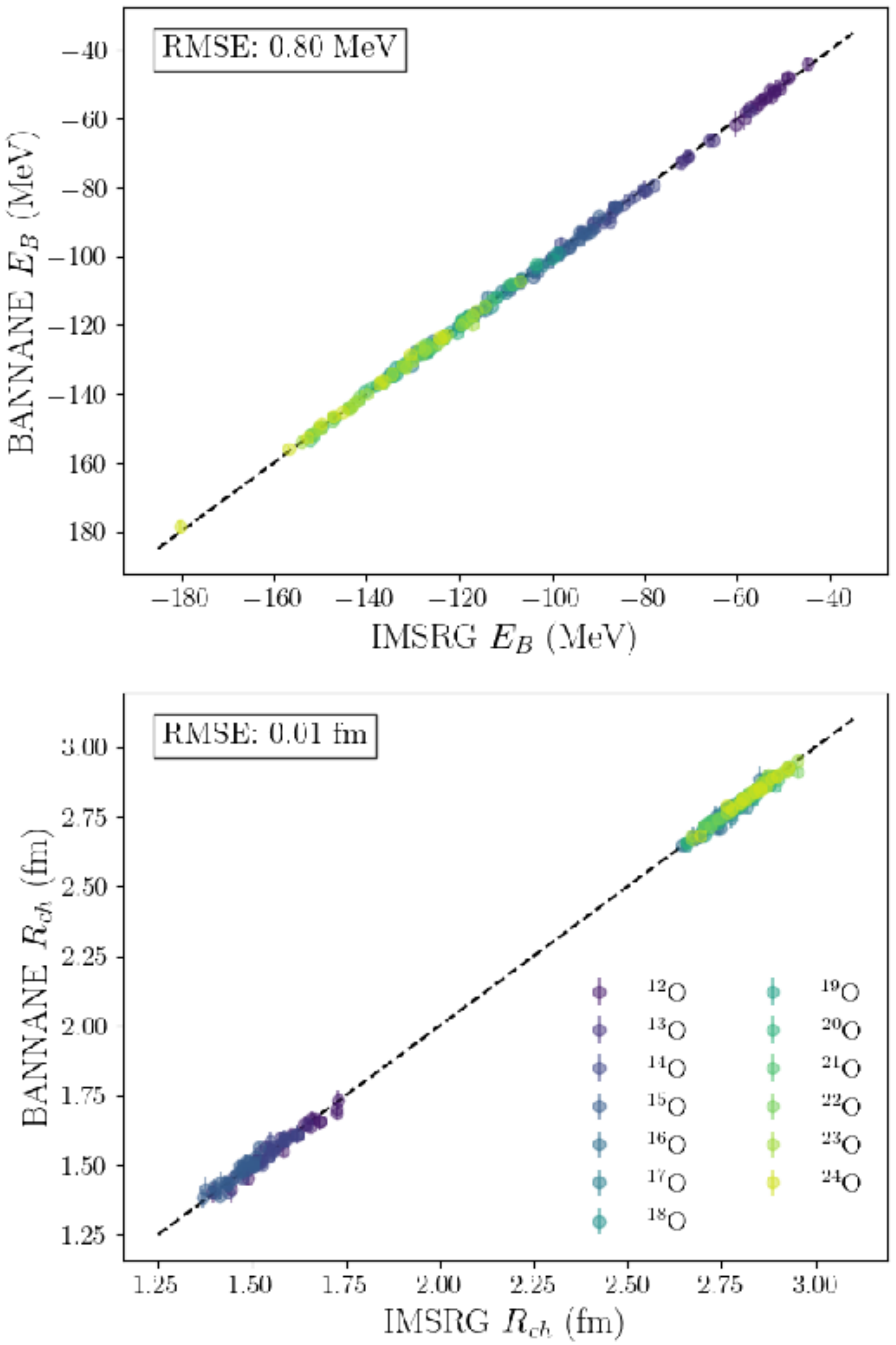
https://frame-architecture-explorer-553167399436.us-west1.run.app/

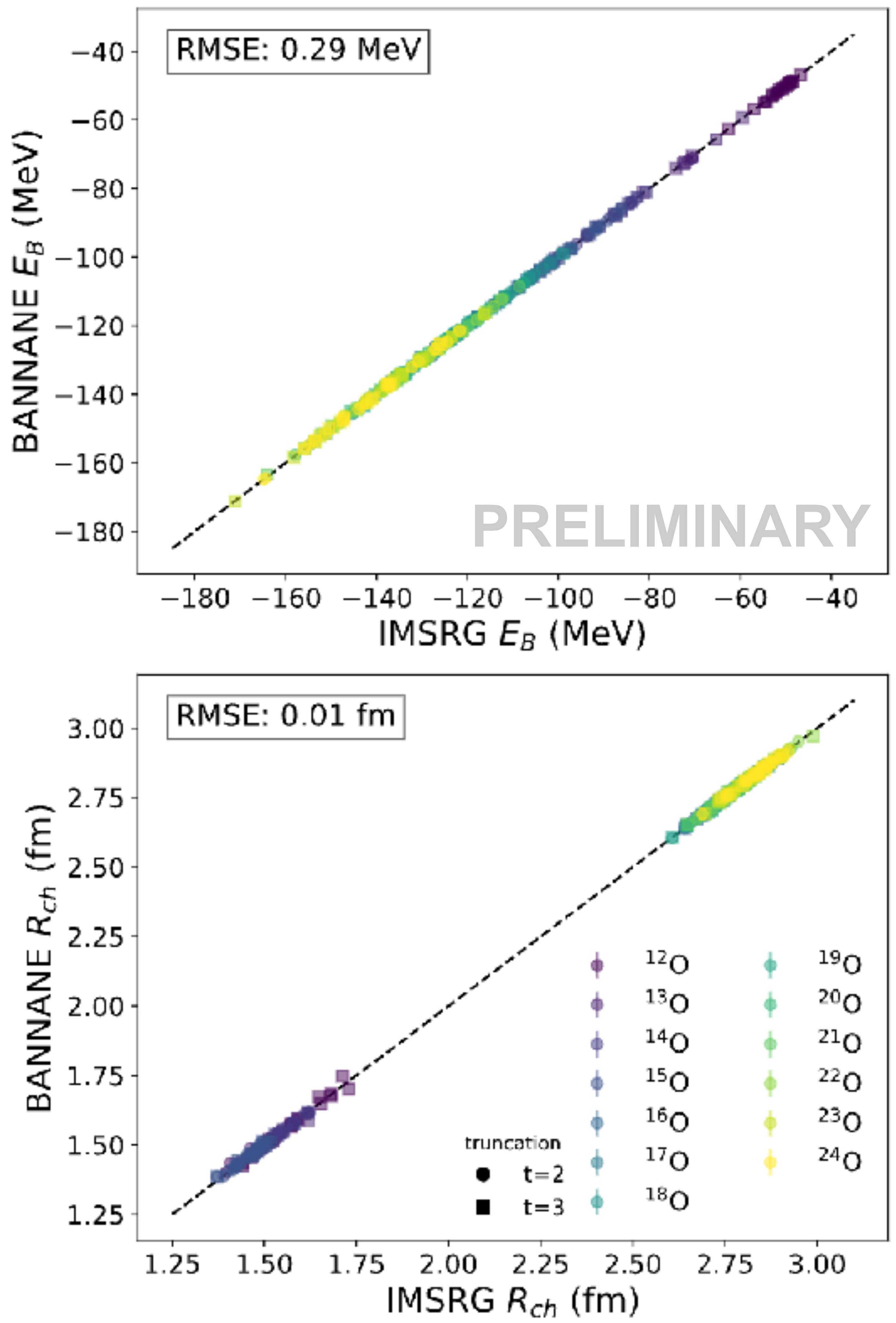
Extrapolating in e_{max}

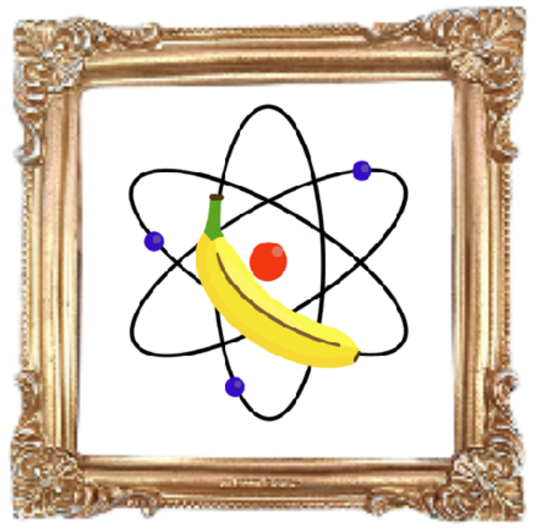


Physics Driven BANNANE!



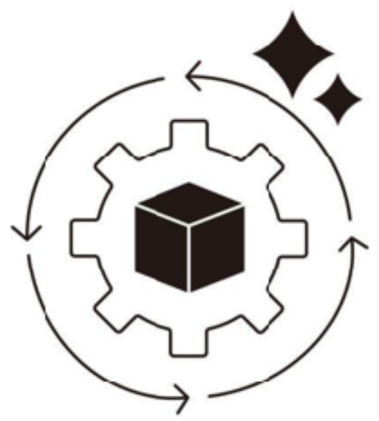






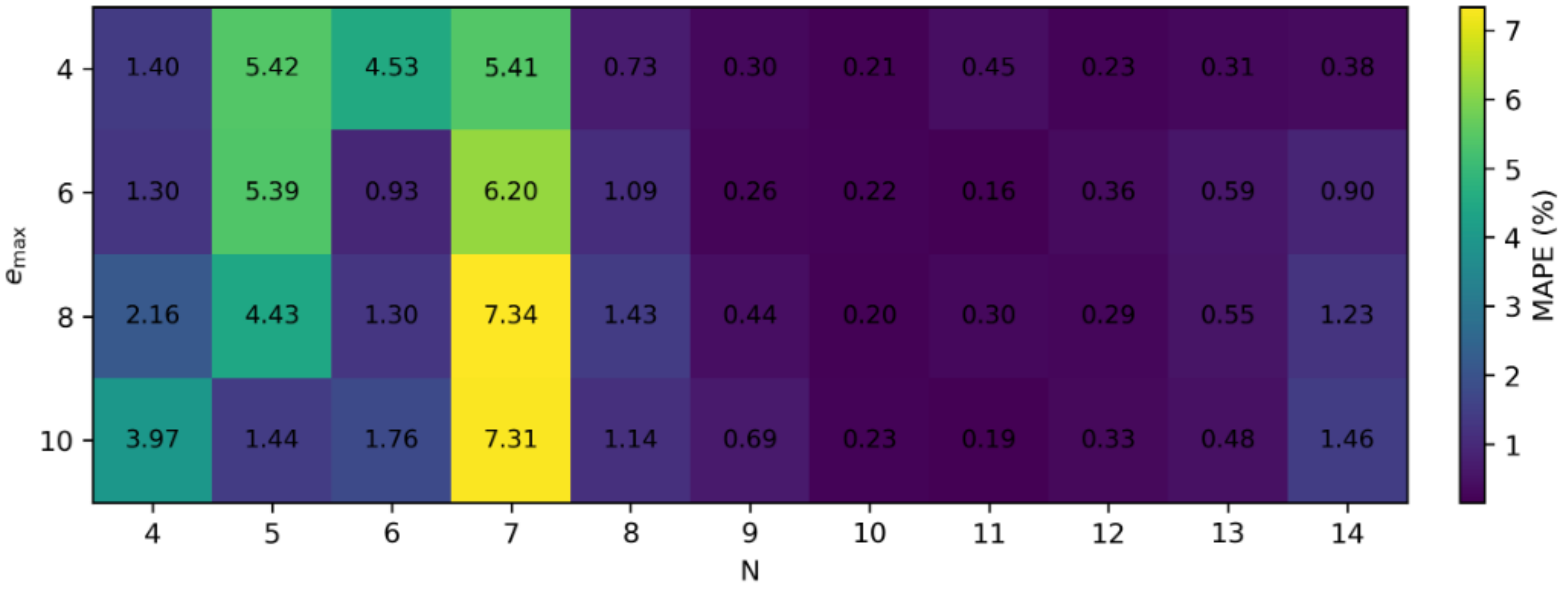
Training cost was reduced by a factor of 5!

Physics Driven BANNANE!



Zero-shot Learning

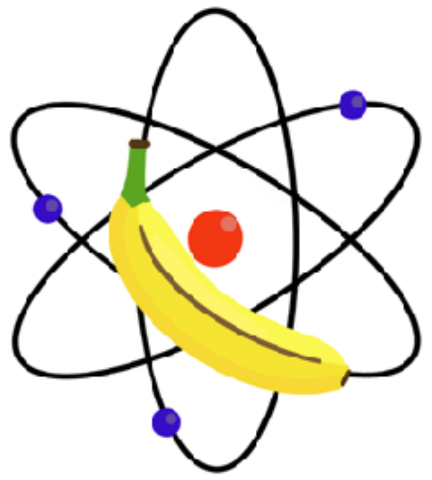
R_{ch}

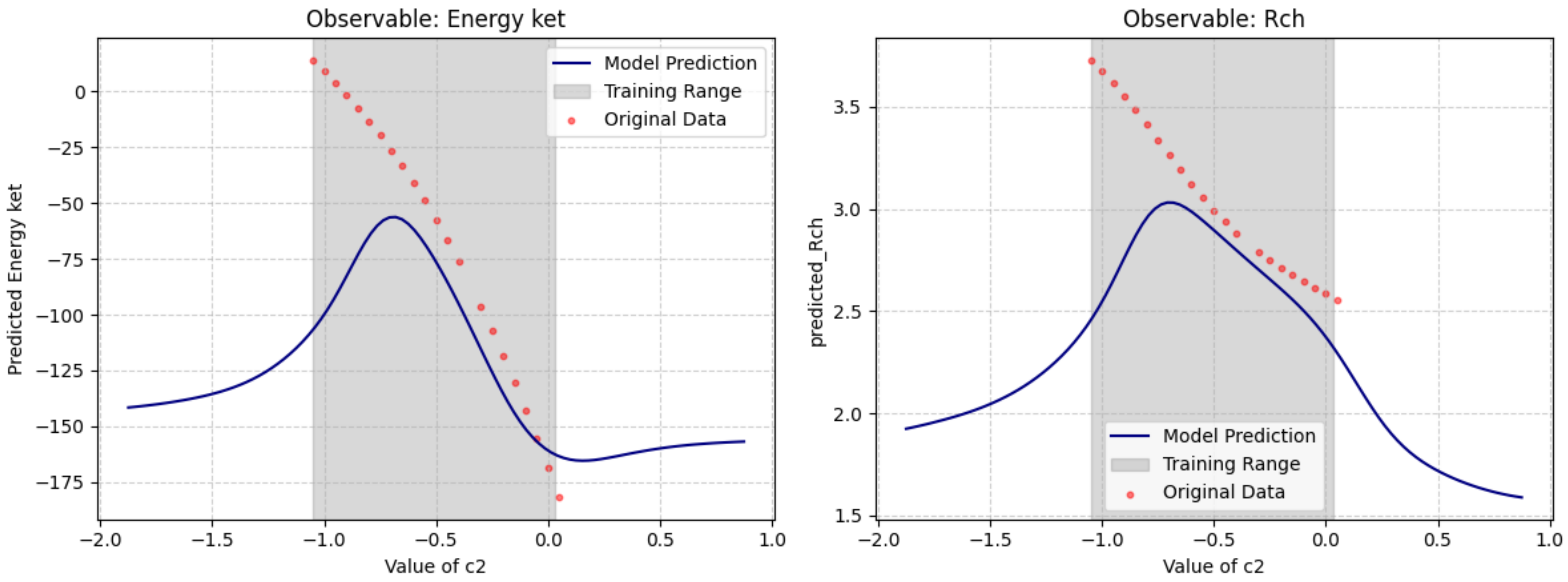


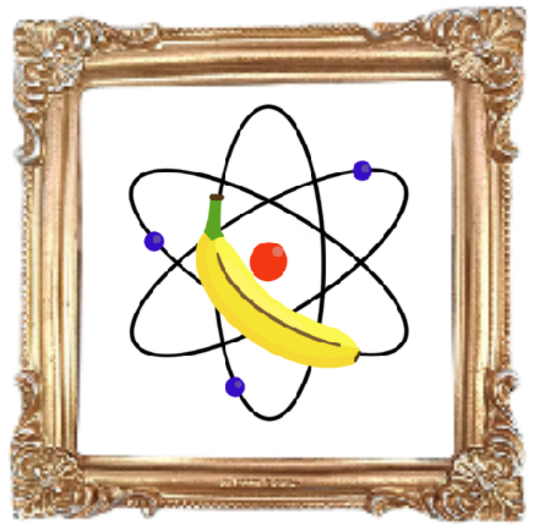
Physics driven version reduced worst zero-shot learning case from 44% error to 7% error!

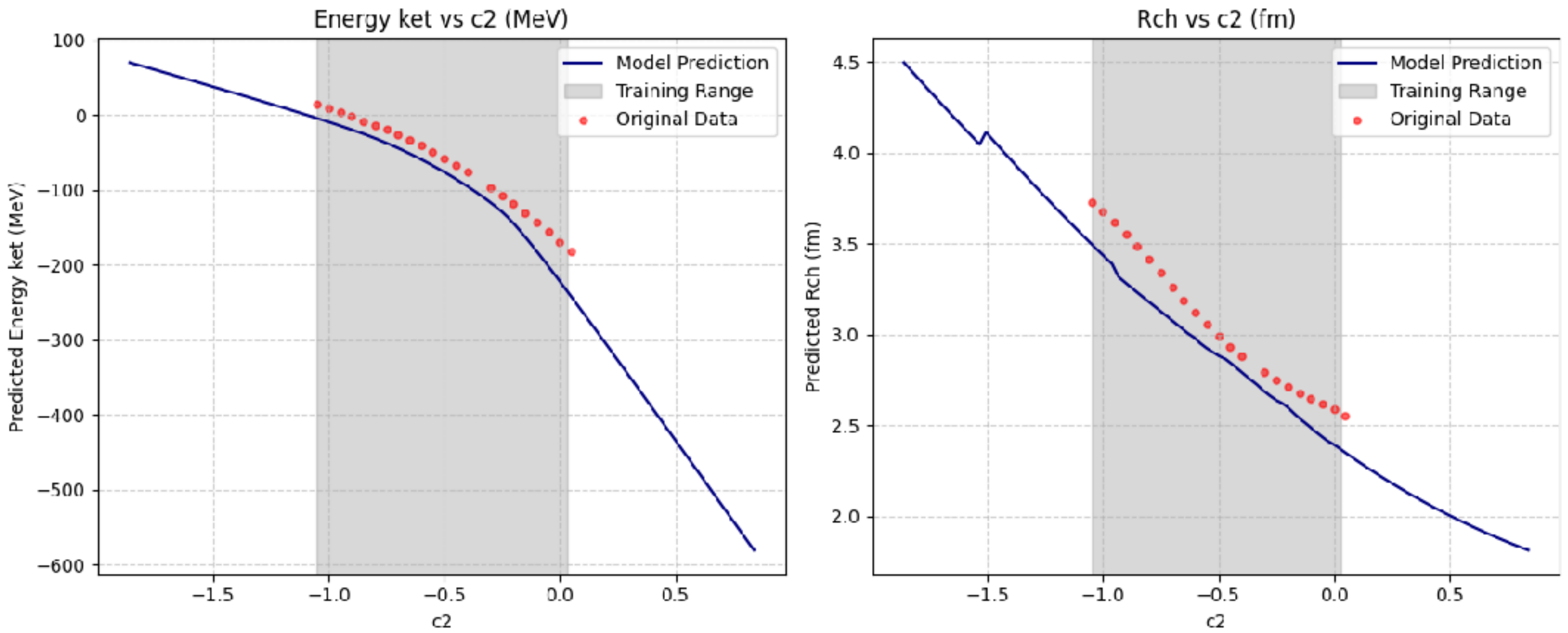
Physics Driven BANNANE!

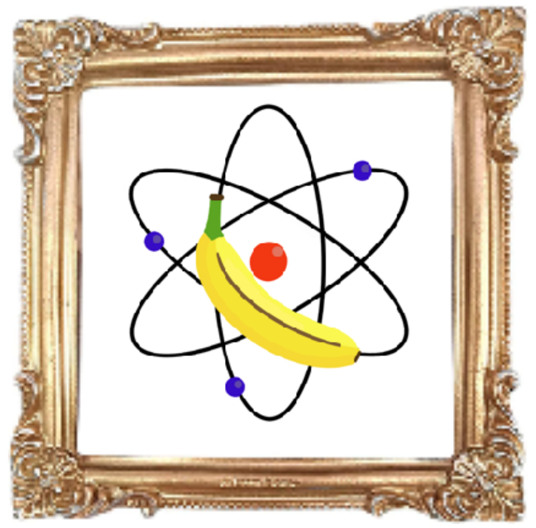
Model Extrapolation vs. Low-Energy Constants (LECs)



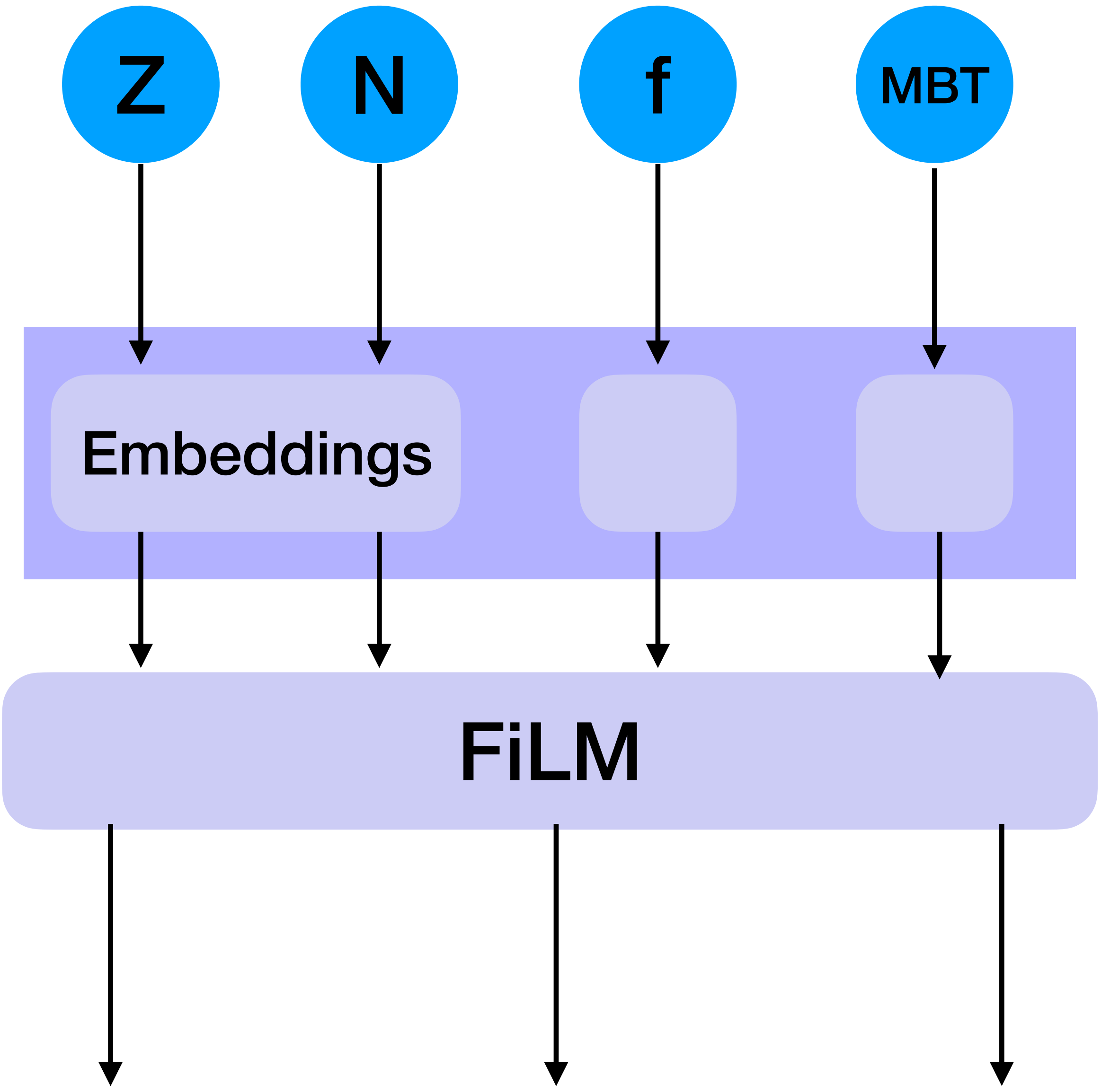


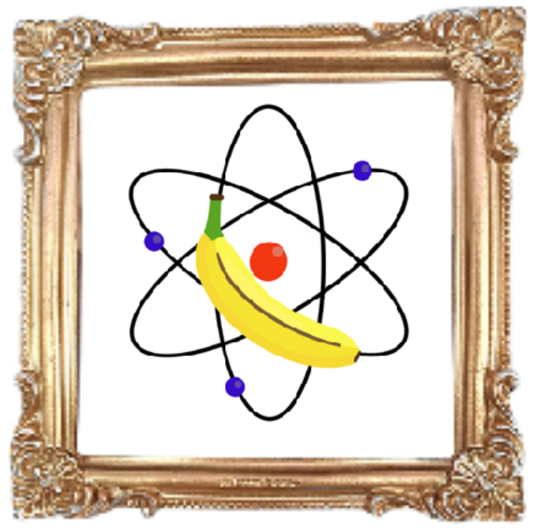






Extrapolating to IMSRG(3)





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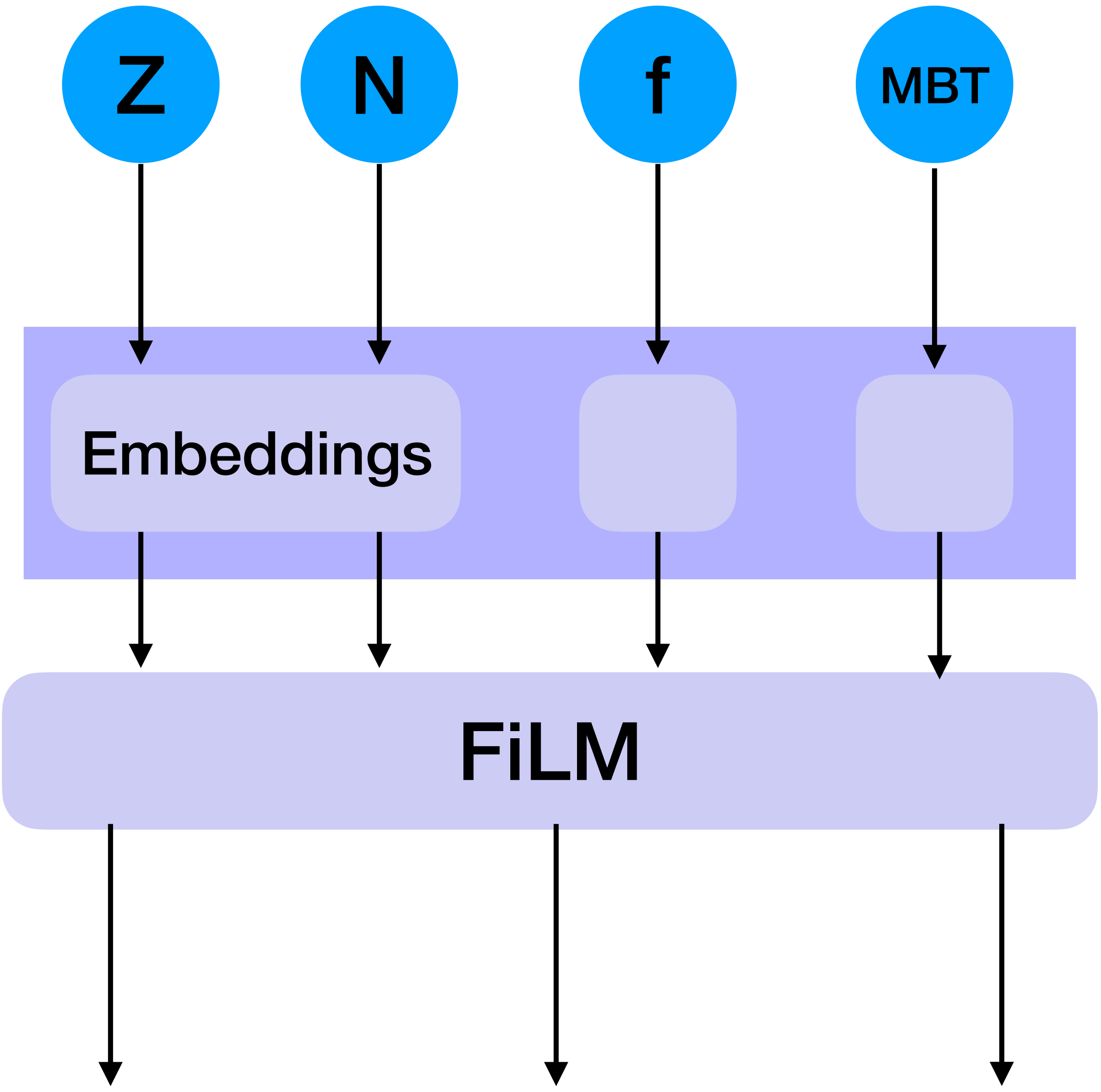

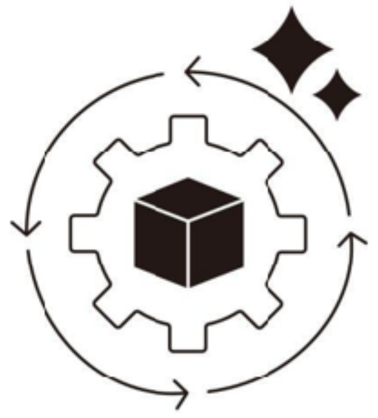

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Difference with model and calculation of IMSRG(3f2) when no IMSRG(3f2) is used to train in a specific isotope.

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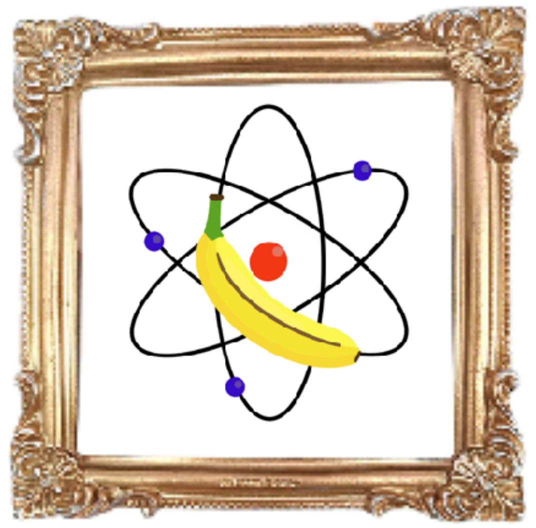
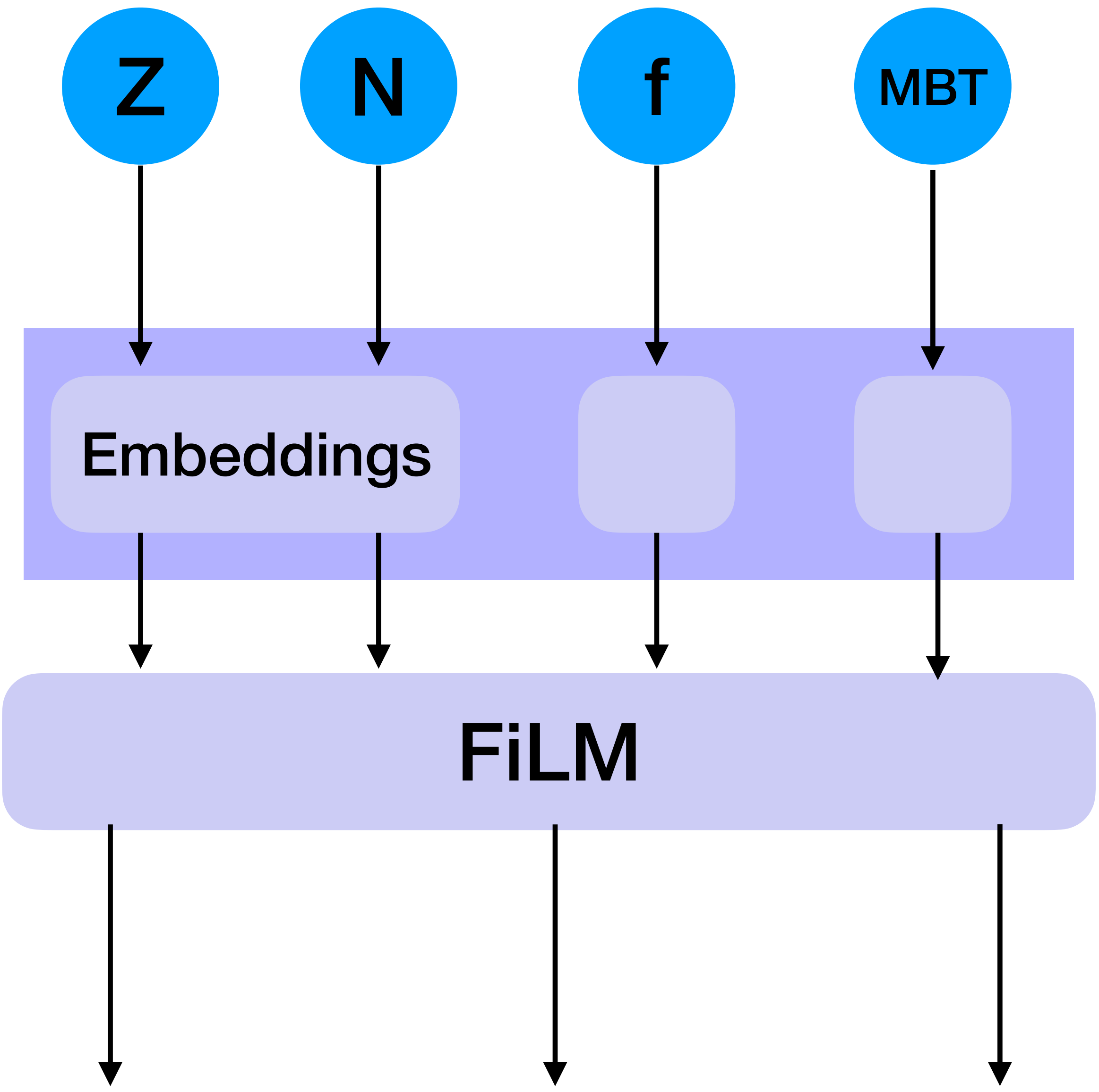

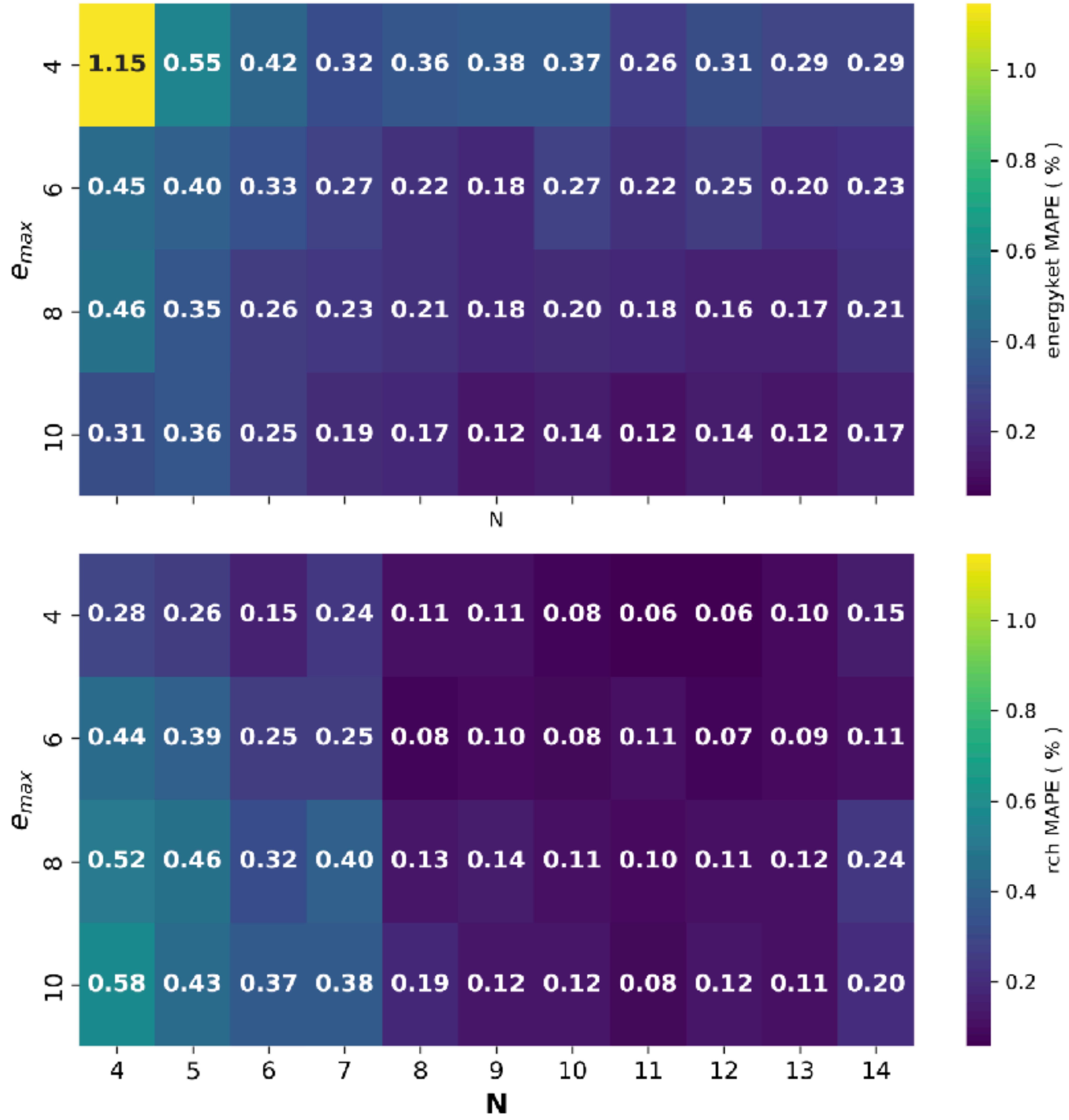

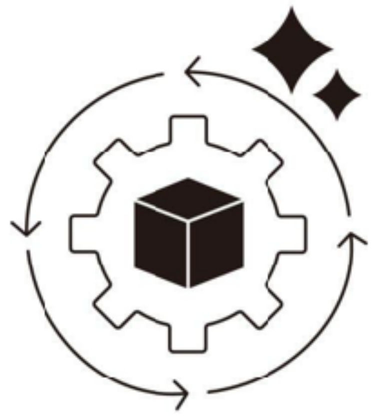

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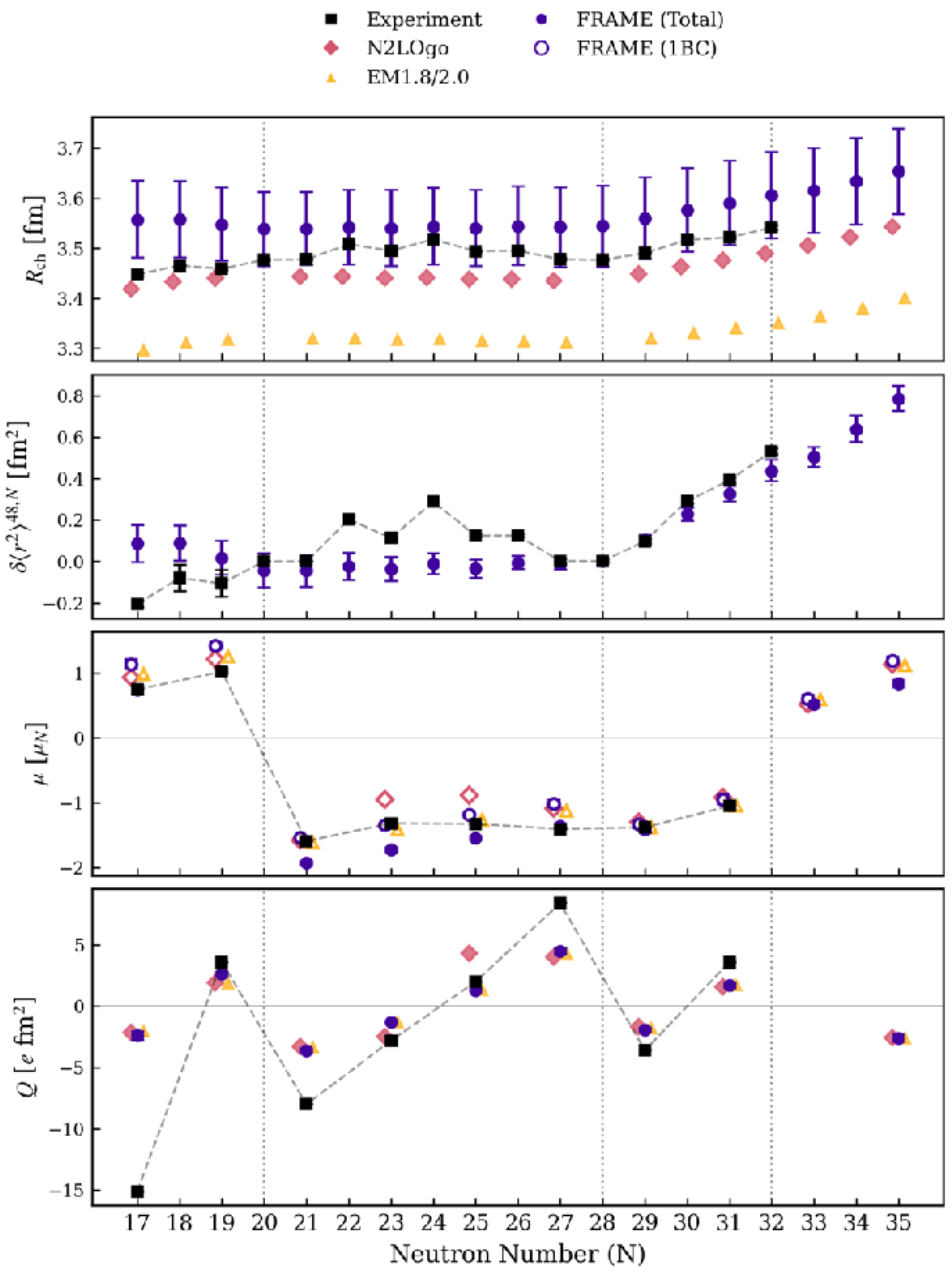
Case study: EM Moments of Ca isotopes

EM Moments of Ca Isotopes



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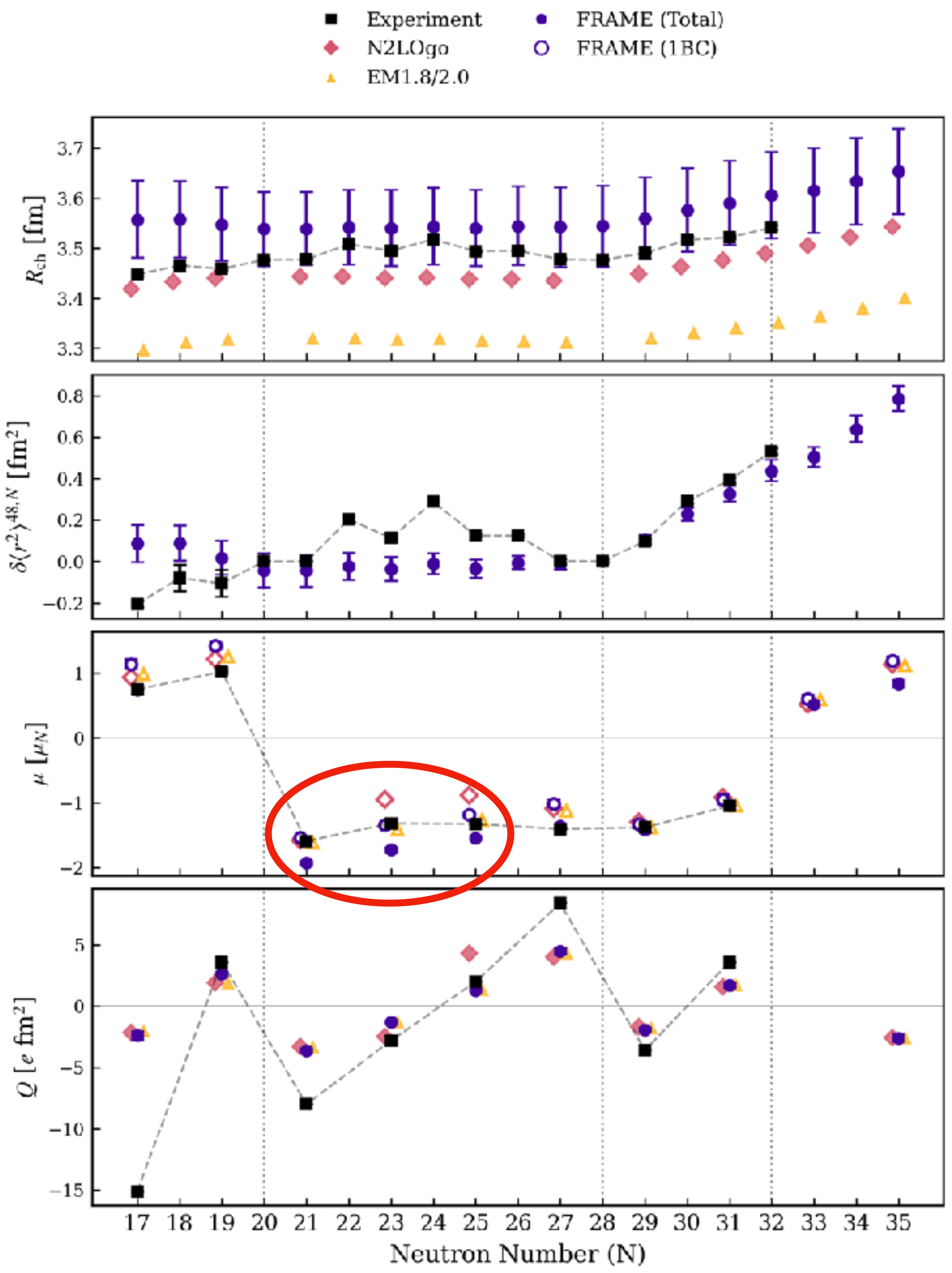

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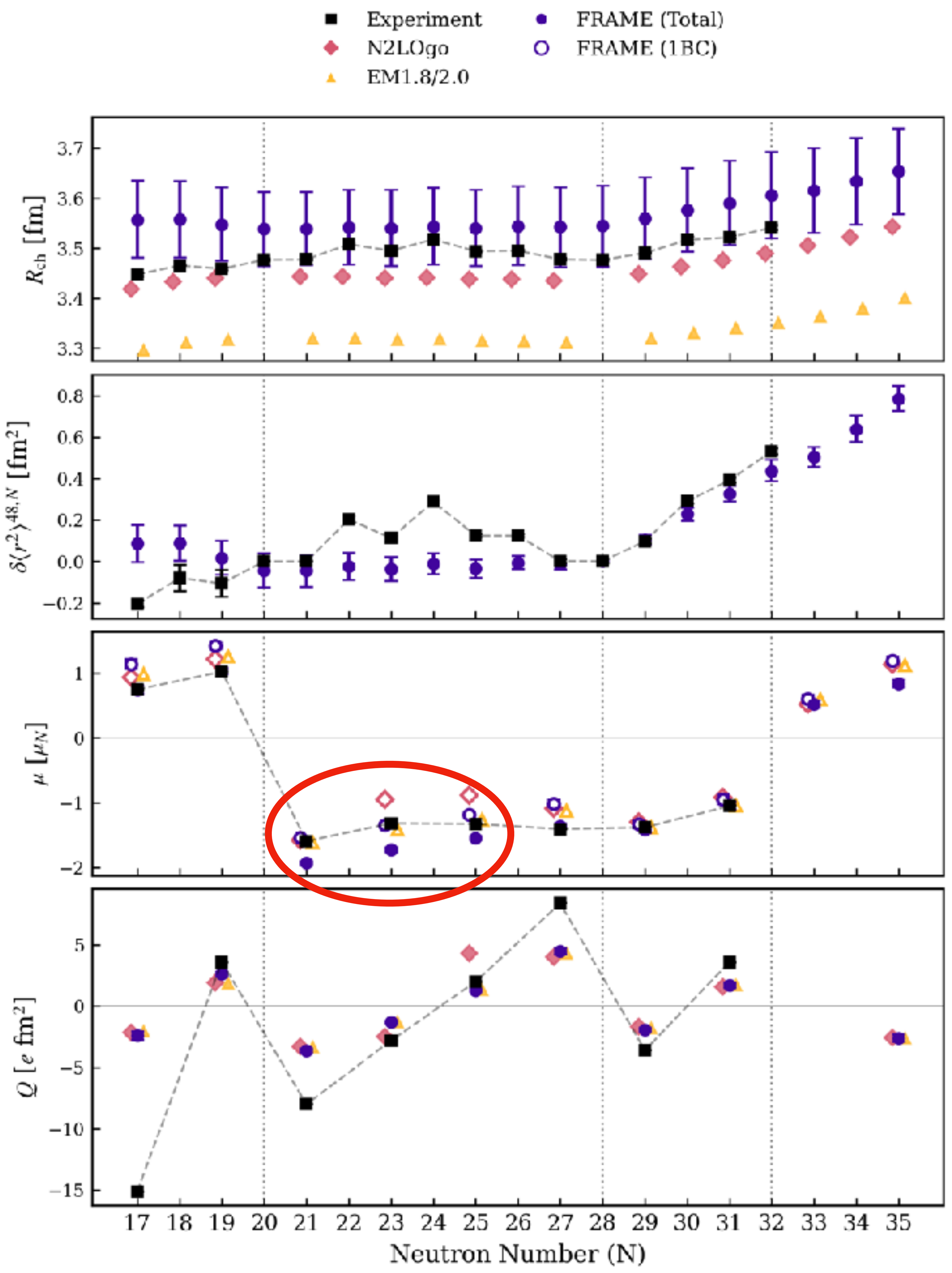
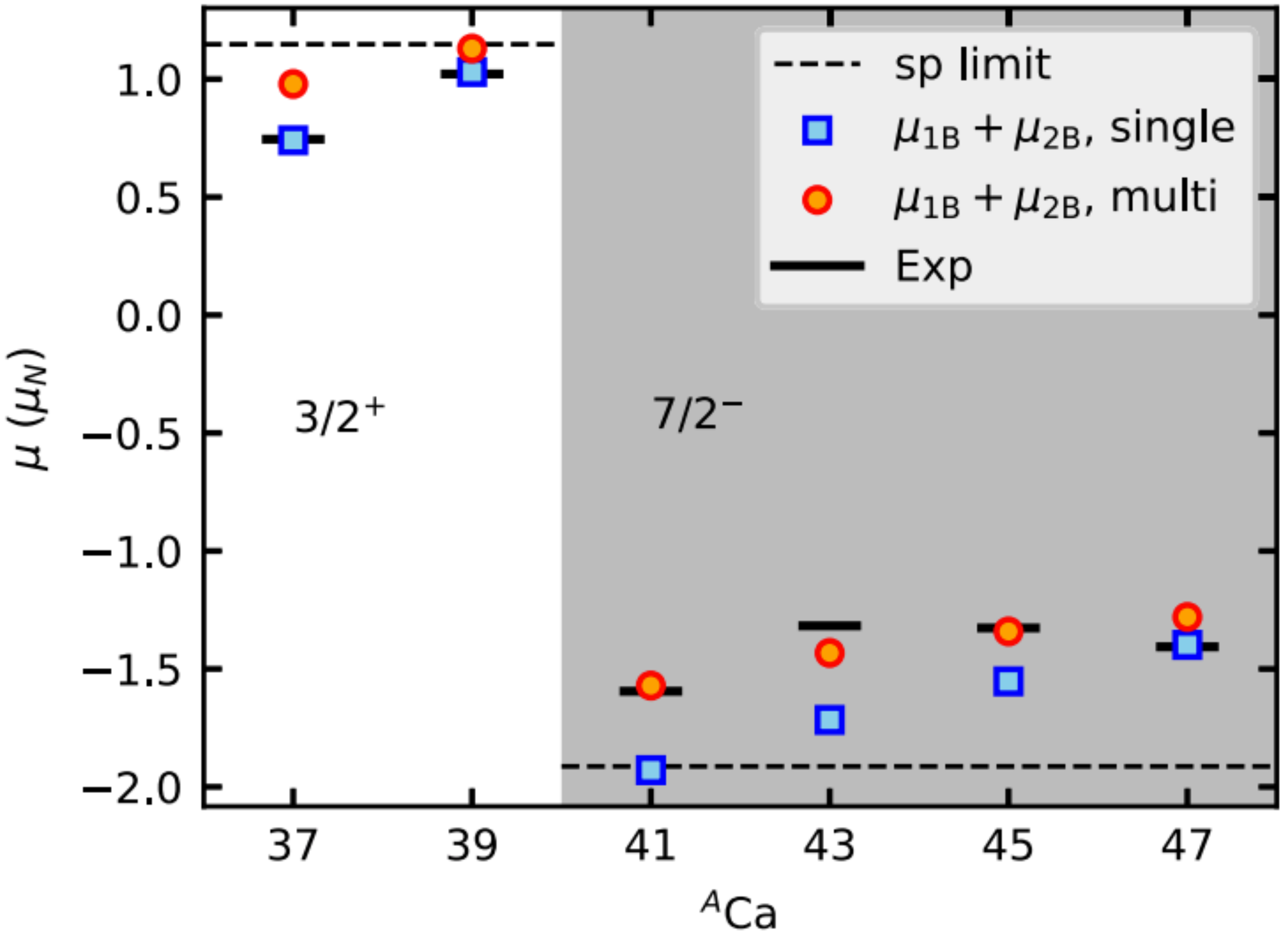
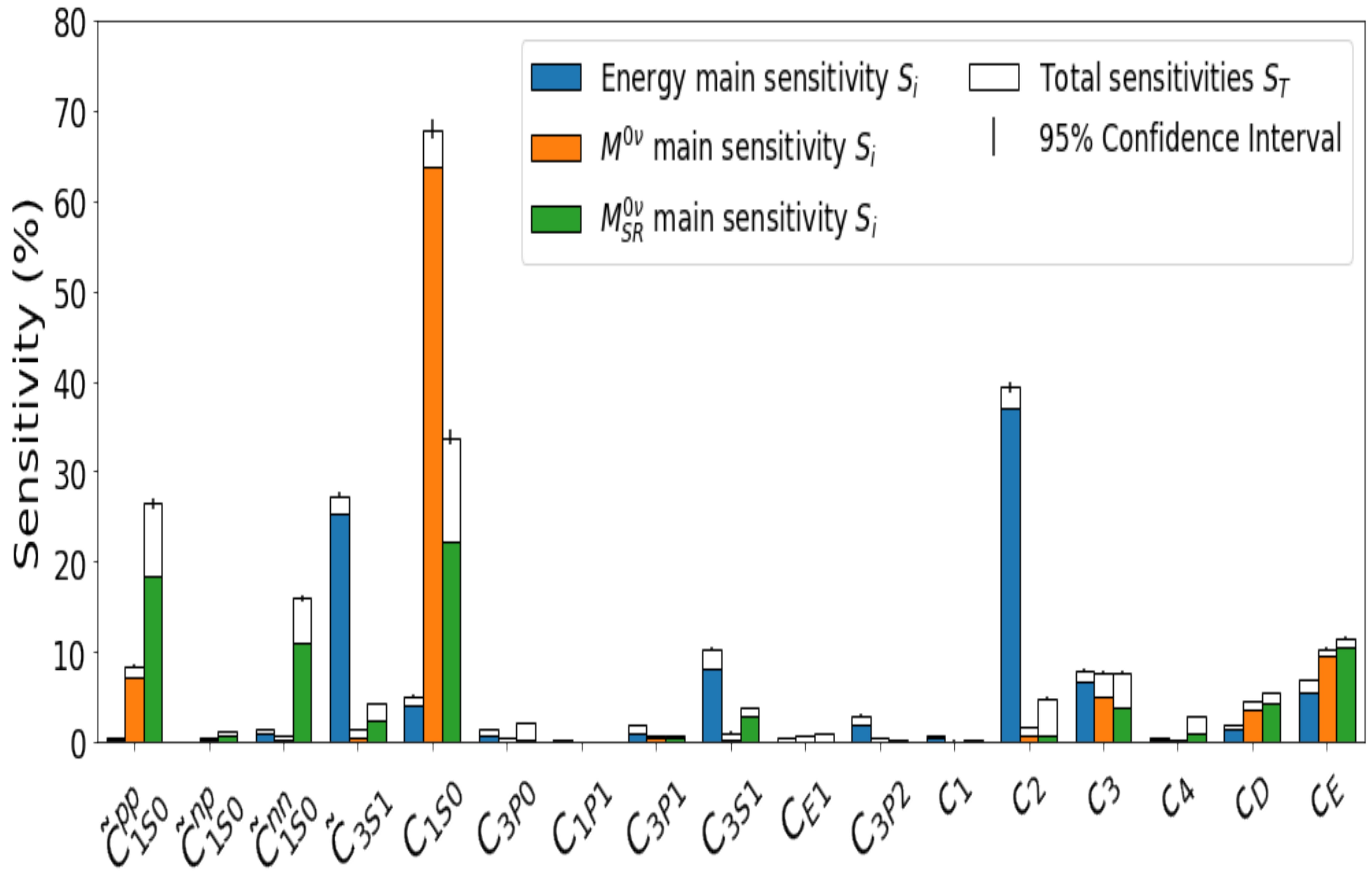


Miyagi et al., Phys. Rev. Lett. **132**, 232503

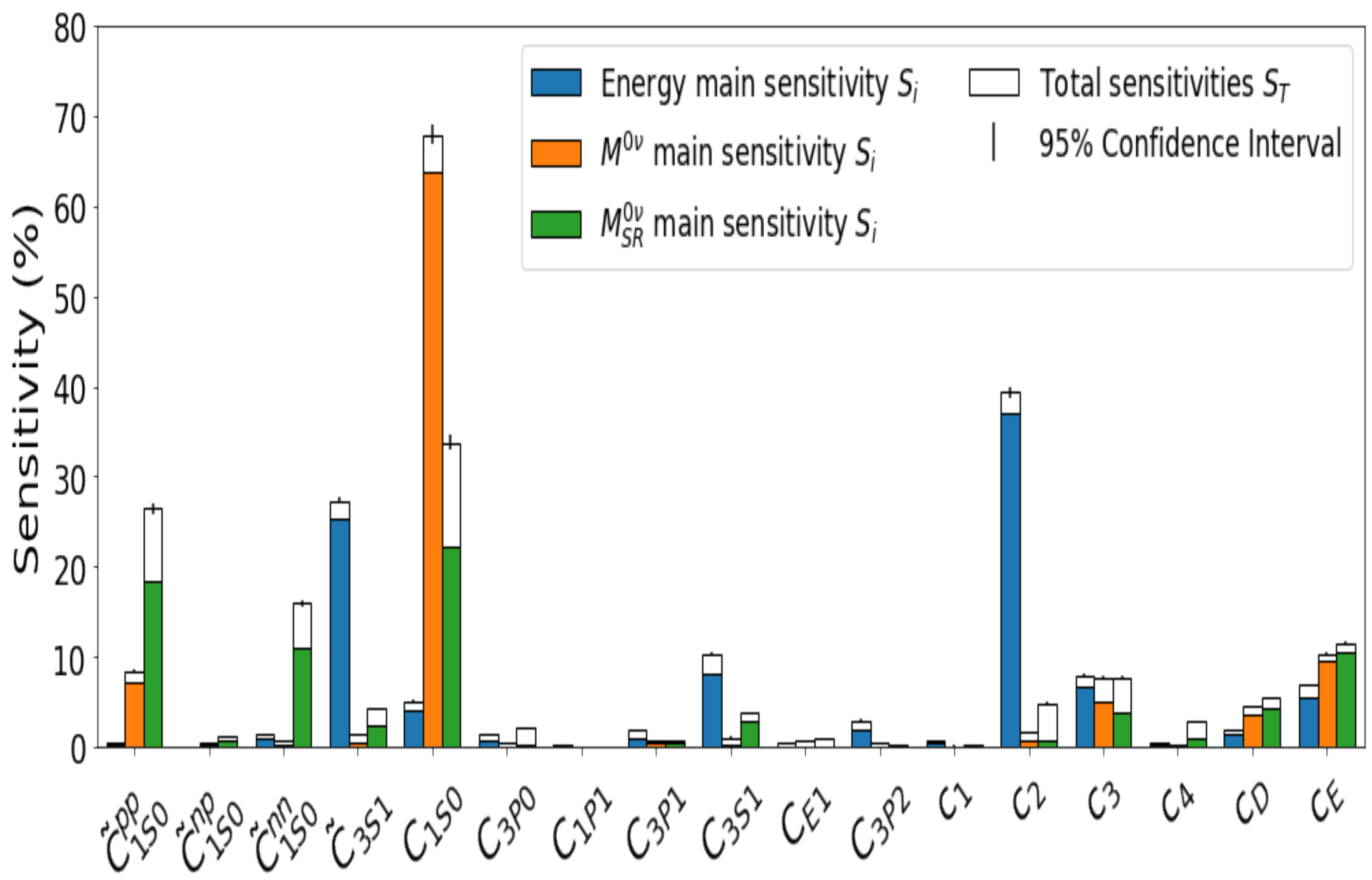


Issues with GSA



Issues with GSA

- Very costly



Issues with GSA

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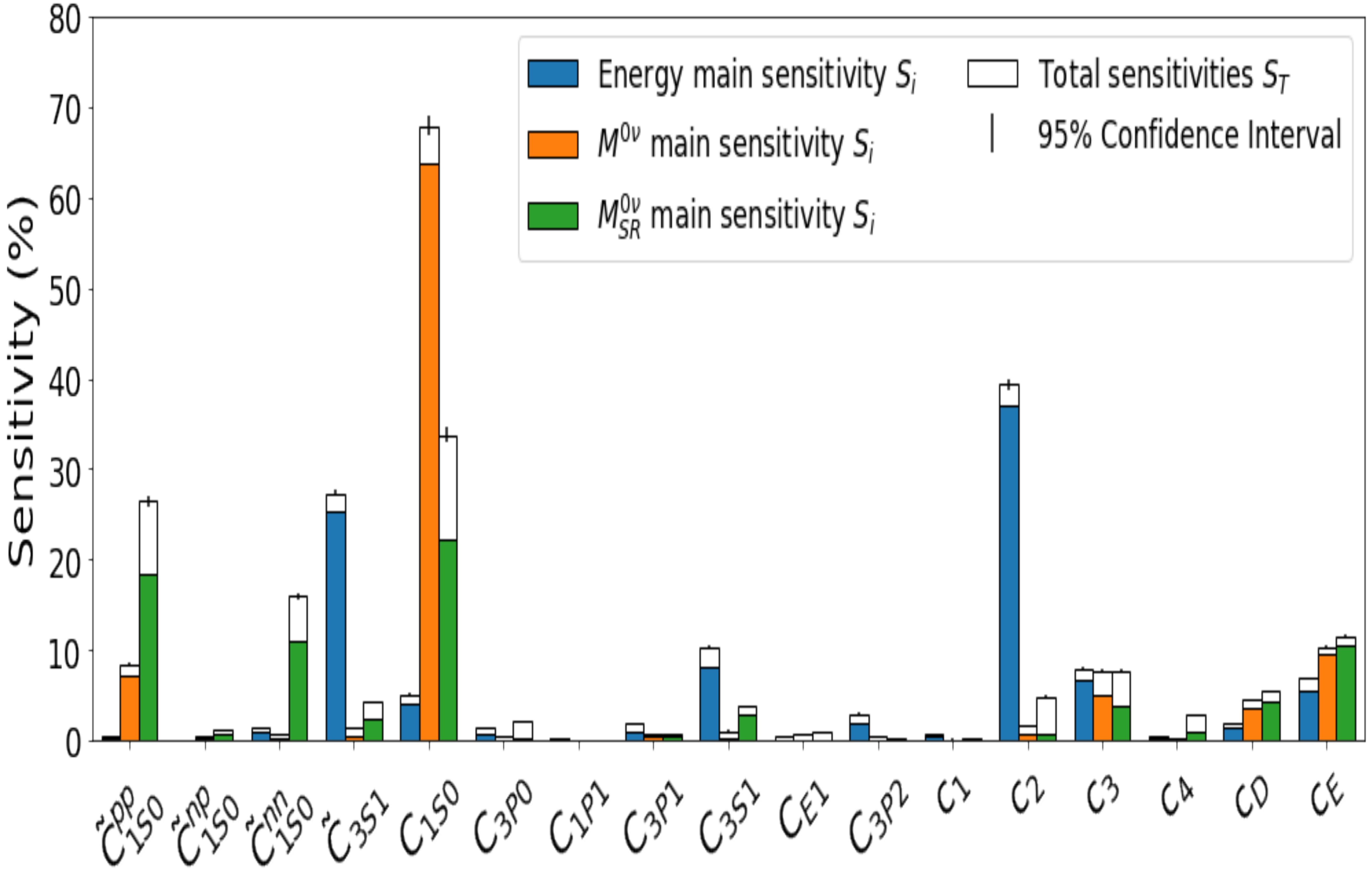
- No indication of how the parameters influence the results



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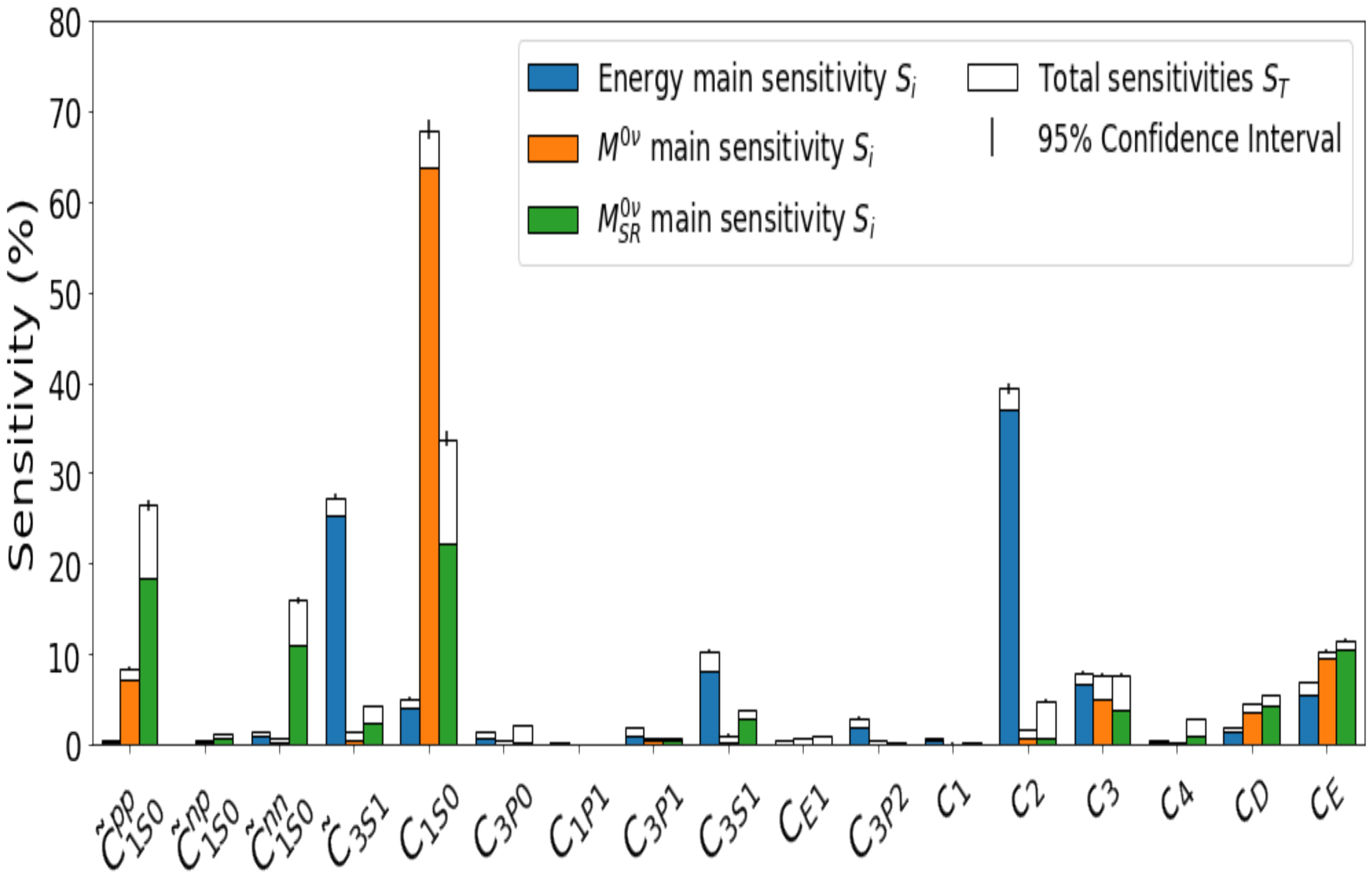

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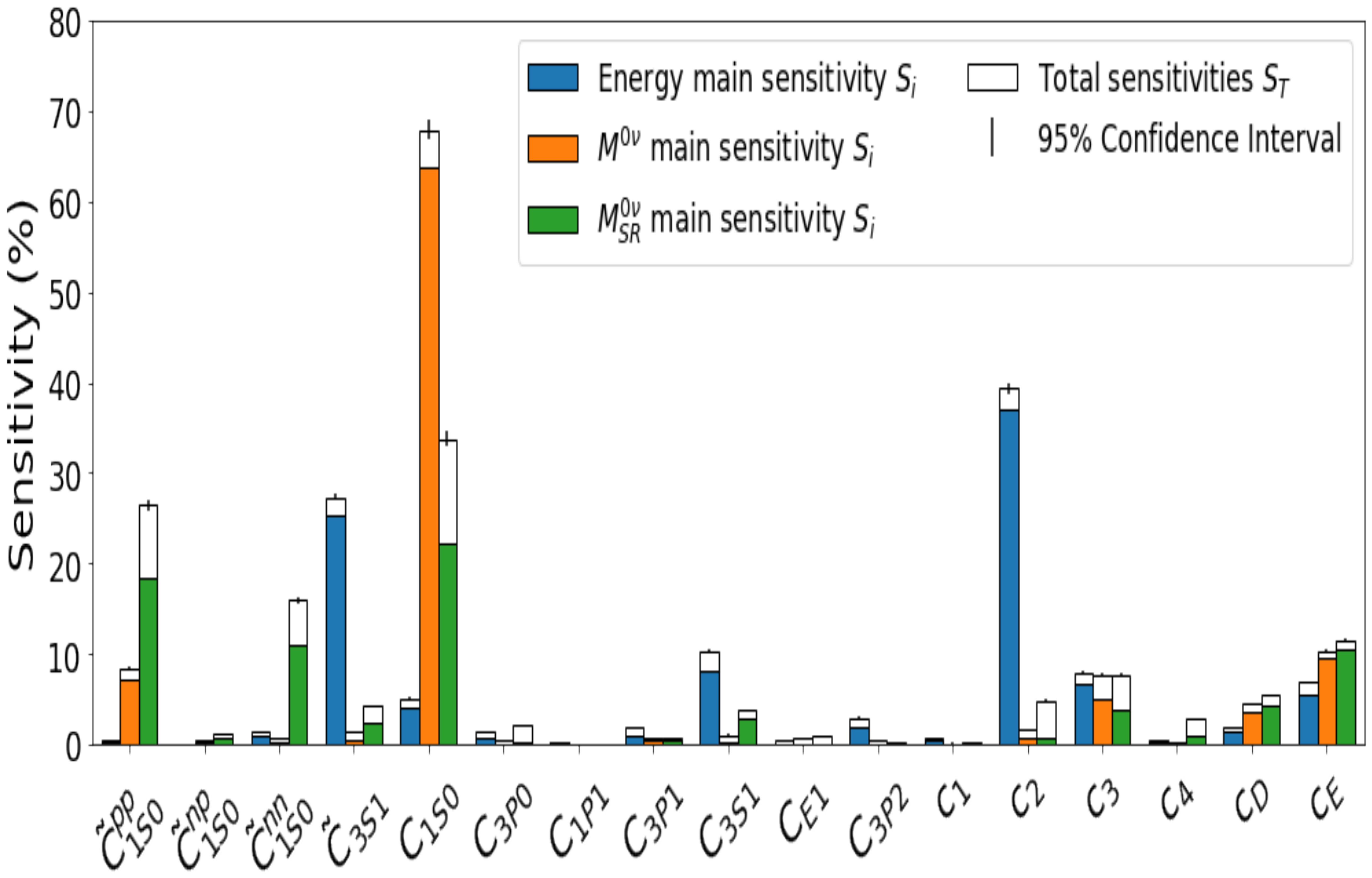
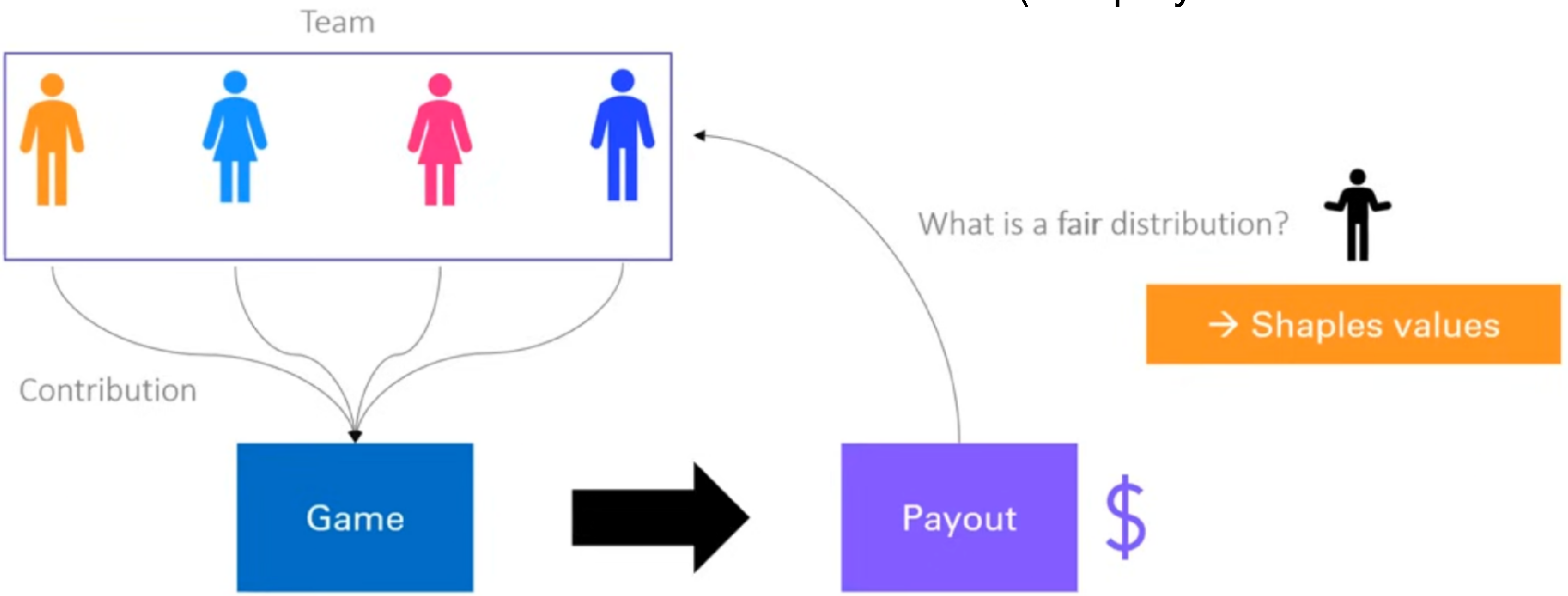


SHAP Values

(SHapely Additive exPlanation)

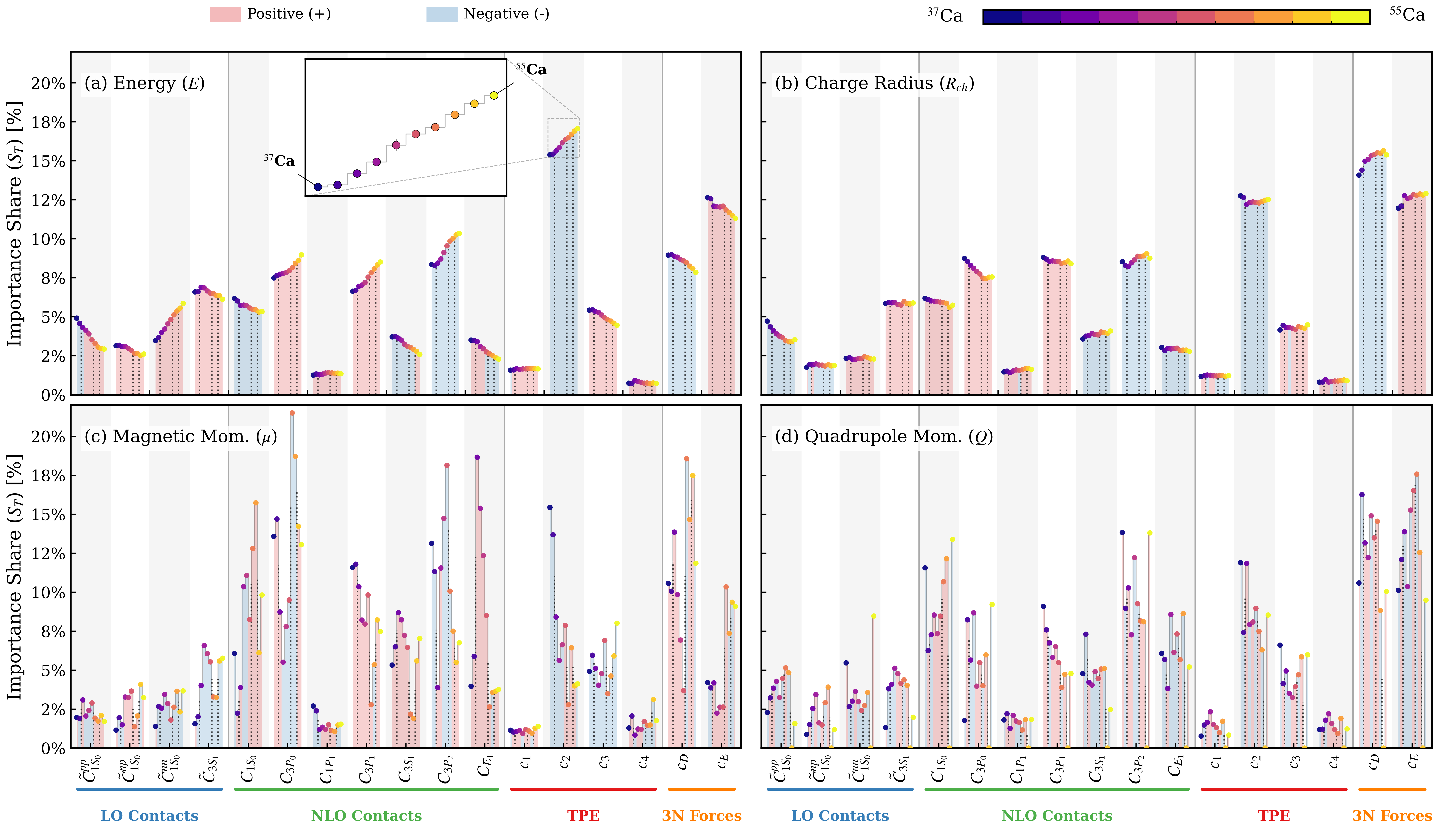


Sobol vs SHAP

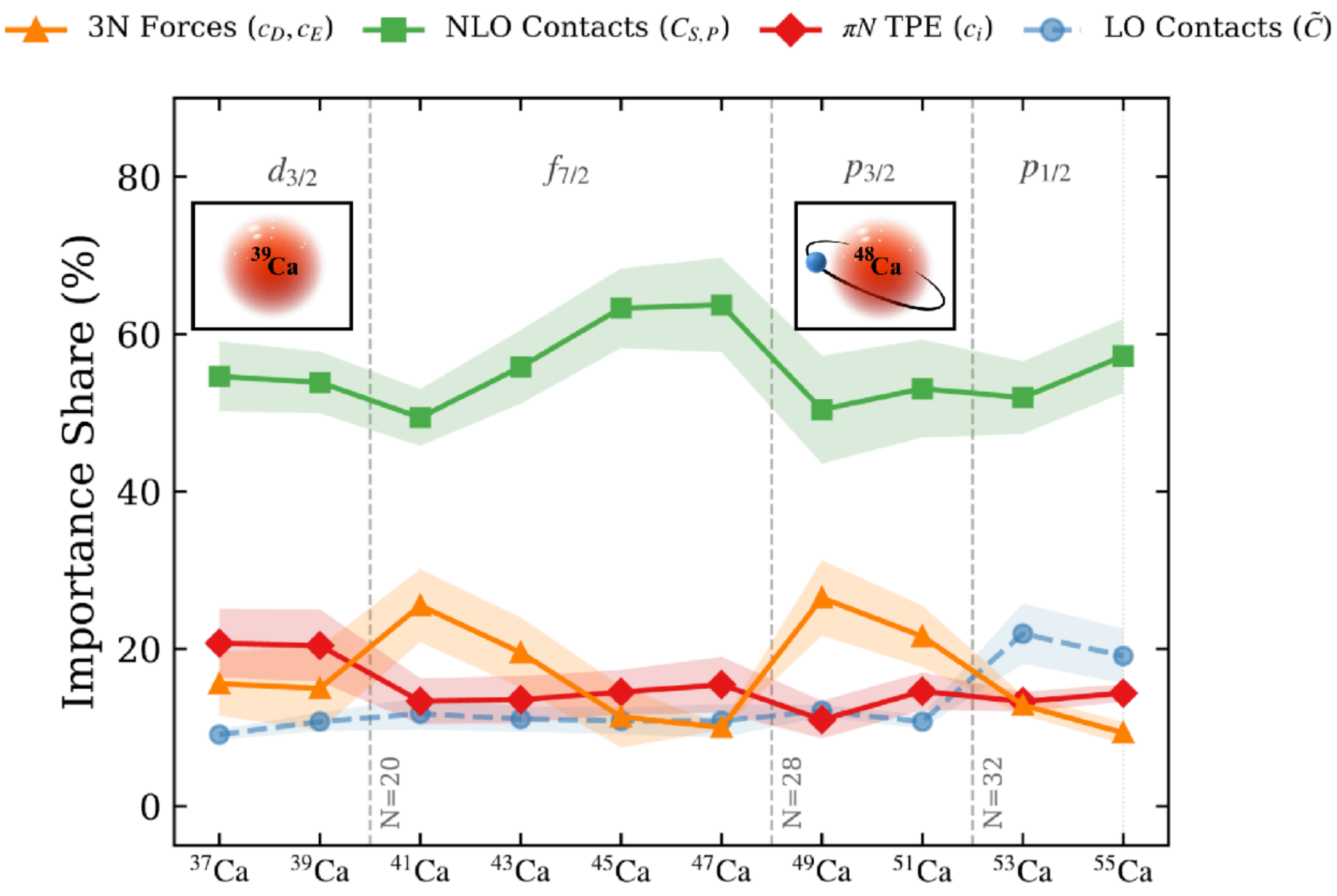
Aspect	Sobol′	SHAP (standard ML usage)
Primary question	Which inputs drive **variance** globally?	Which inputs drive a **specific prediction level** relative to baseline?
Scope	**Global** by design	**Local** per x; global only after aggregation
Units	Fraction of **variance** $[0, 1]$	In **output units** (additive contributions)
Interactions	Explicit $S_{ij}, S_{ijk}, \ldots; S_{T_i} - S_i$ = "all interactions involving i"	Interaction SHAP exists (ϕ_{ij}), but usually you view main ϕ_i or sum of interactions
Input dependence	Assumes **independent** inputs (classic Sobol′)	Can use **interventional** (assumes independence) or **conditional** SHAP (uses empirical dependence); each has trade-offs
Baseline	None (centered by variance)	Explicit baseline $\mathbb{E}[f(X)]$ (or dataset mean)
Cost	$(2 + d)N$ model evals for S_i, S_{T_i} with Saltelli/Jansen	Depends on explainer; TreeSHAP is fast & exact for trees; KernelSHAP is expensive (many coalitions)
Interpretability	"% of uncertainty due to X_i"	"How much X_i pushed this prediction up/down"

SHAP values in Ca Isotopes

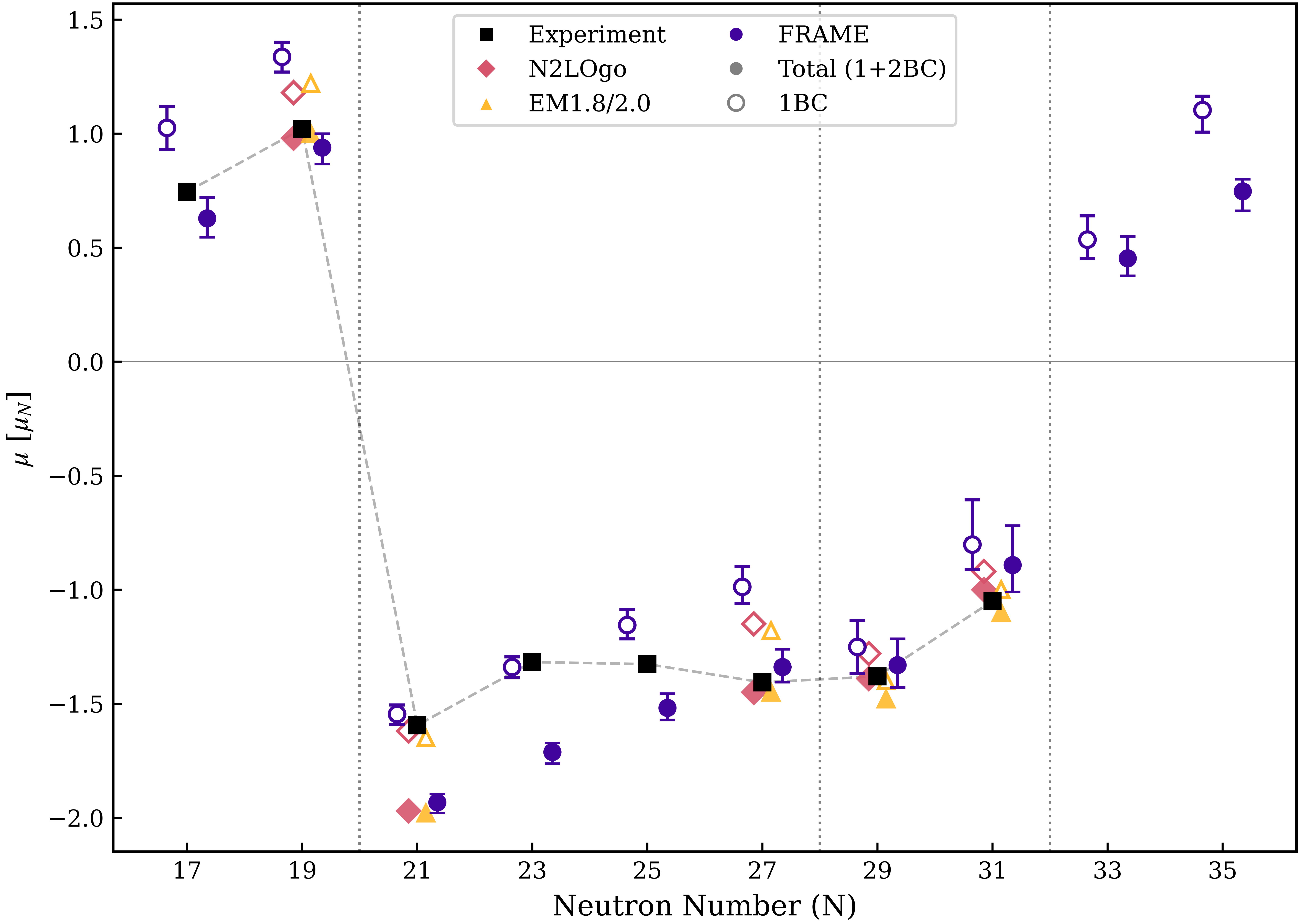
Munoz, **Belley**, et al., arXiv: 2603.26905 (2026)



Forces Through the Shells



Using Emulators to Constrain Forces



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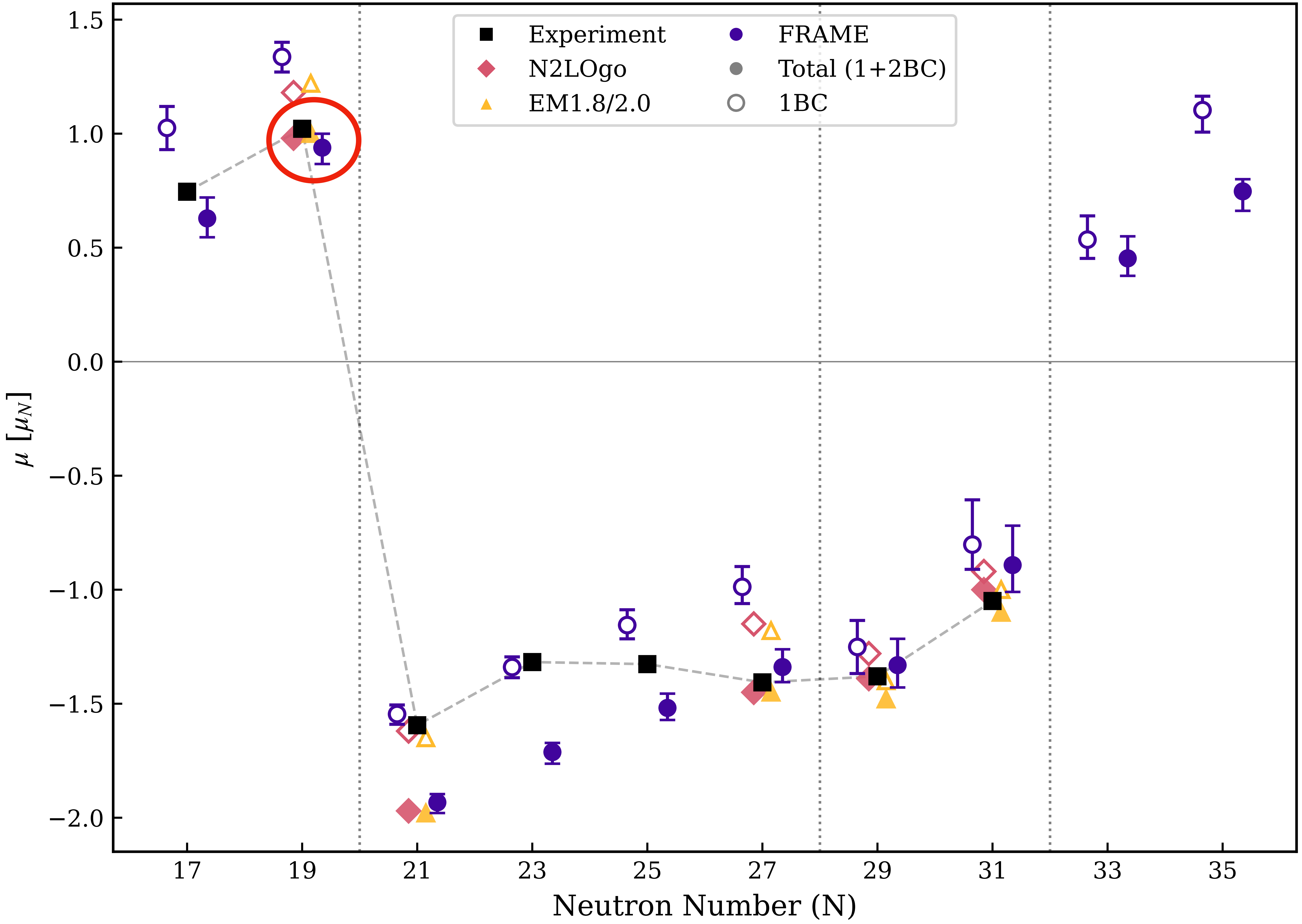

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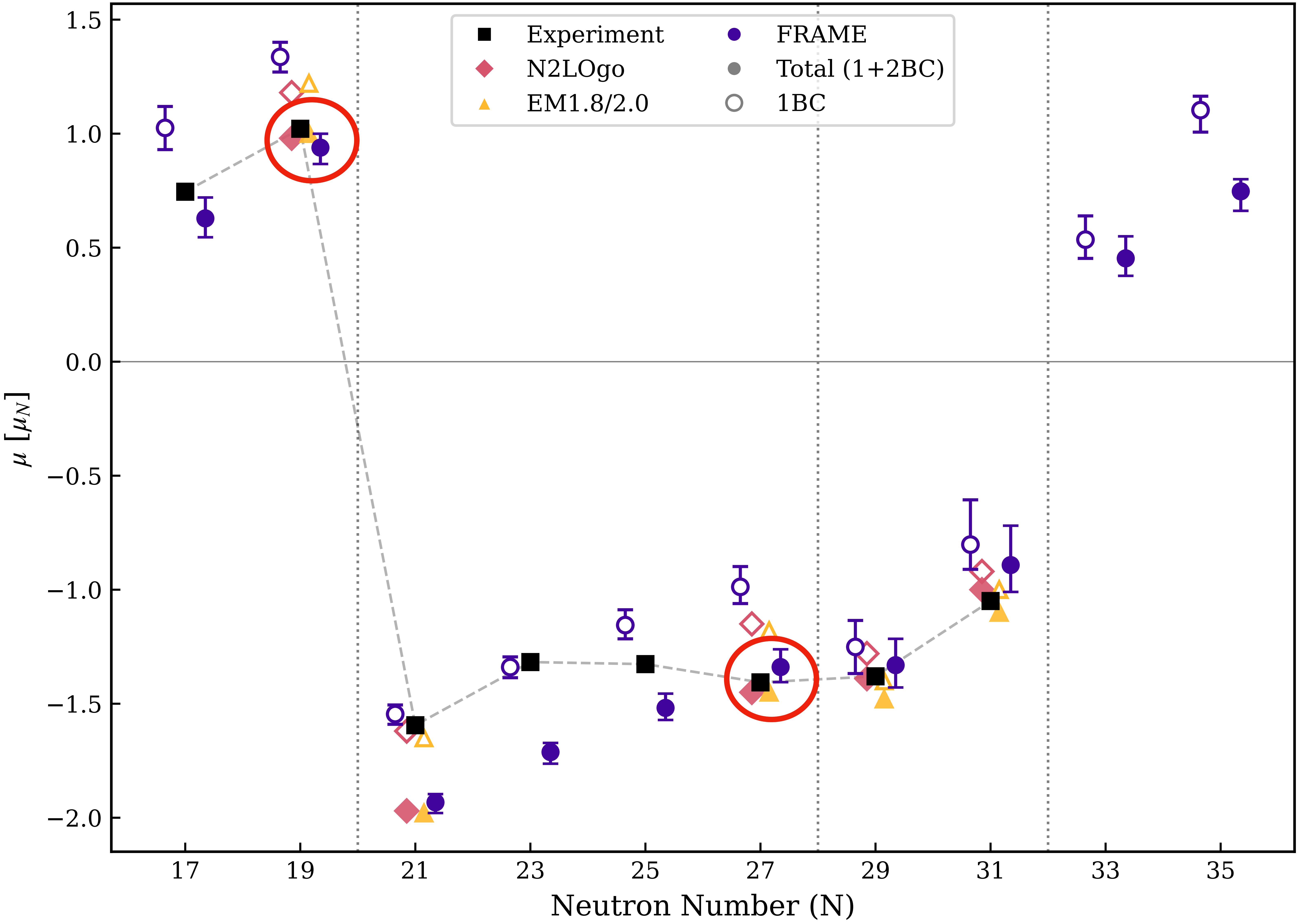

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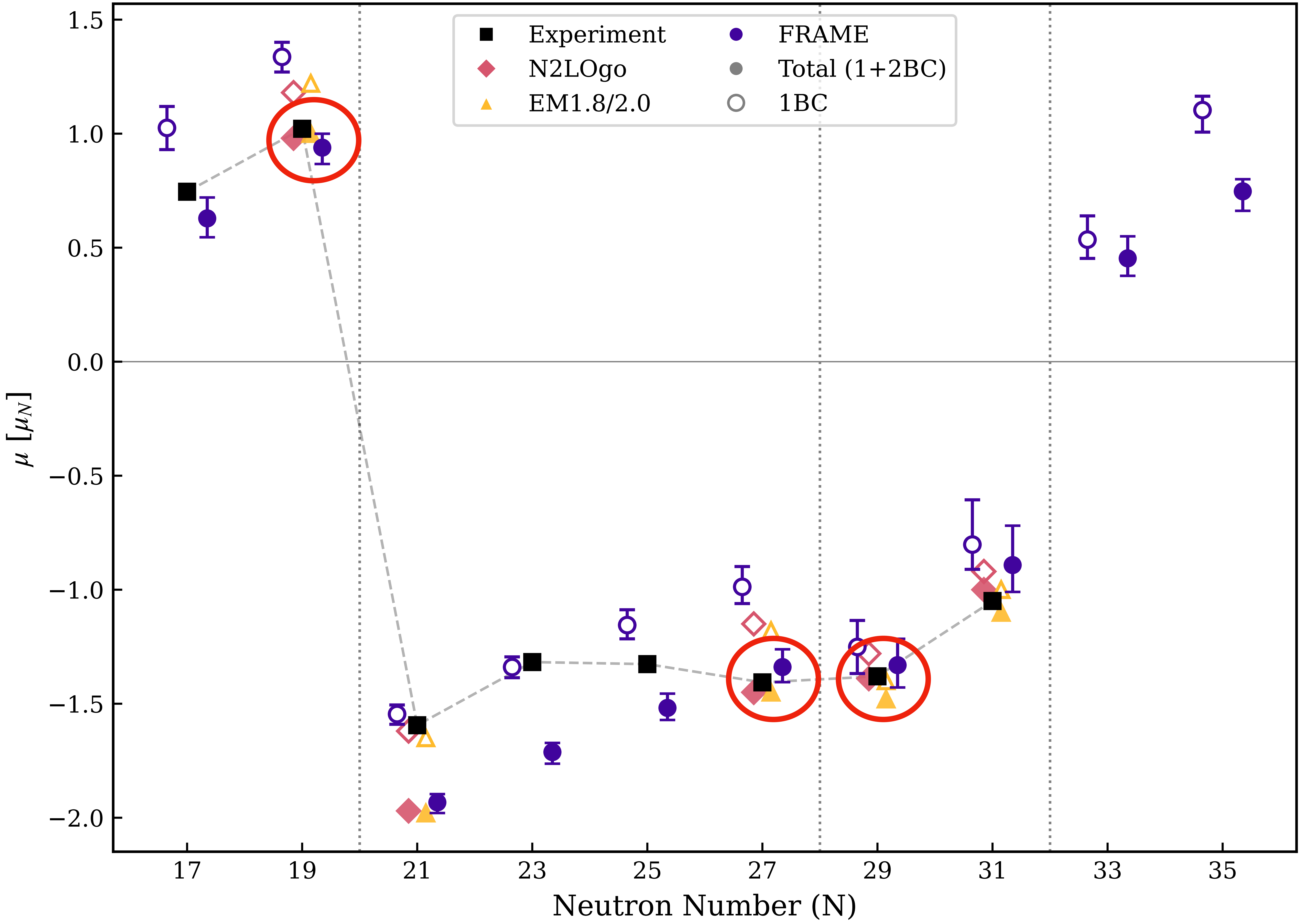
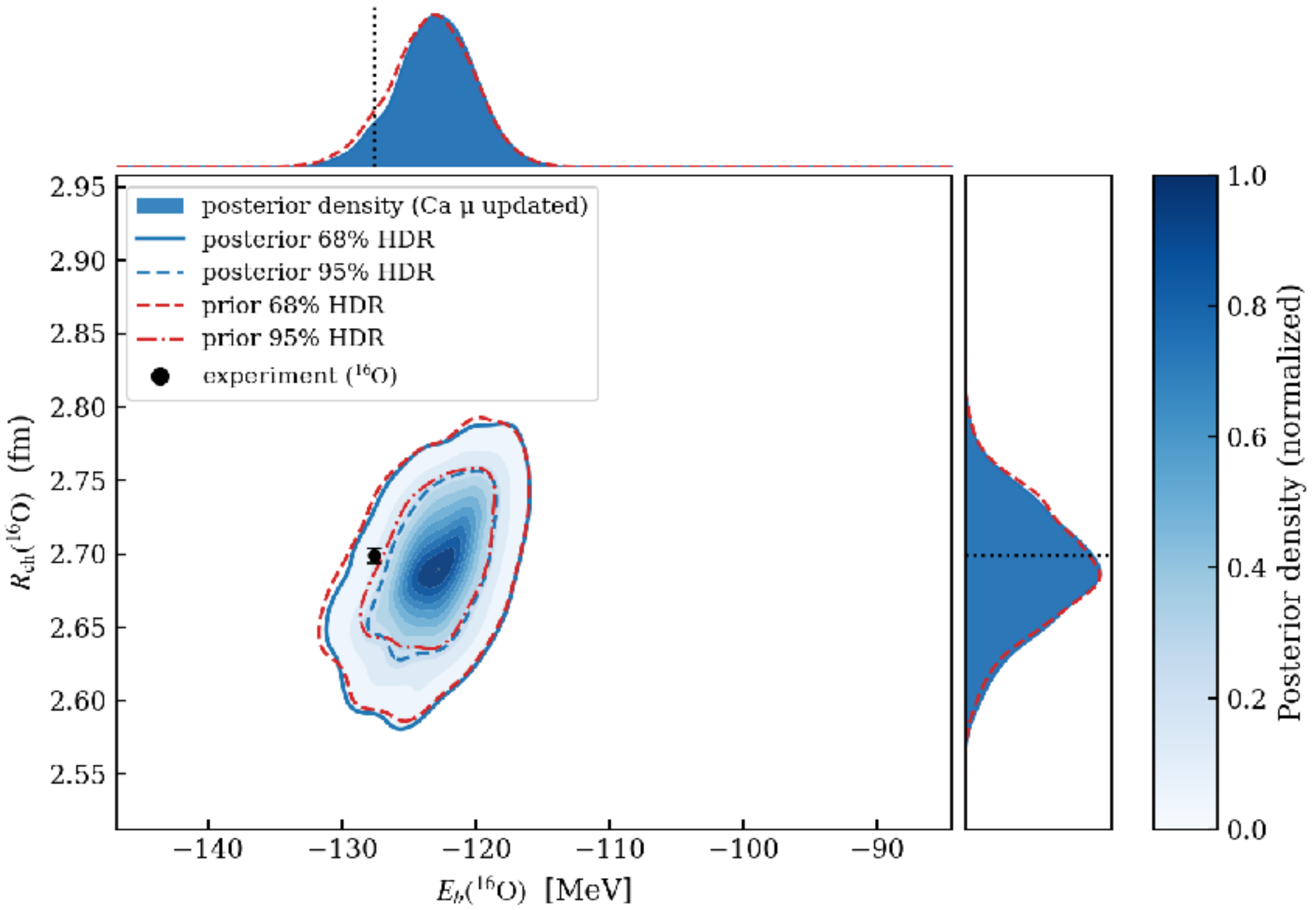
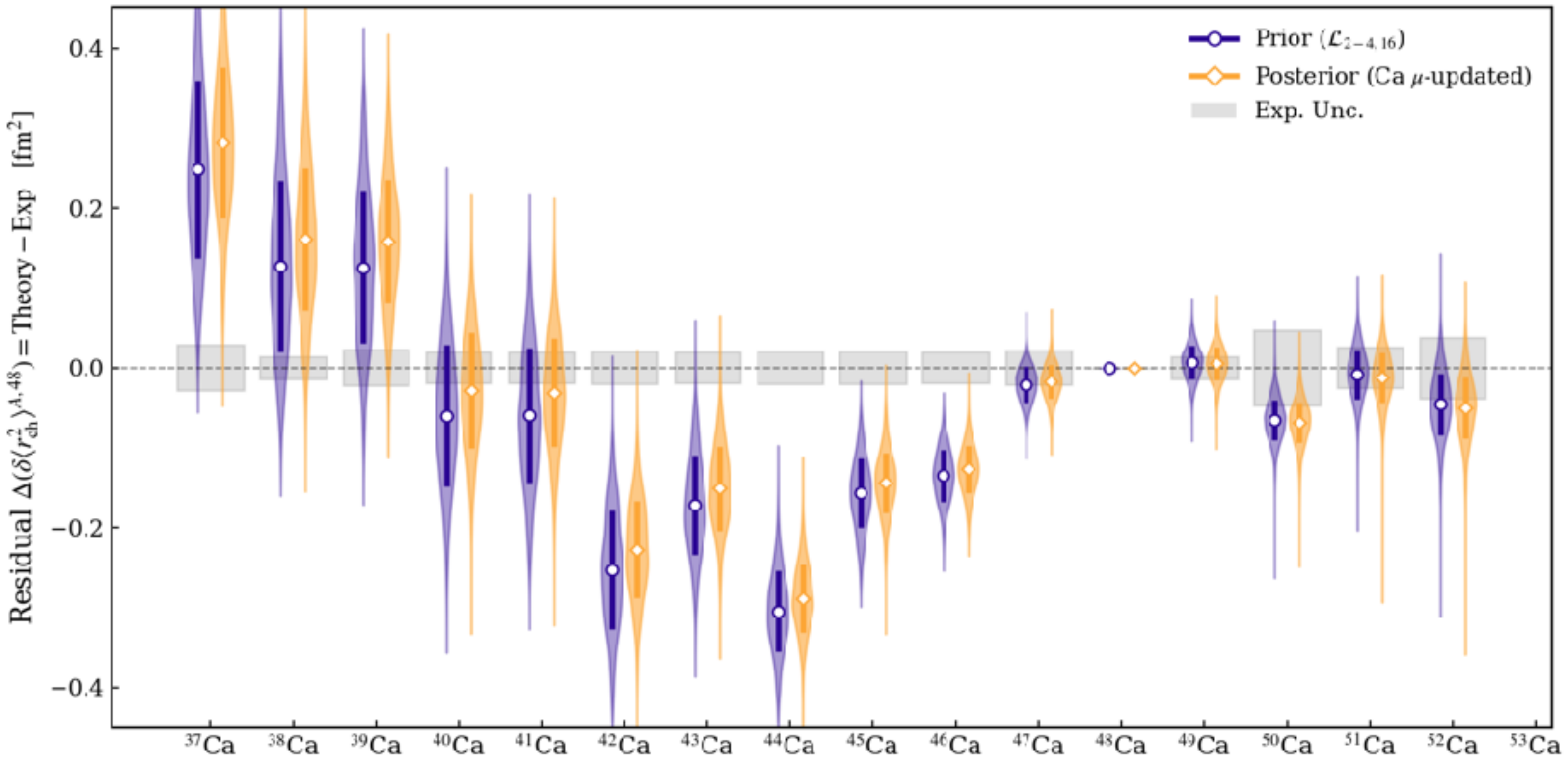


Changes to Likelihood





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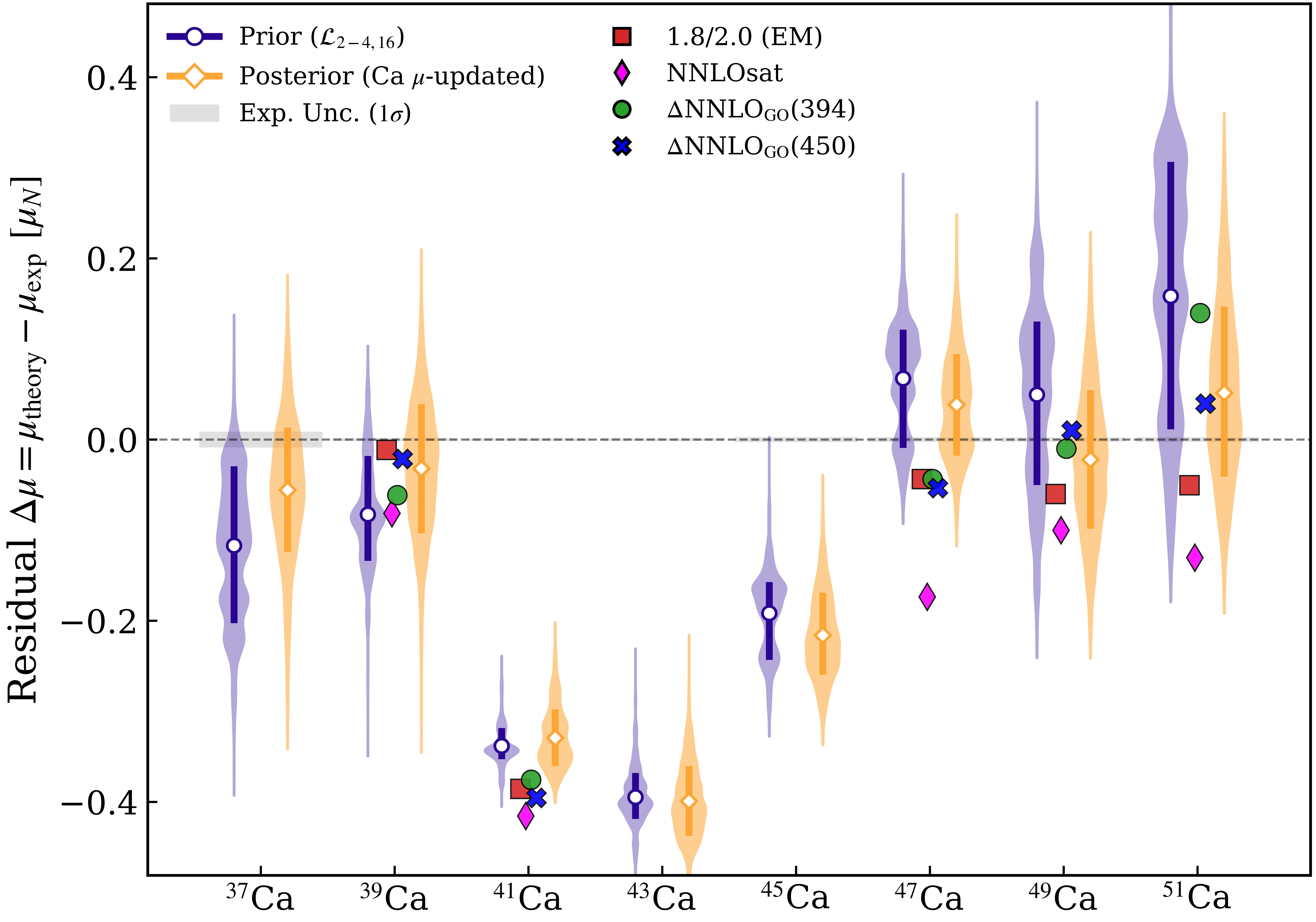

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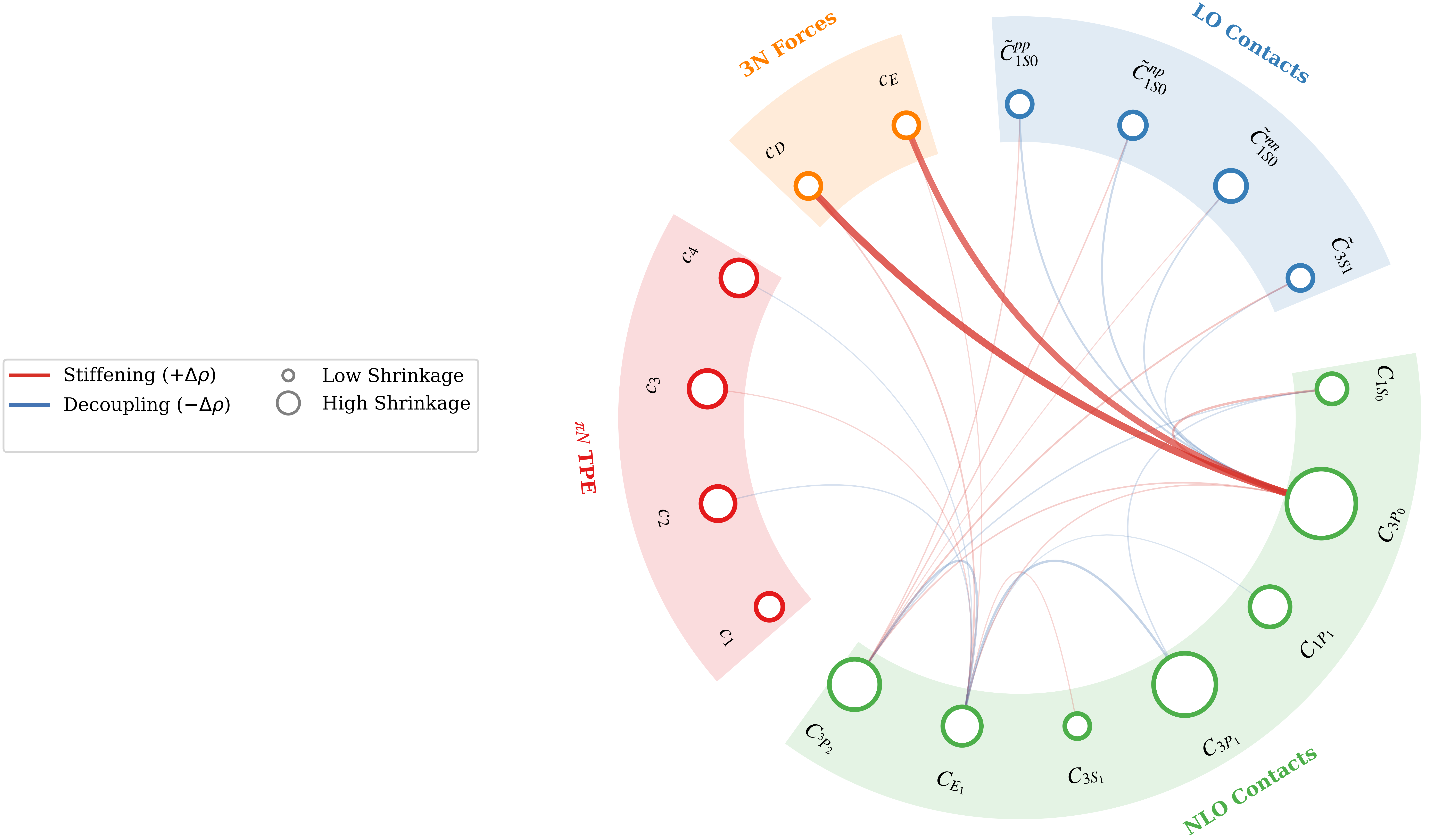

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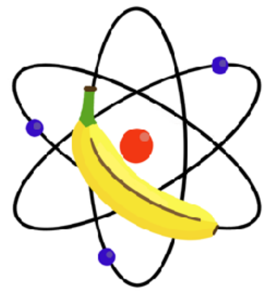
- Created new ML emulator: speed up calculations by a factor of ~10^5. 

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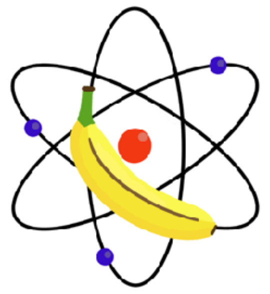
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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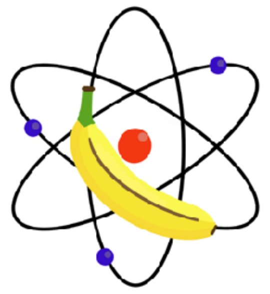
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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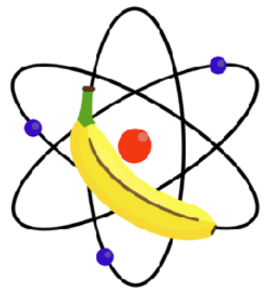
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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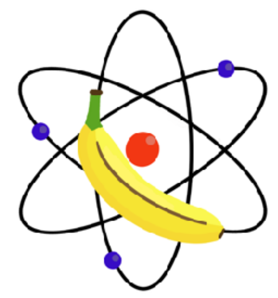
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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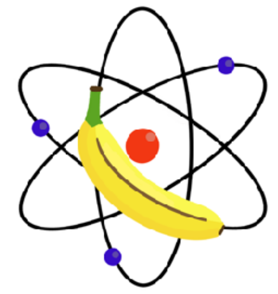
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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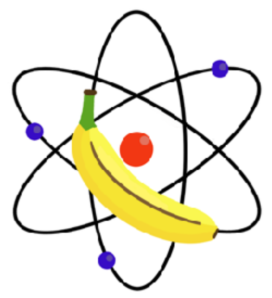
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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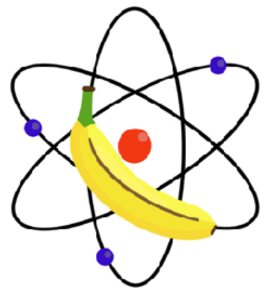
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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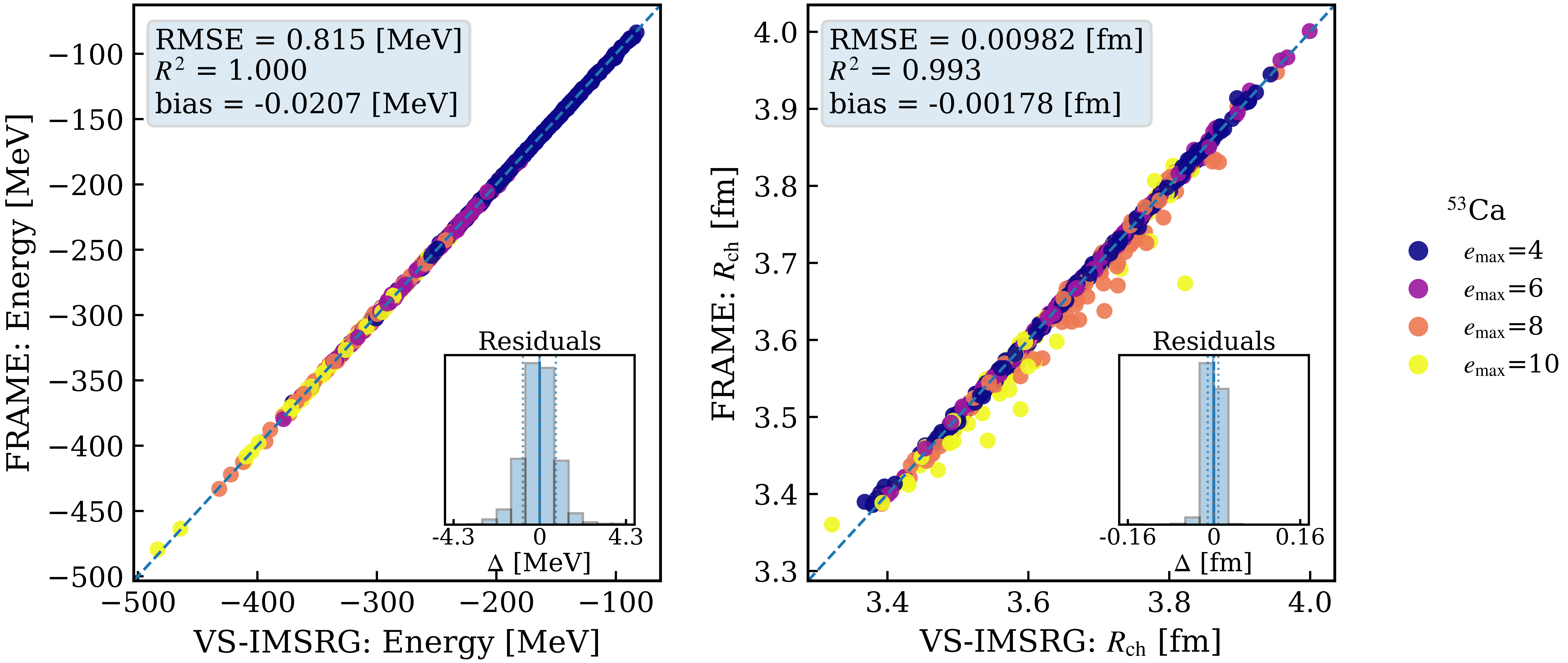
- Use new emulator to quantify uncertainty of many-observables.
- Develop a unified embedding for the nuclear interactions so that they can all be included together.
- Use emulator to get a better understanding of the correlations between different nuclear observables in different nuclei and how they constrain the nuclear forces.

Thank you!

Extrapolation



Correlation between observables