Connecting Nuclear Forces to the Properties of Complex Nuclei

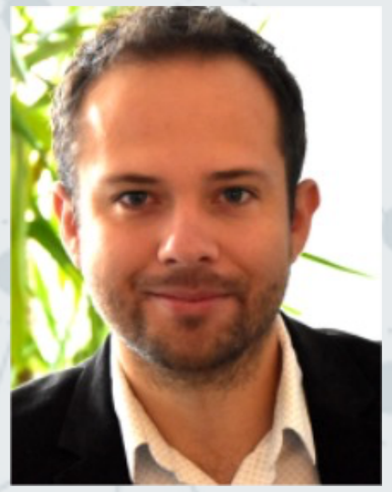
PAINT 2026

Jose Miguel Muñoz Arias

24 February 2026

Acknowledgements

Prof.
Ronald García



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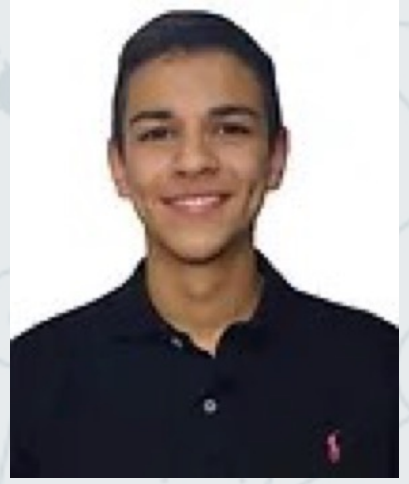

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A. Jadbabaie

C. Konig

Emulators for Many-Body Methods

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

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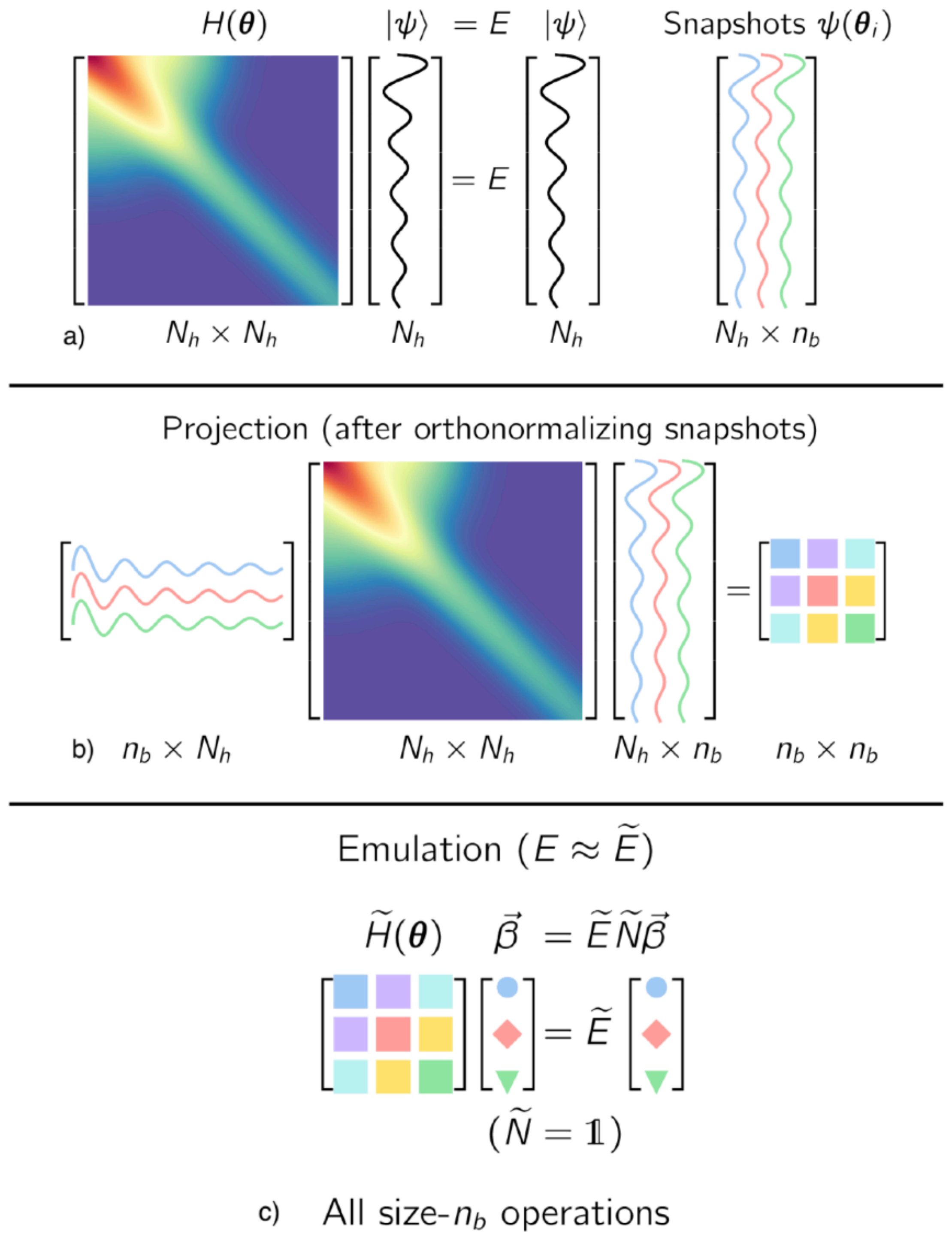
1. Physics driven



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

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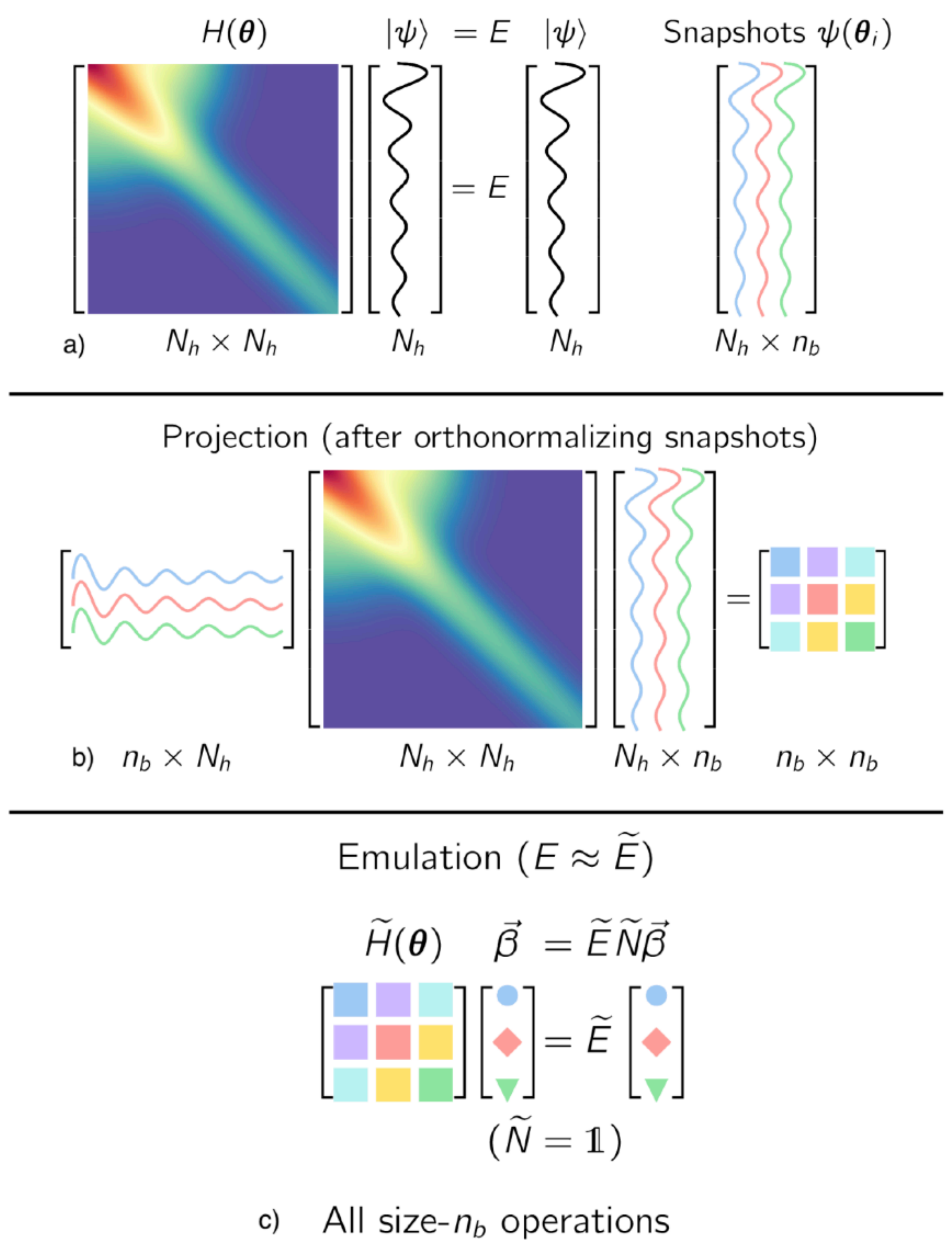
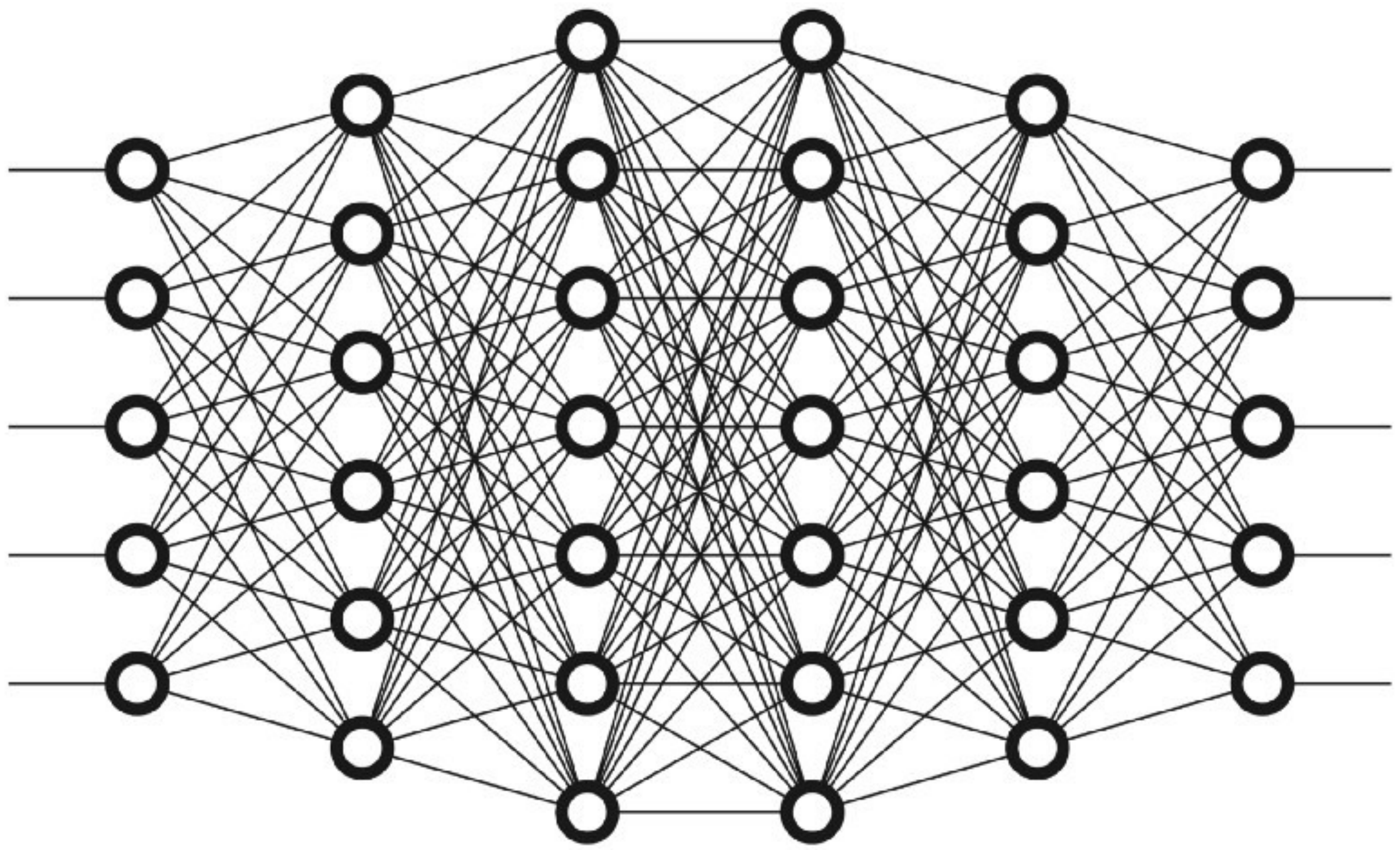


Duguet, et al., Rev. Mod. Phys. **96**, 031002 (2024)

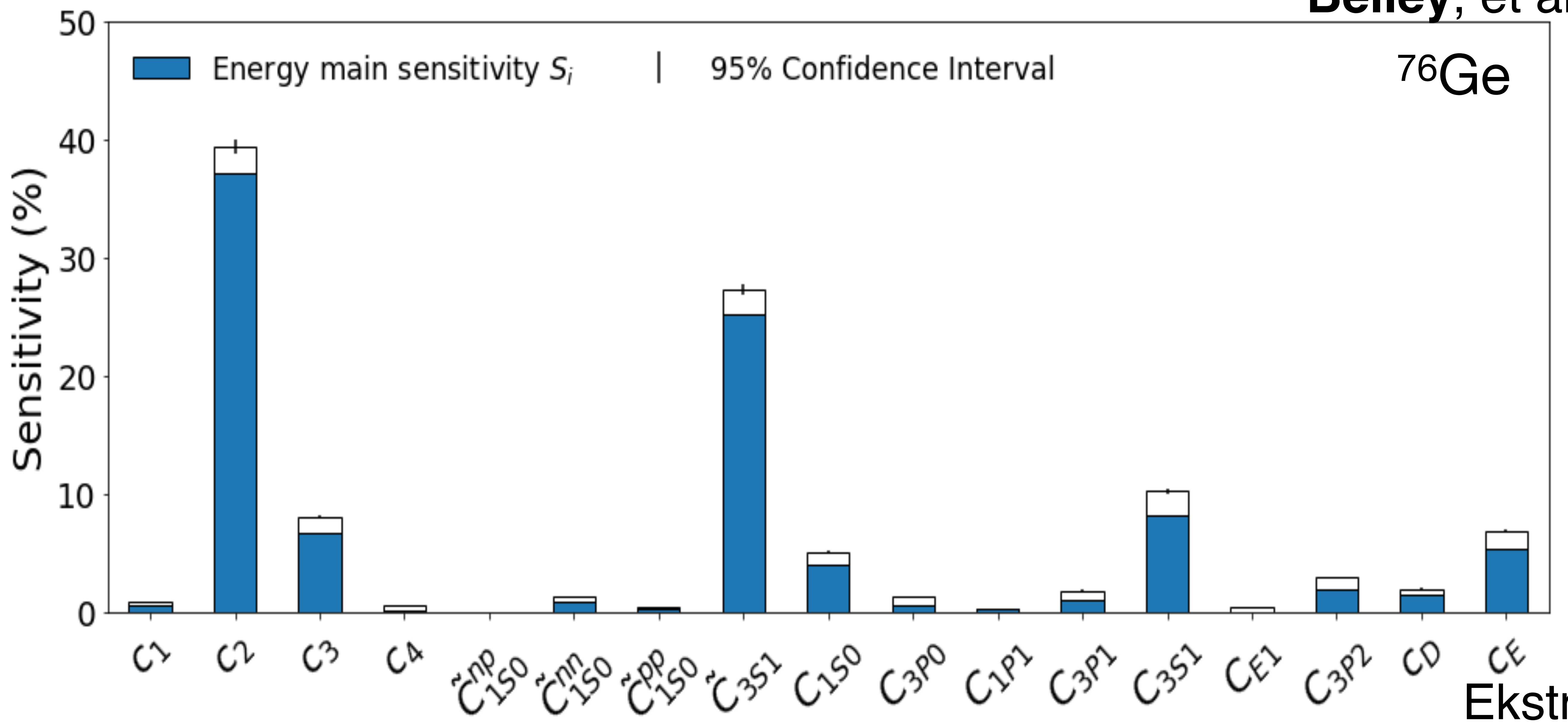
2. Data driven



The MM-DGP Algorithm: GSA

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

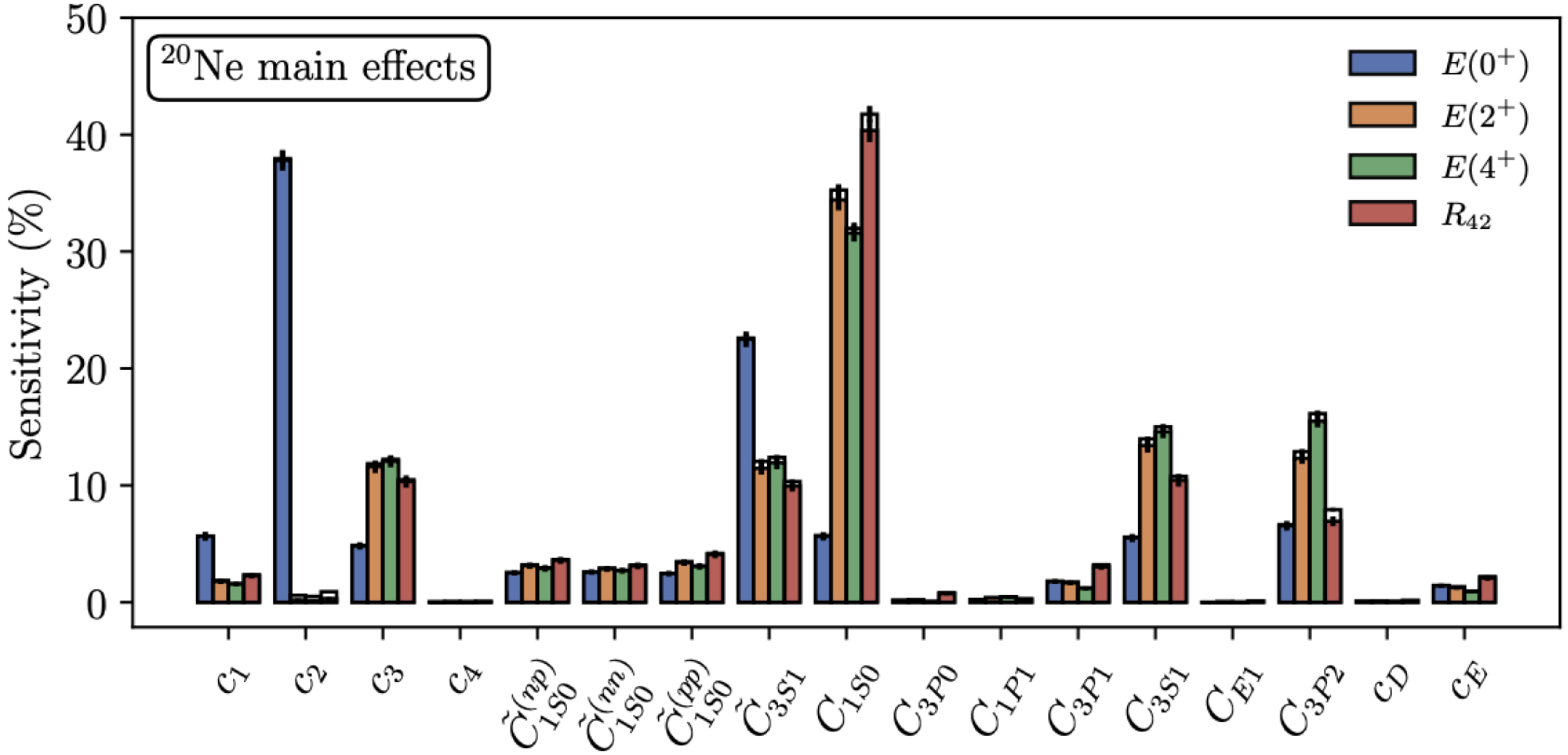
Data driven MM-DGP



vs

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

Physics Driven

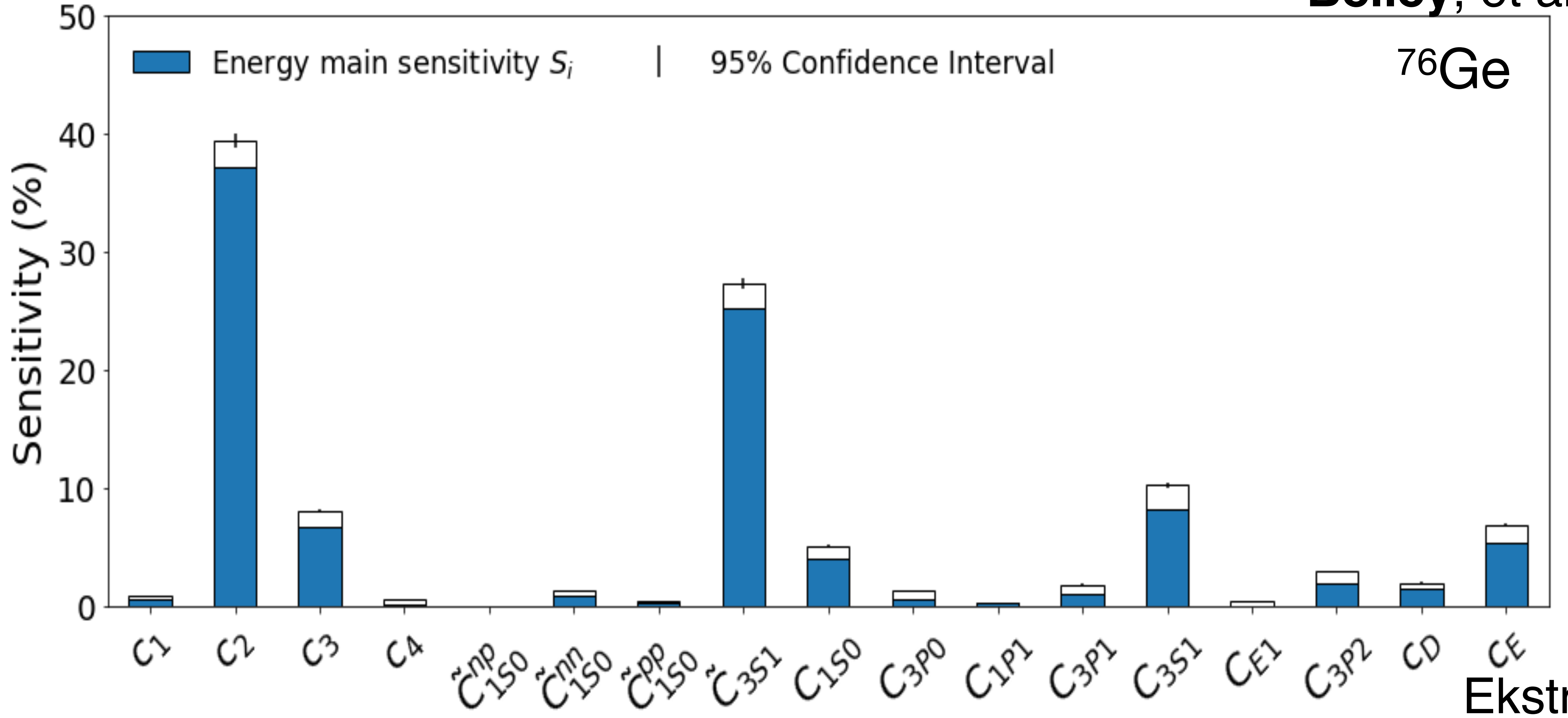


Global emulation

The MM-DGP Algorithm: GSA

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

Data driven MM-DGP



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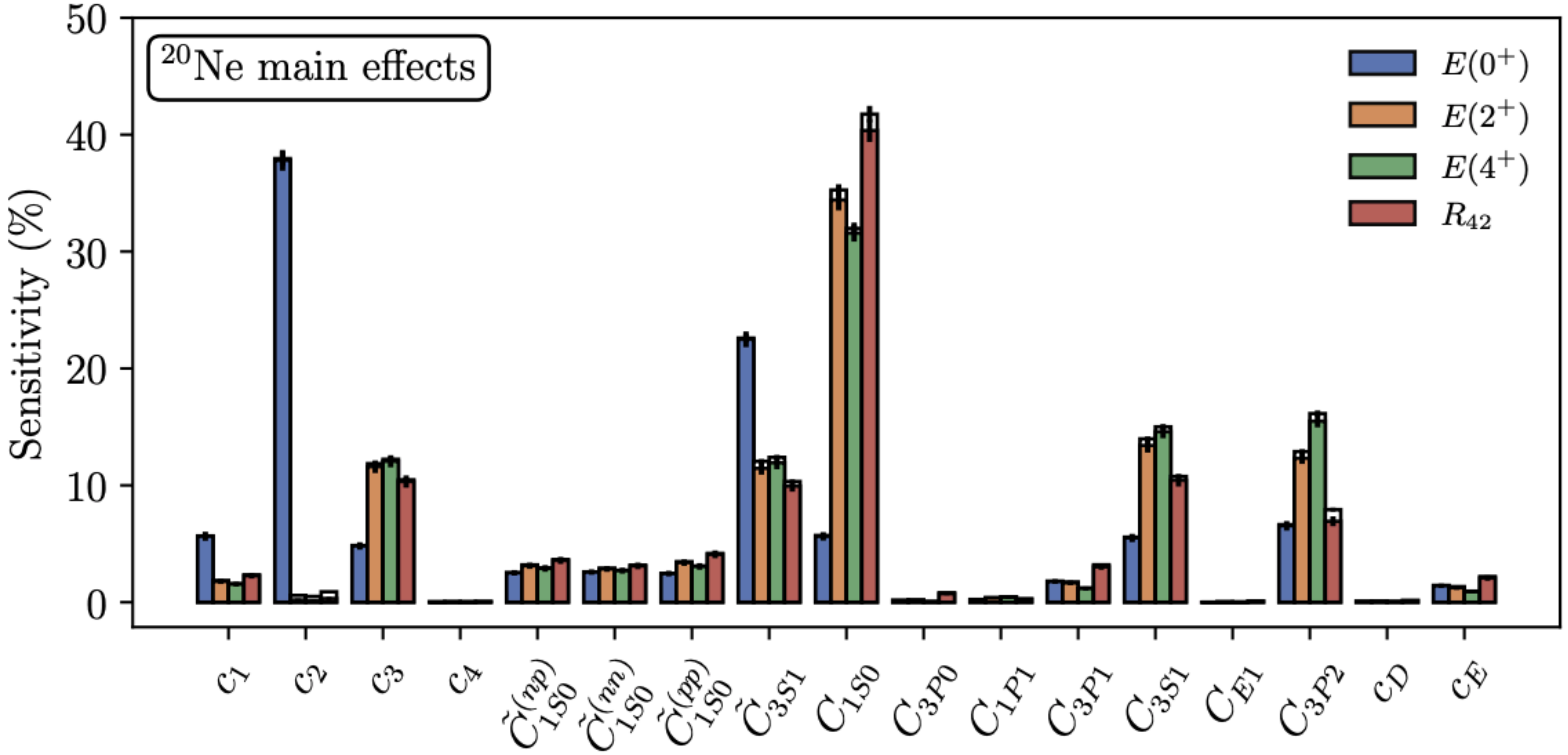

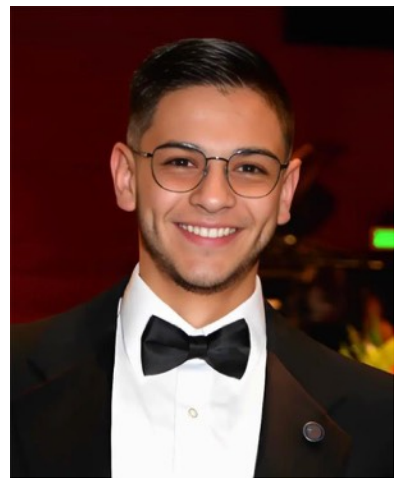

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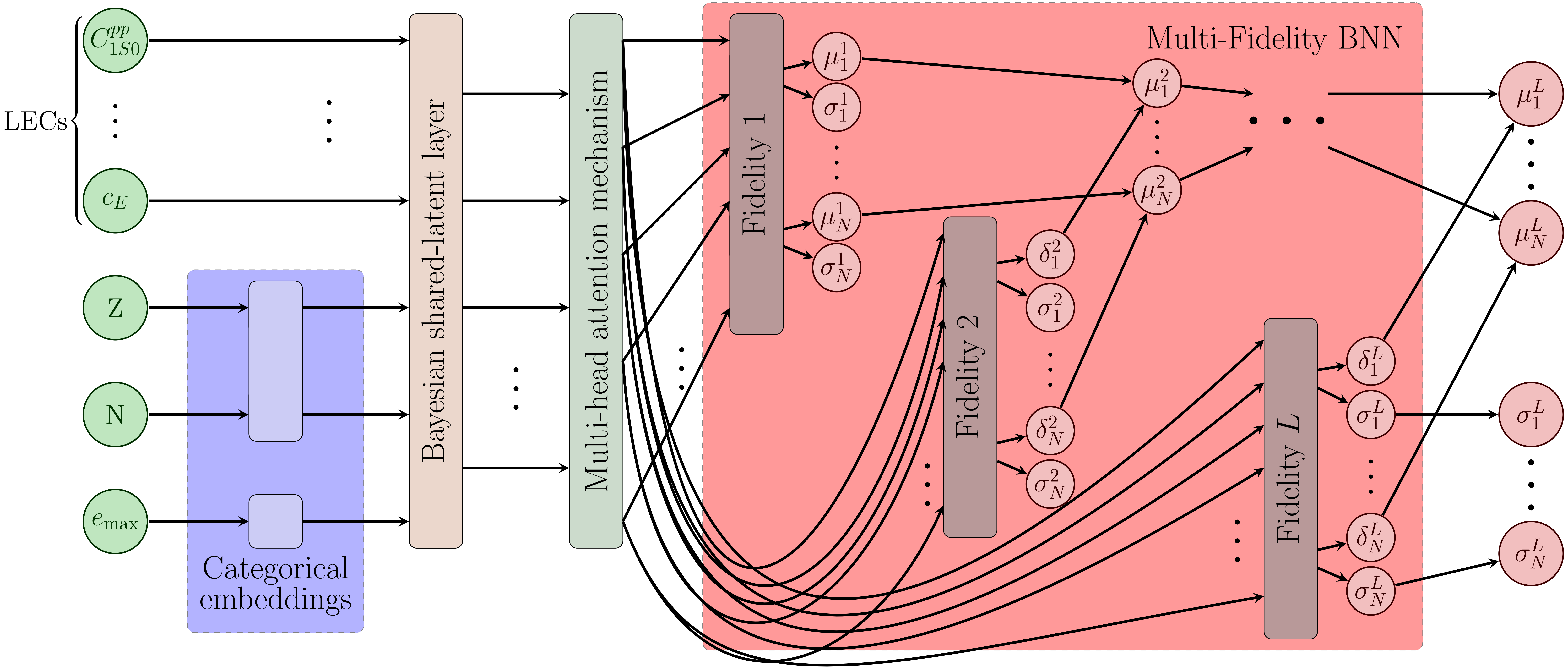
BANNANE

BAyesian Neural Network for Atomic Nuclei Emulation



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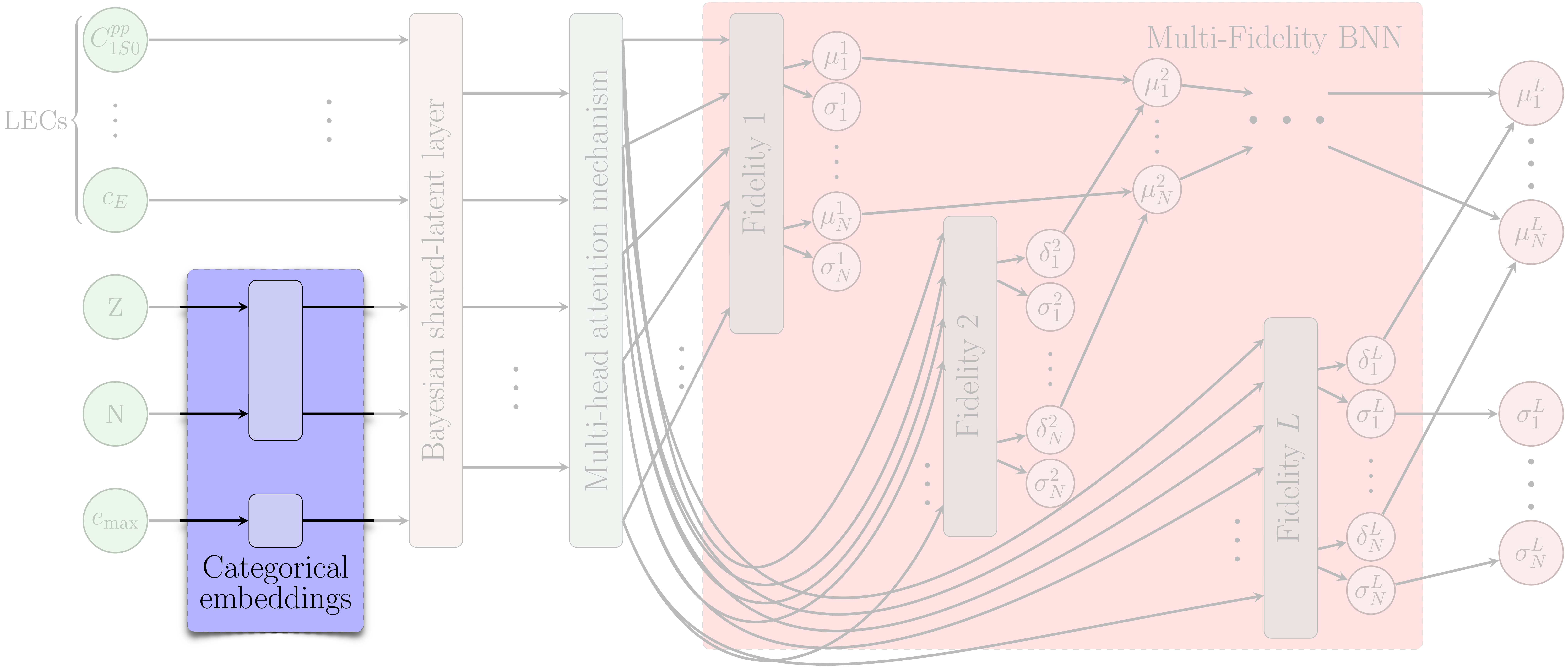

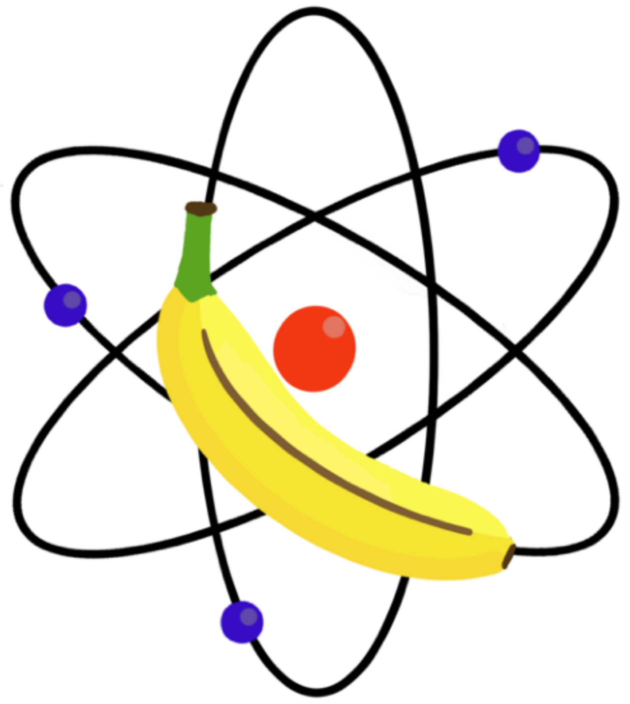

Embeddings

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

- $e_{max} = 4 \rightarrow 6 \rightarrow 8 \rightarrow 10$

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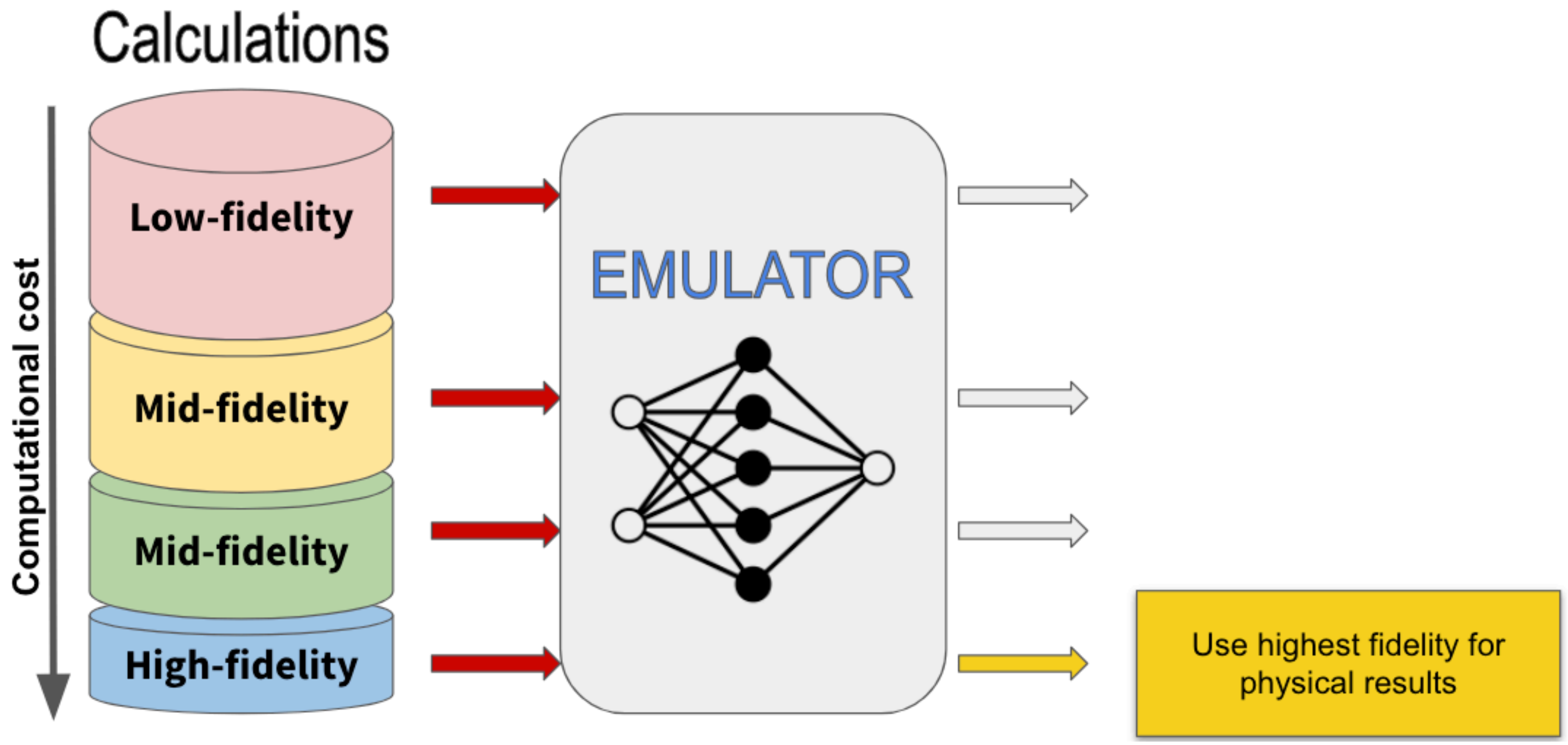

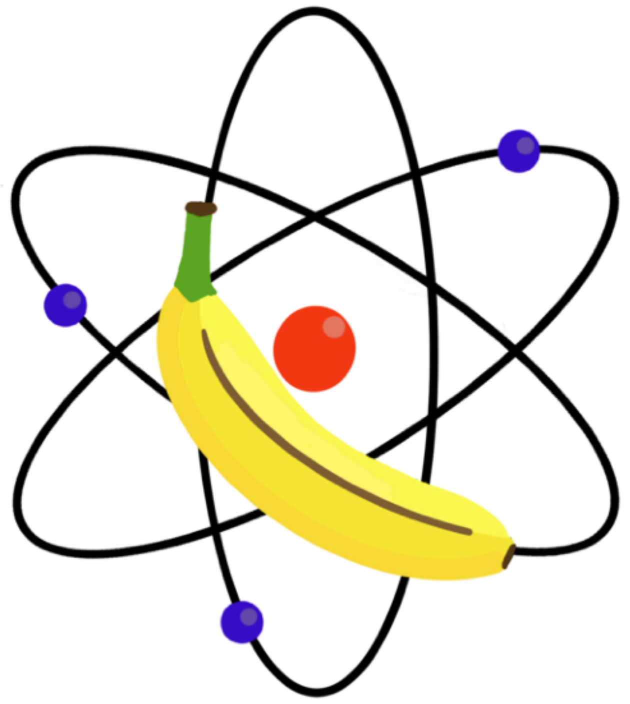

Embeddings

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- $e_{max} = 4 \rightarrow 6 \rightarrow 8 \rightarrow 10$
- **Positions in the nuclear chart: ordering of N and Z**

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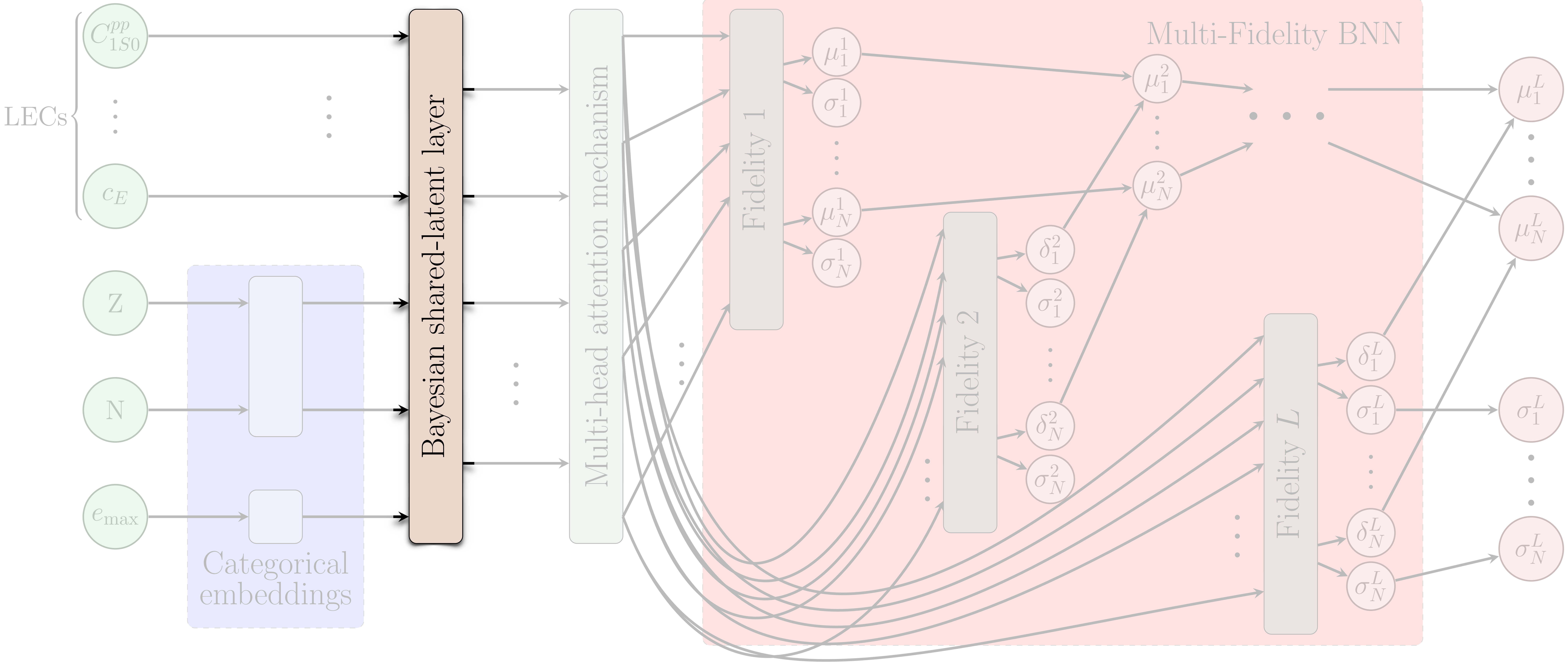

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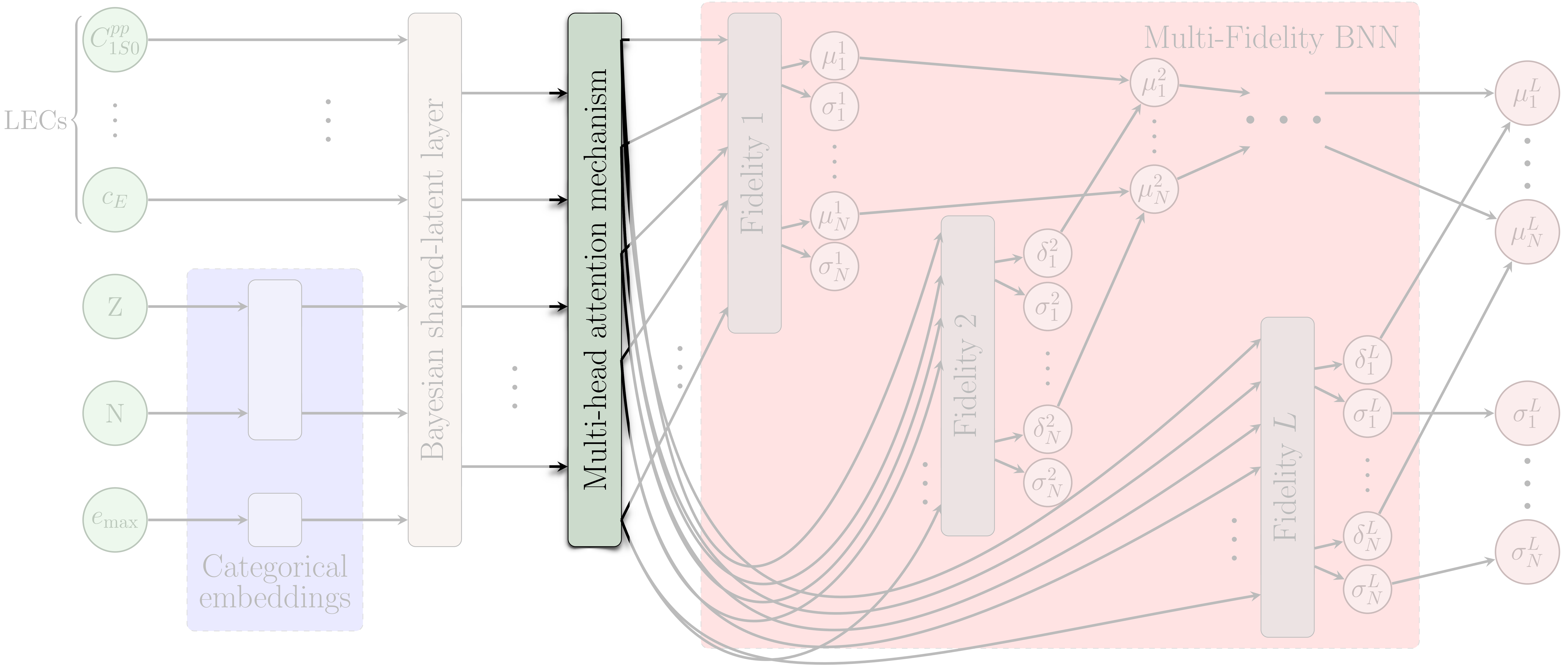
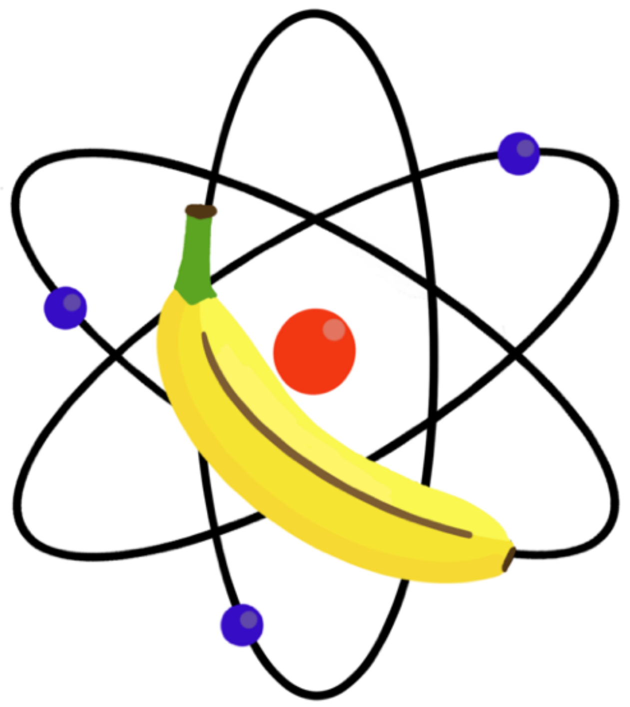
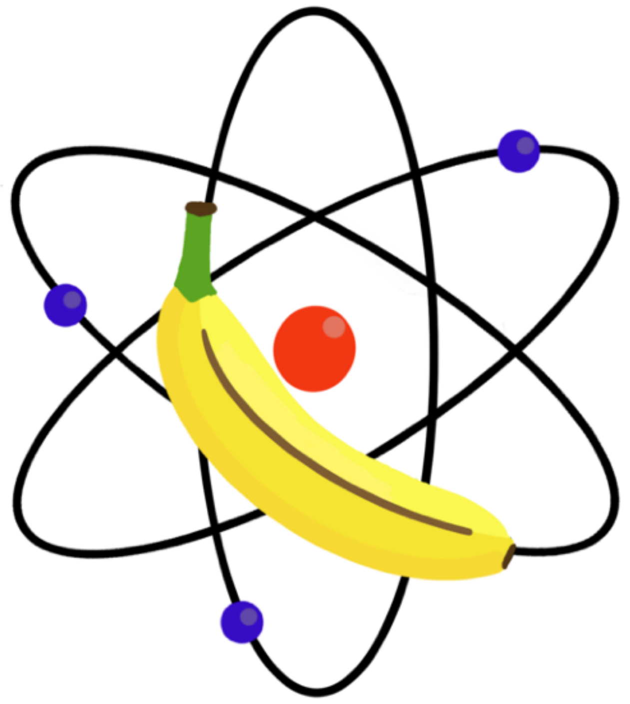




Attention!

- **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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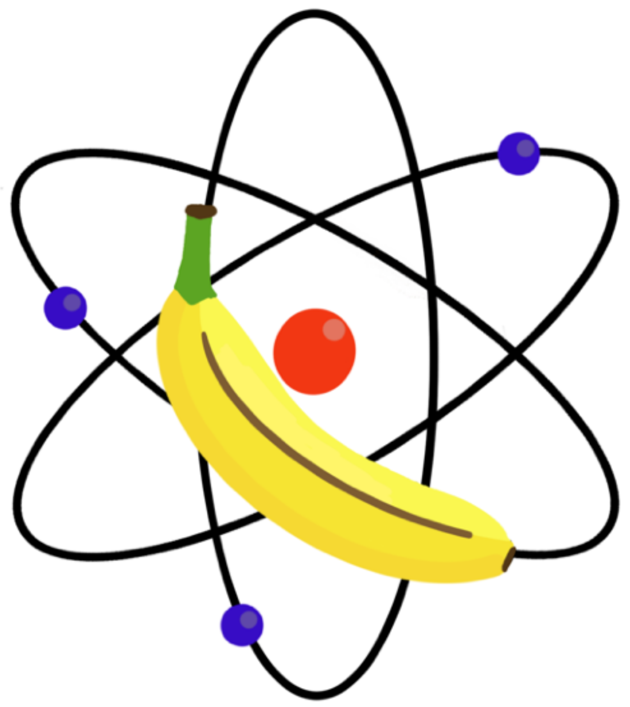
232, 321 citations



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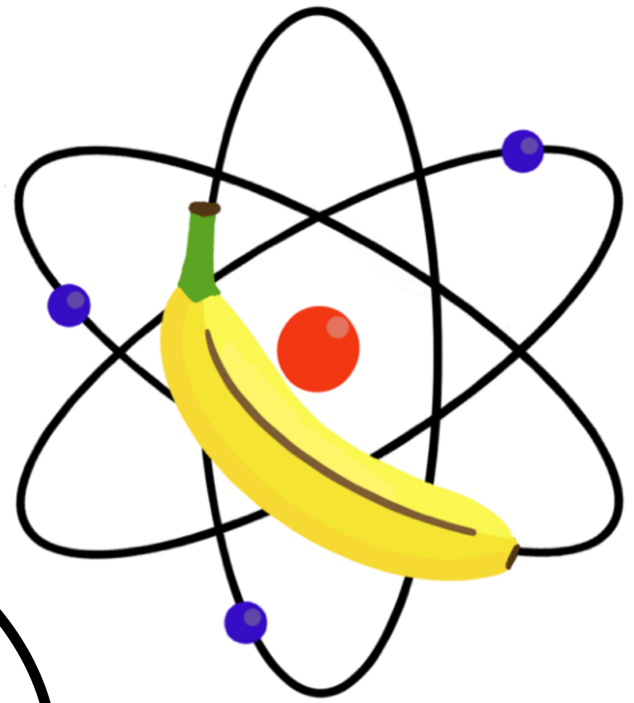
232, 321 citations

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

46, 426 citations



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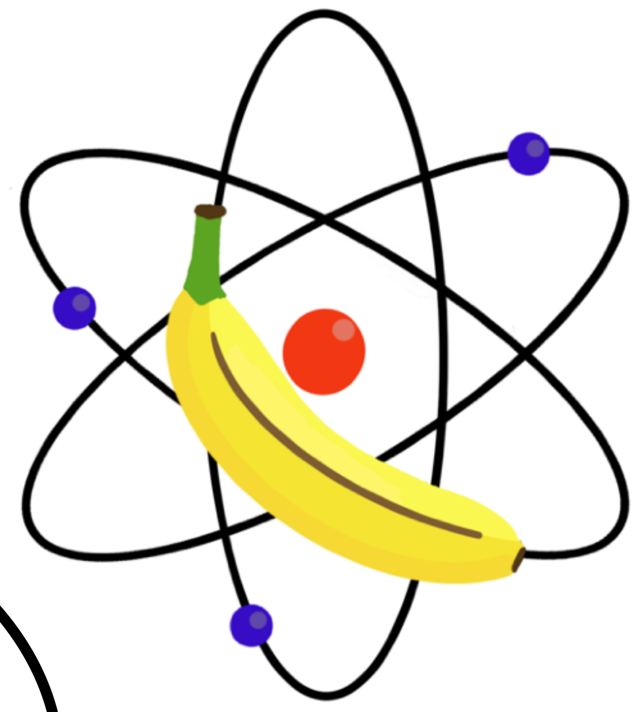

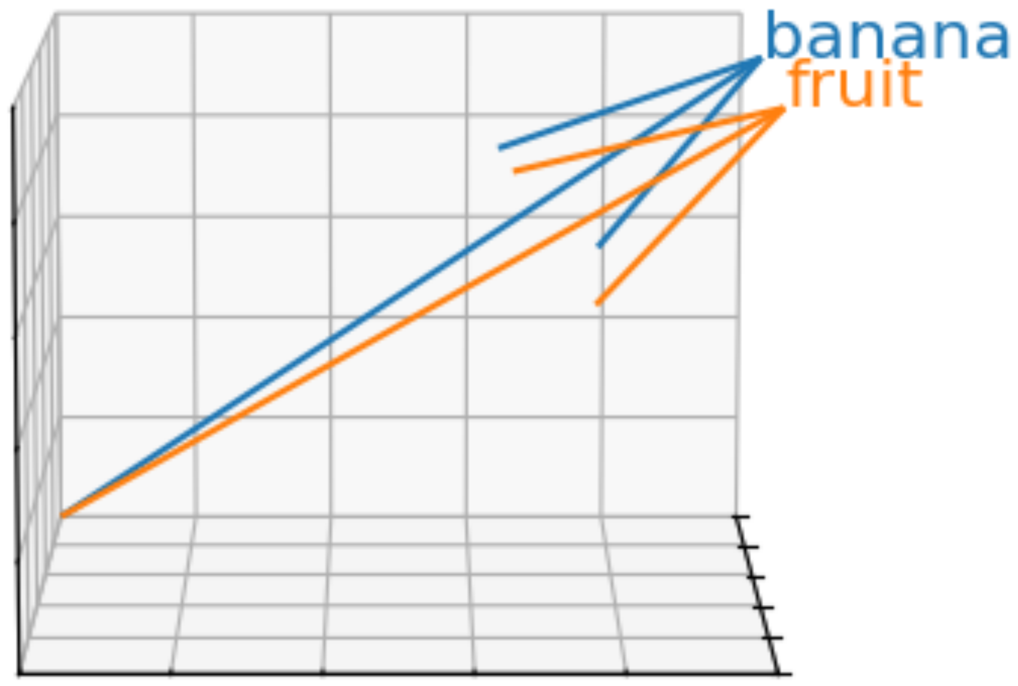

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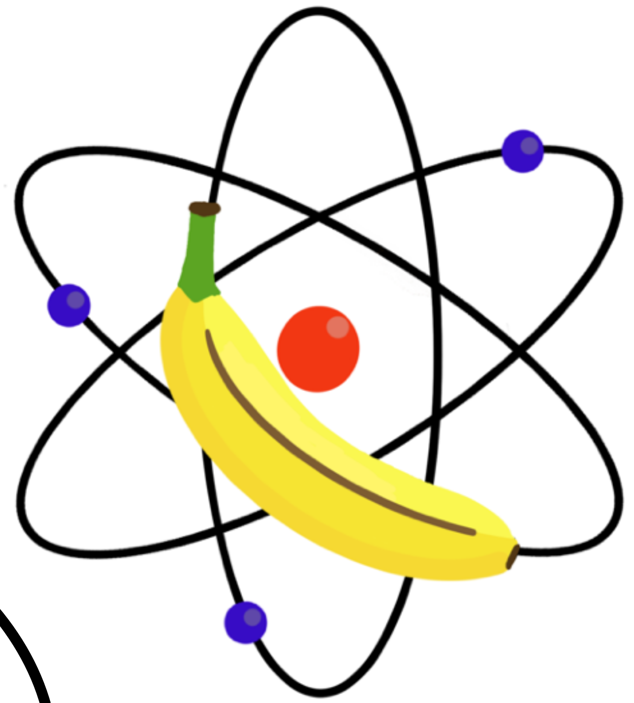

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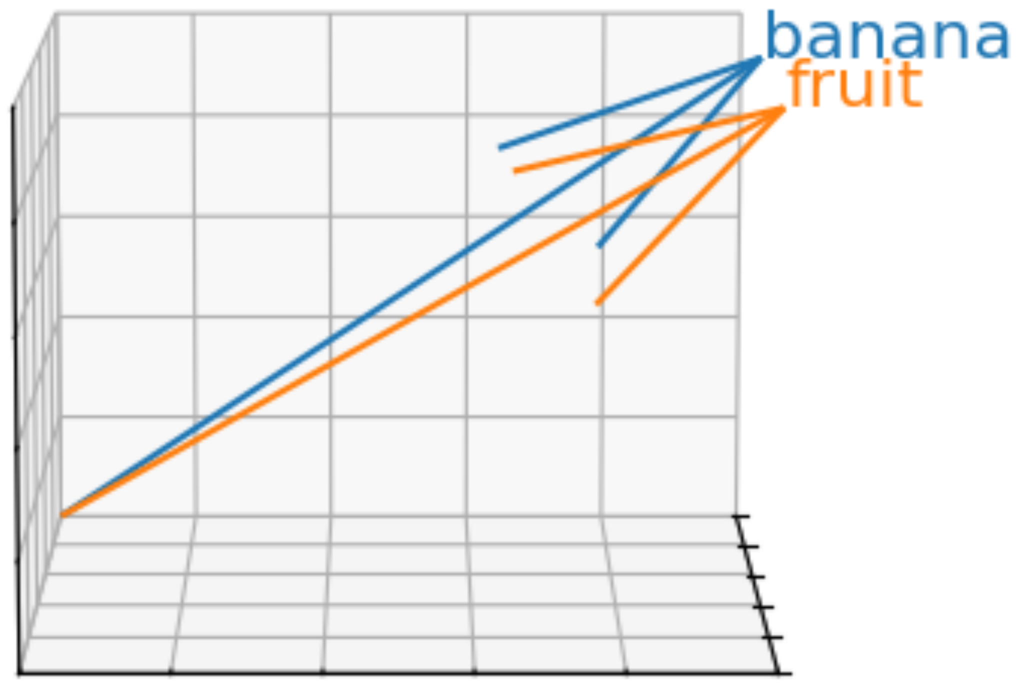

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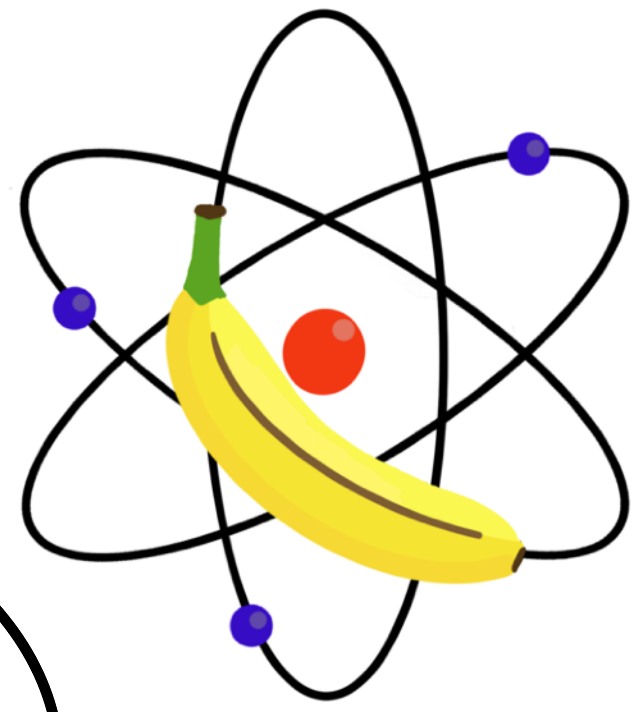

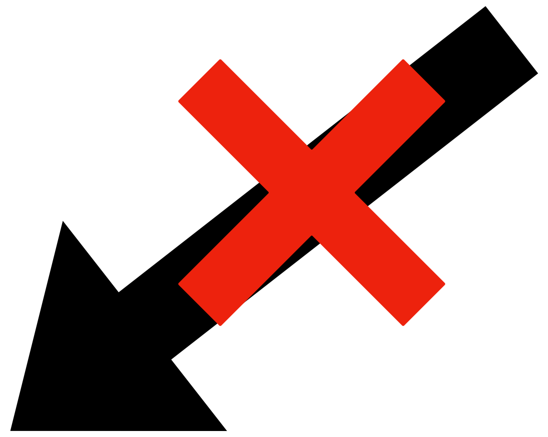

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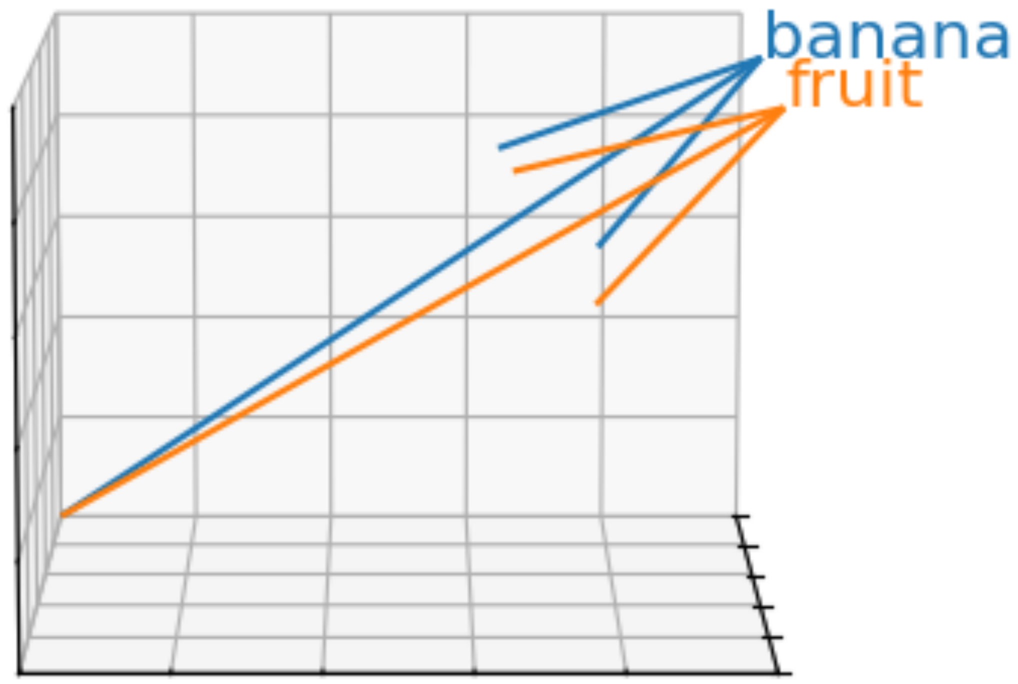

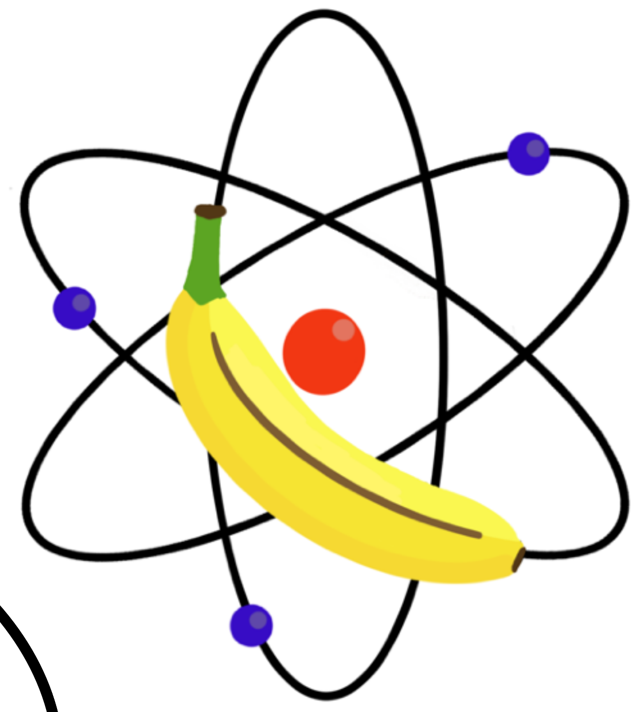

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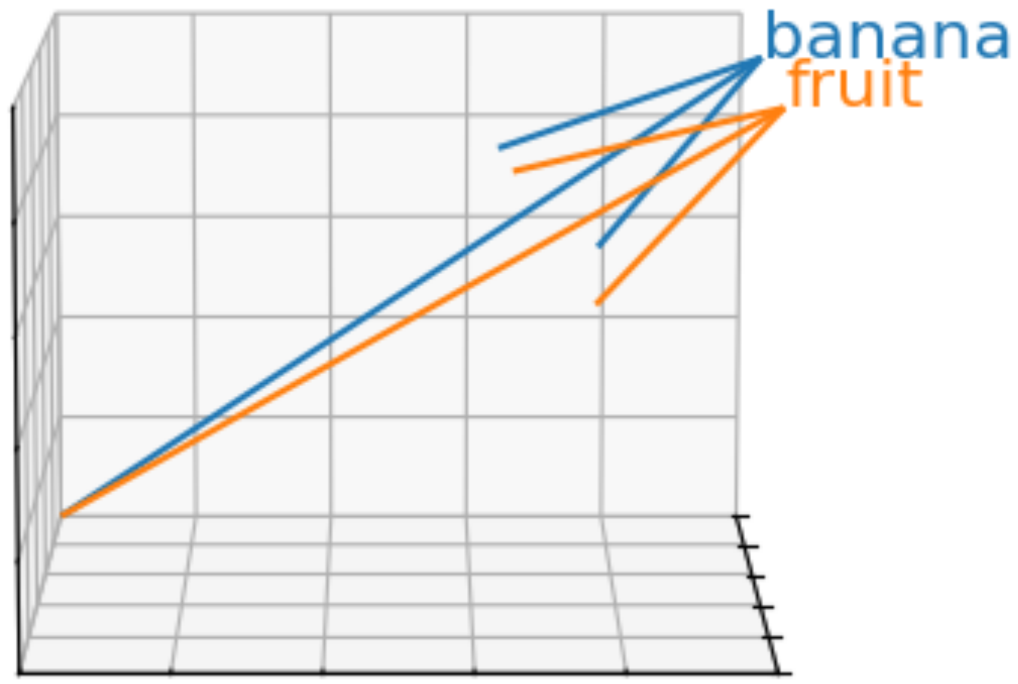

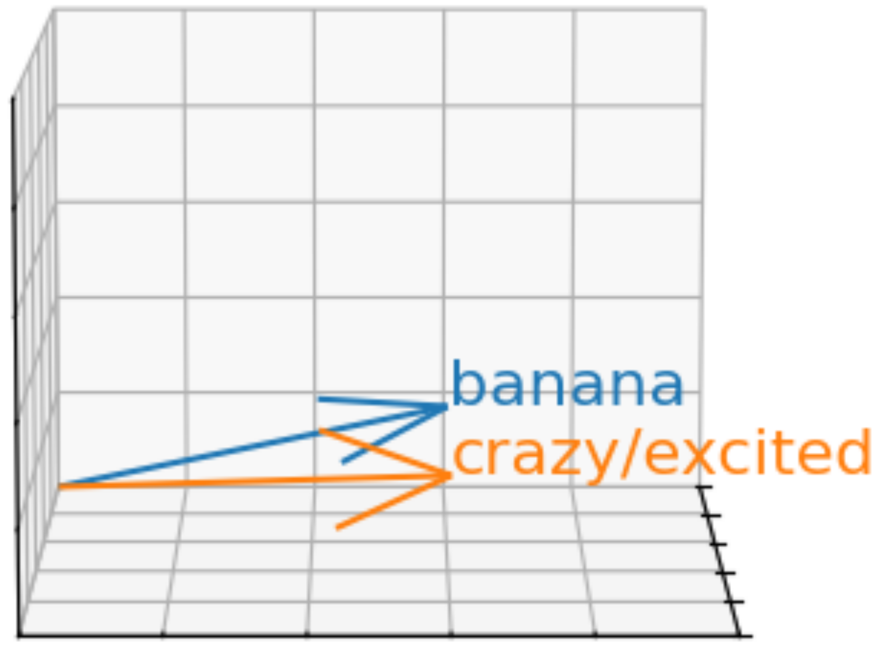

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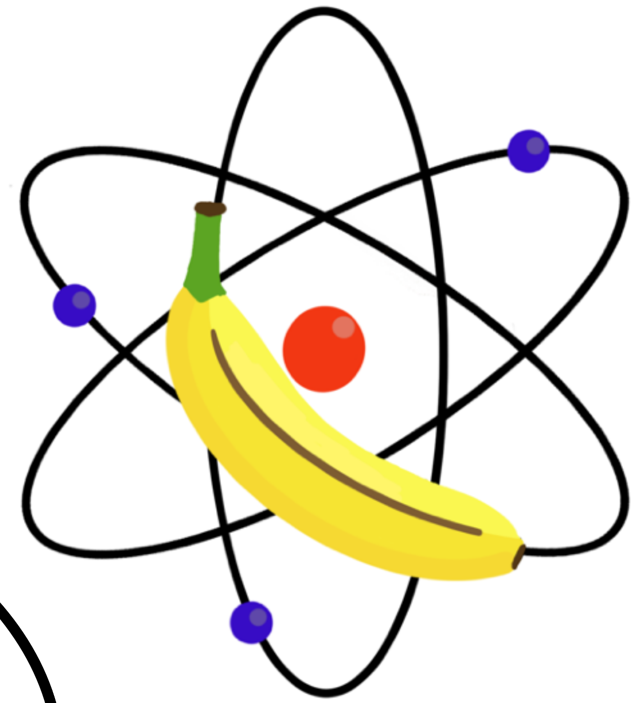

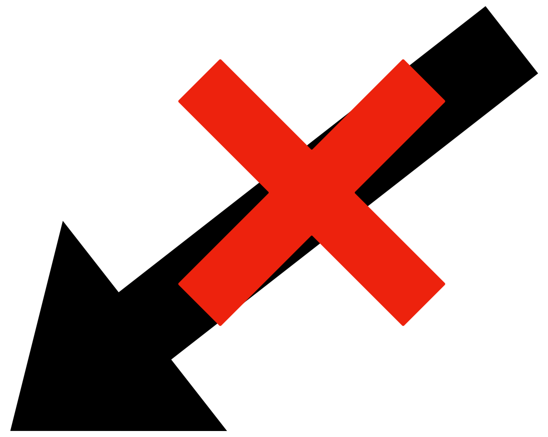

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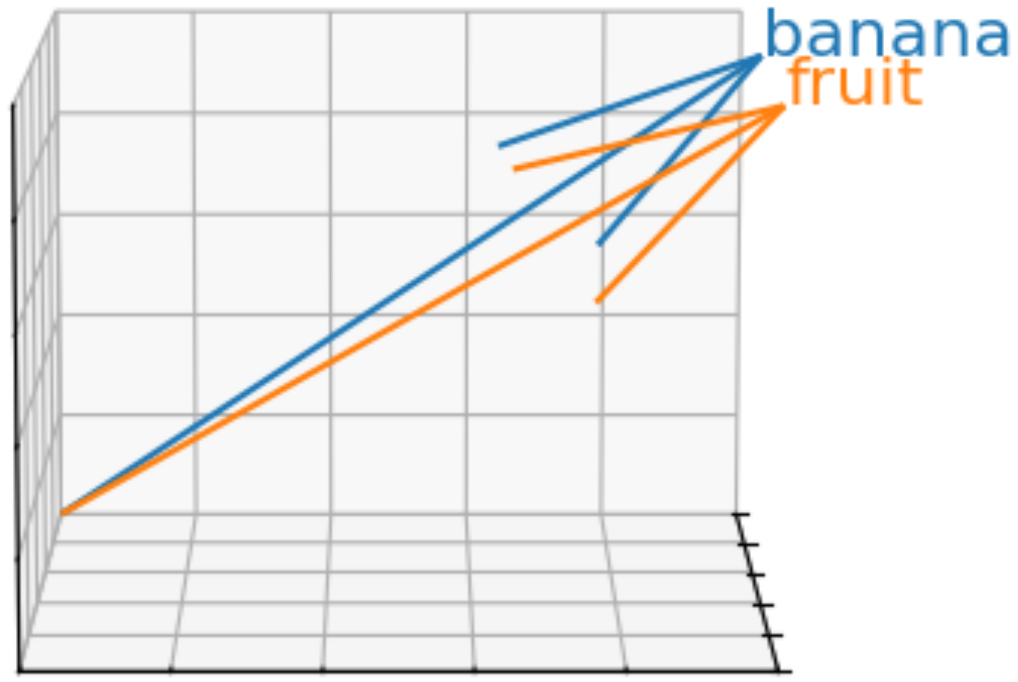

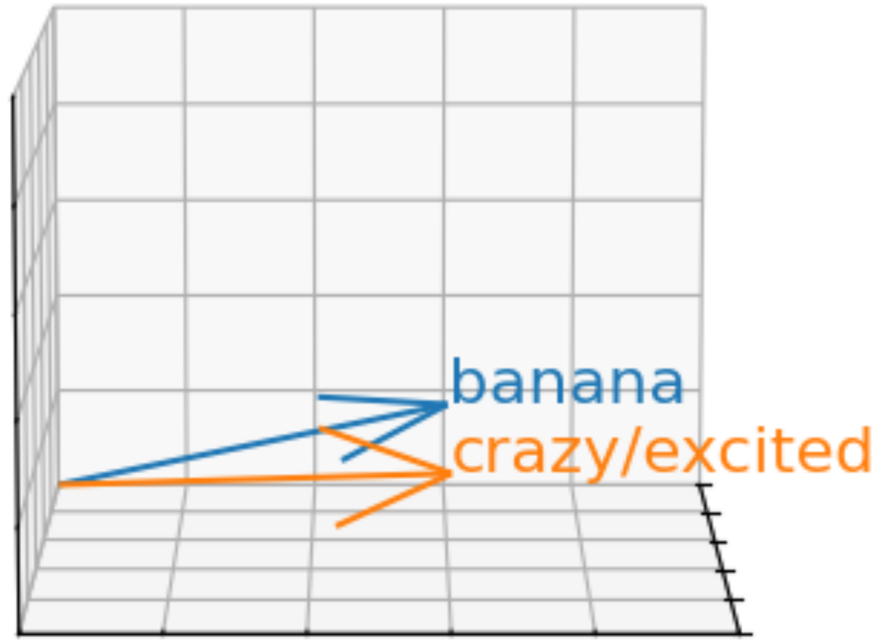

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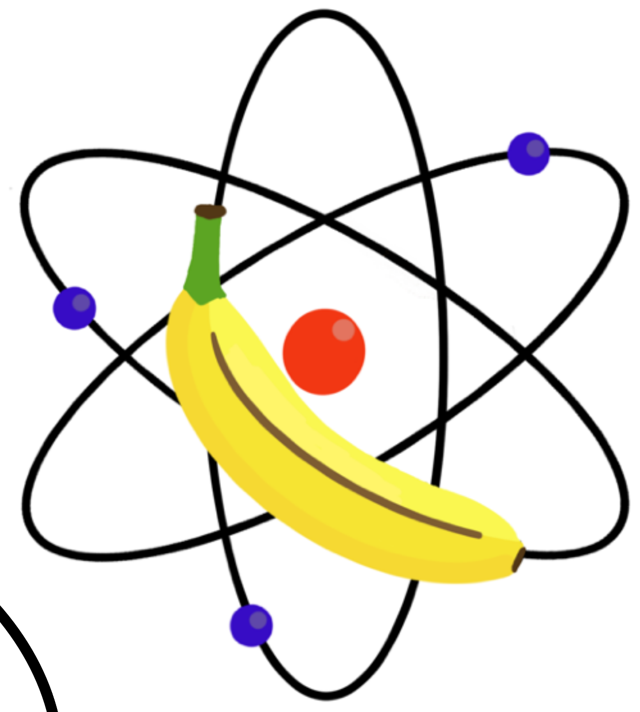

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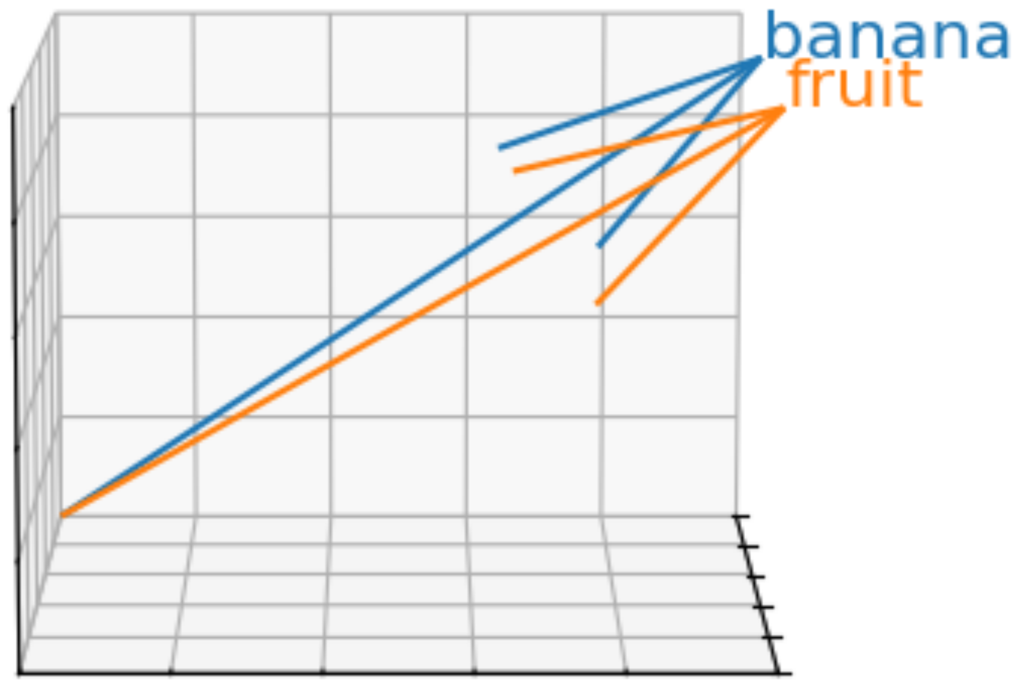

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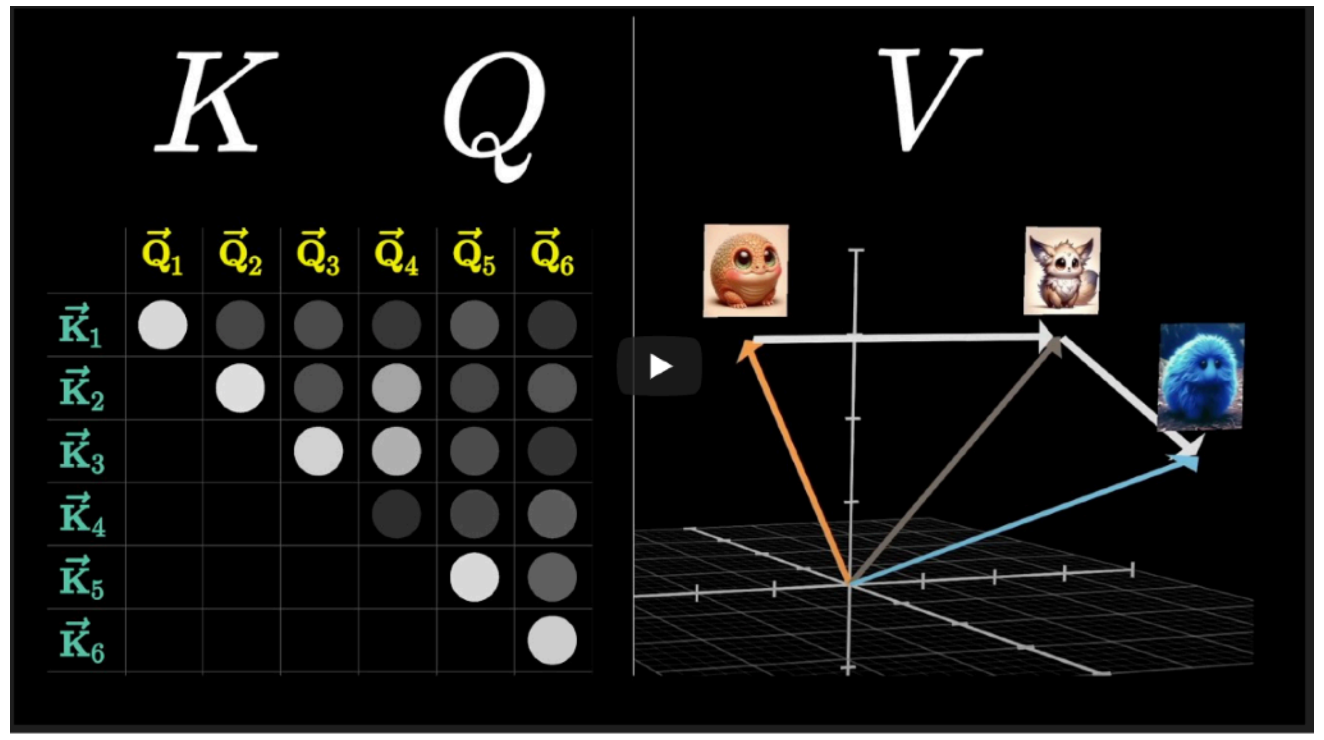
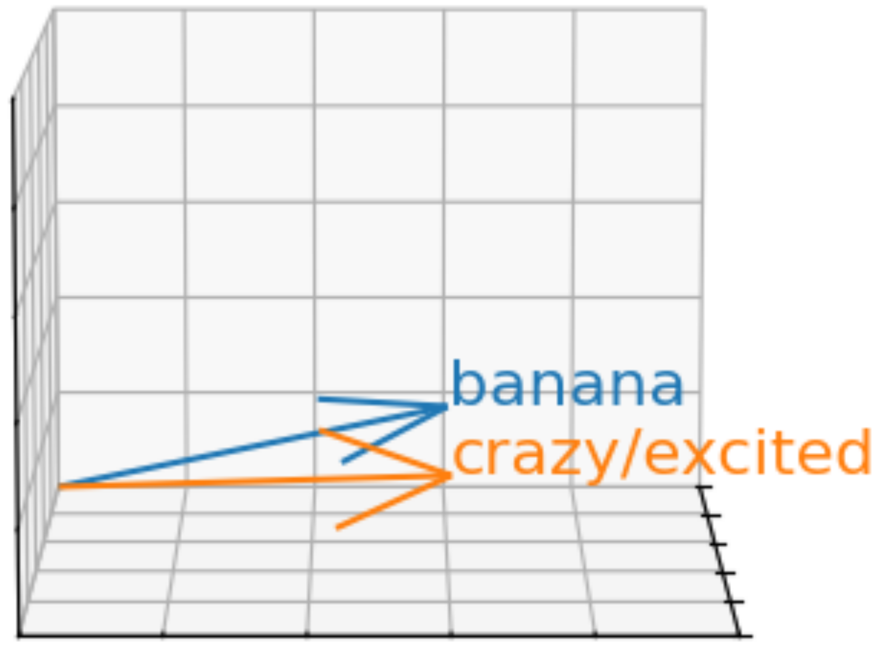
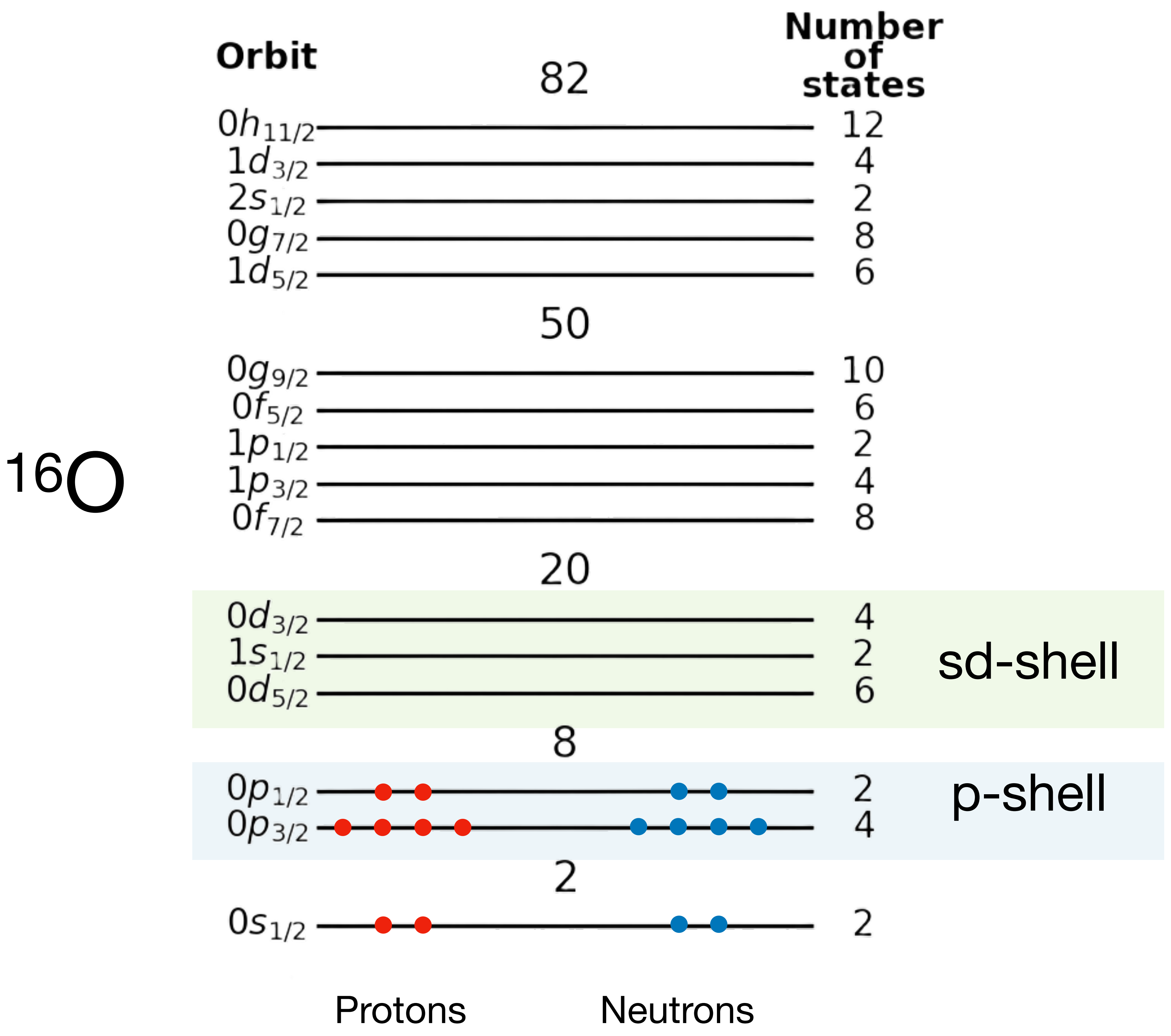
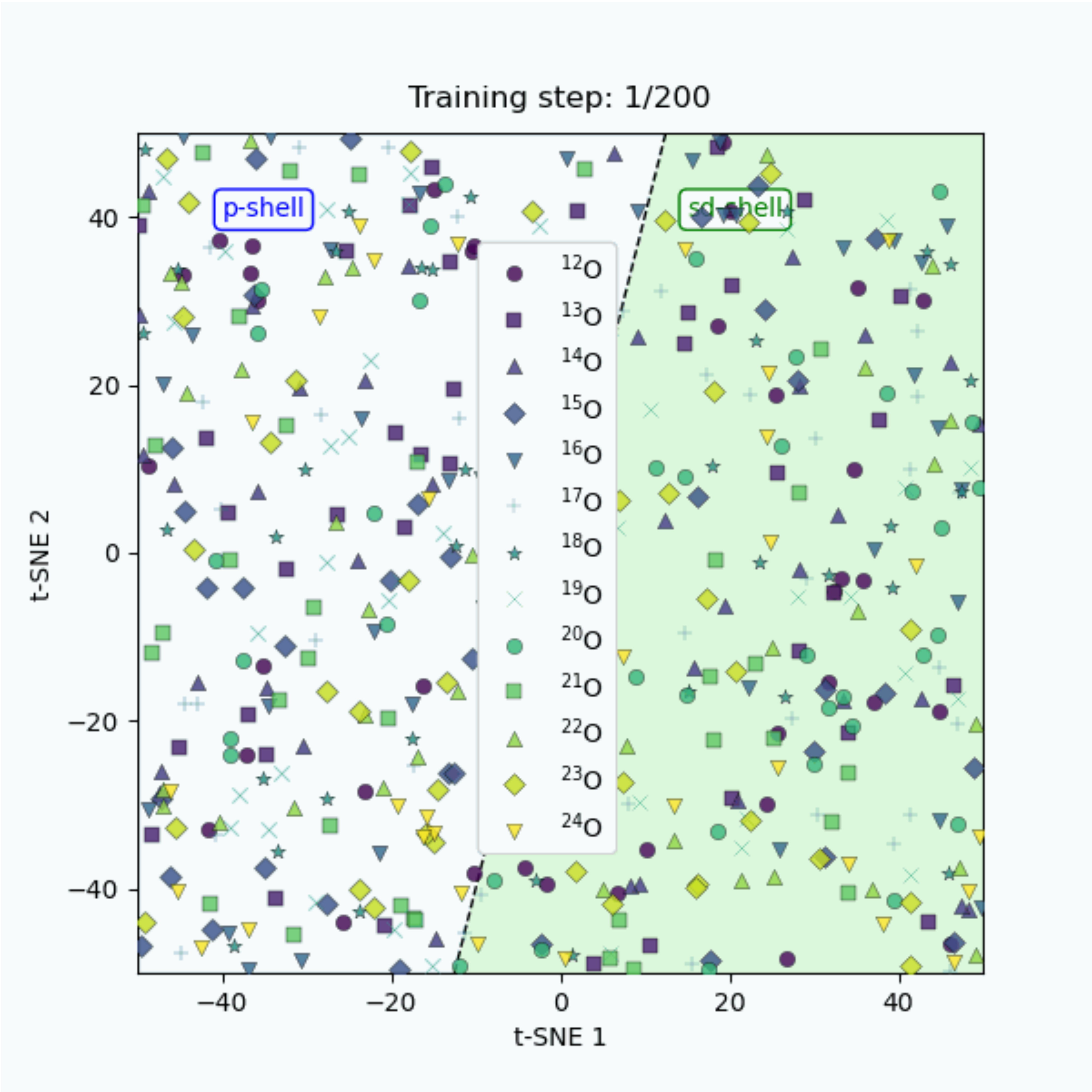




Visualizing the Embeddings

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





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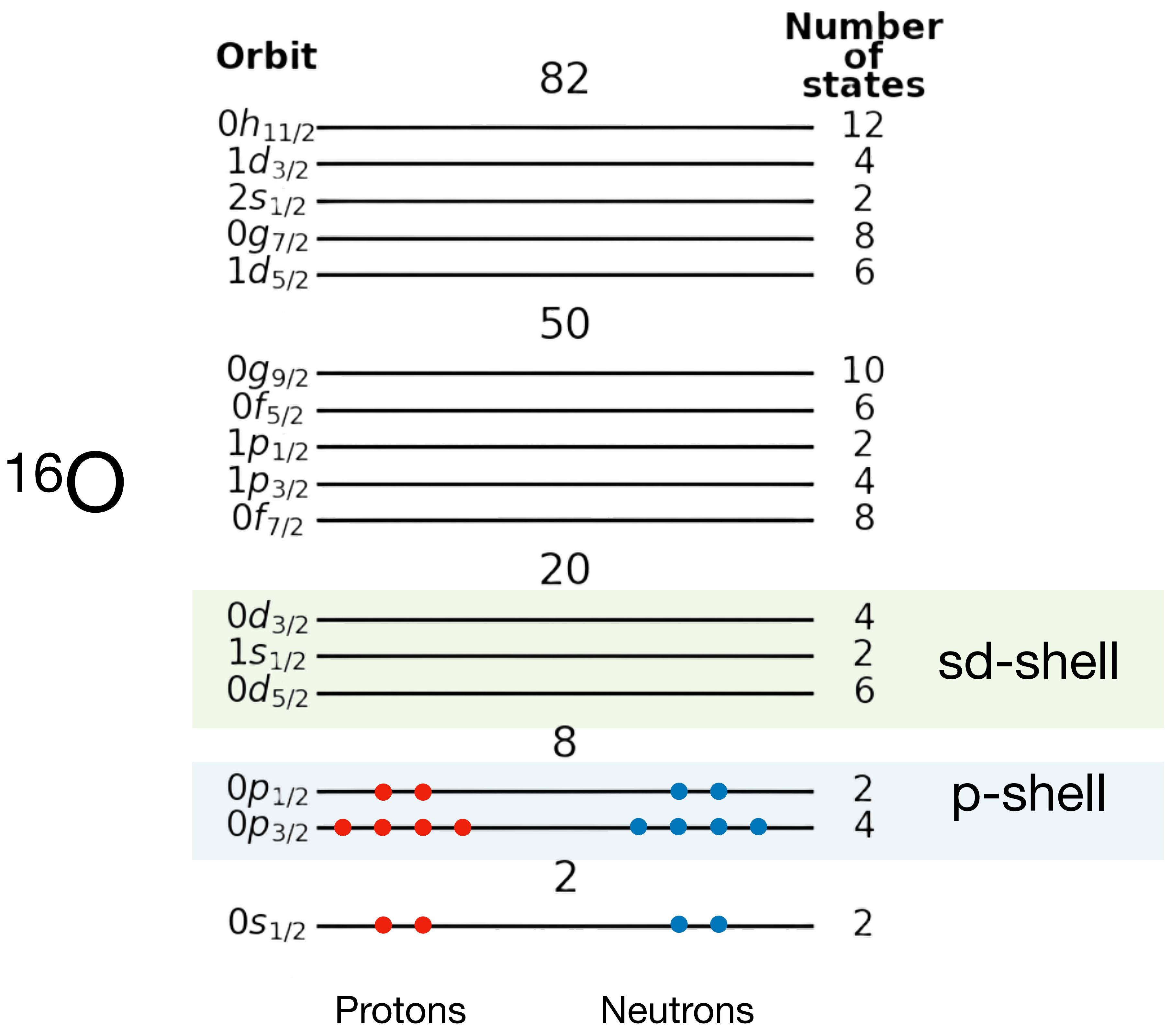

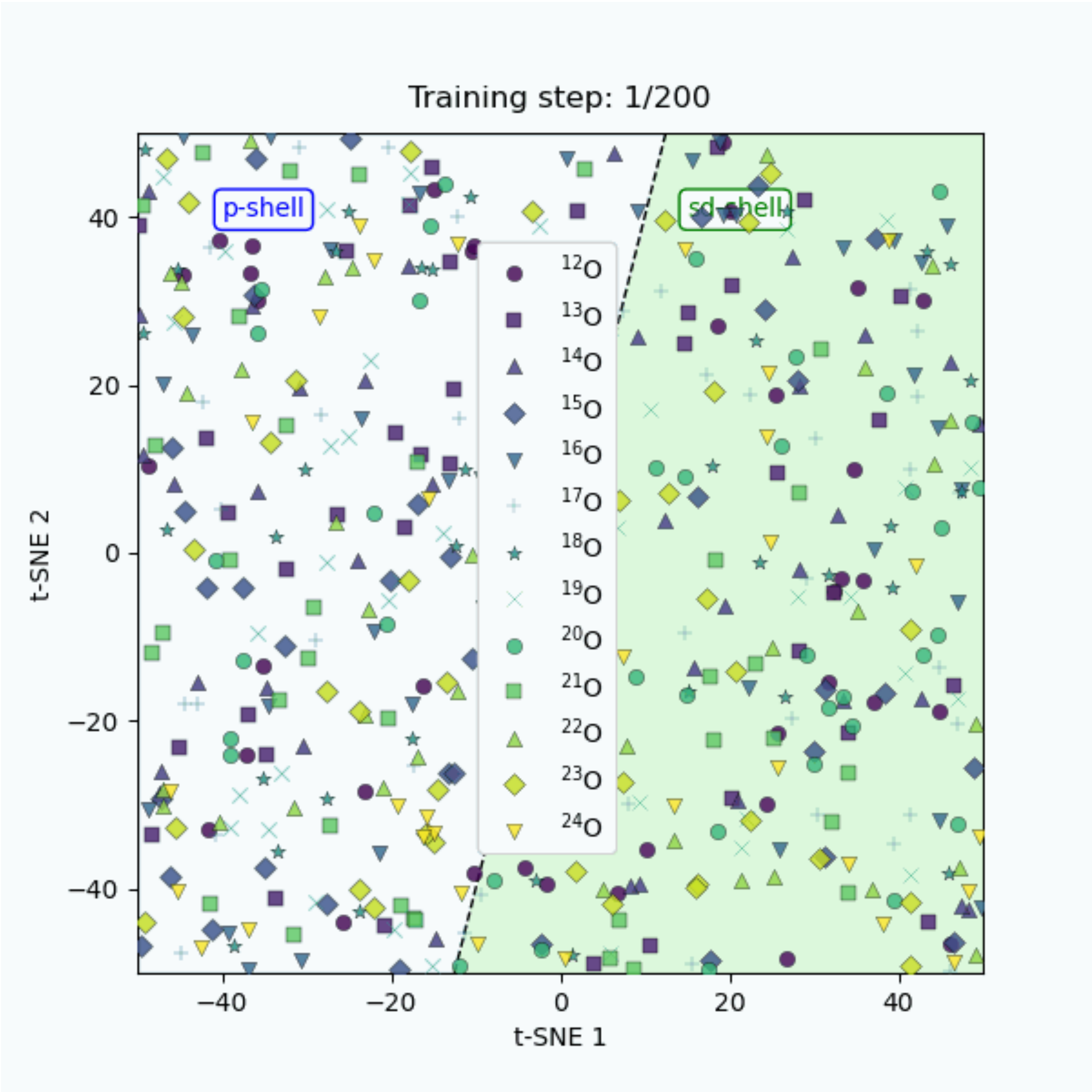

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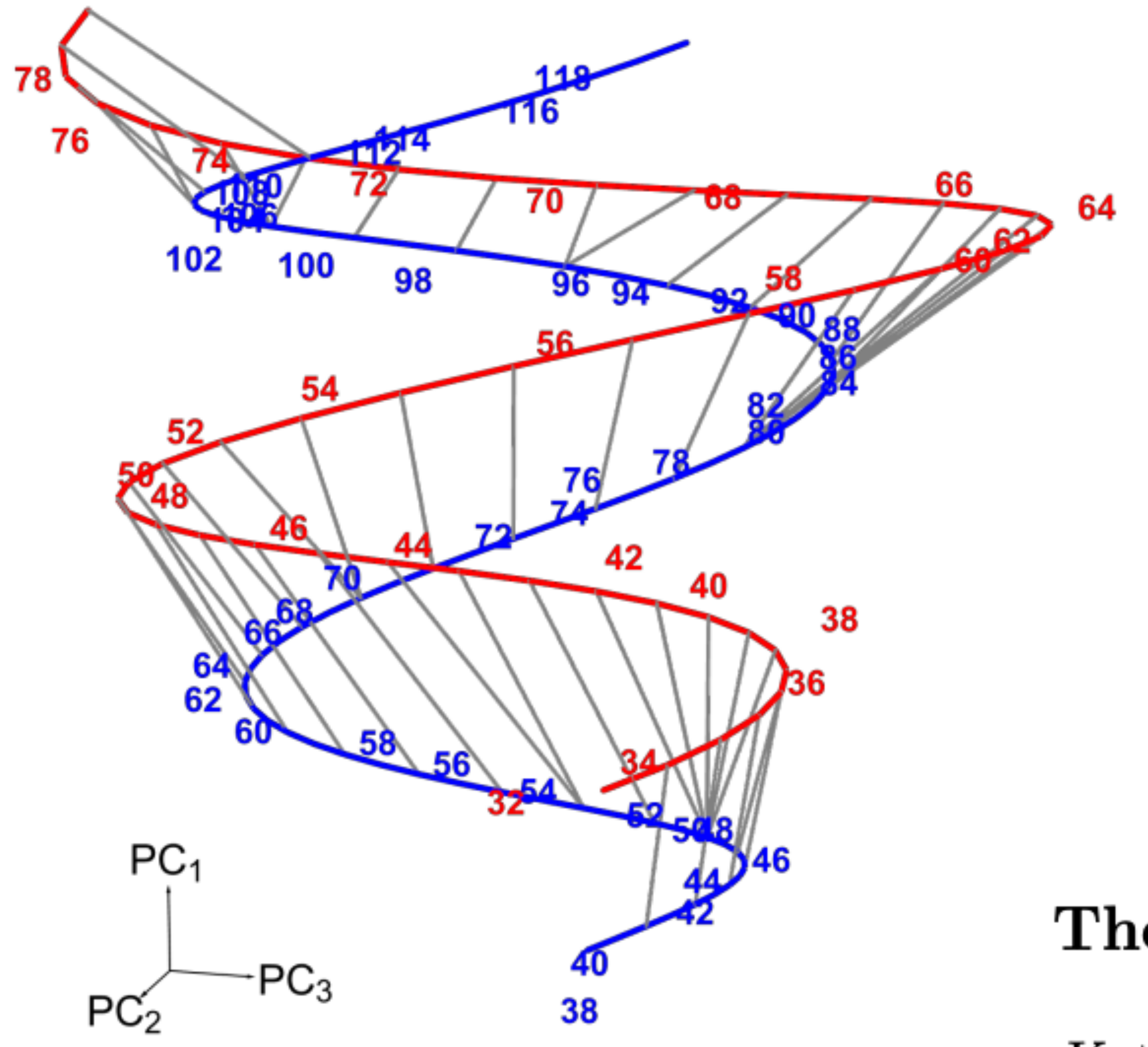
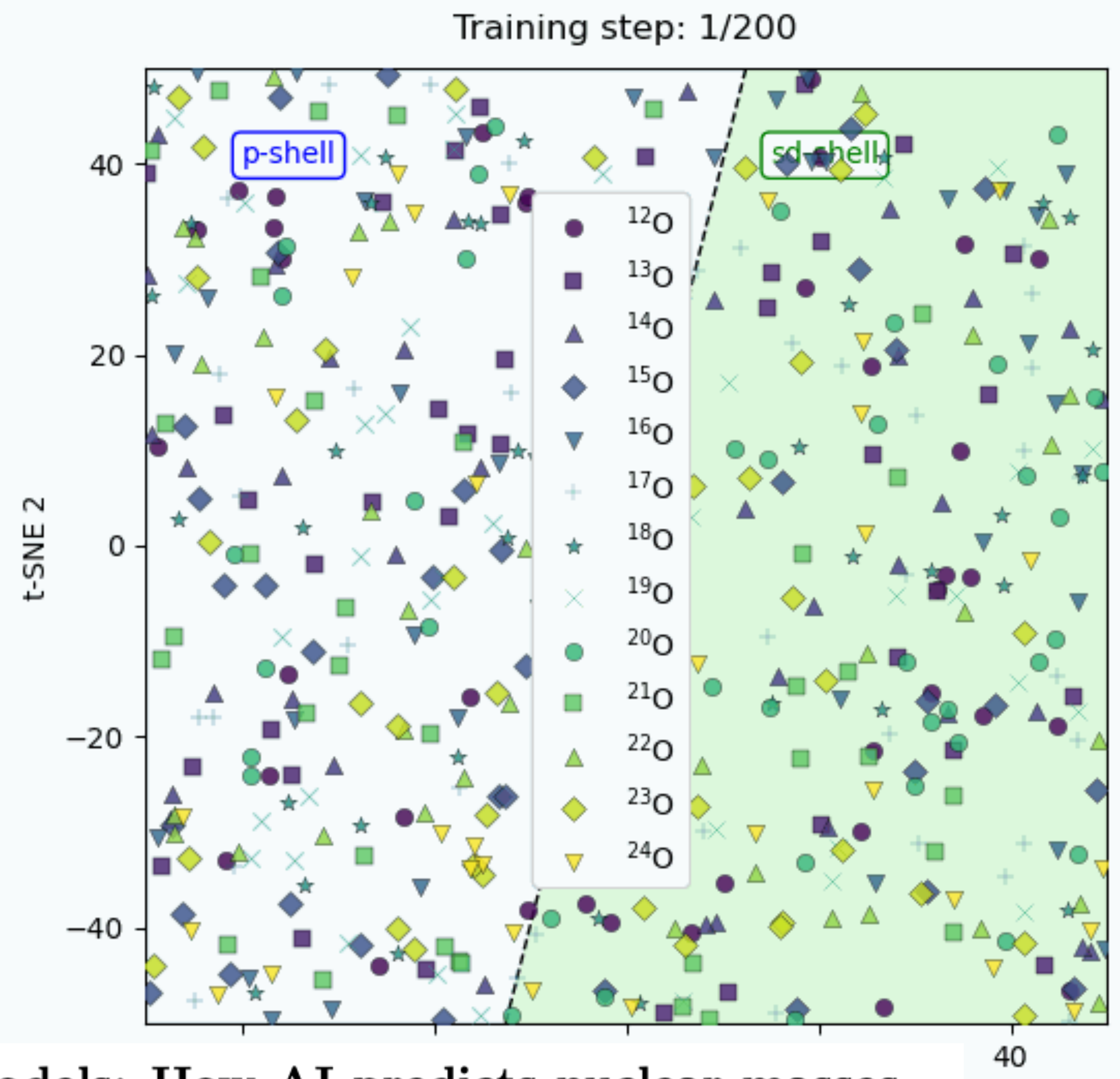
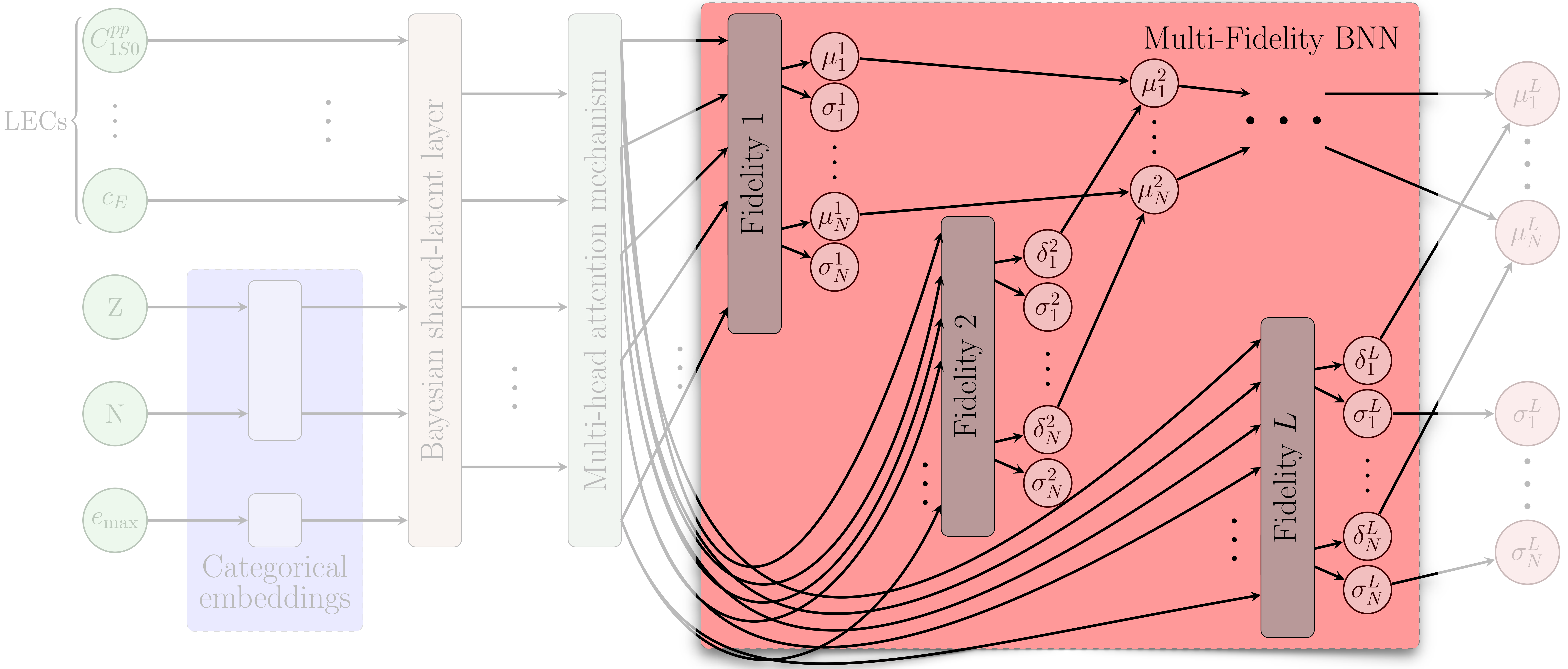




The DNA of nuclear models: How AI predicts nuclear masses

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

BAyesian Neural Network for Atomic Nuclei Emulation



Results

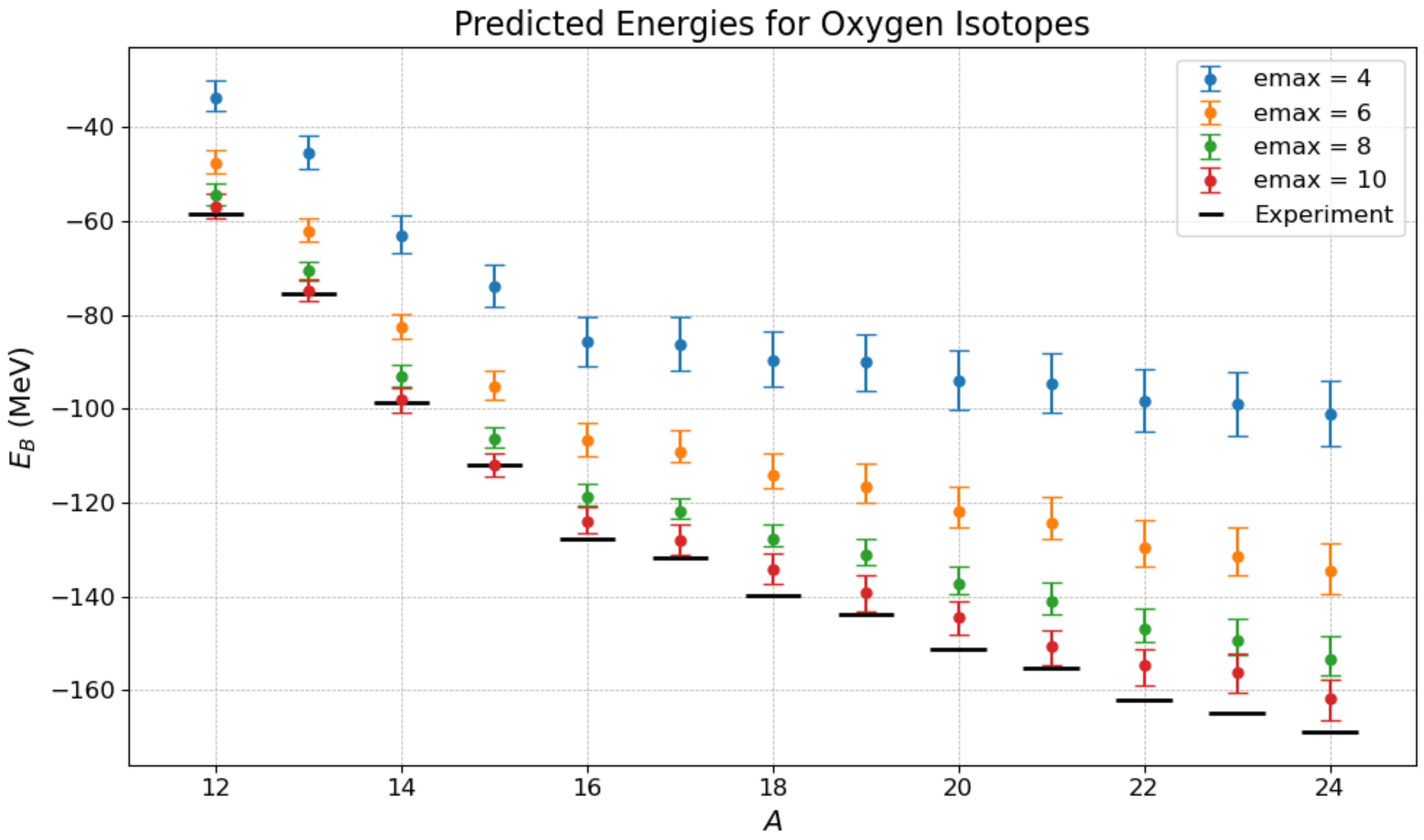
Emulating Multiple Isotopes

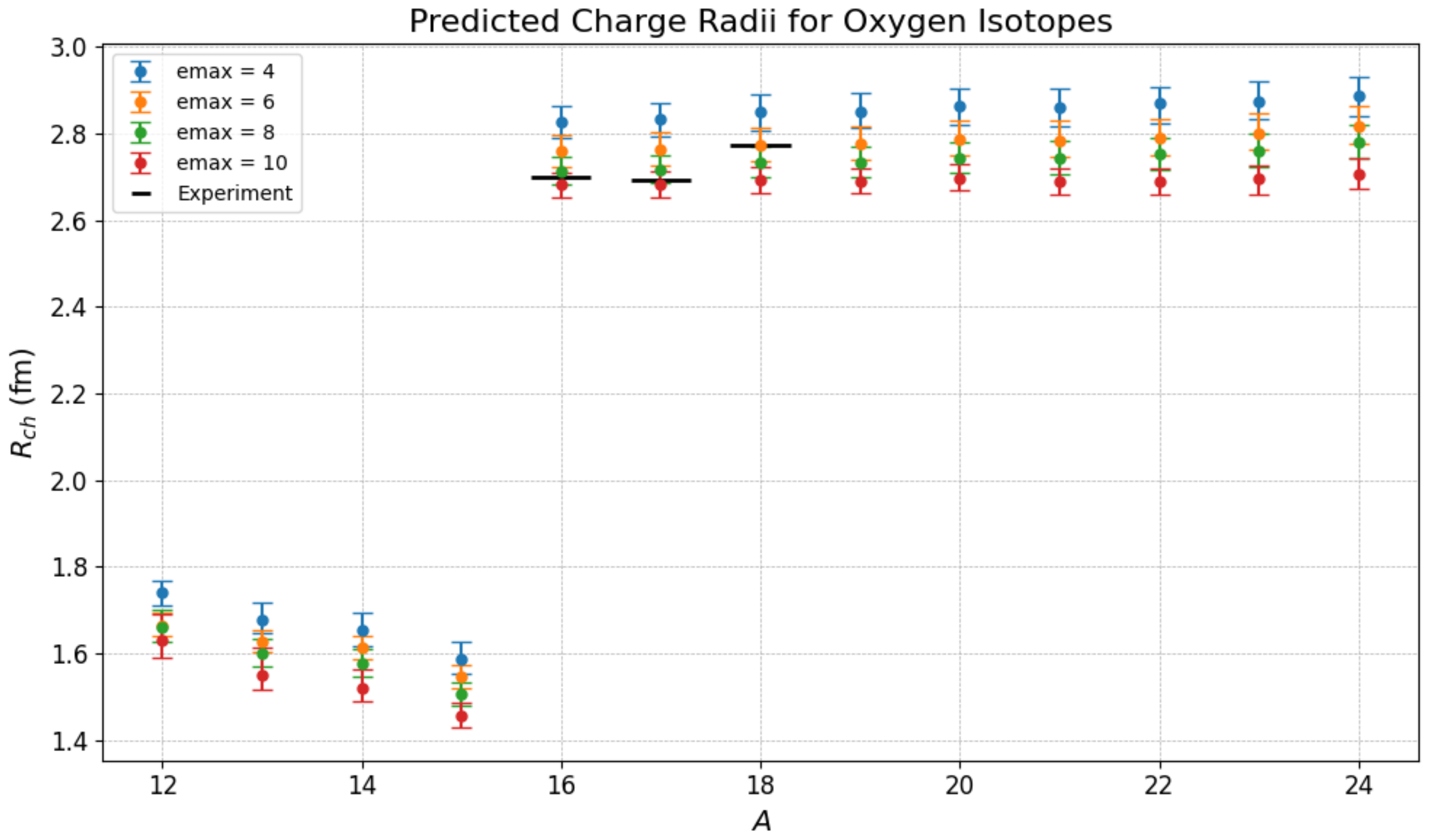
Belley, et al.,Phys. Rev. Lett. **136**, 082501 (2026)

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

Emulating Multiple Isotopes

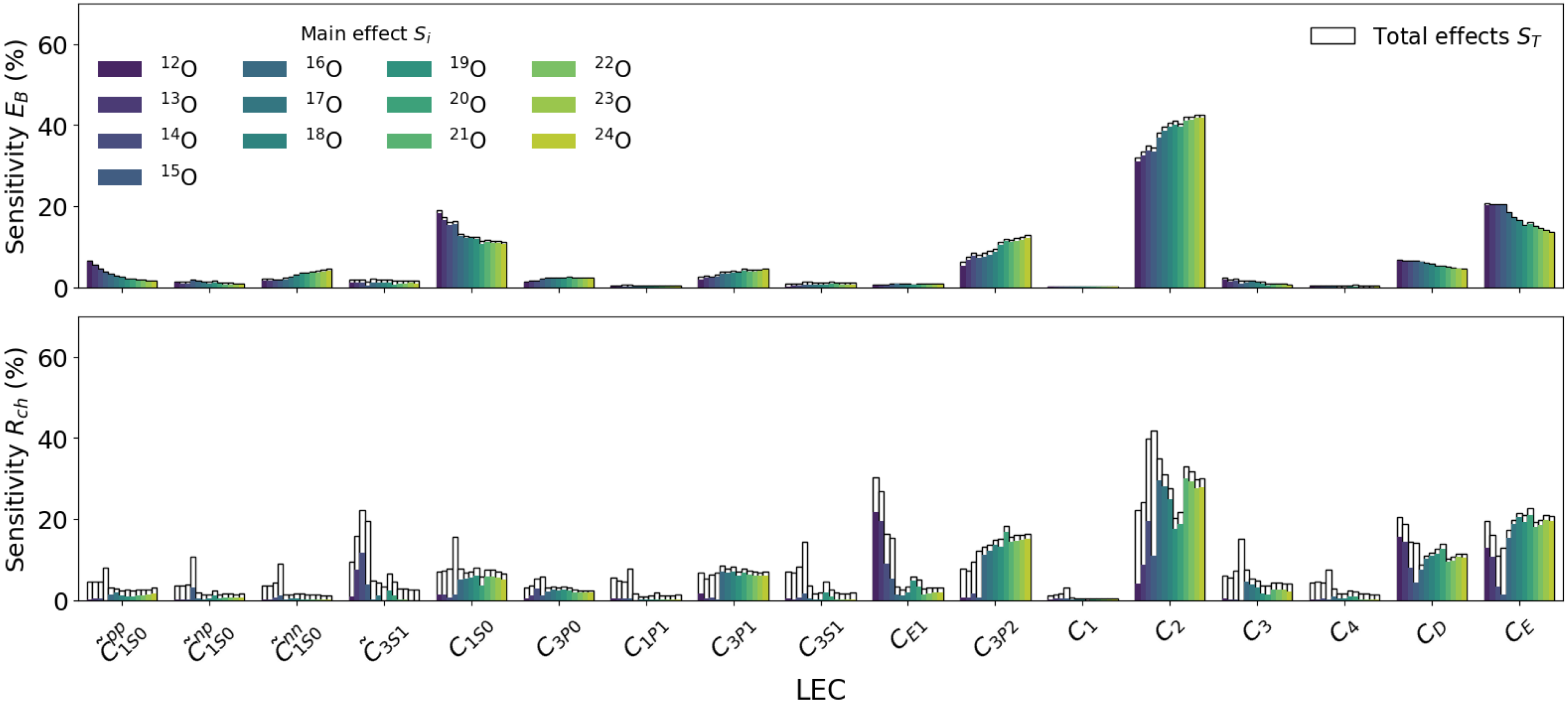
Belley, et al.,Phys. Rev. Lett. **136**, 082501 (2026)





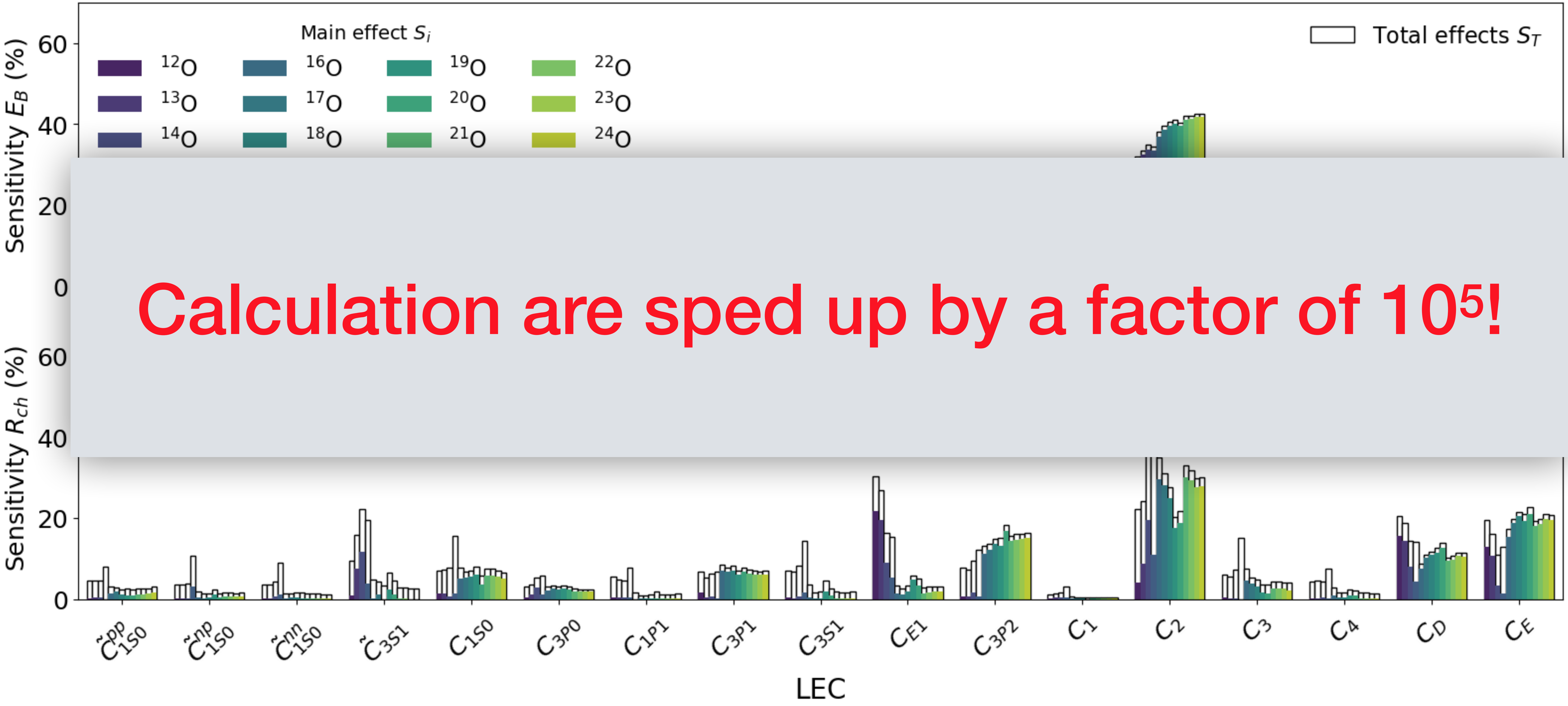
Combining this with UQ technique, we can predict observables with associated uncertainties over the full isotopic chains in a few minutes.

Emulating Multiple Isotopes



Global sensitivity analysis is consistent with other emulators!

Emulating Multiple Isotopes



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

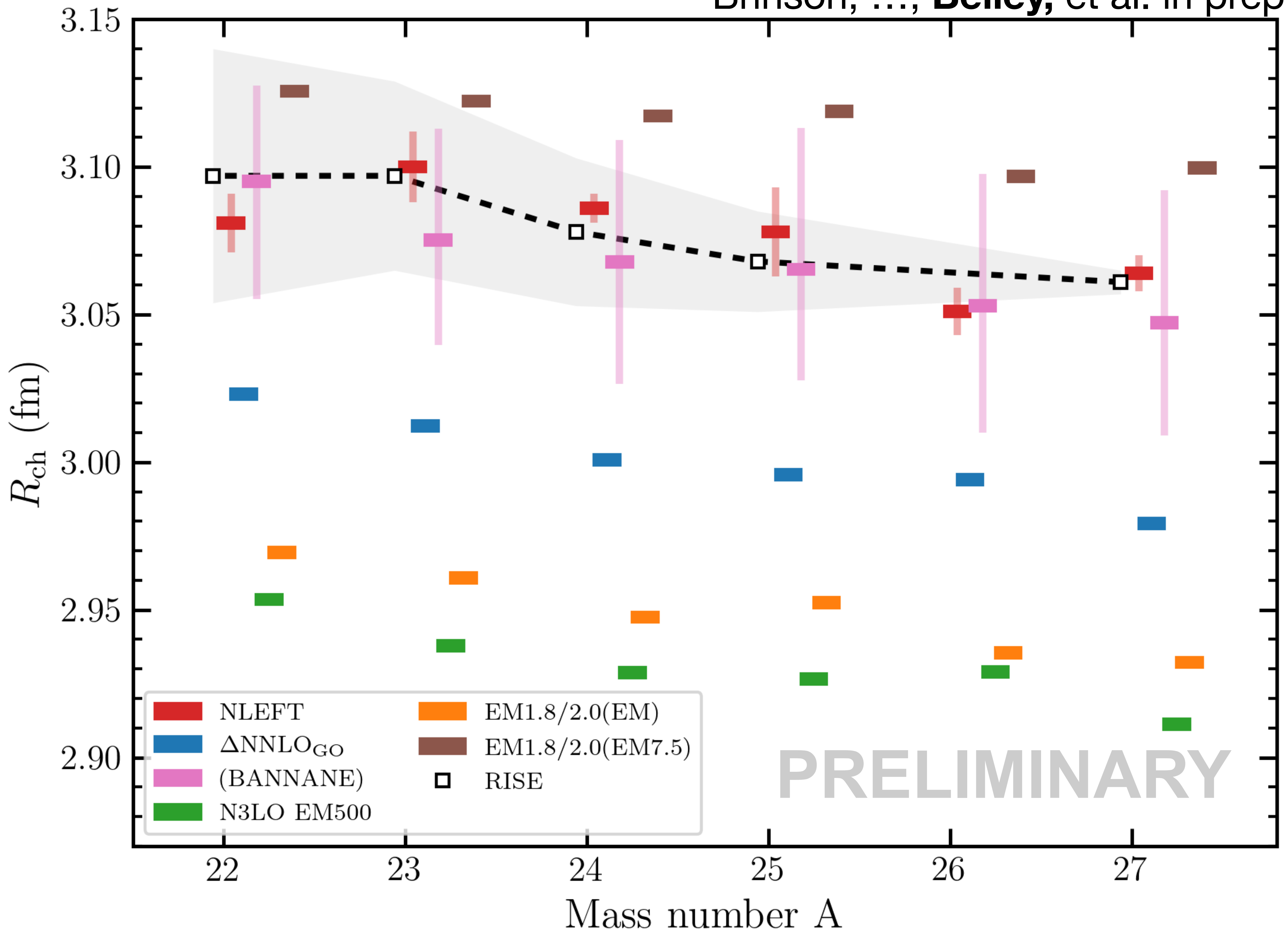
Global sensitivity analysis is consistent with other emulators!

BANNANE with Experiments

Collaboration with the Resonant ionization Spectroscopy Experiment (RiSE) at BECOLA facility at FRIB

- Study charge radii of Aluminum isotopes.
- BANNANE is used to understand the trends across the isotopic chain from theory point of view.

Brinson, …, **Belley,** et al. in prep

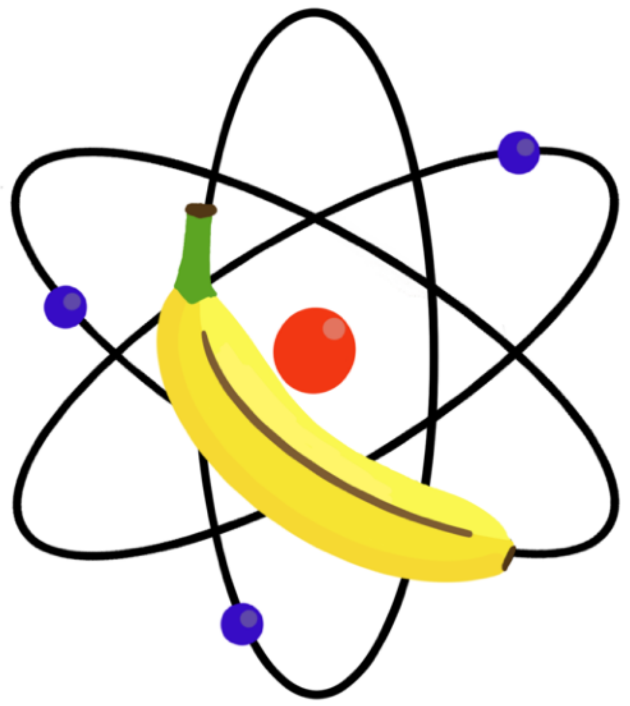


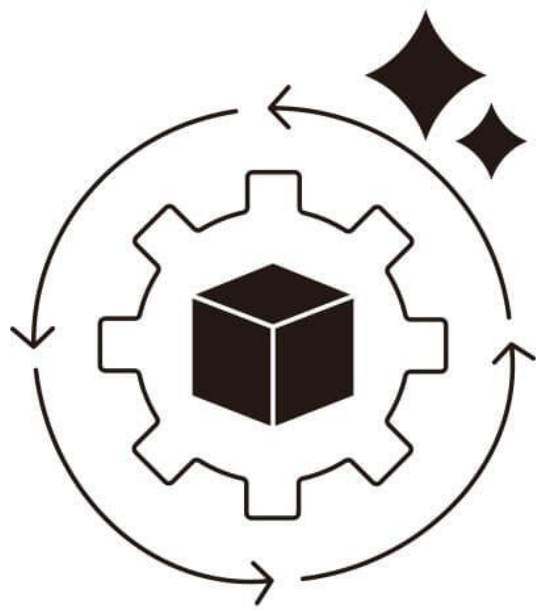
BECOLA

FRIB

Challenges

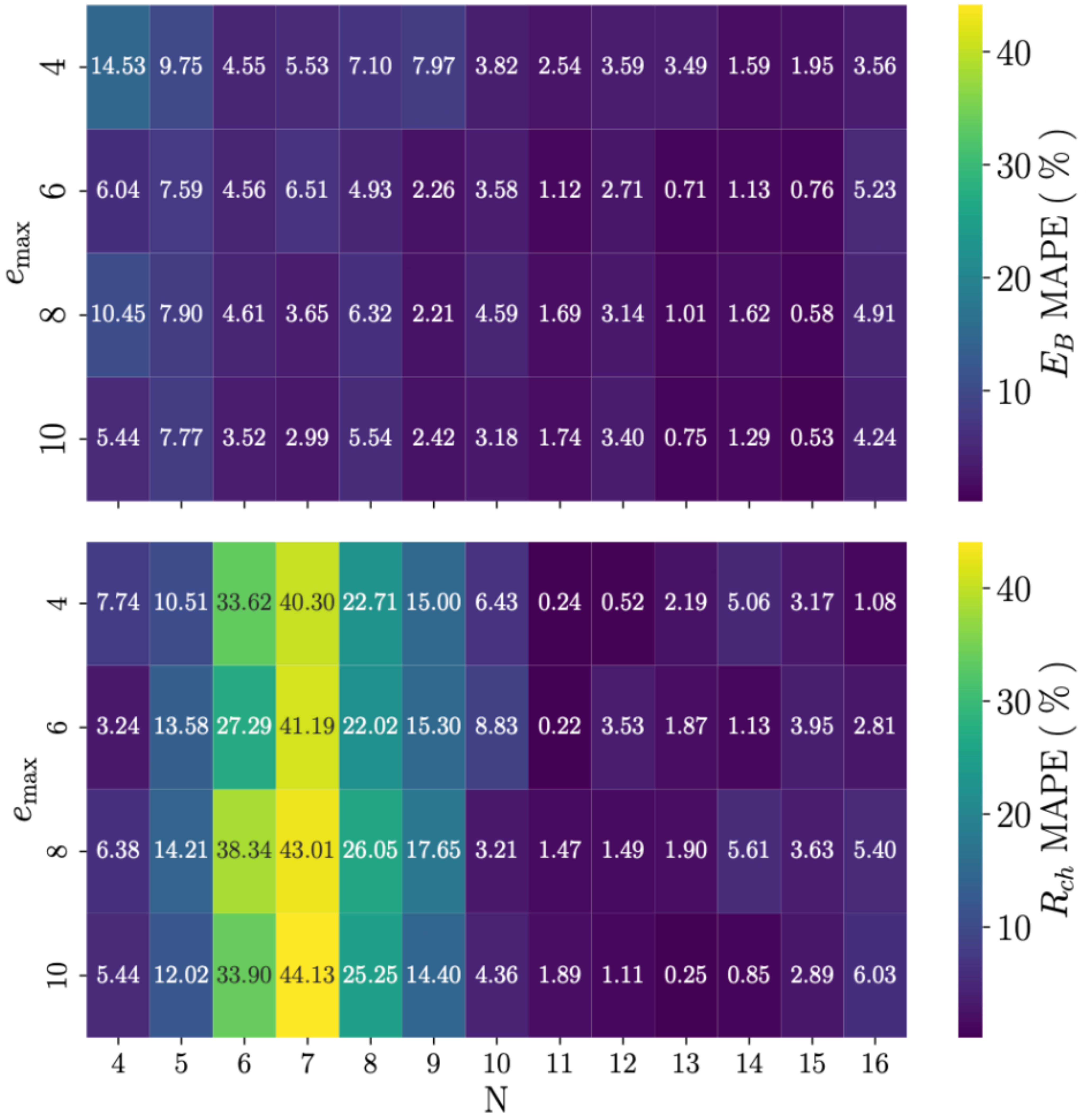
Emulating To Unseen Data





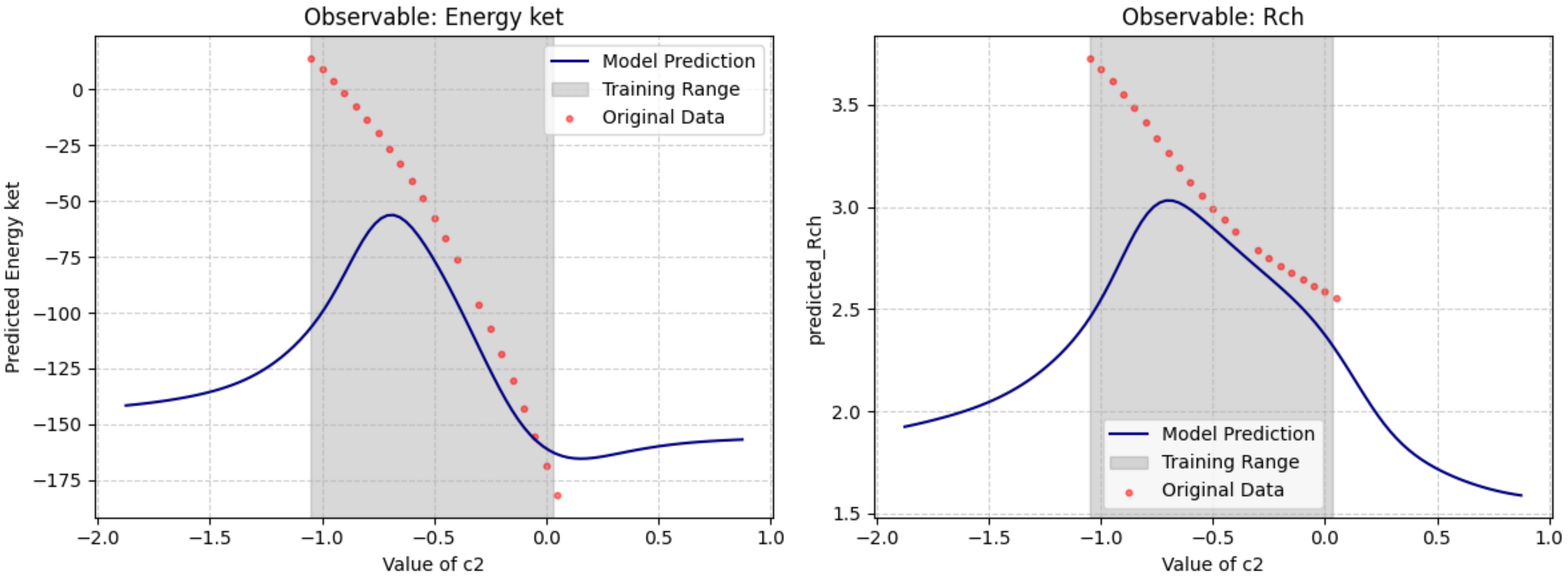
Zero-shot Learning

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)



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Physics driven **Data driven**

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Reduce Basis Methods

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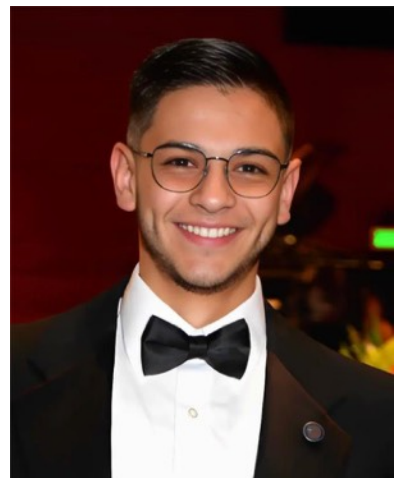
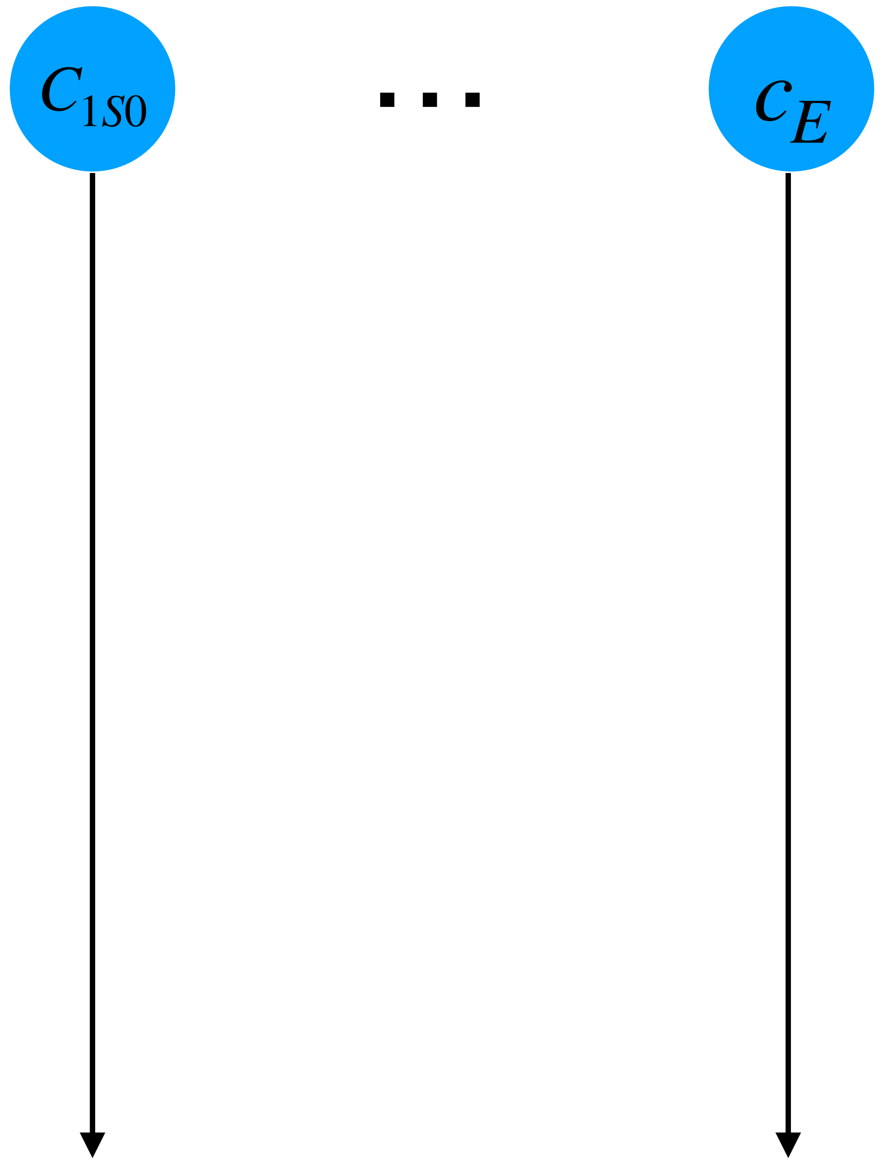
Physics Driven BANNANE?

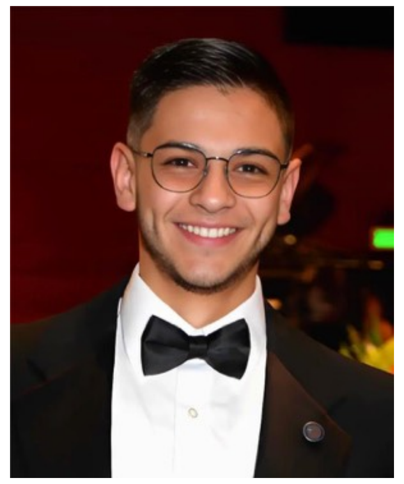


Jose Miguel Muñoz Arias

Parametric Matrix Models



Physics Driven BANNANE?



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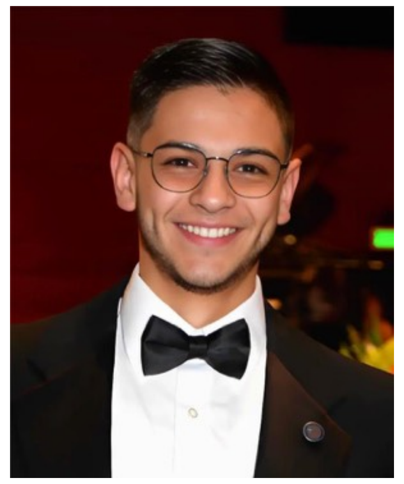
Parametric Matrix Models

C_{1S0} $\cdots$ c_E

$$M \quad = P_0 + C_{1S0}P_{1S0} + \ldots + c_E P_E$$

Physics Driven BANNANE?

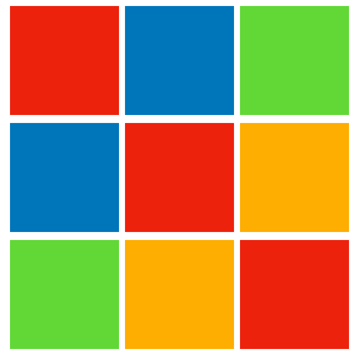


Jose Miguel Muñoz Arias

Parametric Matrix Models

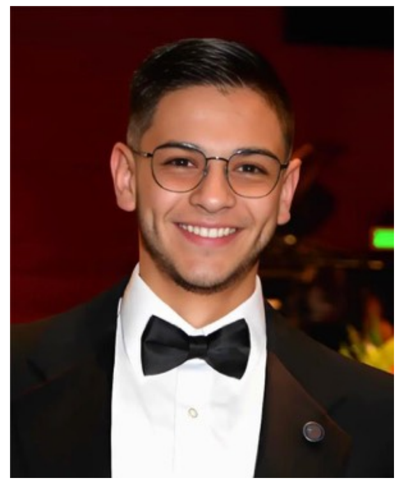
C_{1S0} $\cdots$ c_E

Hermitian matrix

$P_i =$ 

$$M = P_0 + C_{1S0}P_{1S0} + \ldots + c_E P_E$$

Physics Driven BANNANE?

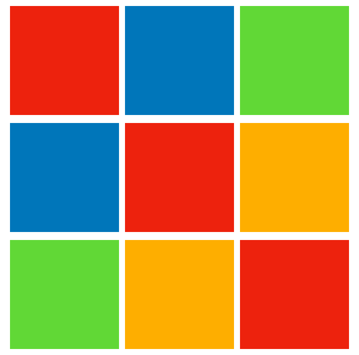


Jose Miguel Muñoz Arias

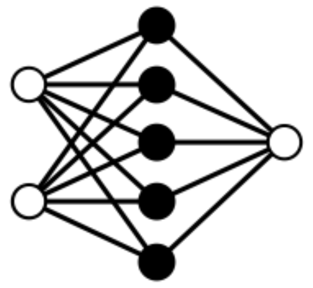
Parametric Matrix Models

C_{1S0} … c_E

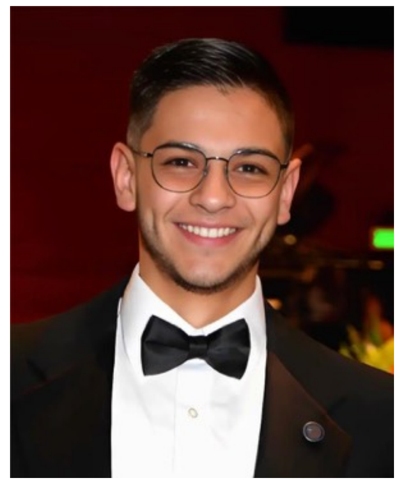
Hermitian matrix

$P_i =$ 

$$M = P_0 + C_{1S0} P_{1S0} + \ldots + c_E P_E$$



Physics Driven BANNANE?

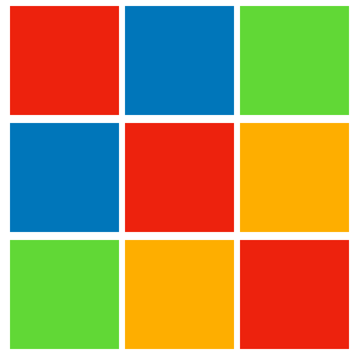


Jose Miguel Muñoz Arias

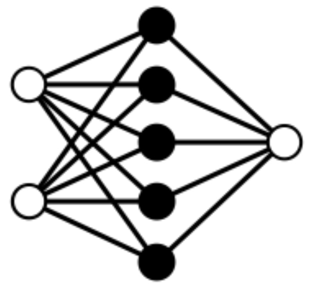
Parametric Matrix Models

C_{1S0} $\cdots$ c_E

Hermitian matrix

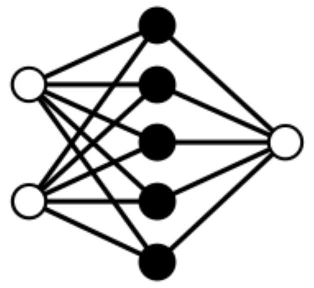
$P_i =$ 

$$M \quad = P_0 + C_{1S0}P_{1S0} + \ldots + c_E P_E$$



$$M|v_j\rangle = E_j|v_j\rangle$$

$$O = \langle v_j | S | v_j \rangle$$



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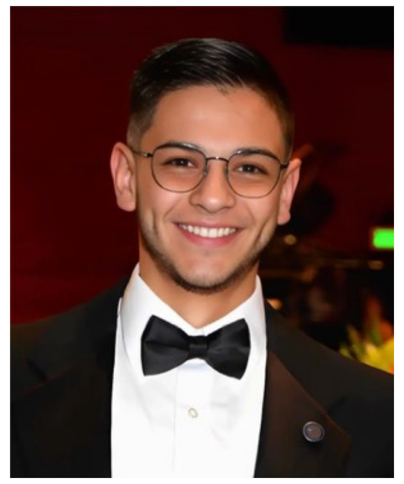
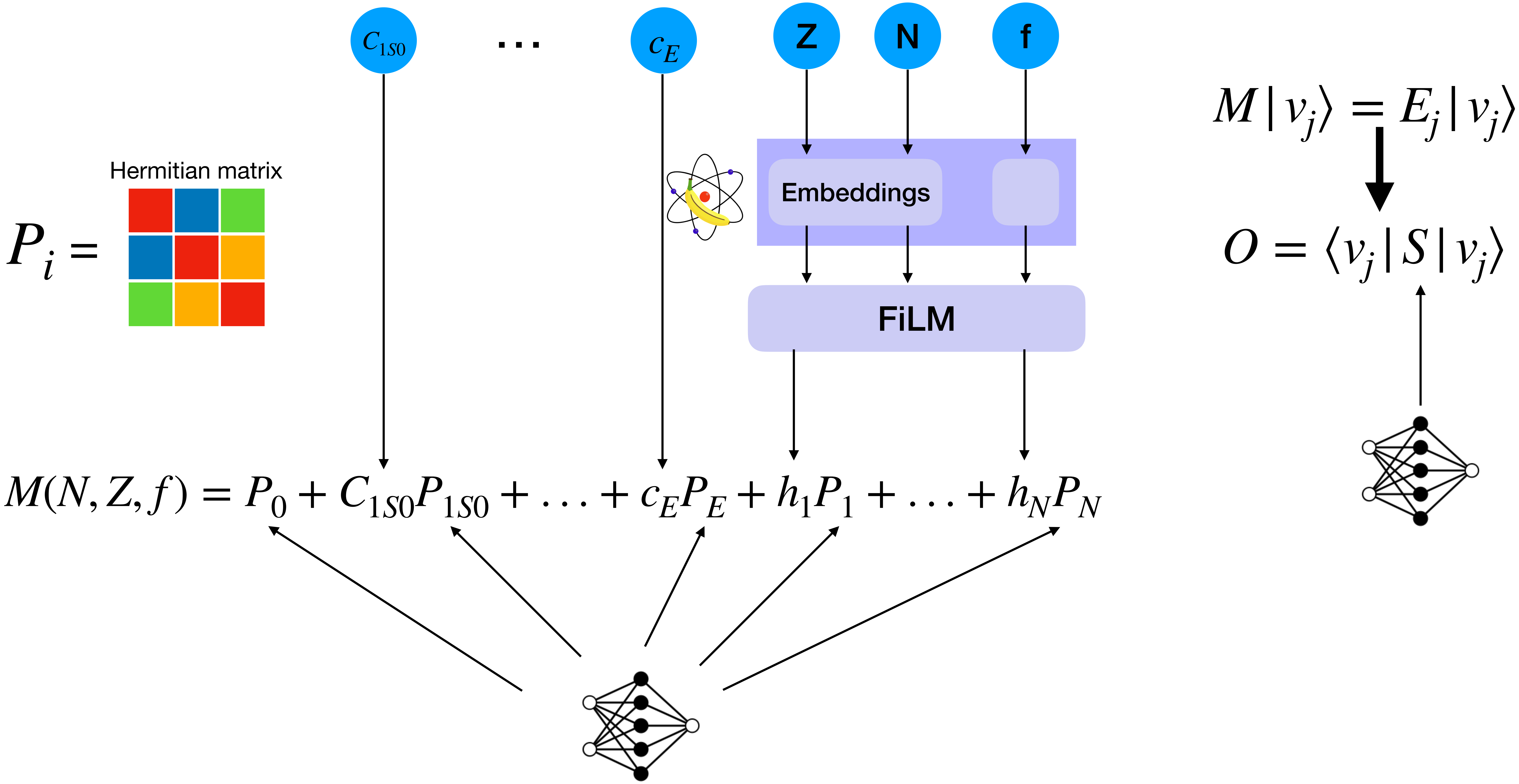
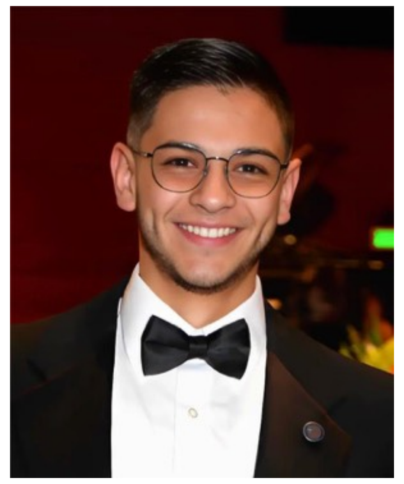


Jose Miguel Muñoz Arias

Parametric Matrix Models



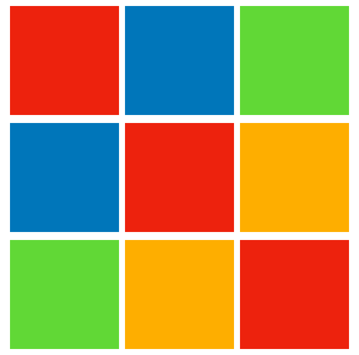
Physics Driven BANNANE?

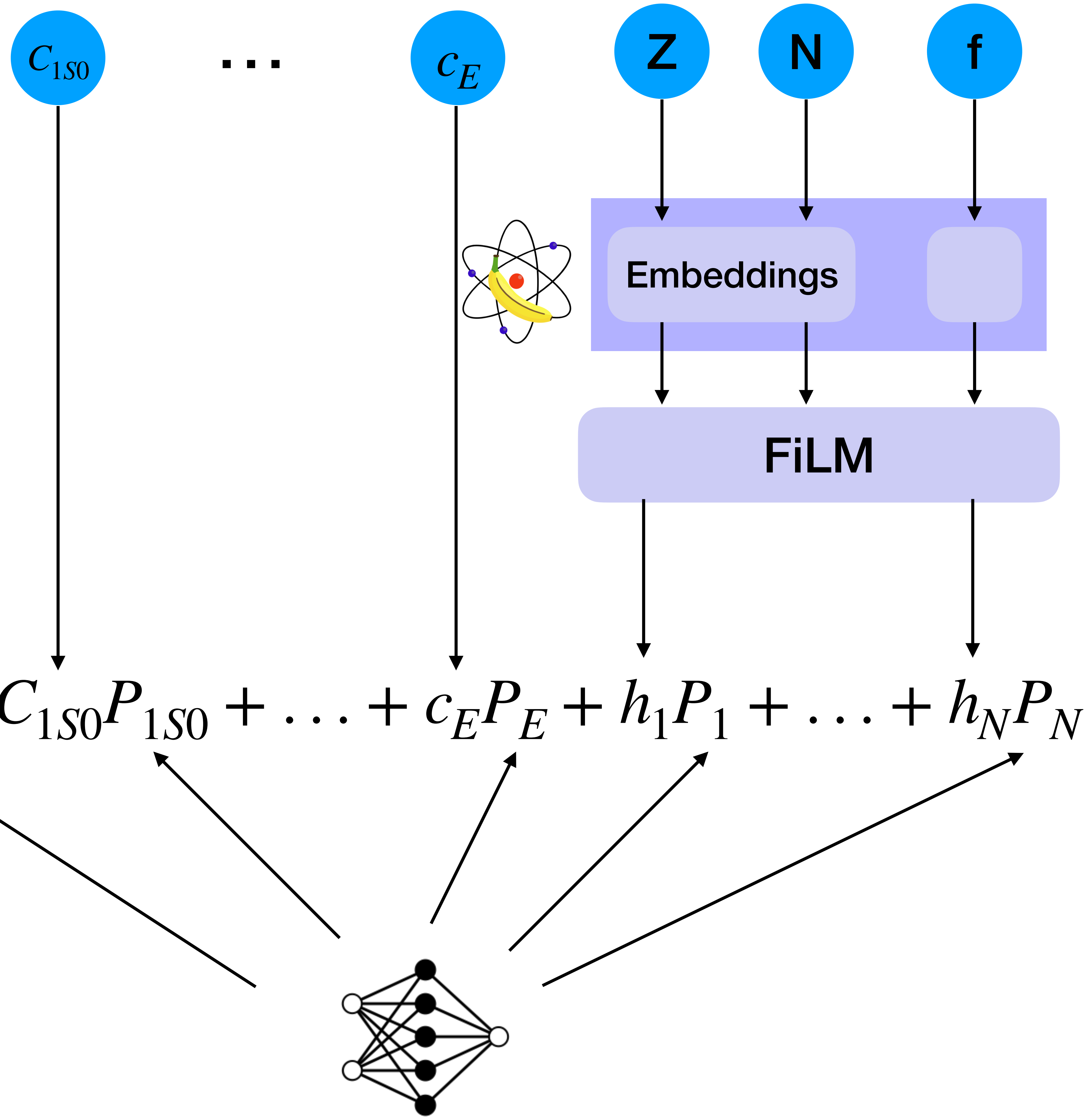


Jose Miguel Muñoz Arias

Parametric Matrix Models

Hermitian matrix

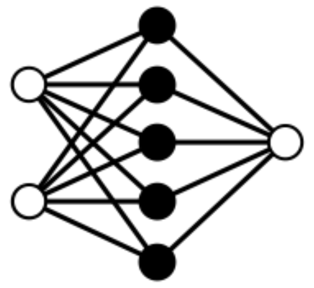
$P_i =$ 



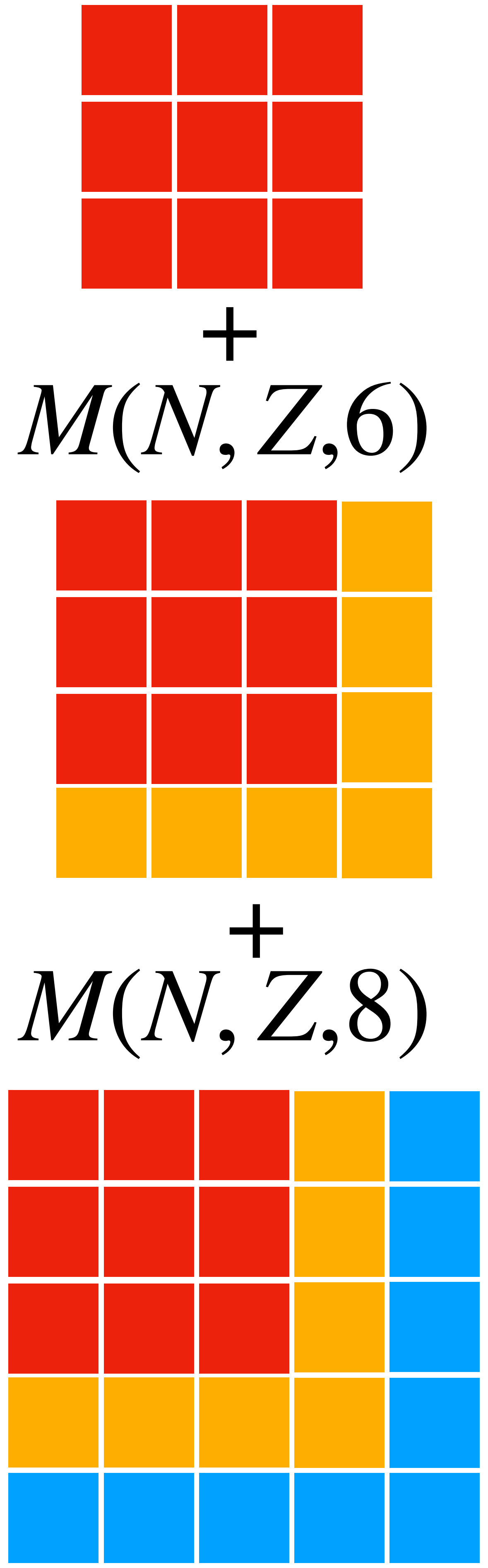
$$M(N,Z,f) = P_0 + C_{1S0}P_{1S0} + \ldots + c_E P_E + h_1 P_1 + \ldots + h_N P_N$$

$$M|v_j\rangle = E_j|v_j\rangle$$

$$O = \langle v_j|S|v_j\rangle$$



$M(N,Z,4)$



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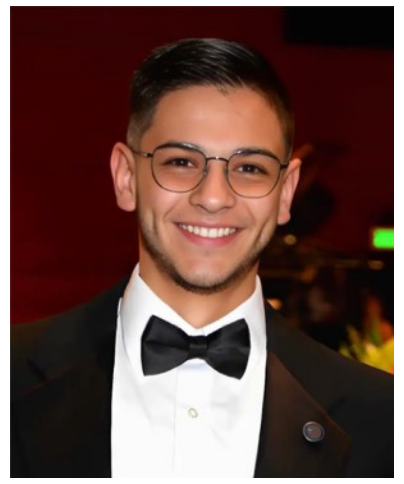
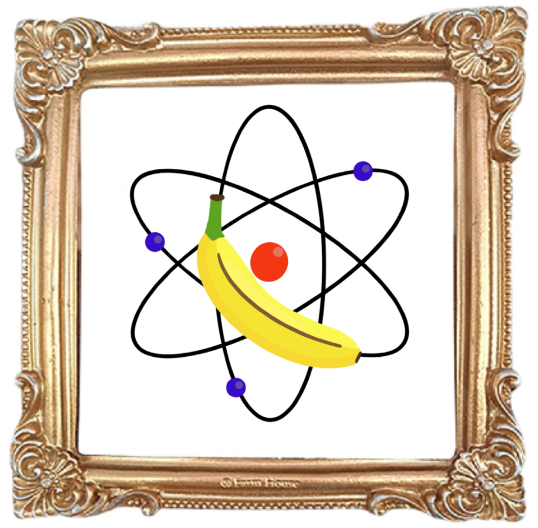
Physics Driven BANNANE?

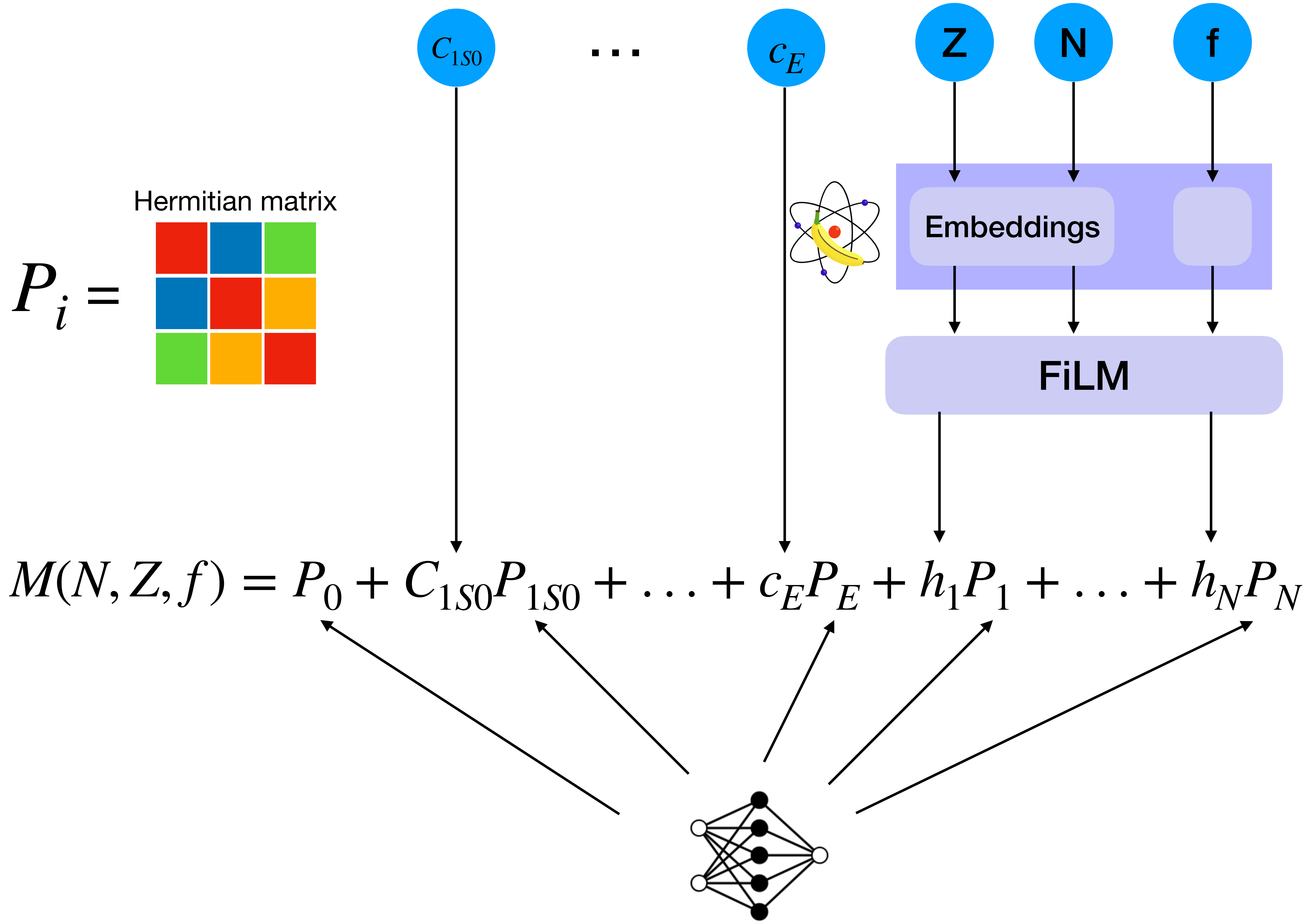


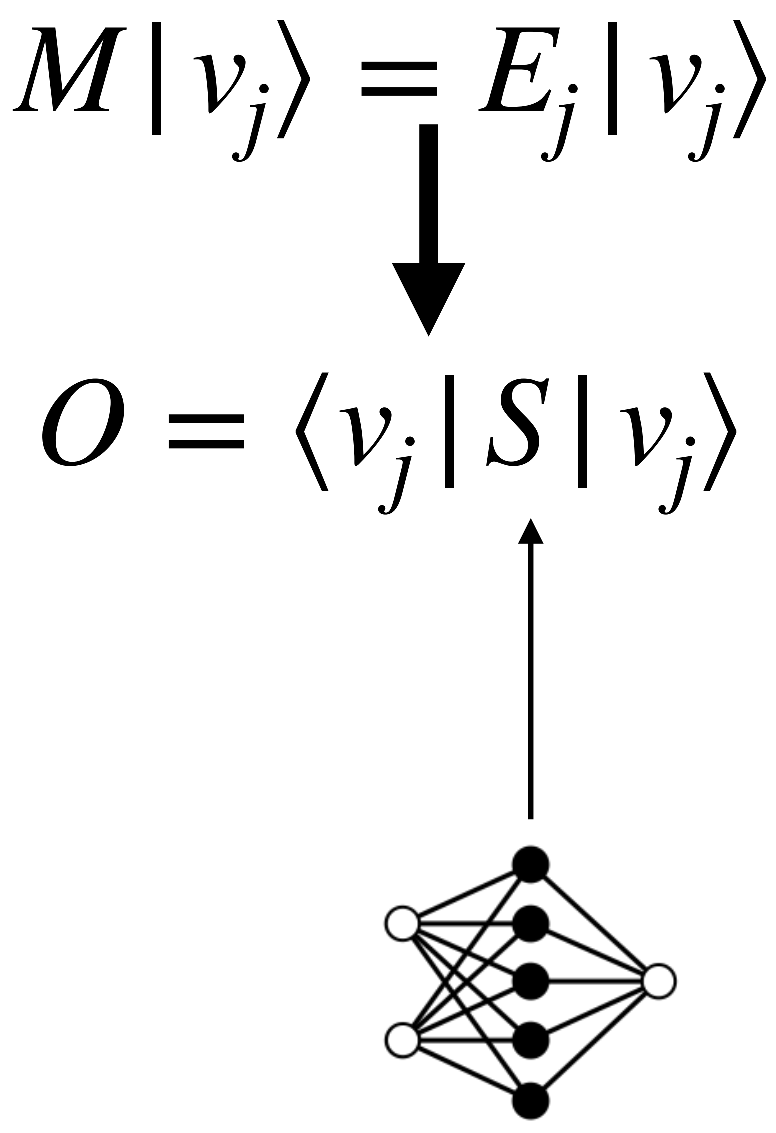
Jose Miguel Muñoz Arias

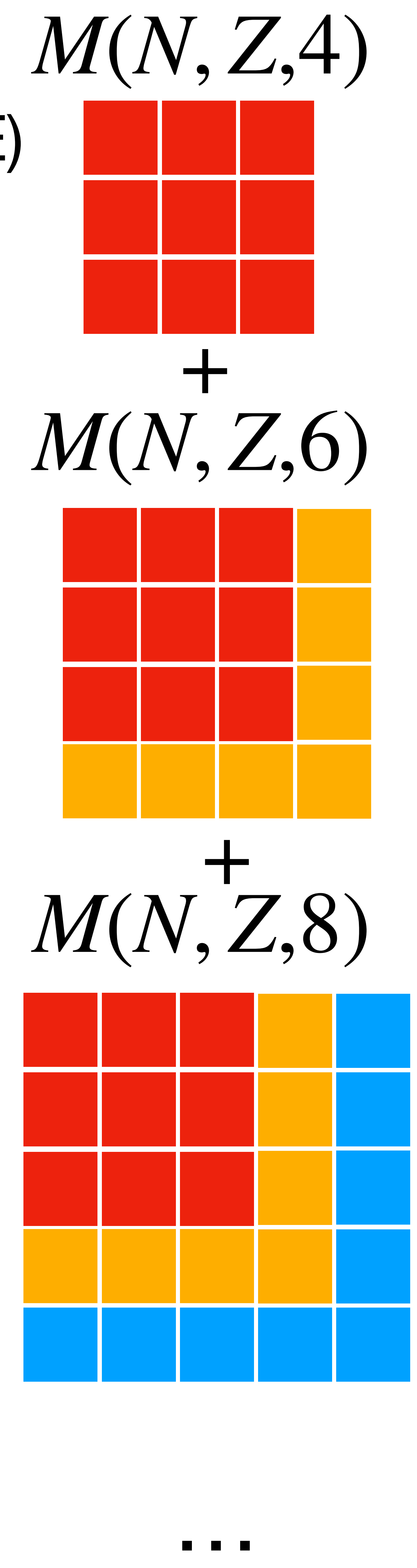


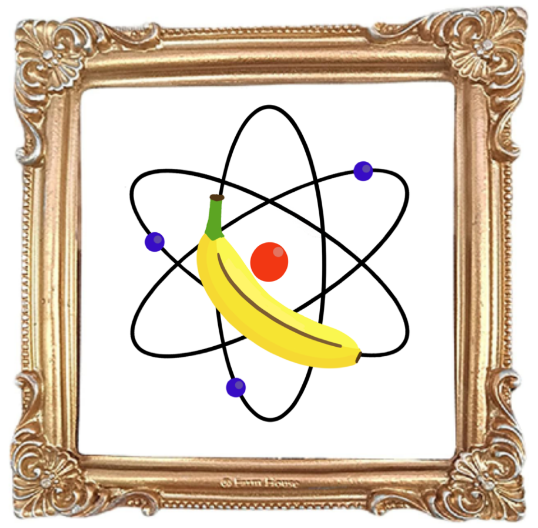
Feature Resolved Affine Matrix Emulator (FRAME)

Parametric Matrix Models

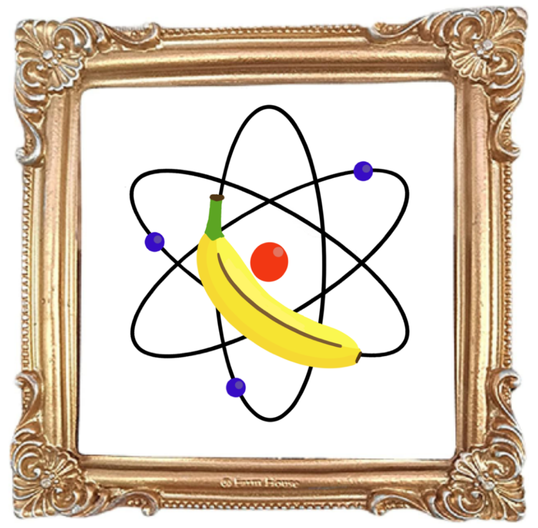






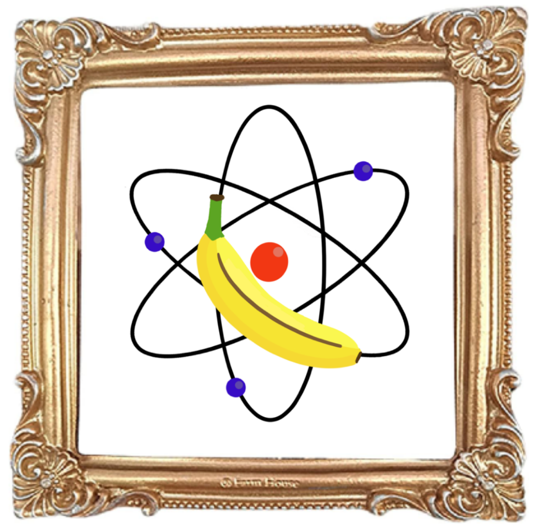


Anchor and Refinement



Anchor and Refinement

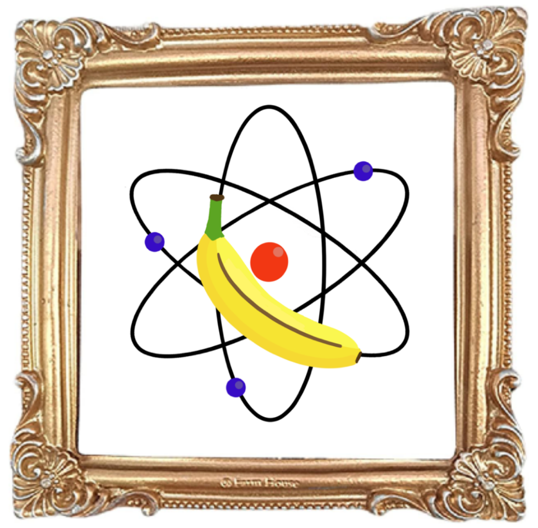
$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^{f} \xi(f; N, Z, \alpha)\Delta M_p]$$



Anchor and Refinement

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

Anchor: Matrix at the lowest fidelity

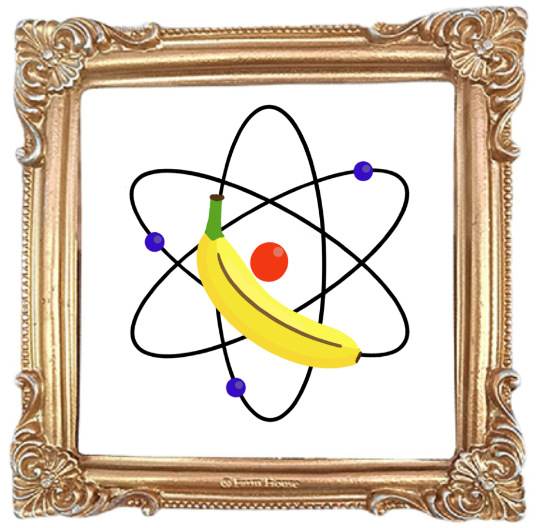


Anchor and Refinement

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

Anchor: Matrix at the lowest fidelity

Refinement: Corrections from higher fidelities



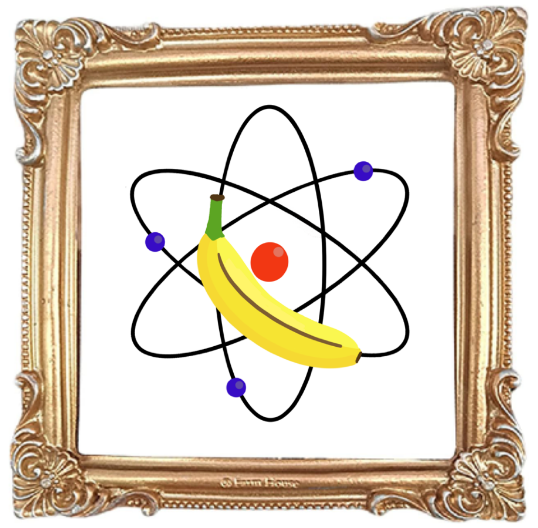
Anchor and Refinement

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

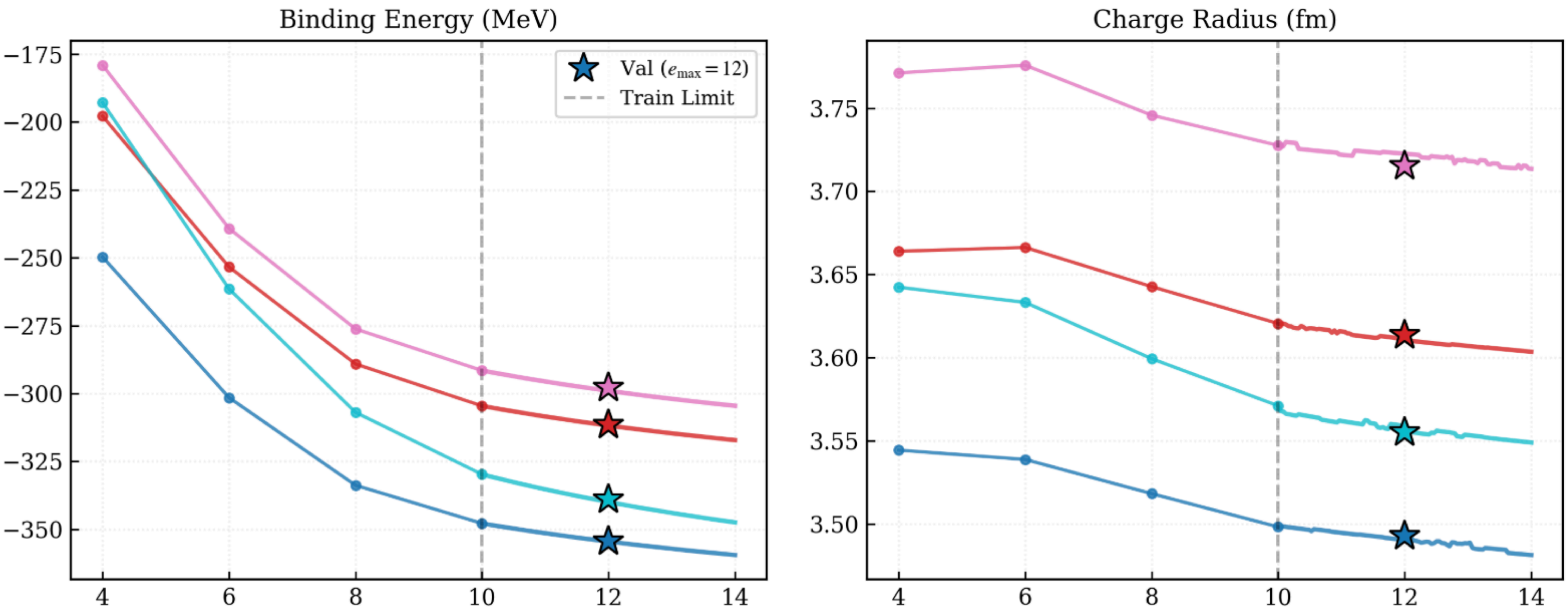
Anchor: Matrix at the lowest fidelity

Refinement: Corrections from higher fidelities

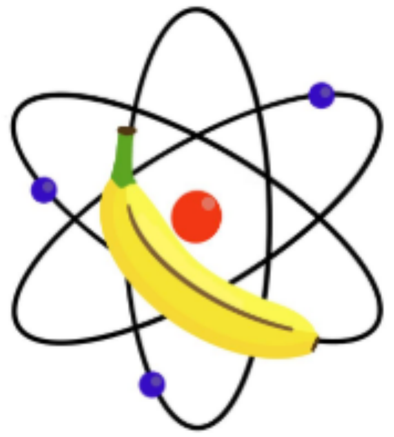
https://frame-architecture-explorer-553167399436.us-west1.run.app/

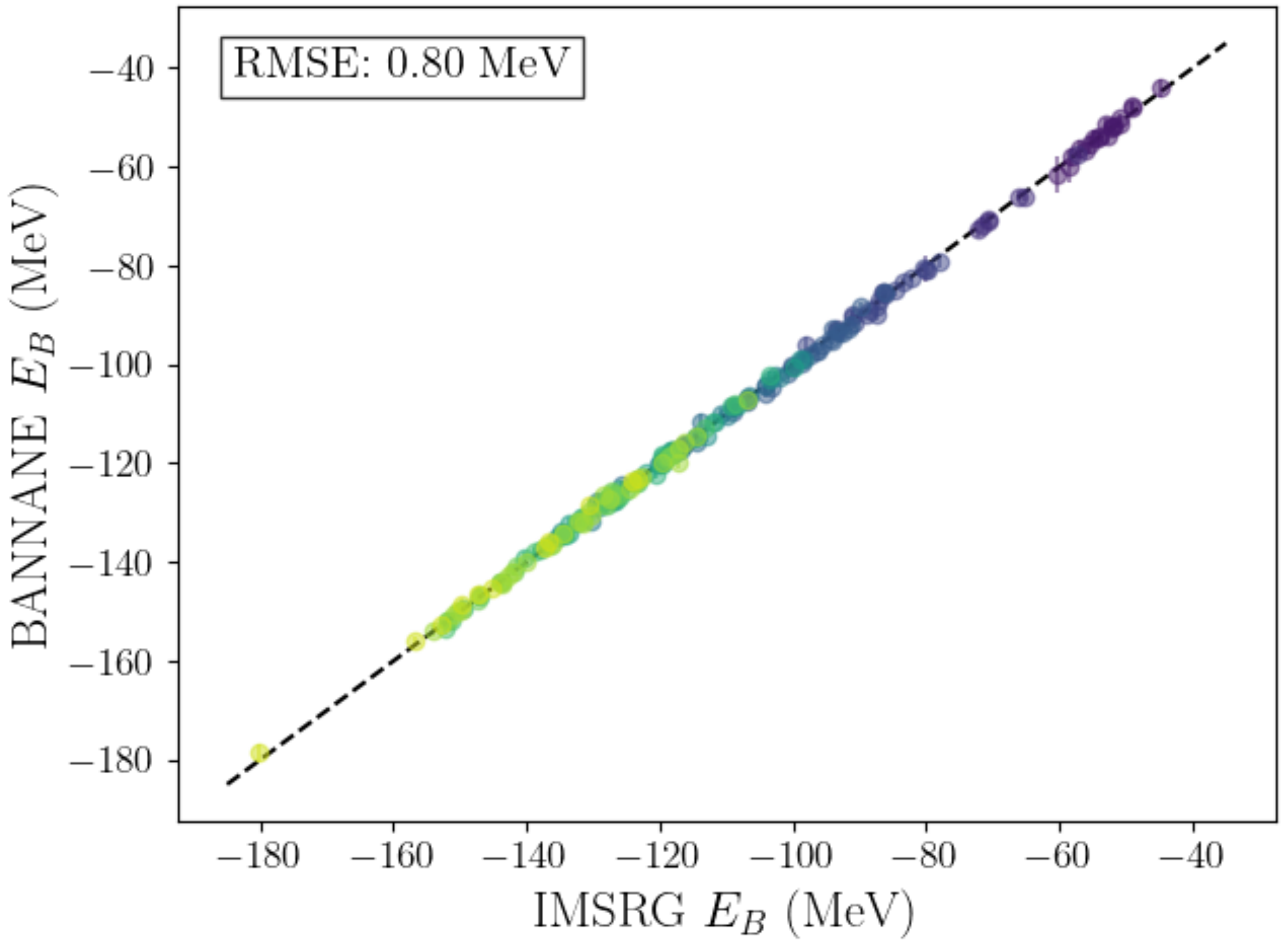


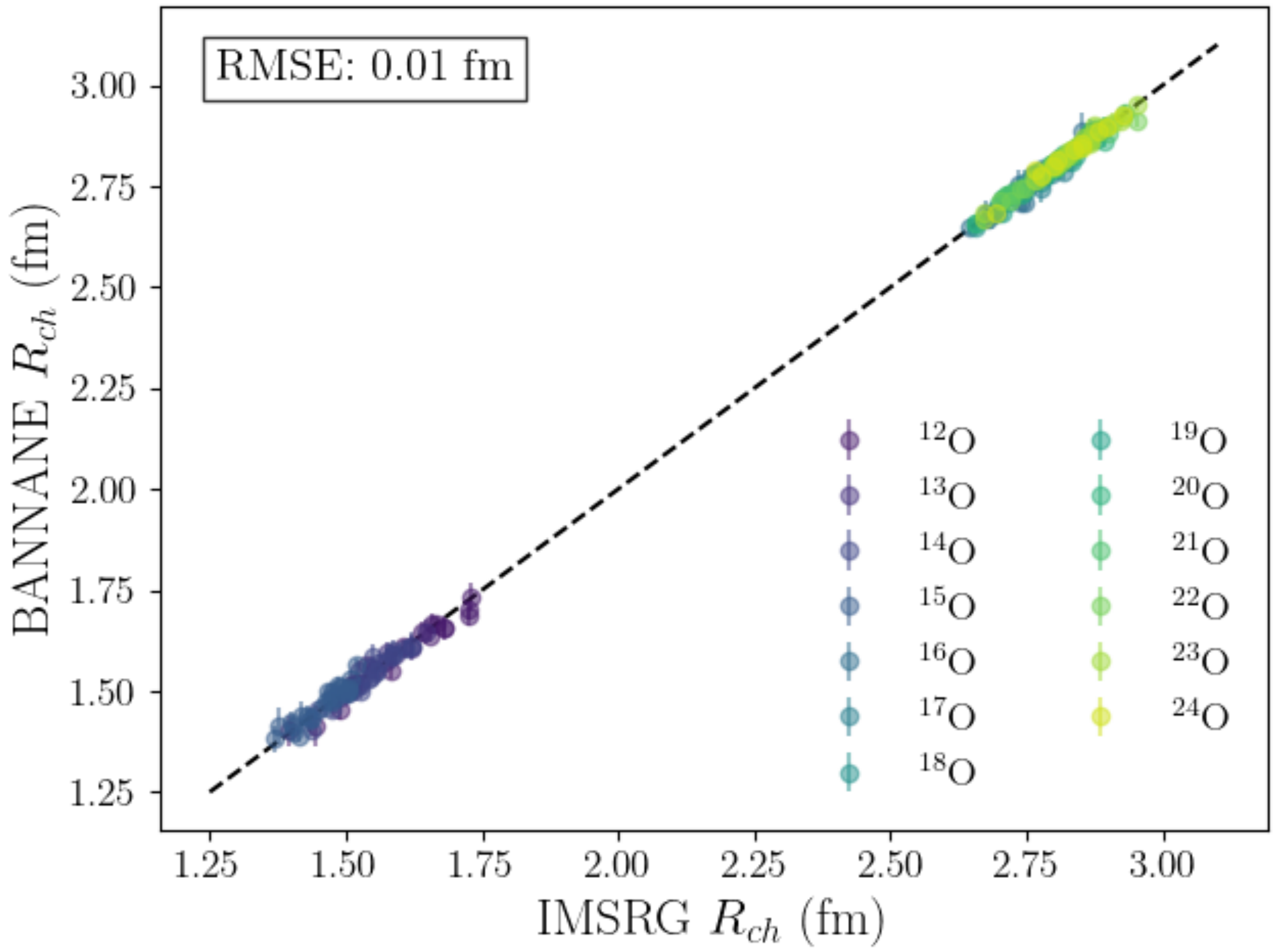
Extrapolating in e_{max}

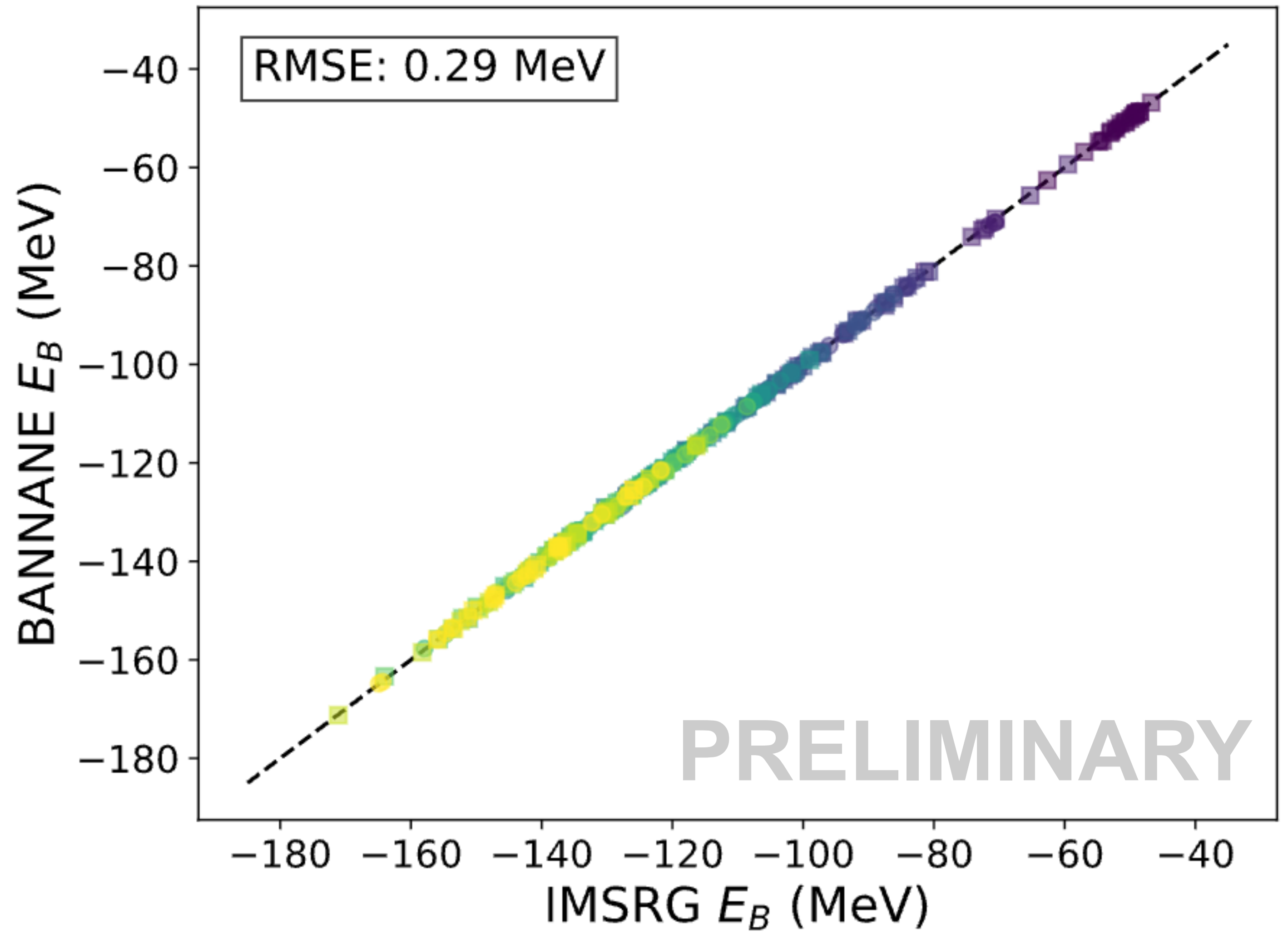


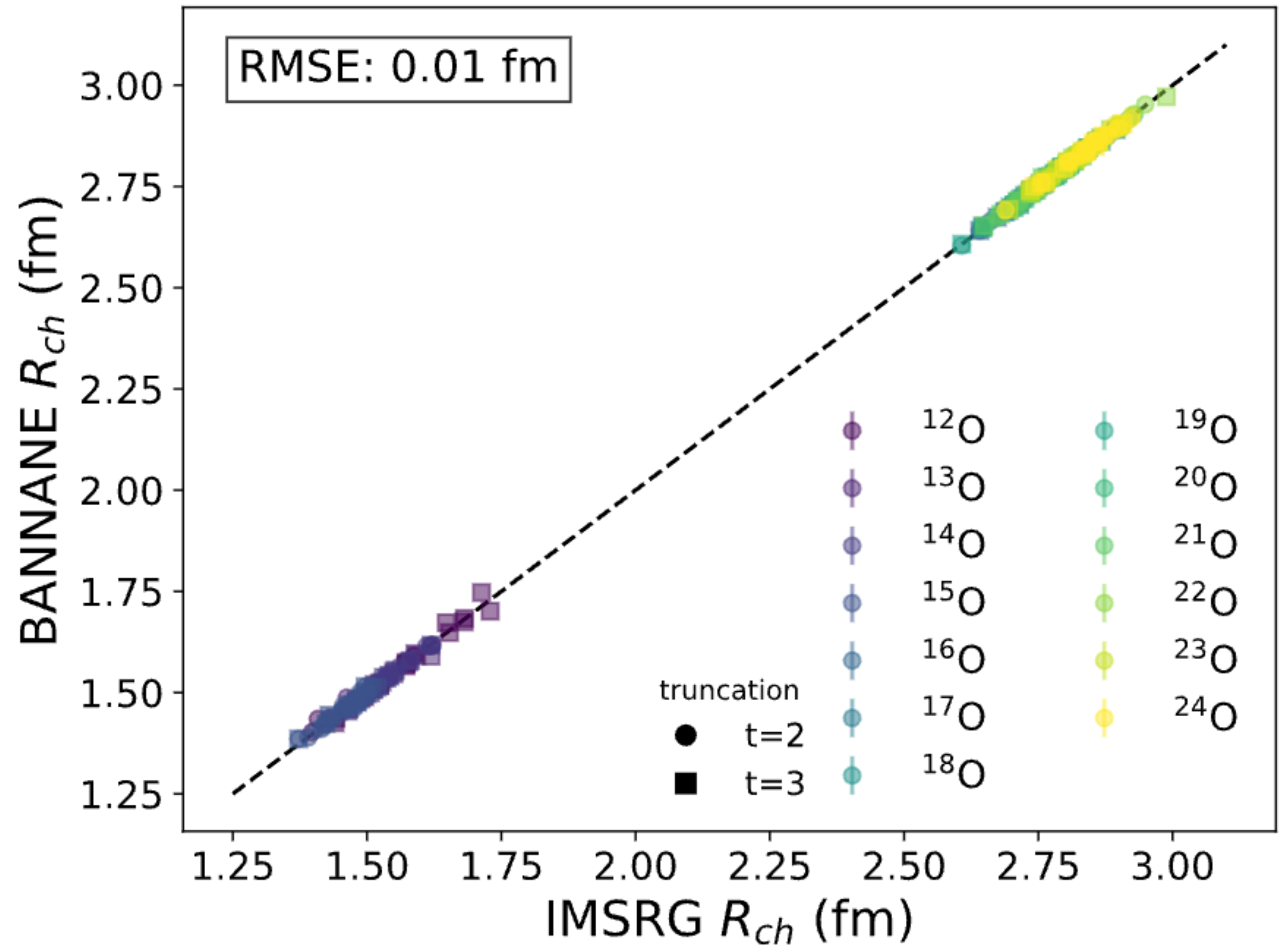
Physics Driven BANNANE!

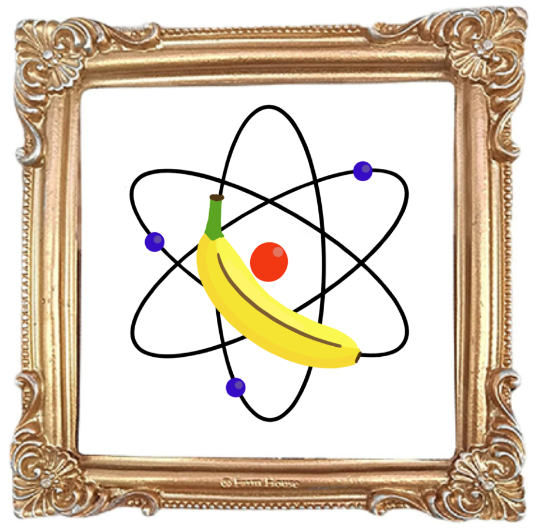








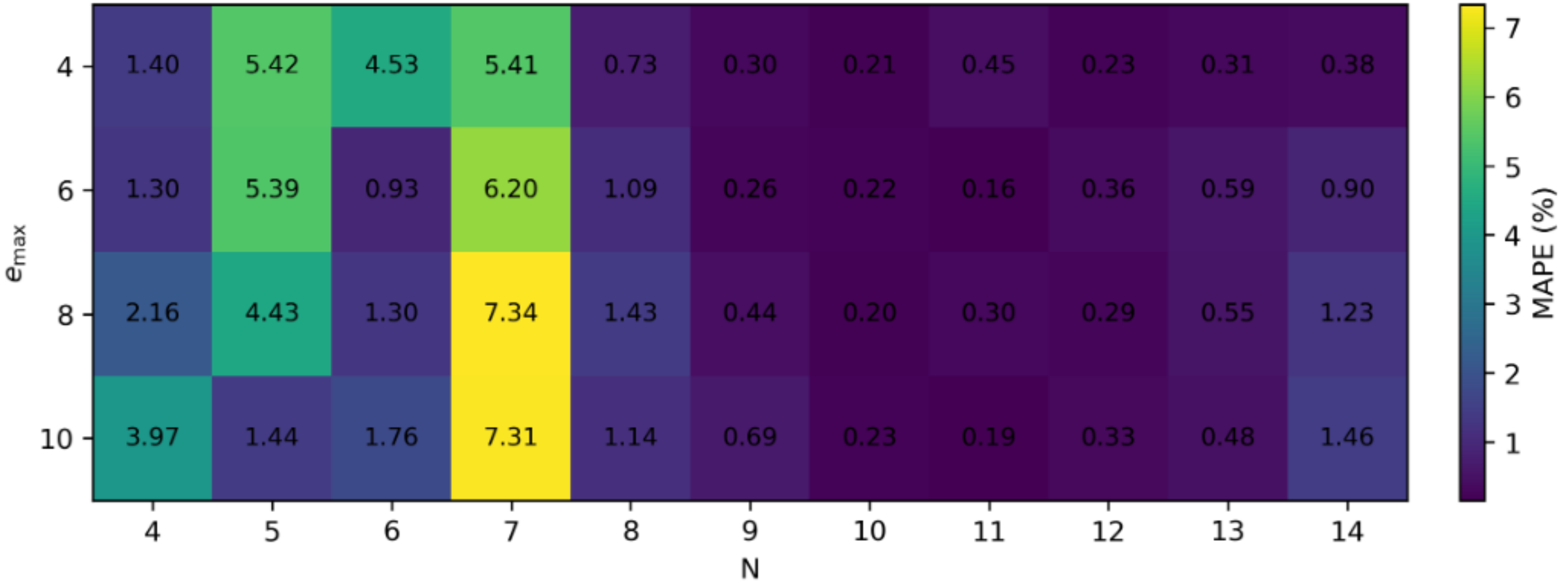


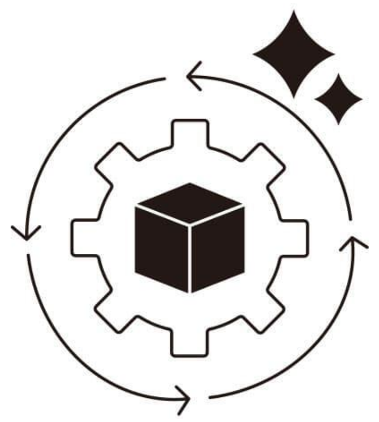


Training cost was reduced by a factor of 5!

Physics Driven BANNANE!

R_{ch}



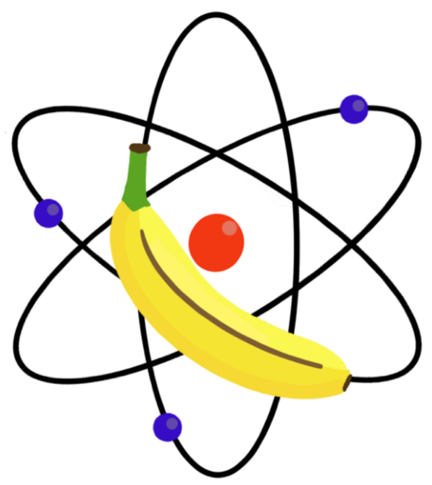


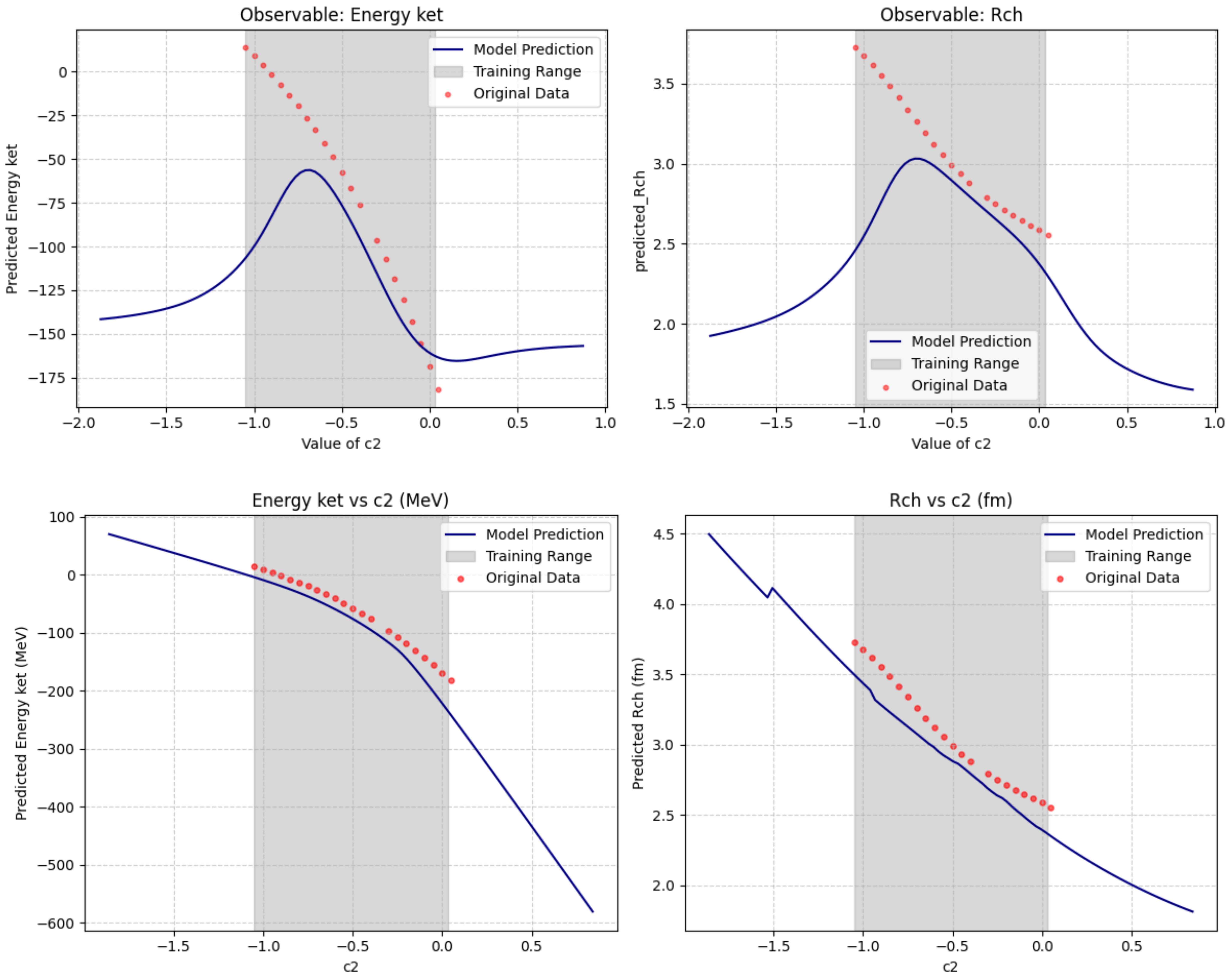
Zero-shot Learning

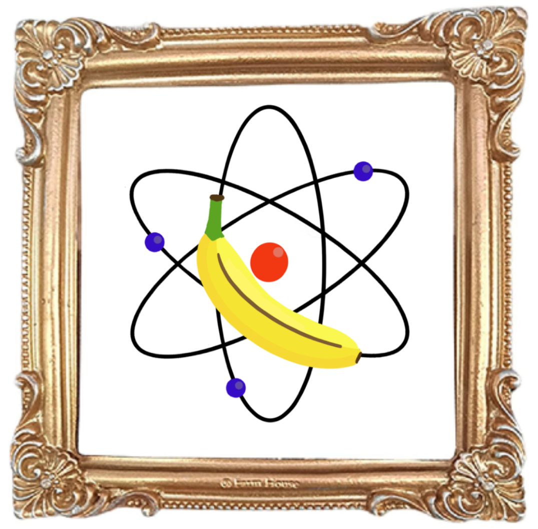
Physics driven version reduced worst zero-shot learning case from 44% error to 7% error!

Physics Driven BANNANE!

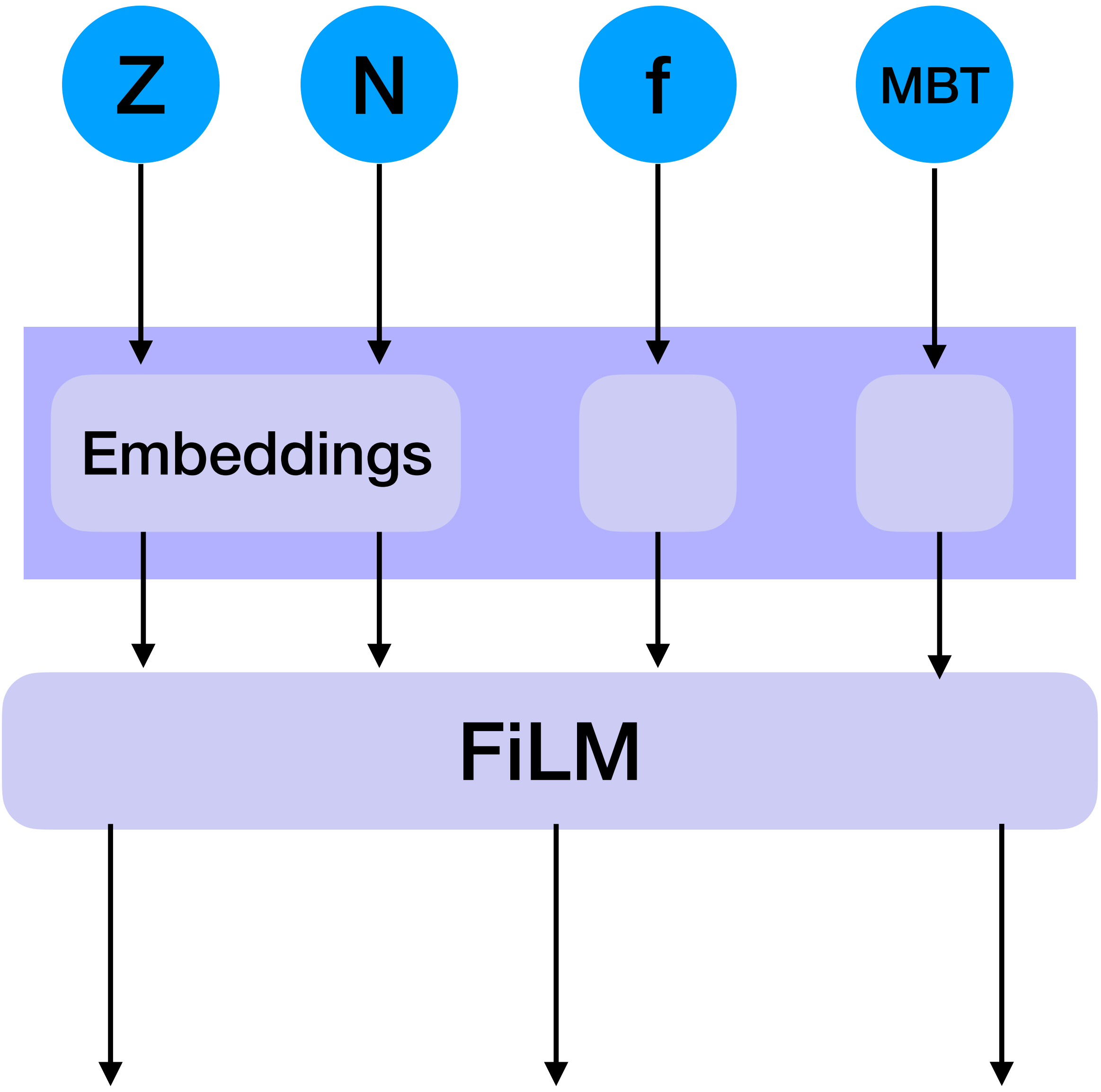
Model Extrapolation vs. Low-Energy Constants (LECs)



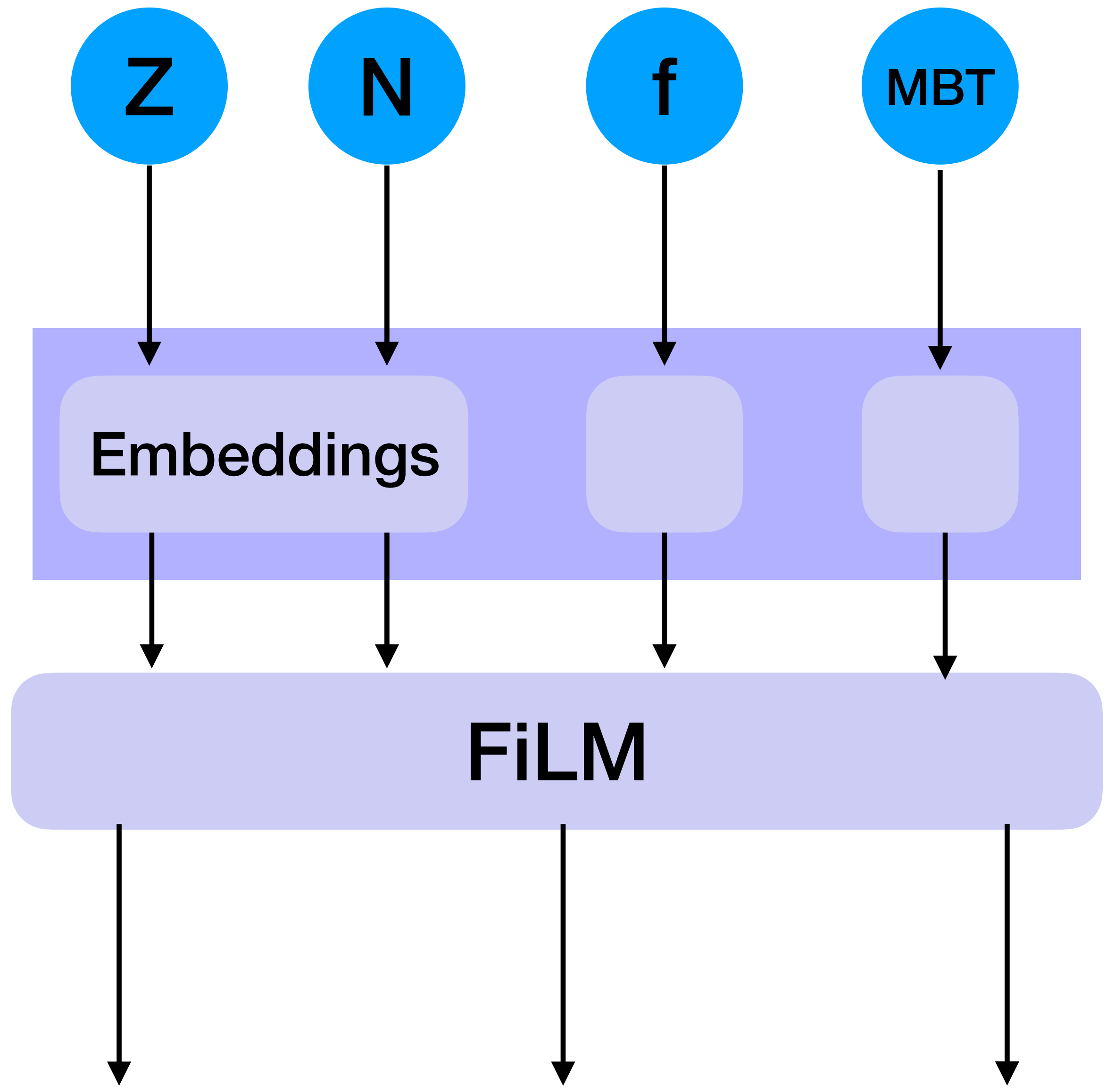


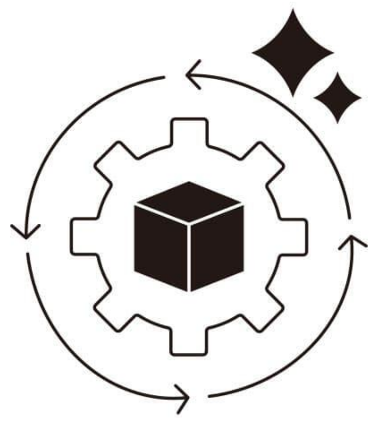


Extrapolating to IMSRG(3)



Extrapolating to IMSRG(3)

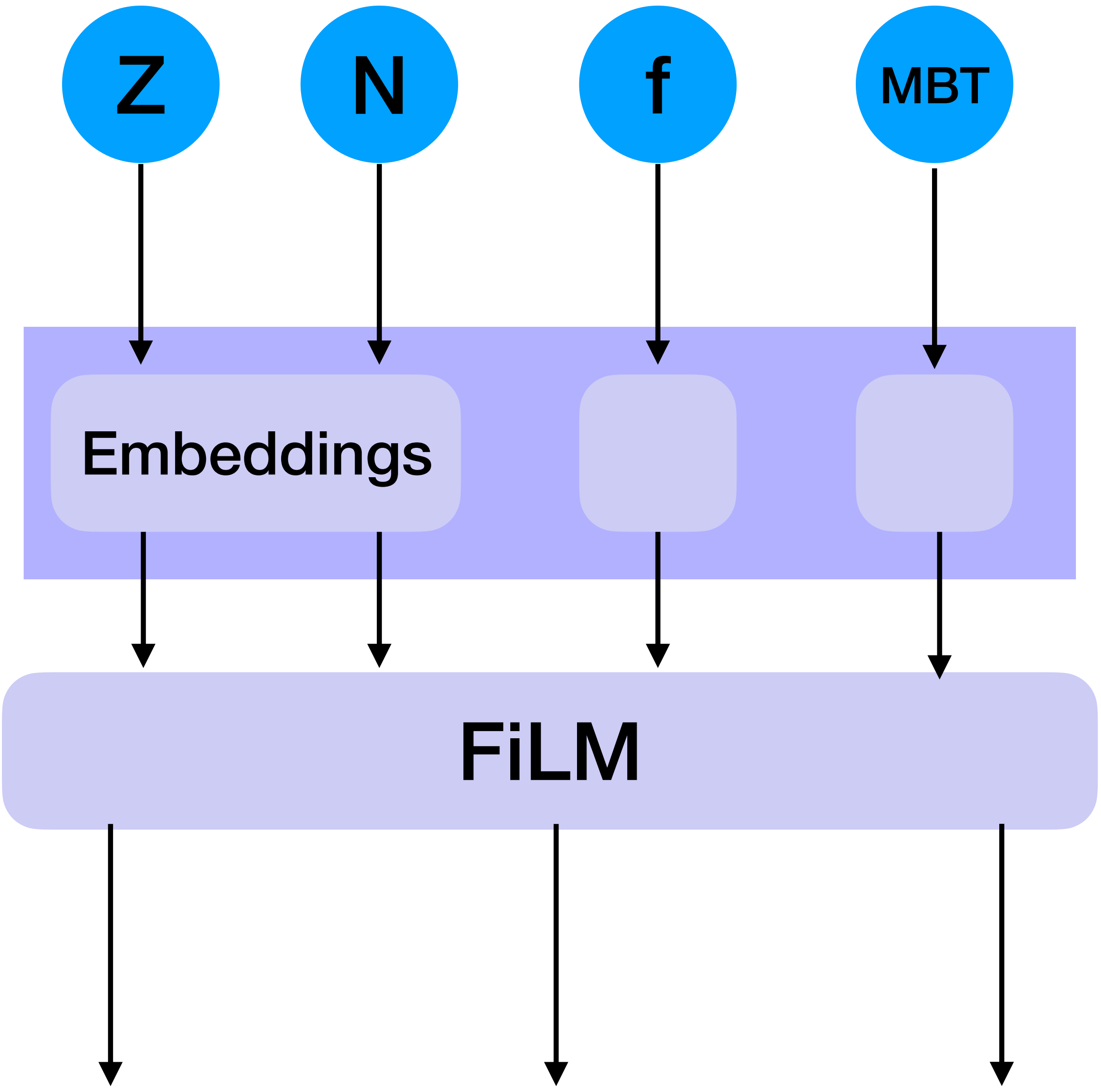


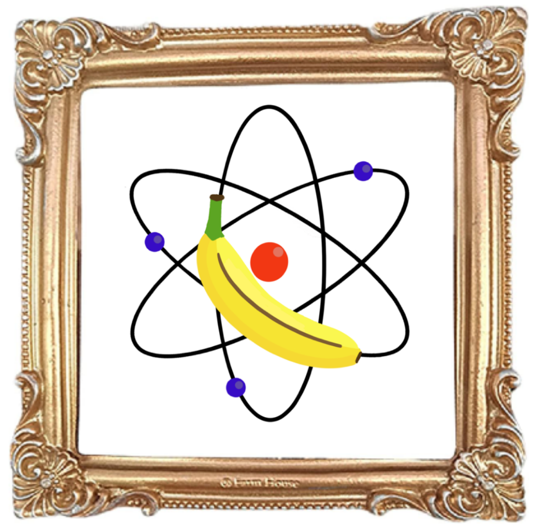


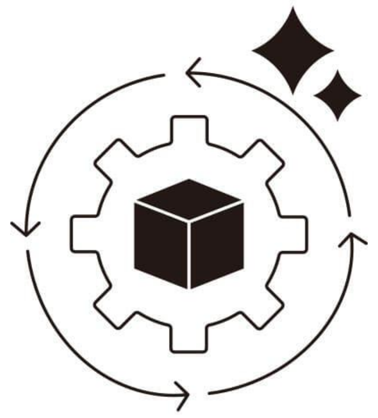
Zero-shot Learning

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

Extrapolating to IMSRG(3)







Zero-shot Learning

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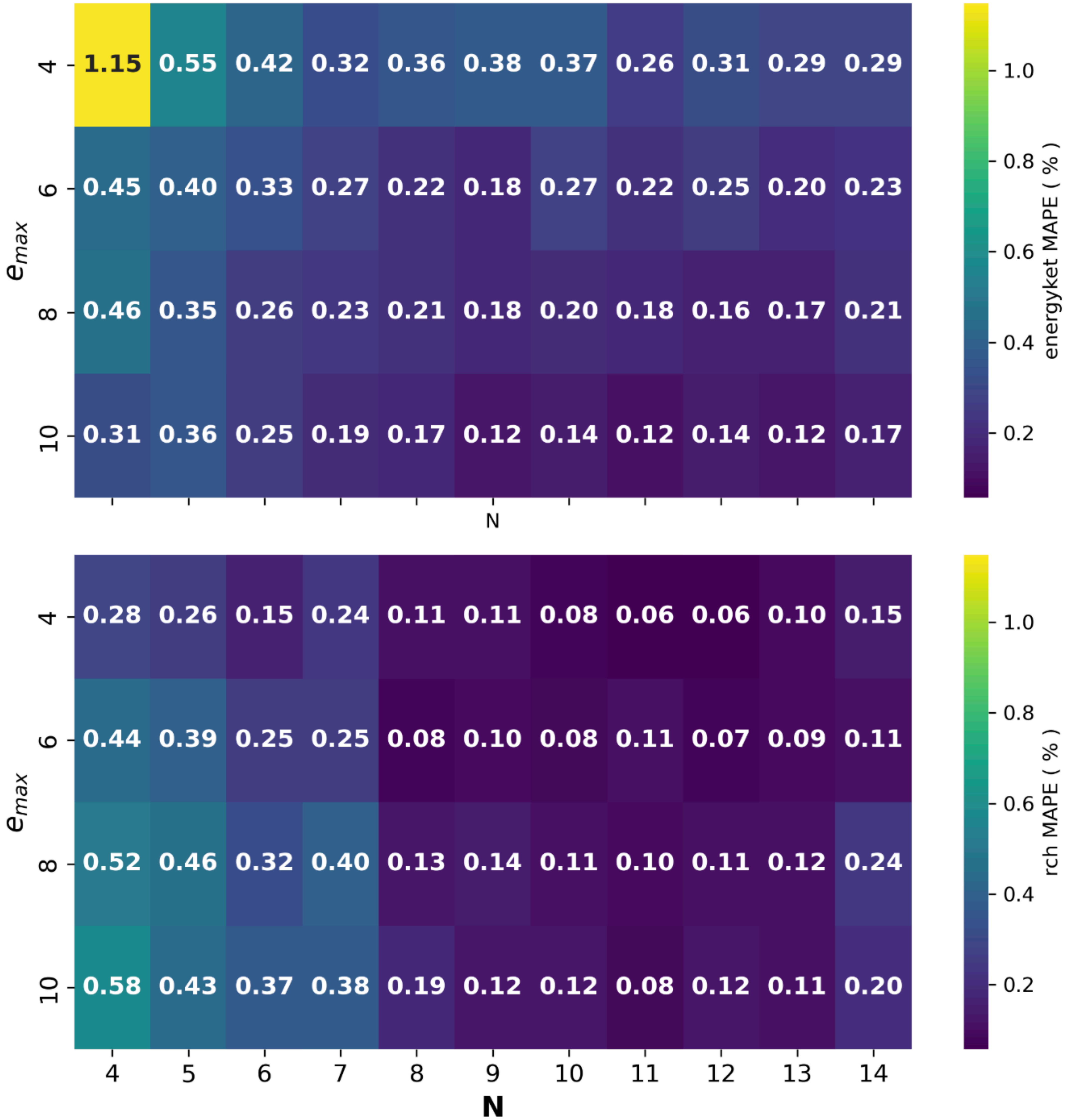
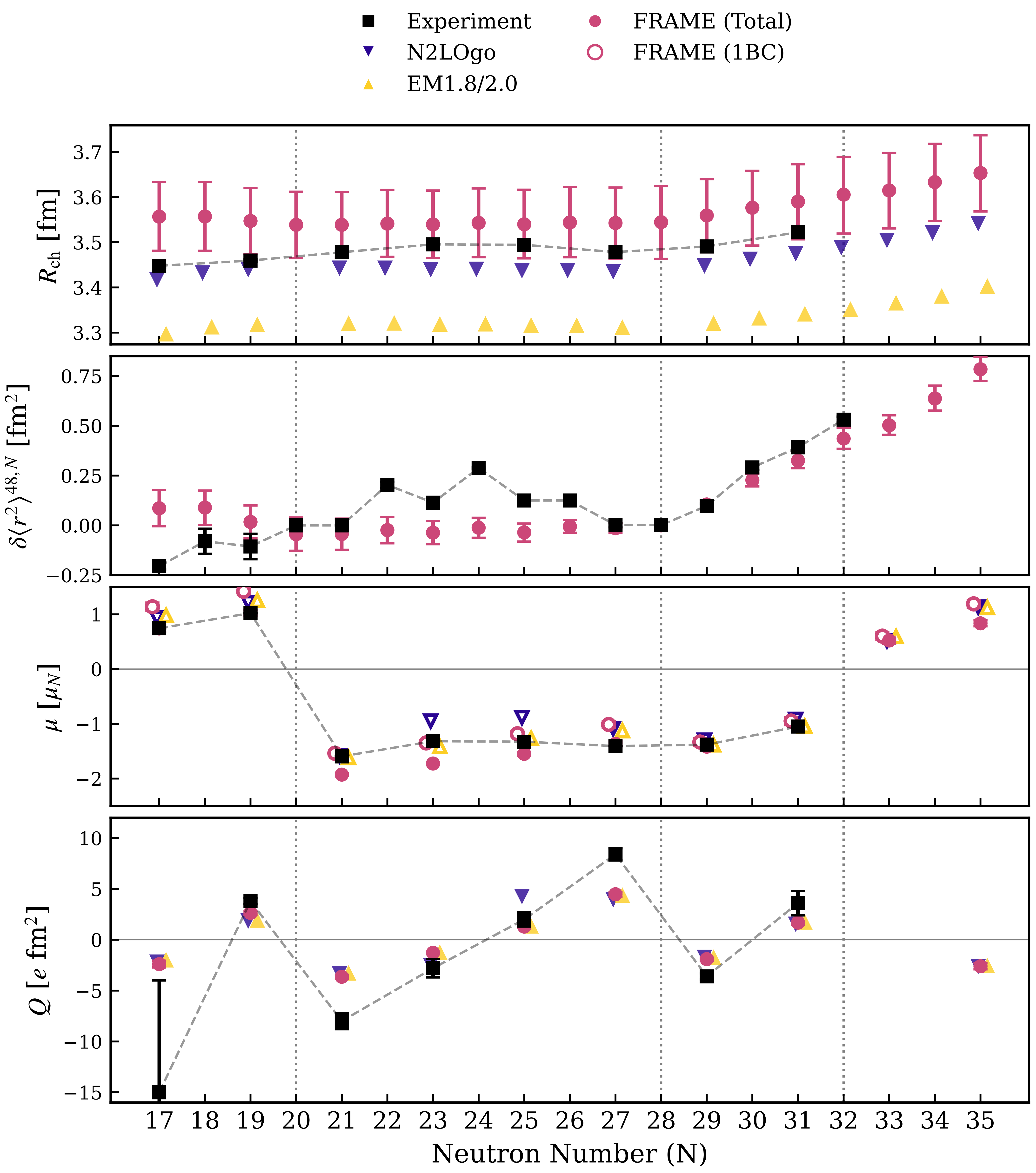
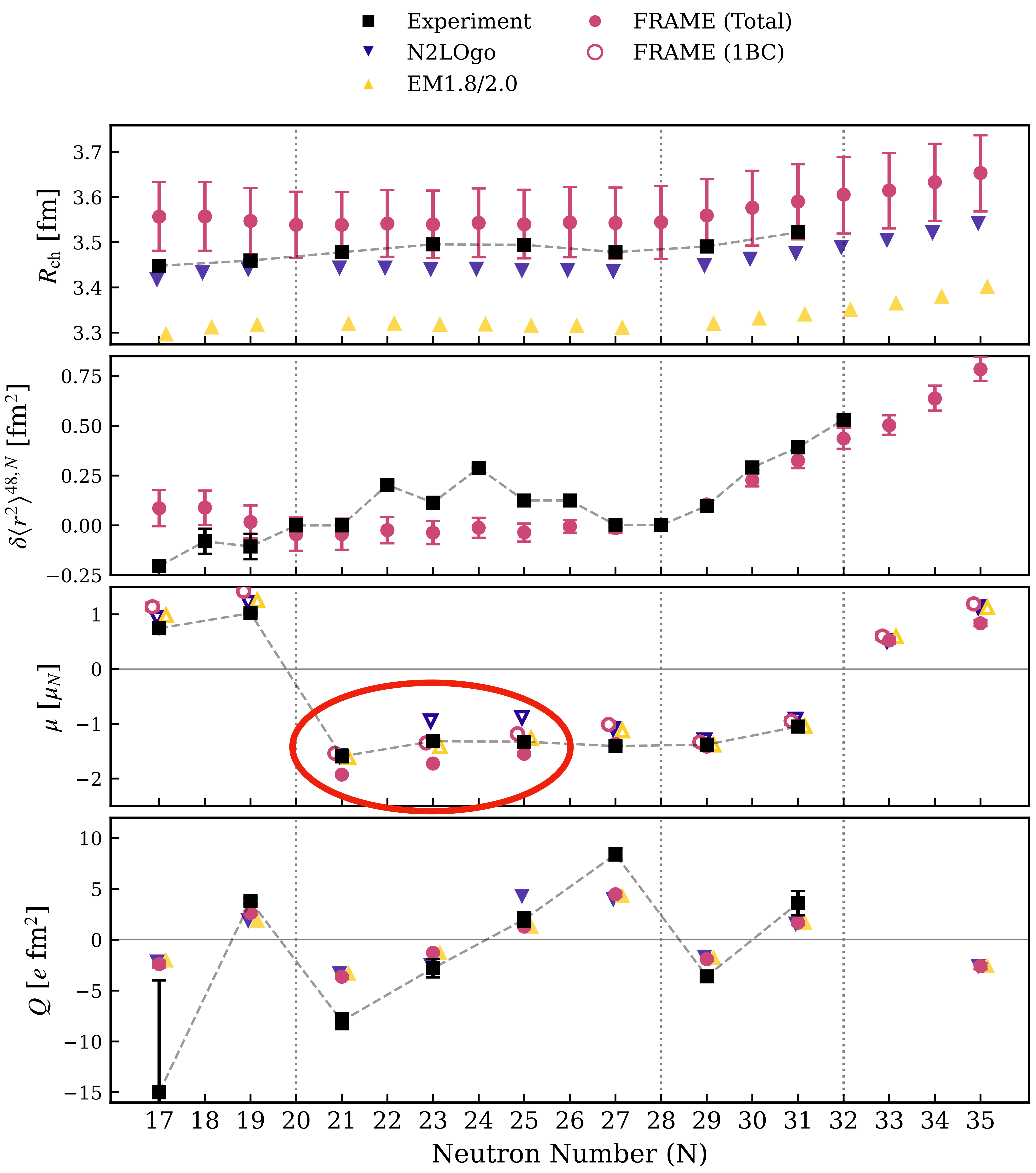


Case study: EM Moments of Ca isotopes

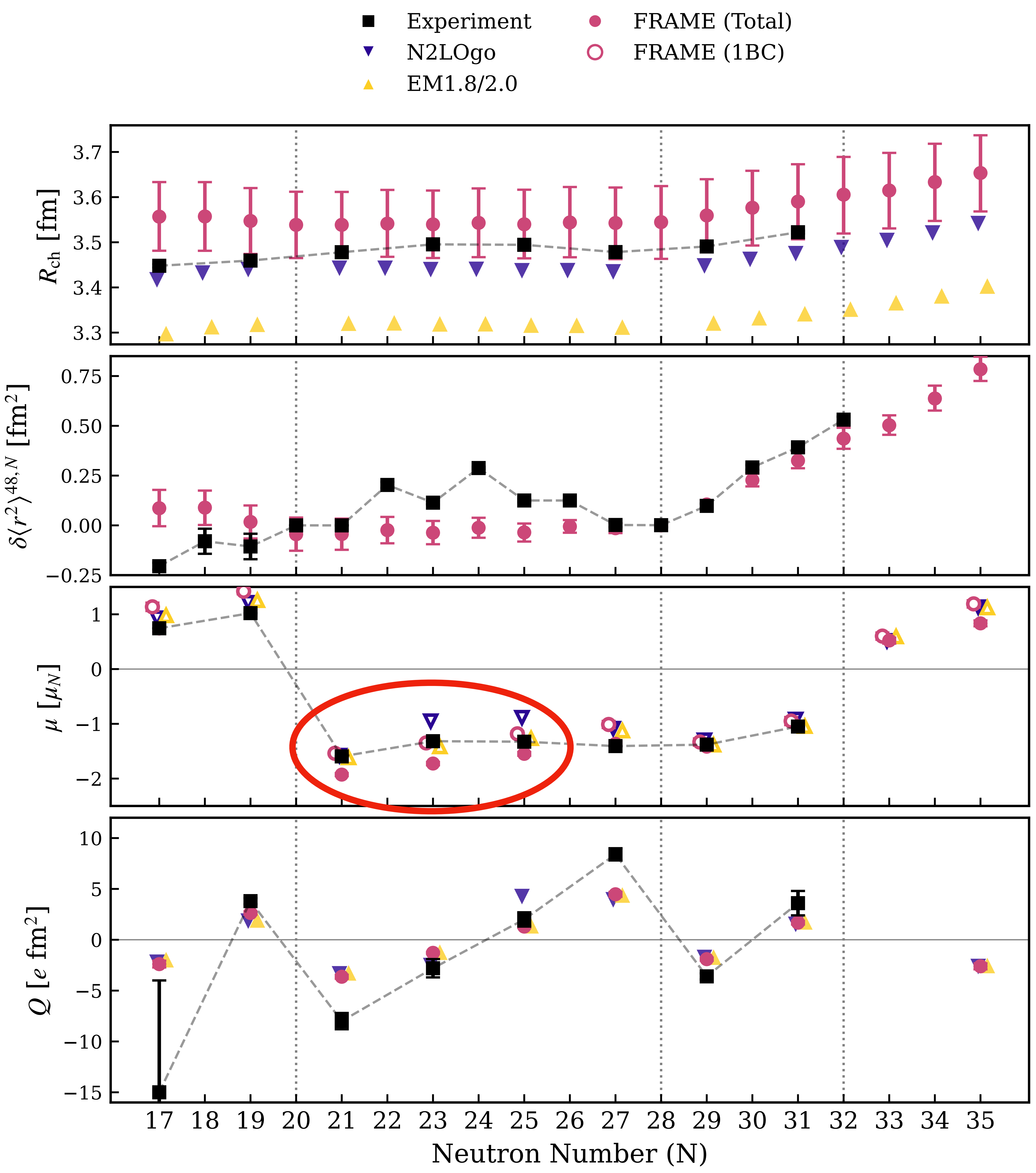
EM Moments of Ca Isotopes



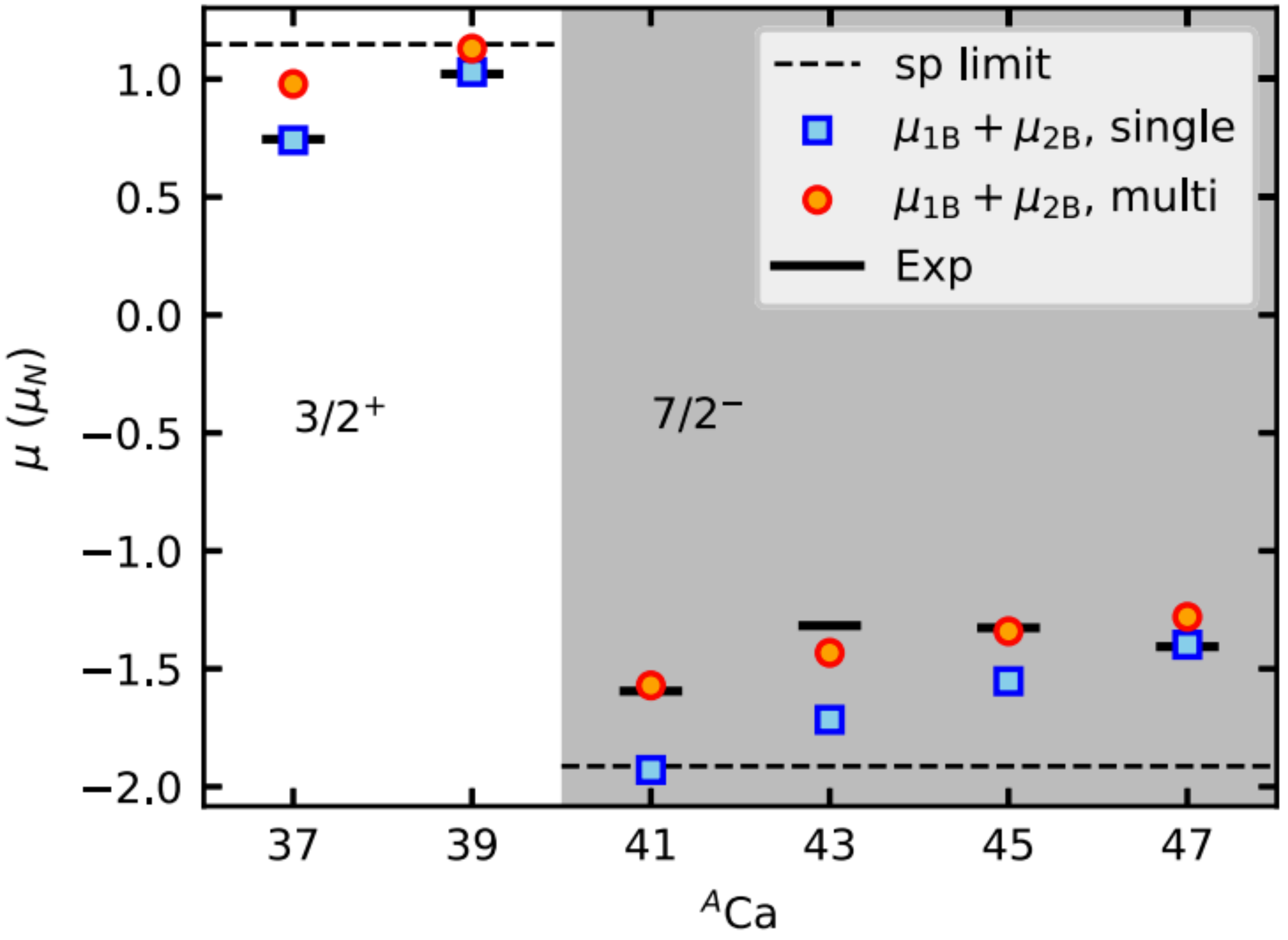
EM Moments of Ca Isotopes



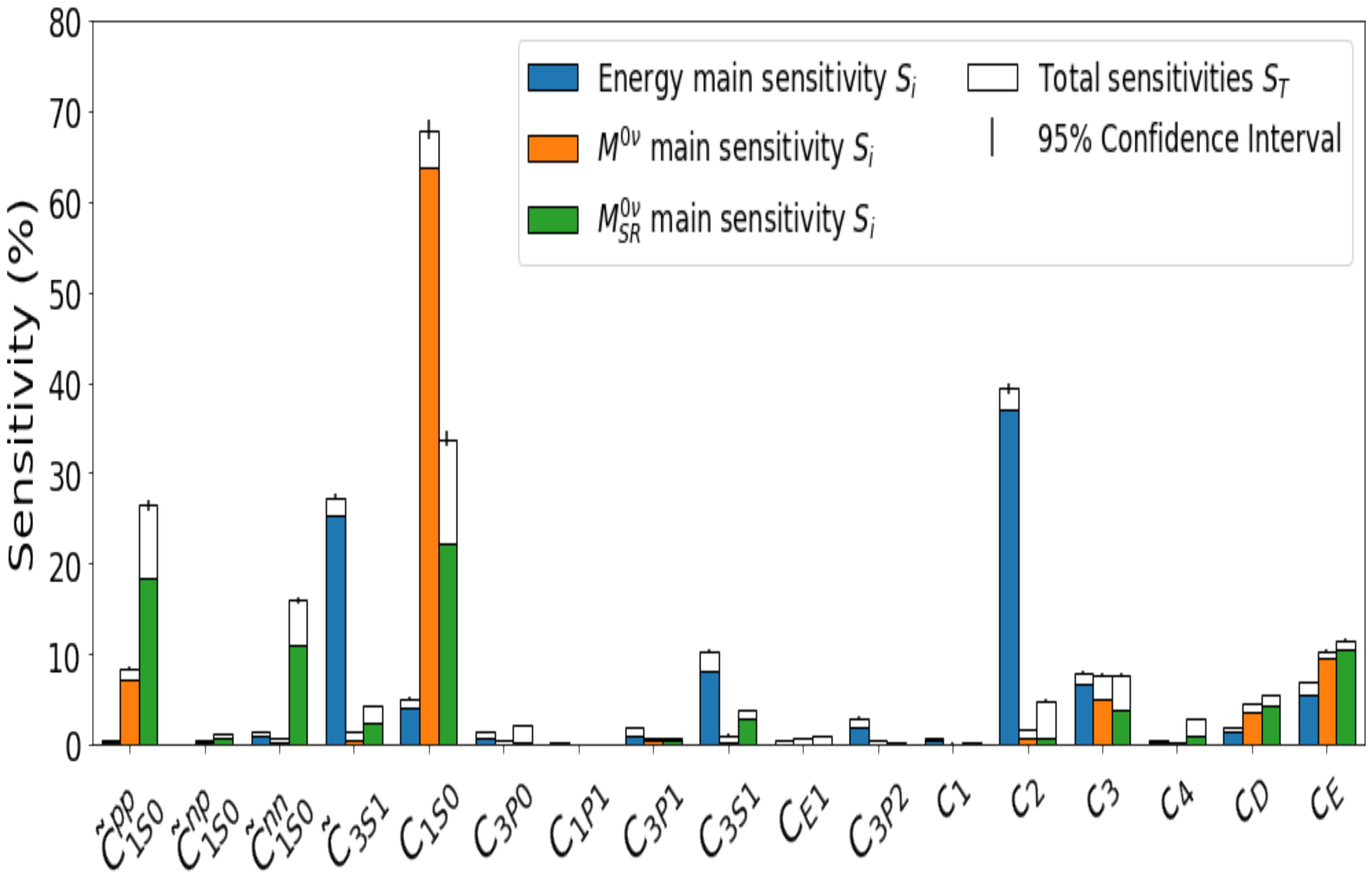
EM Moments of Ca Isotopes



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

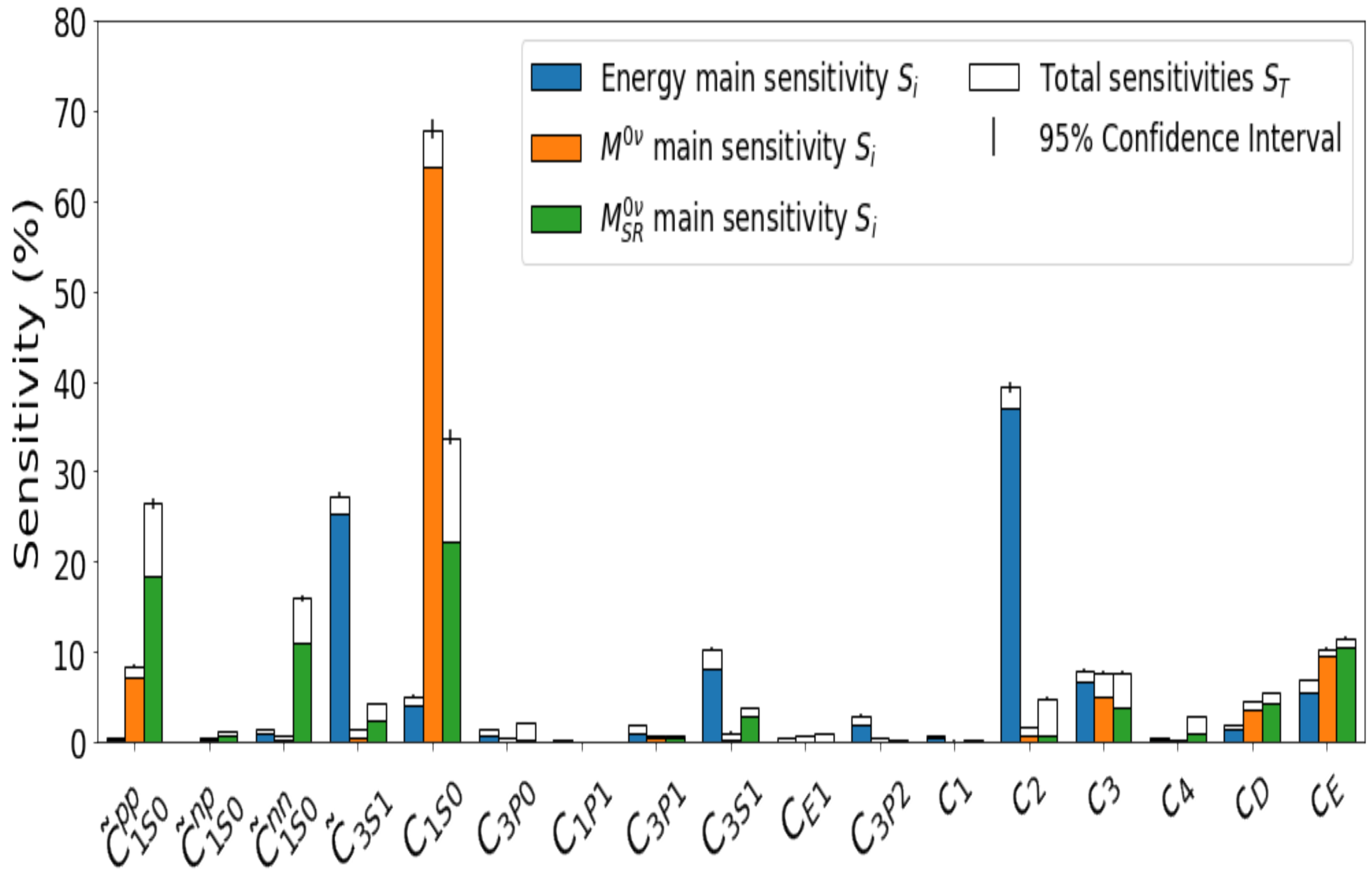


Issues with GSA



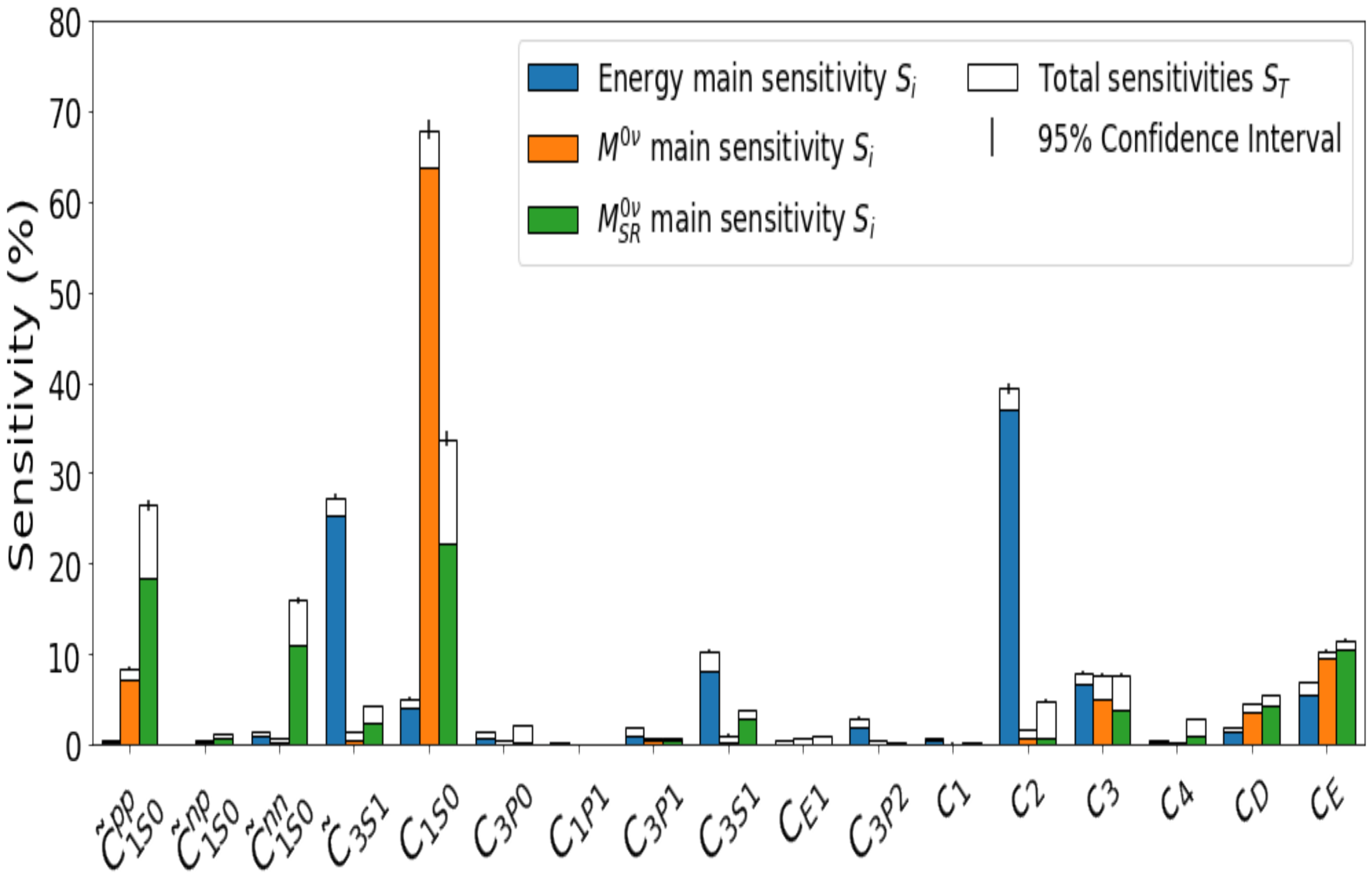
Issues with GSA

- Very costly



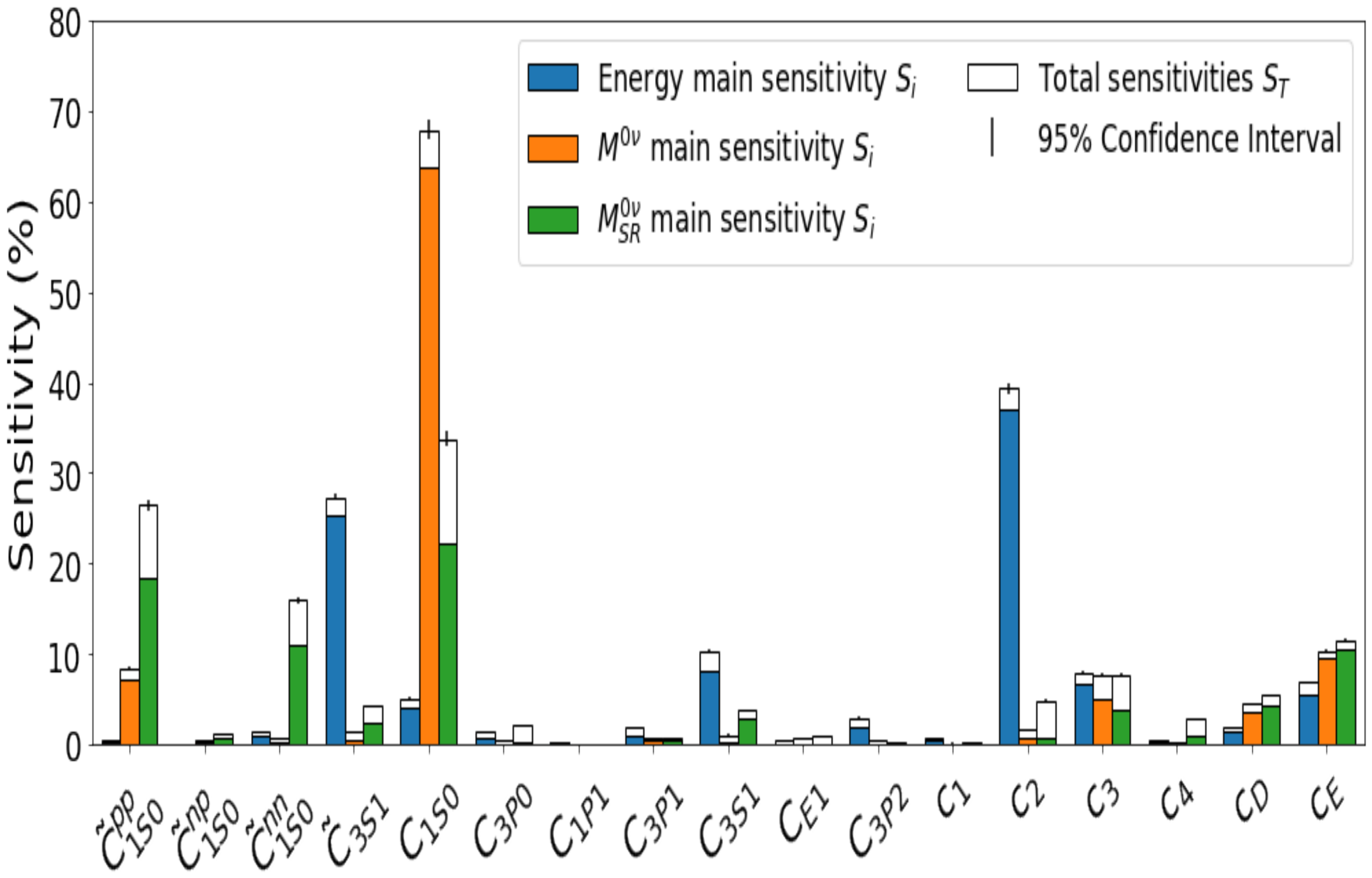
Issues with GSA

- Very costly
- No indication of how the parameters influence the results



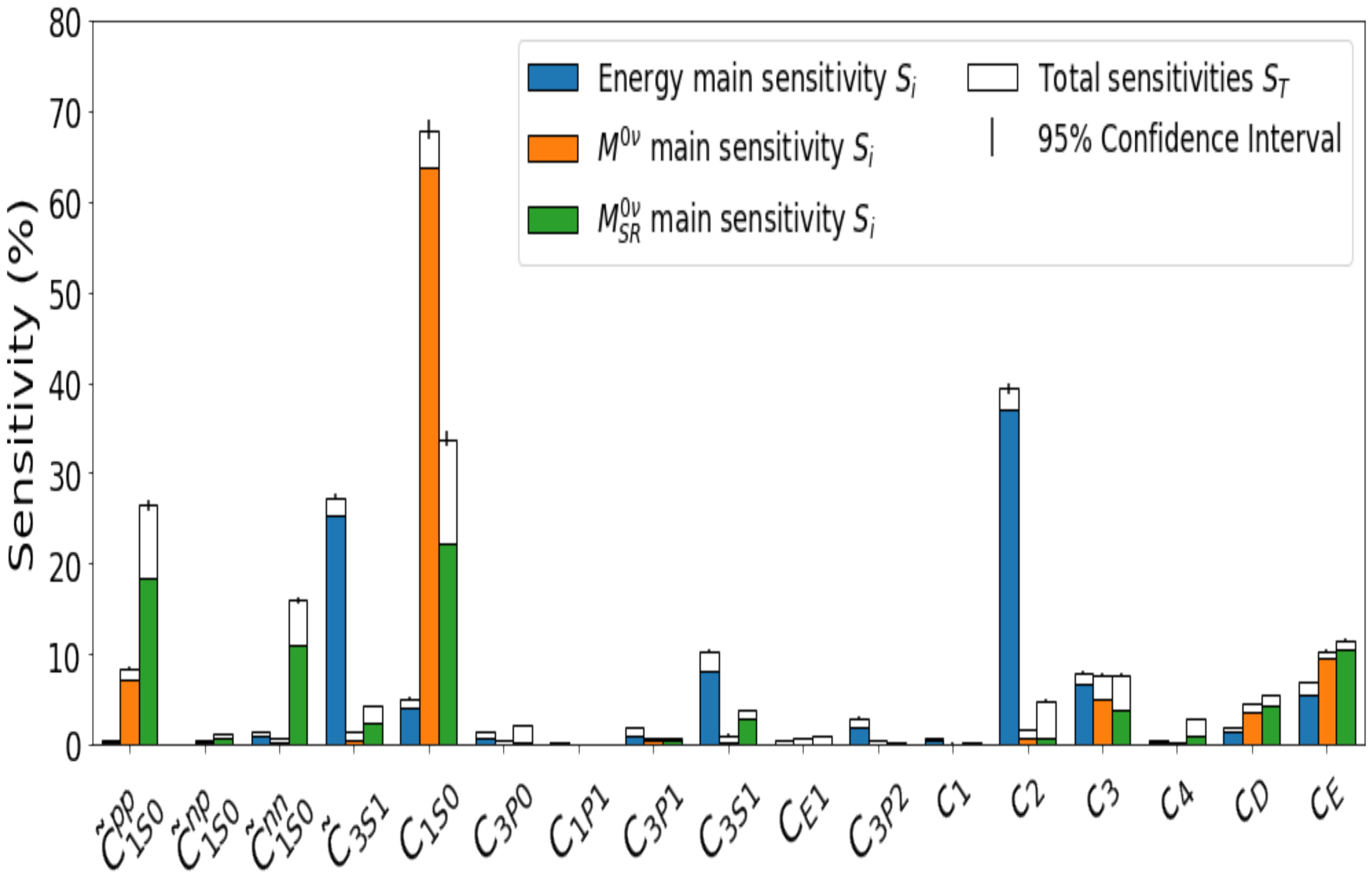
Issues with GSA

- Very costly
- No indication of how the parameters influence the results
- Initial range of the prior influence the final sensitivity



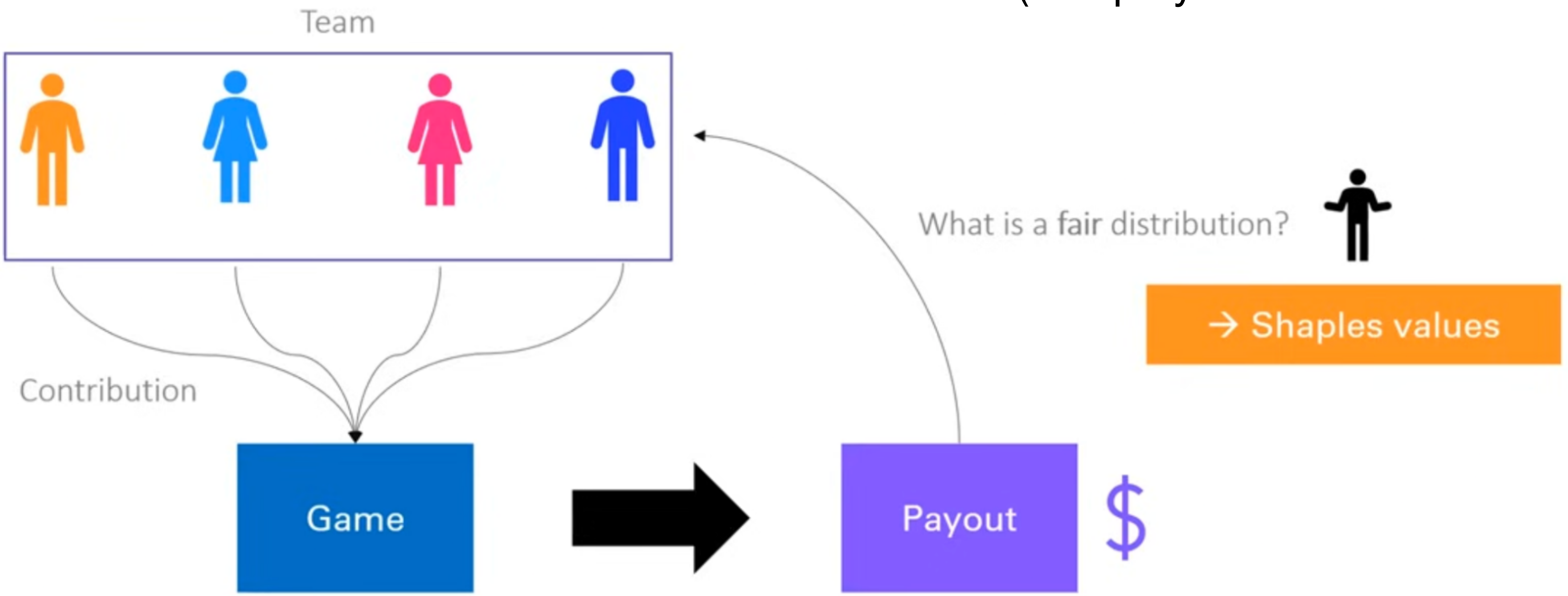
Issues with GSA

- Very costly
- No indication of how the parameters influence the results
- Initial range of the prior influence the final sensitivity
- “Bad” samples impact sensitivity as much as “good” samples



SHAP Values

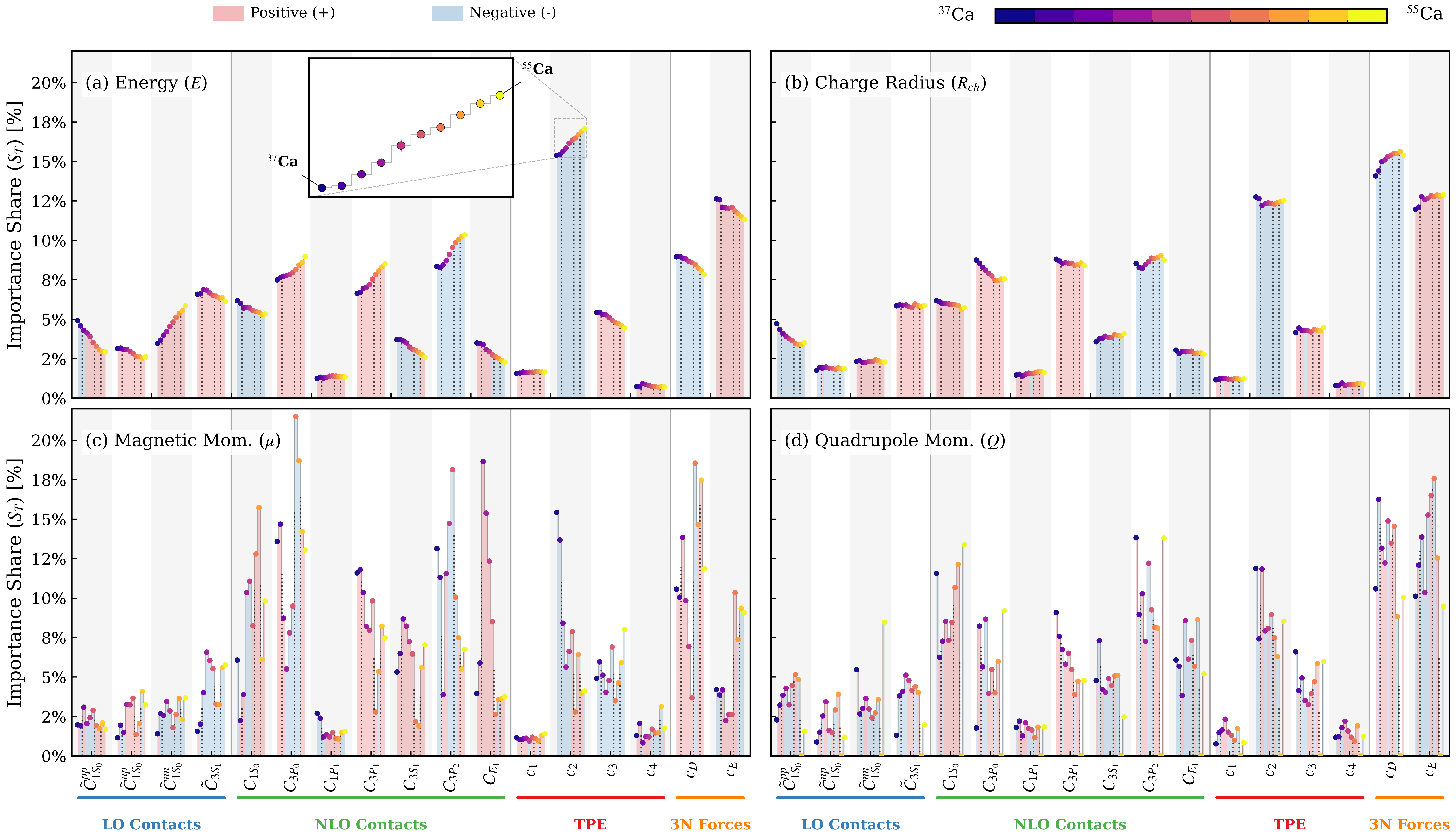
(SHapely Additive exPlanation)



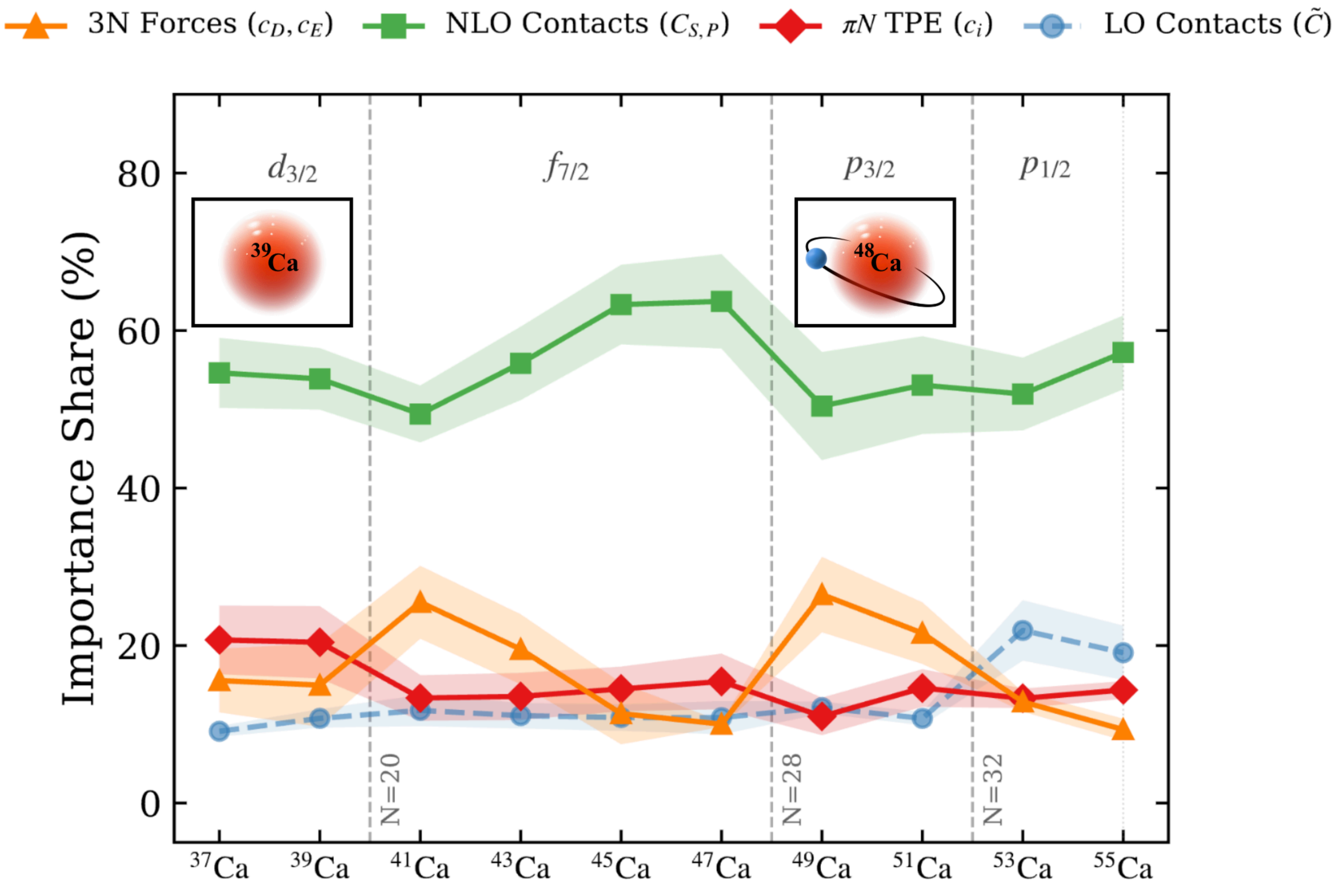
Sobol vs SHAP

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"

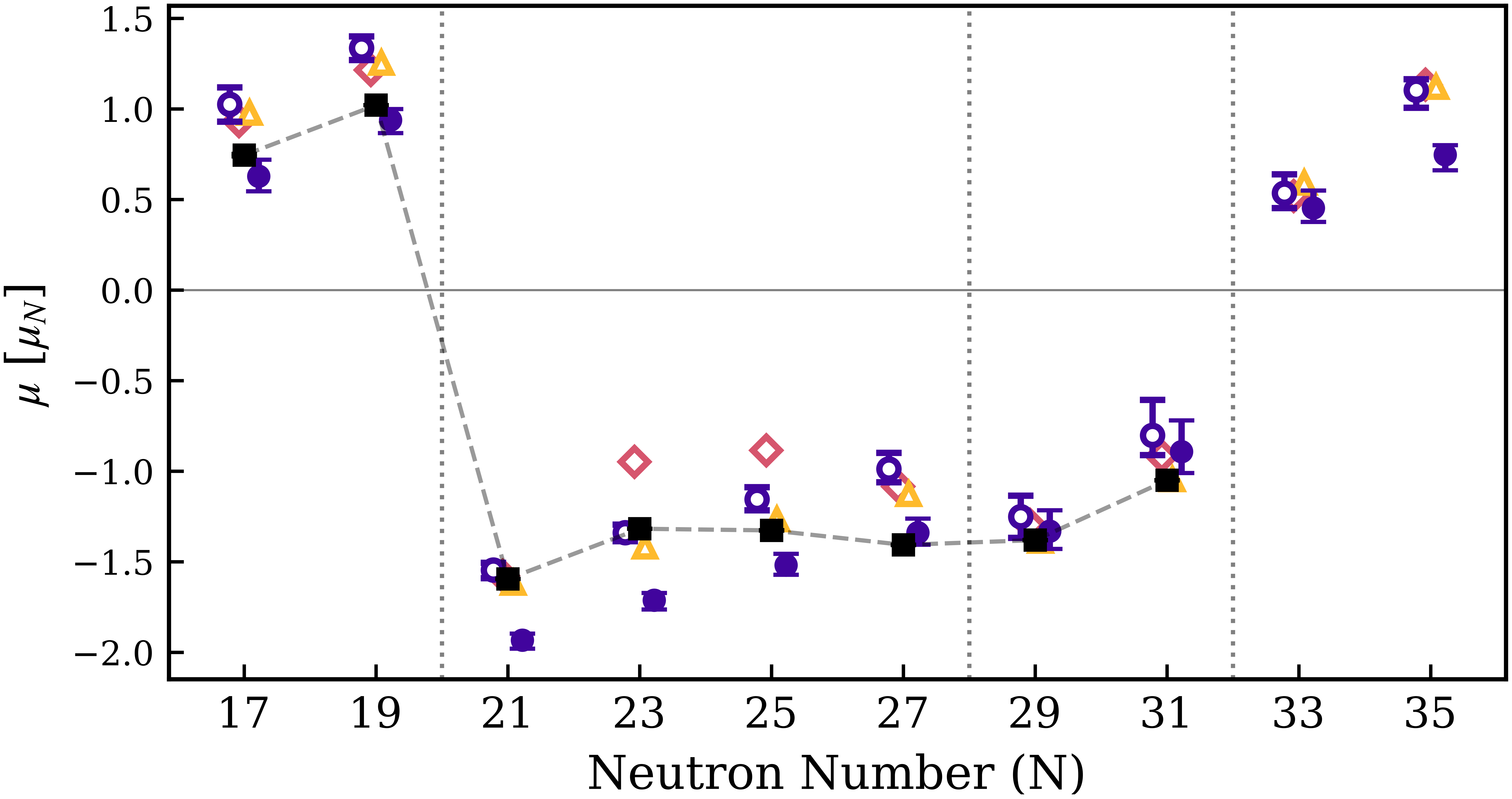
SHAP values in Ca Isotopes



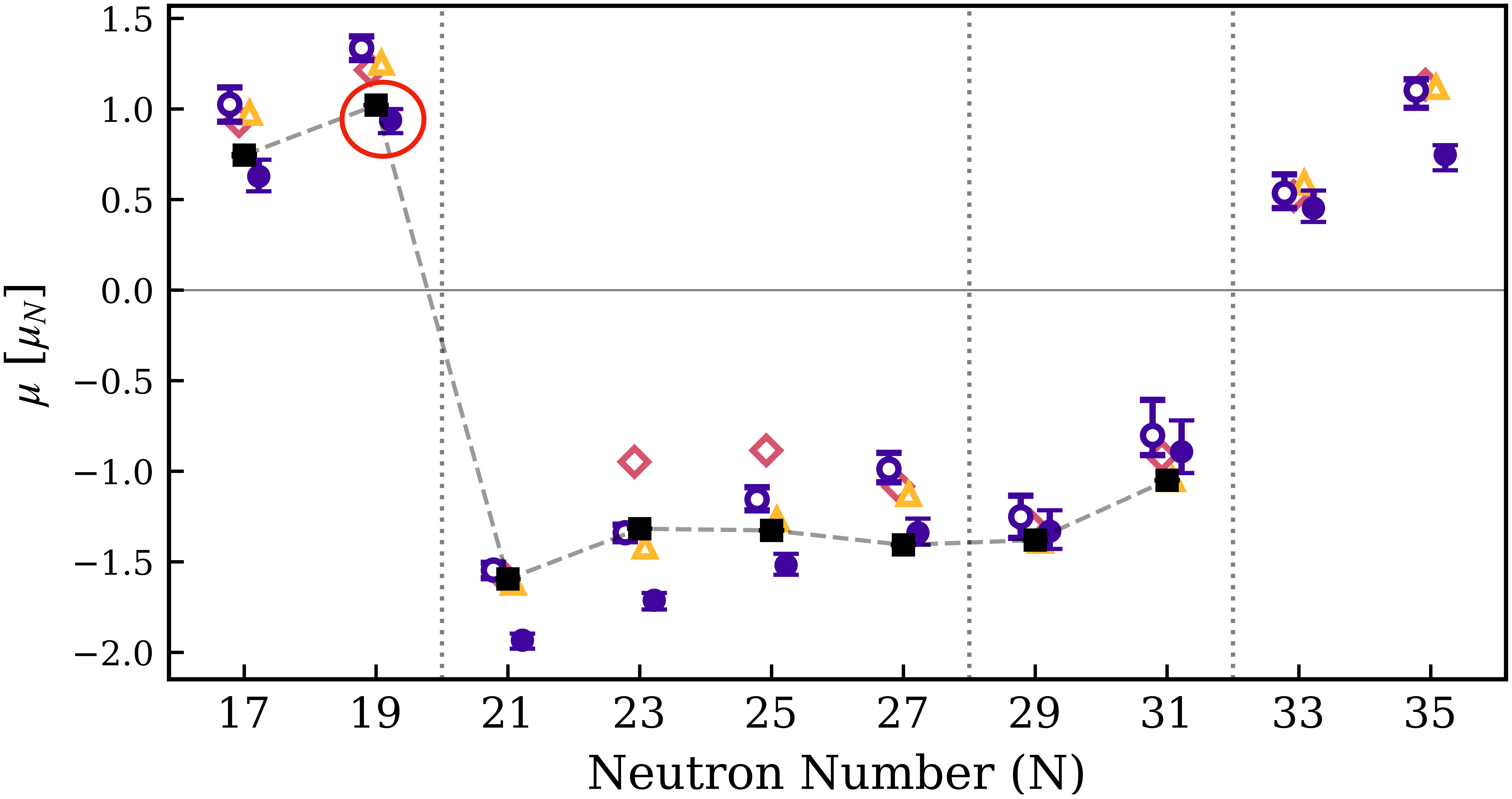
Forces Through the Shells



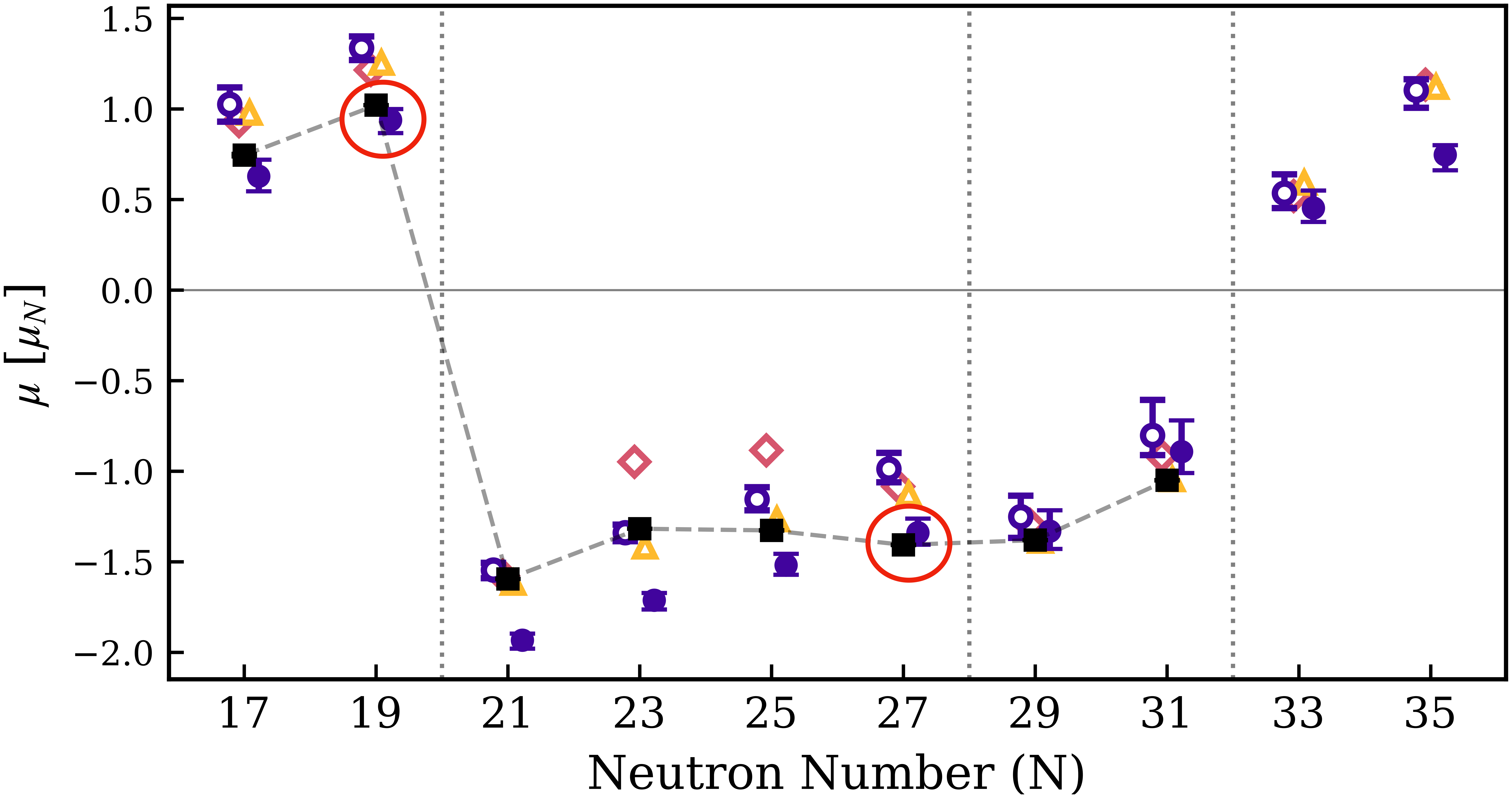
Using Emulators to Constrain Forces



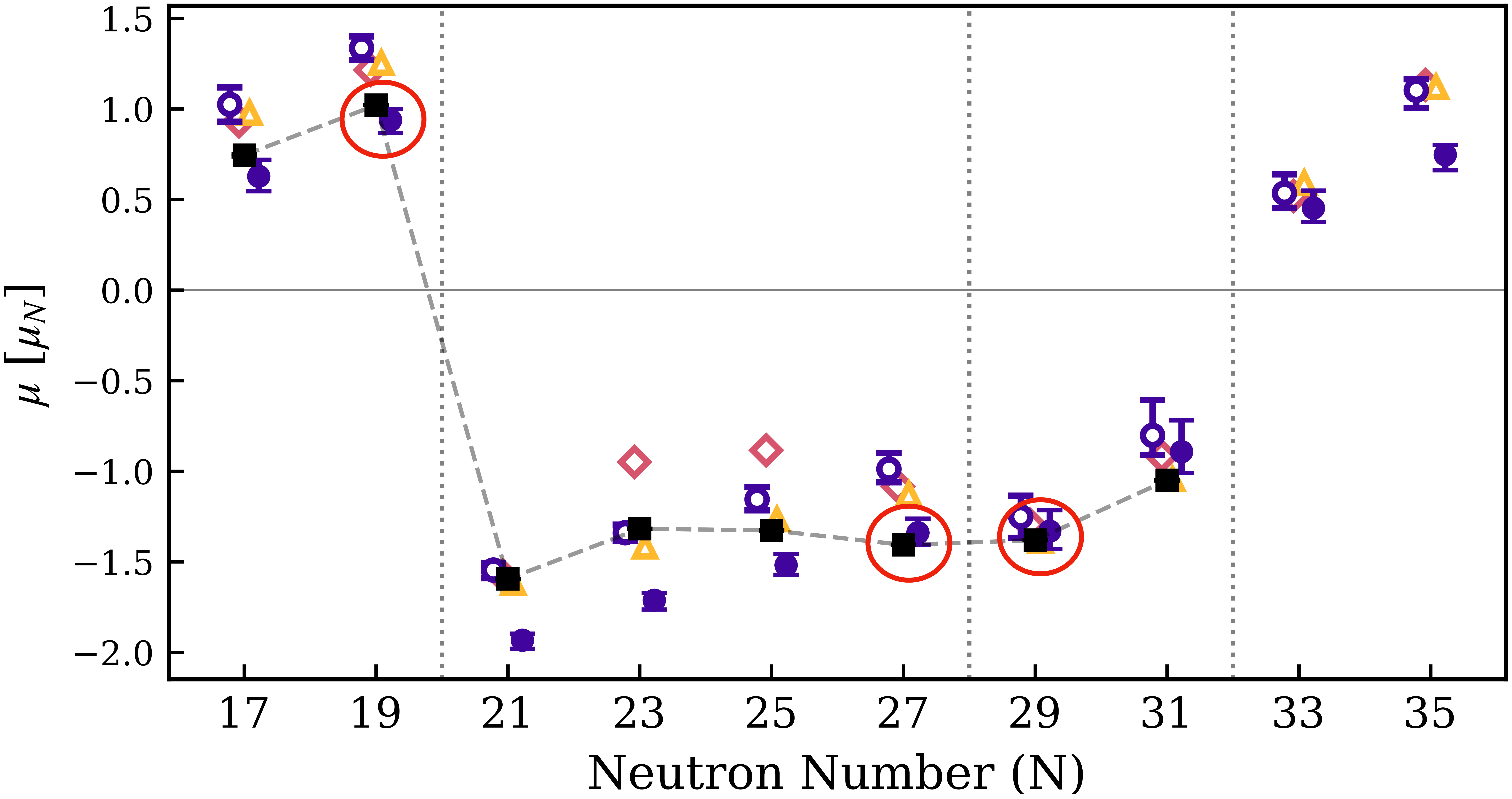
Using Emulators to Constrain Forces



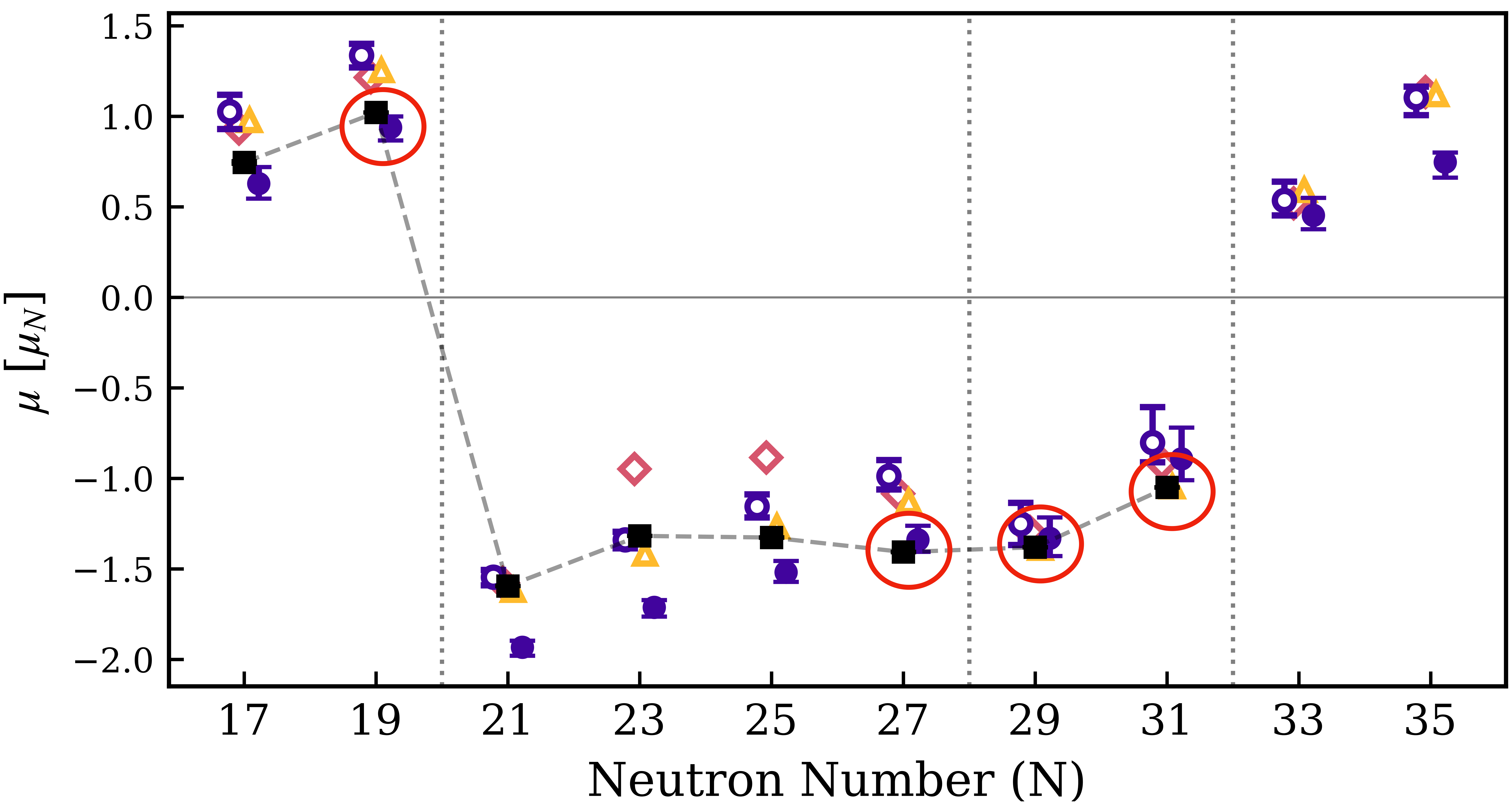
Using Emulators to Constrain Forces



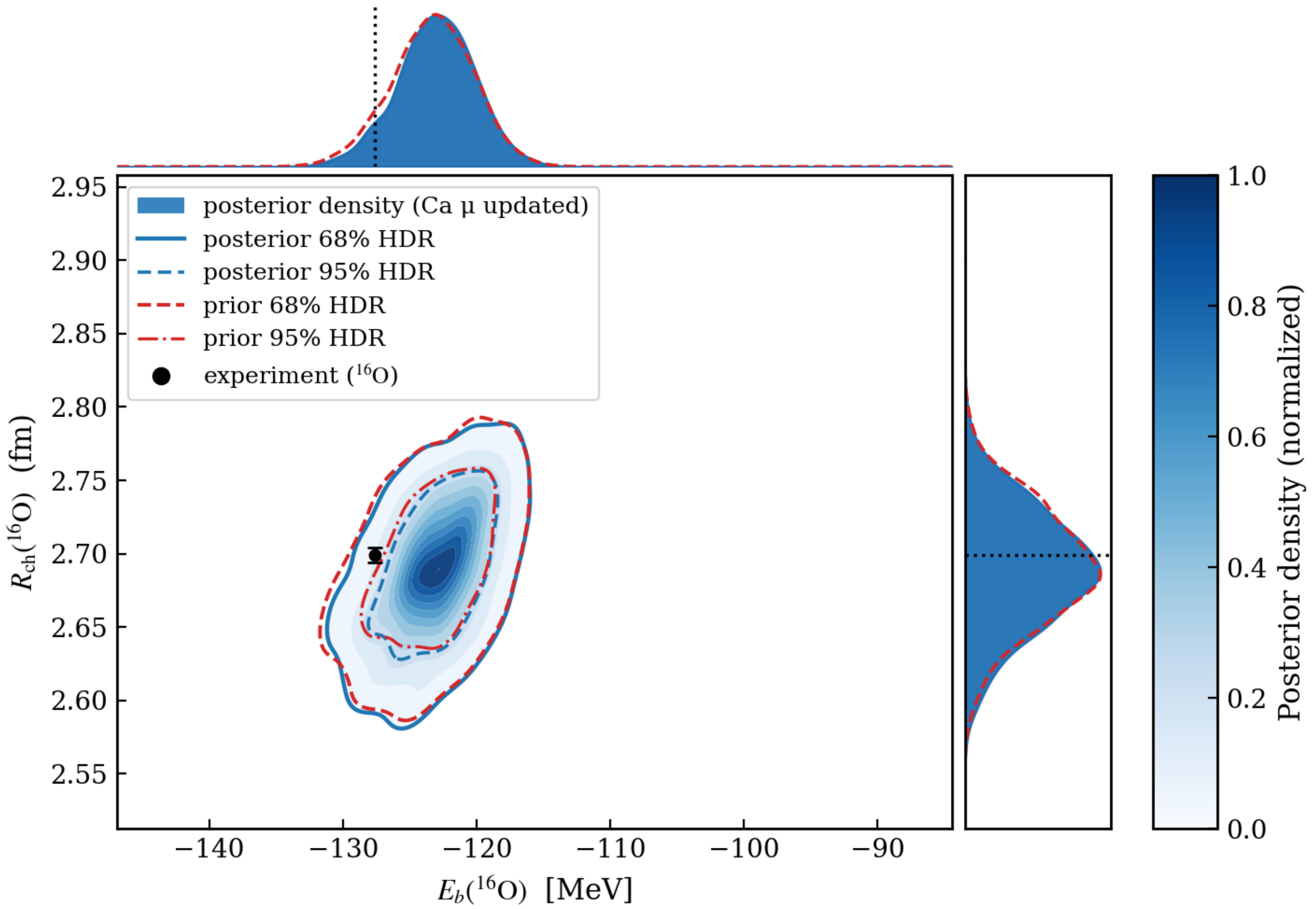
Using Emulators to Constrain Forces

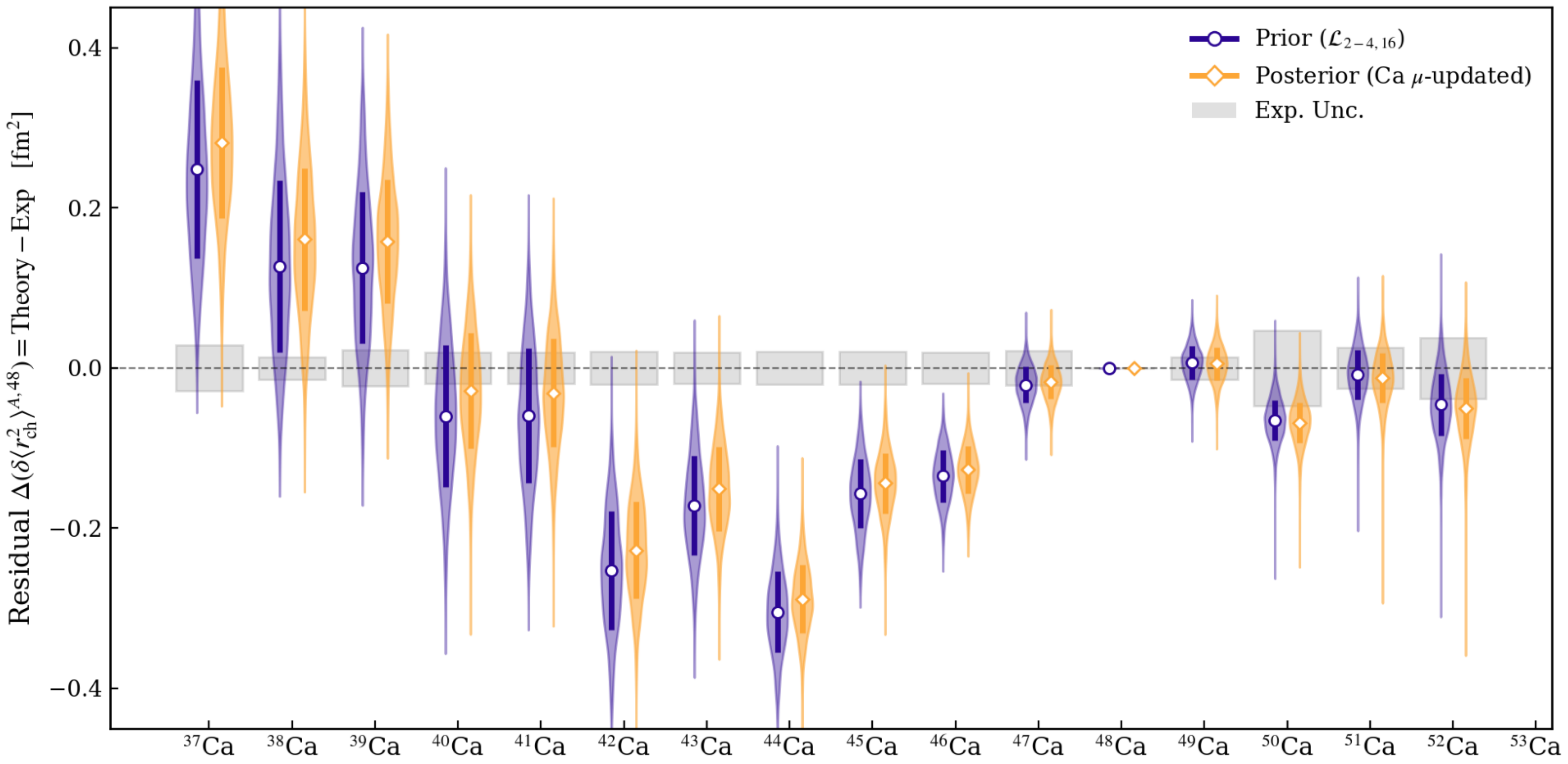


Using Emulators to Constrain Forces

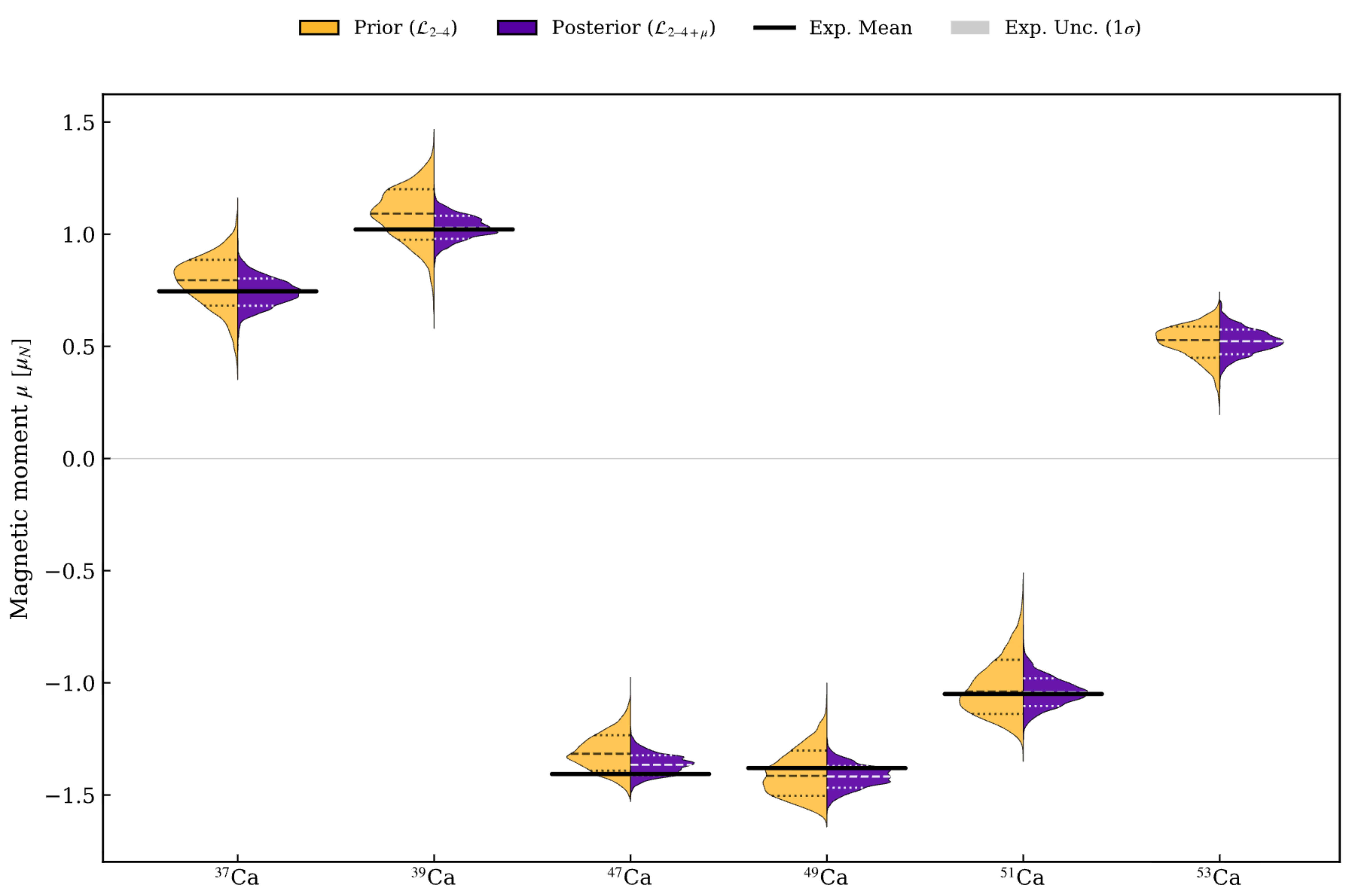


Changes to Likelihood





Reducing Uncertainties



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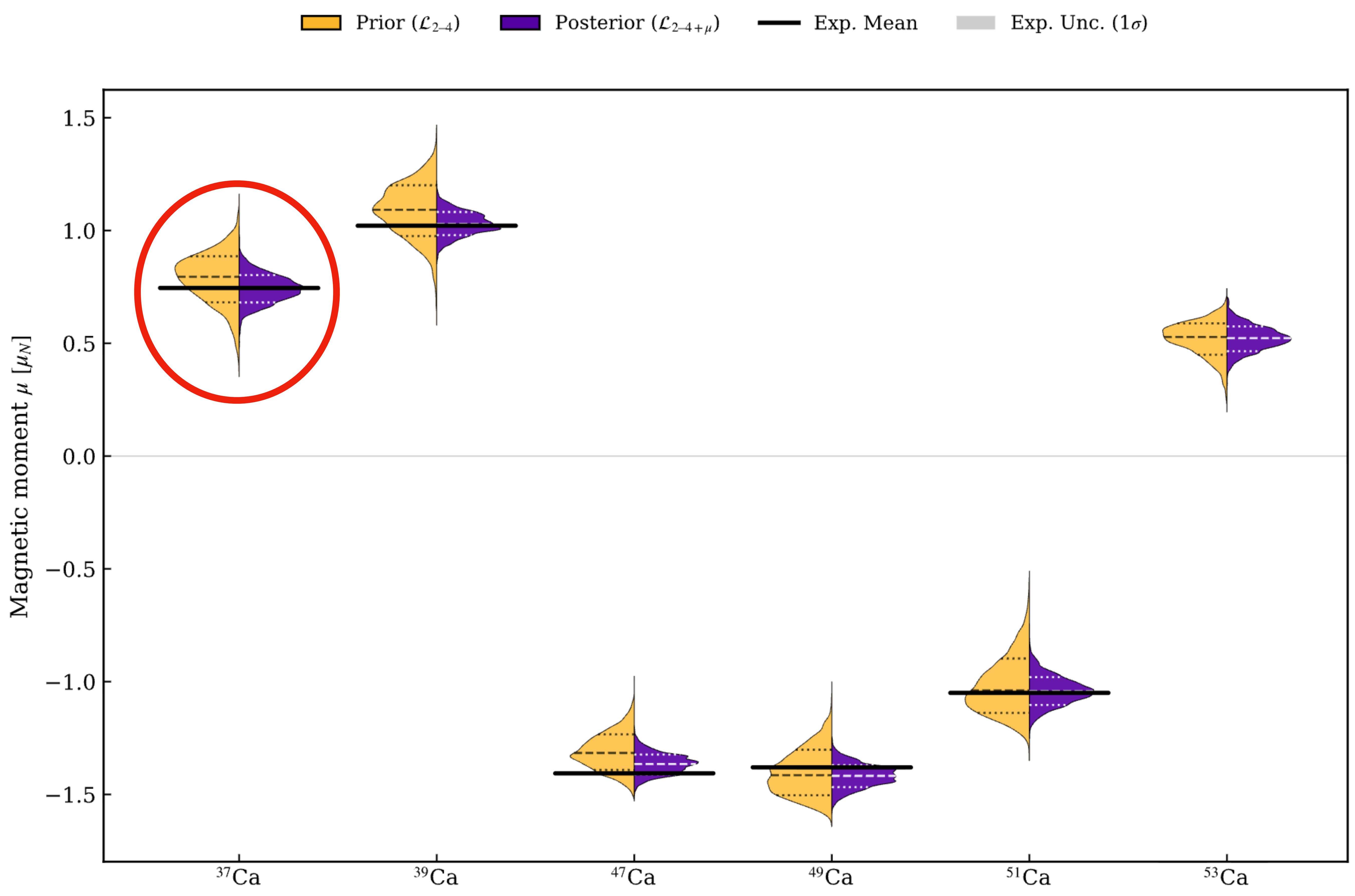

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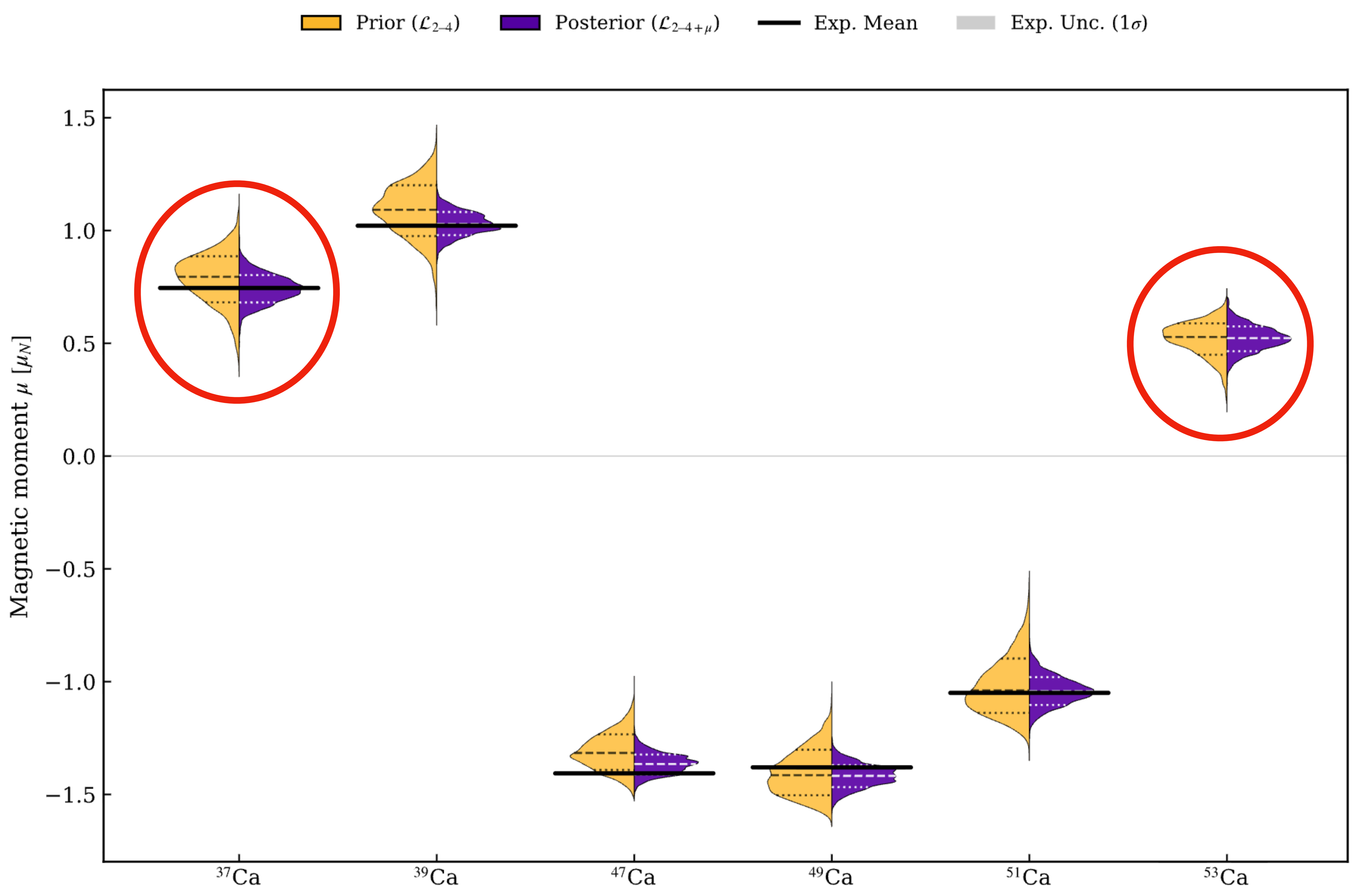

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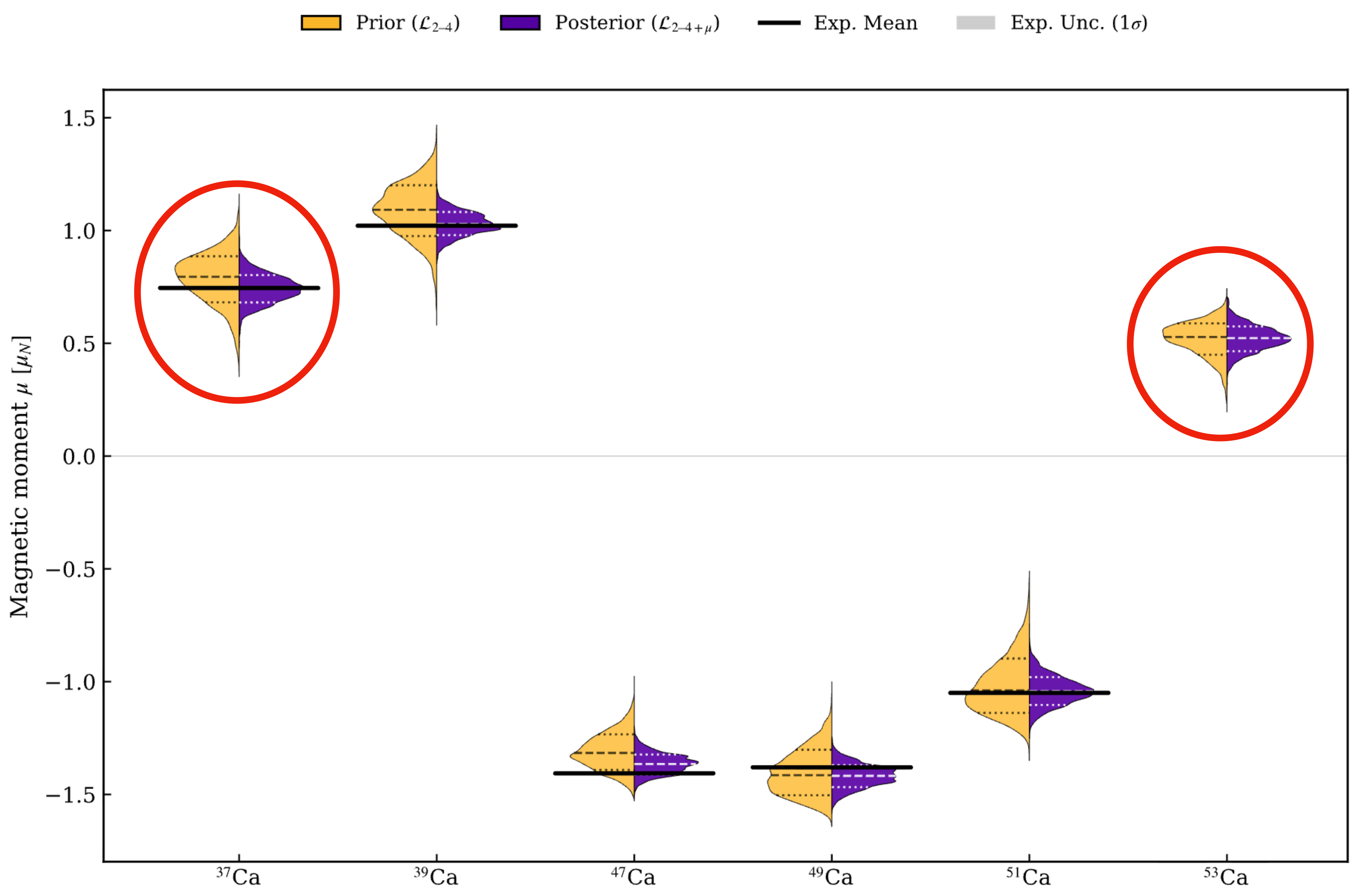

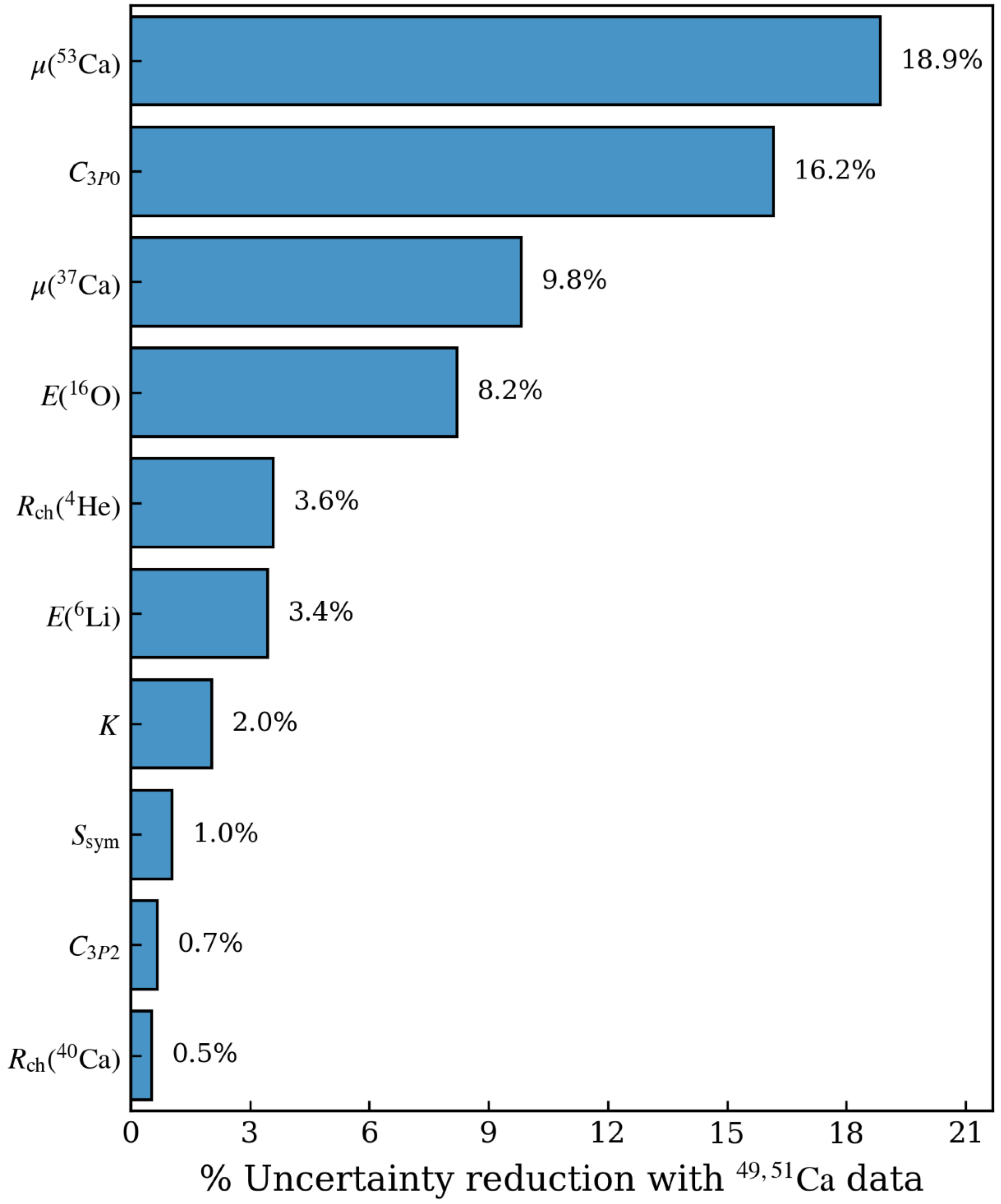

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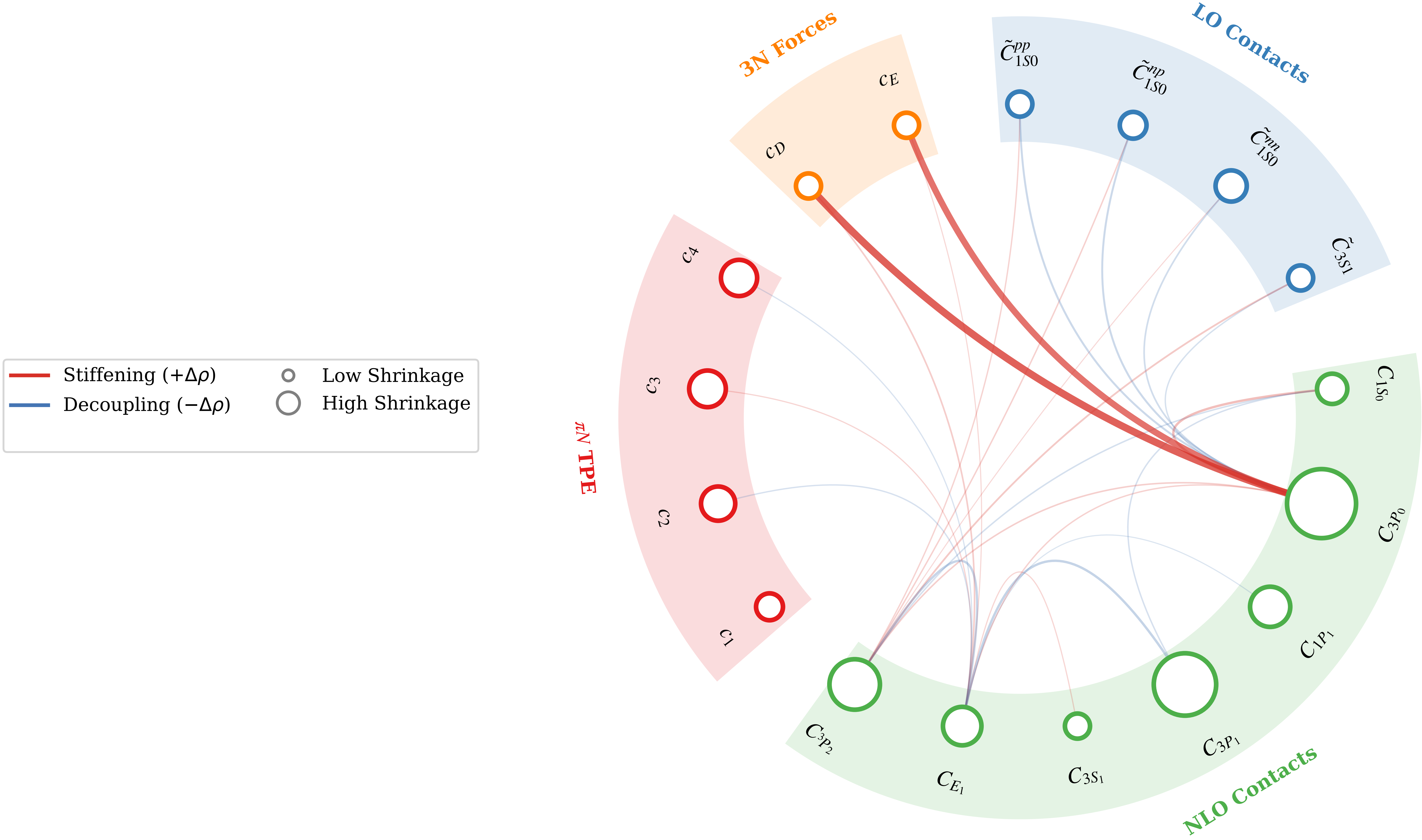

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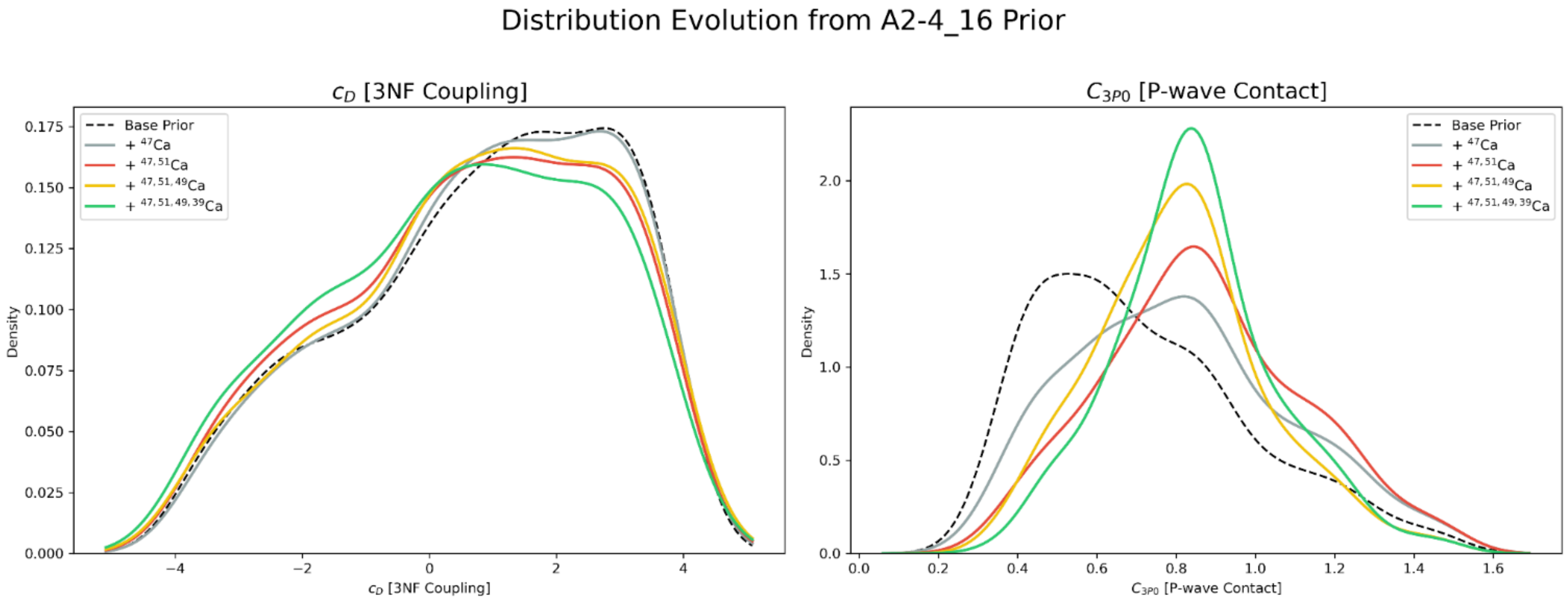
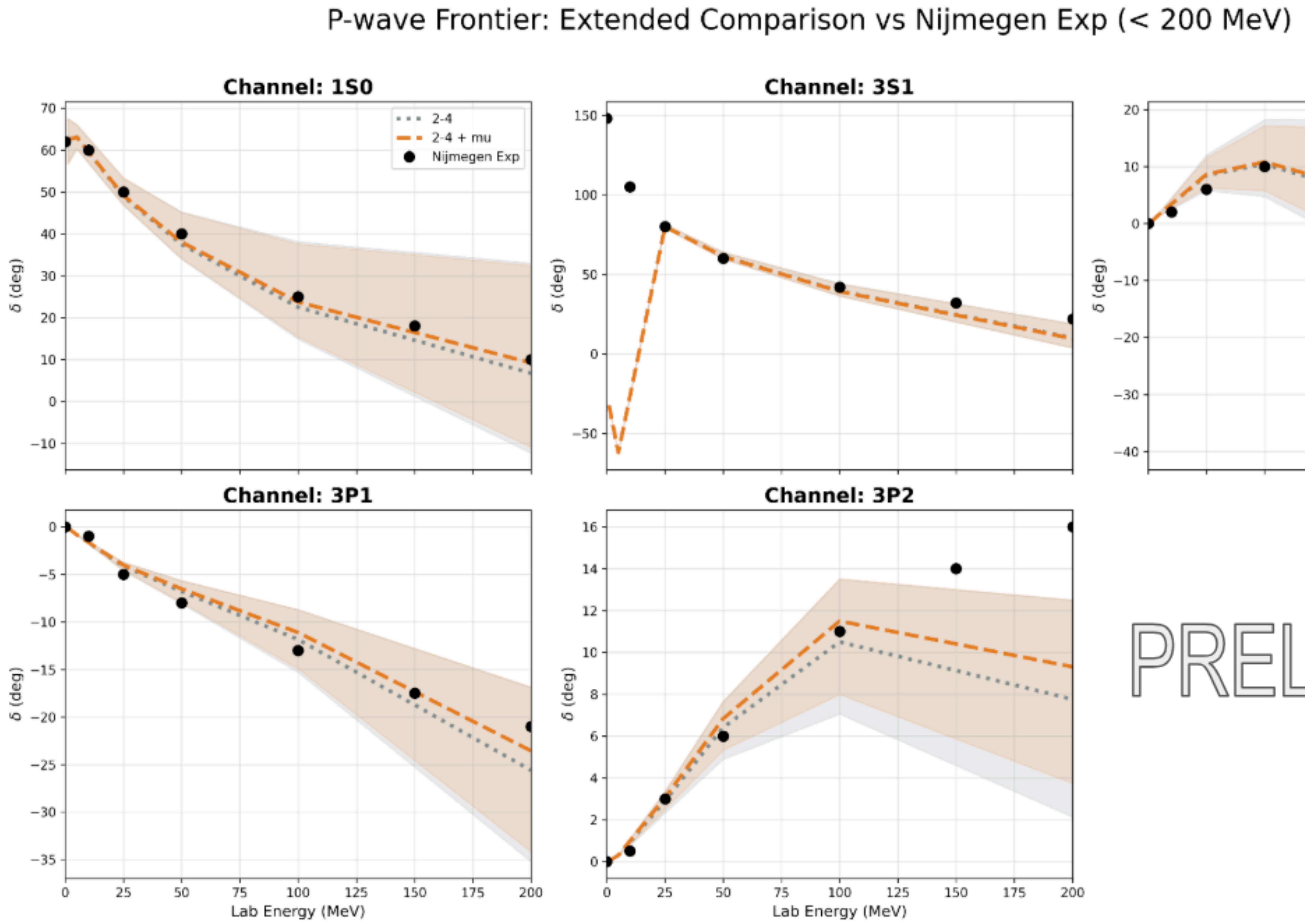


Improvements of phase-shifts



PRELIMINARY

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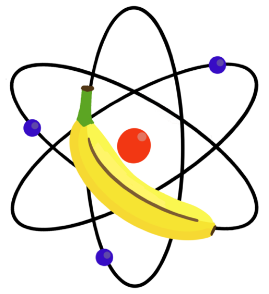
- Created new ML emulator: speed up calculations by a factor of ~10^5. 

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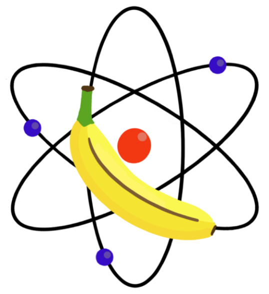
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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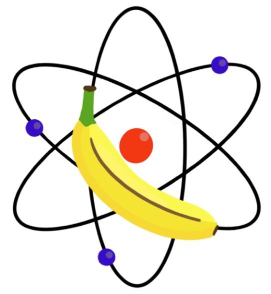
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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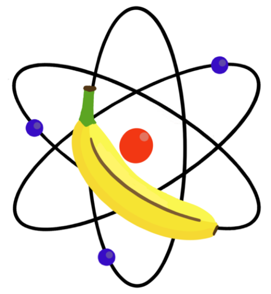
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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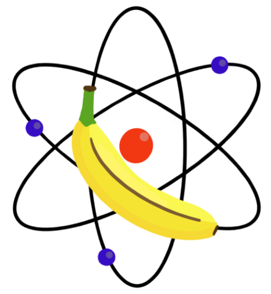
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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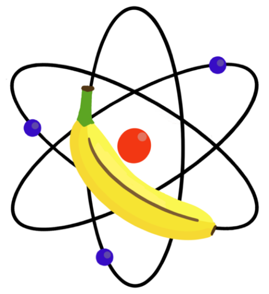
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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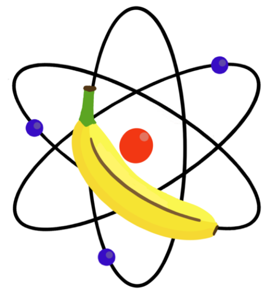
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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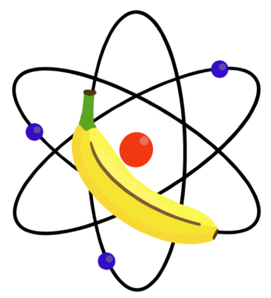
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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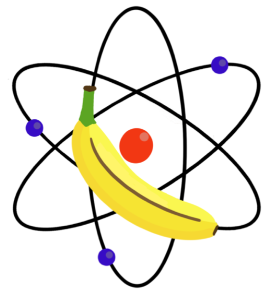
- Created new ML emulator: speed up calculations by a factor of $\sim 10^5$. 
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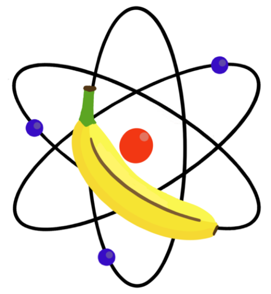
- Created new ML emulator: speed up calculations by a factor of ~10^5. 
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