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THE UNIVERSITY OF BRITISH COLUMBIA

Towards reliable nuclear matrix elements for neutrinoless double beta decay

Antoine Belley

New physics searches at the precision frontier,

INT 2023

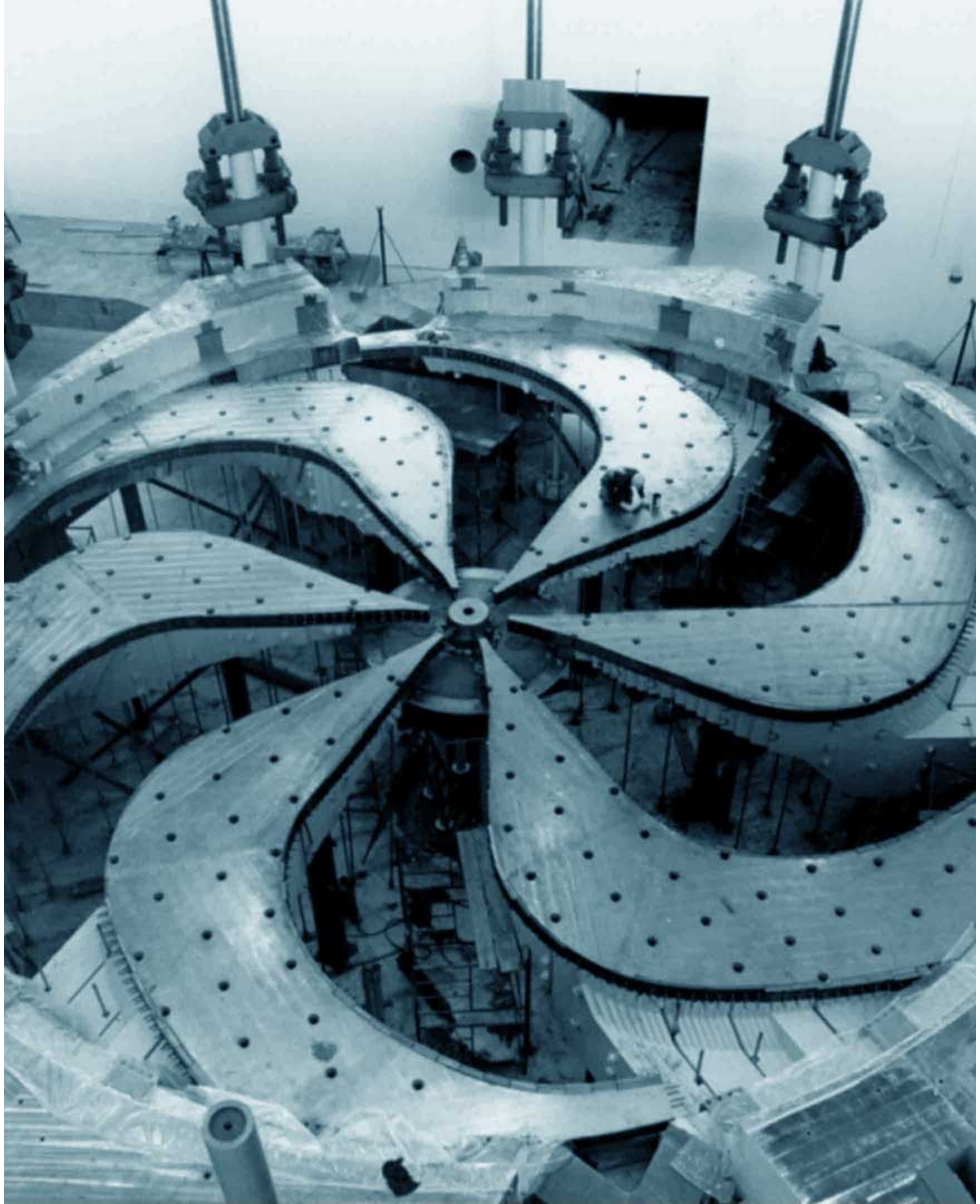
Collaborators: Jack Pitcher, Takayuki Miyagi, Ragnar Stroberg, Jason Holt

CINP ICPN

NSERC CRSNG

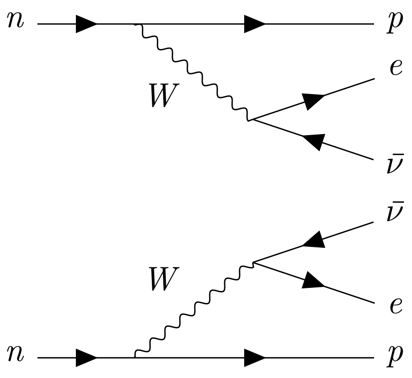
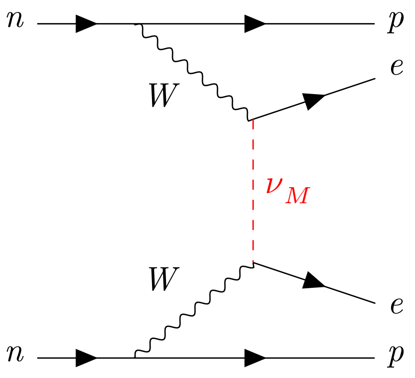
Arthur B. McDonald Canadian Astroparticle Physics Research Institute

NRC·CNRC



Discovery, accelerated

2νββ vs 0νββ

Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2 M^{0\nu}_F + M^{0\nu}_T - 2g_{\nu\nu}M^{0\nu}_{CT}$
LNV	No	Yes!
Observed	Yes	No

*NME : Nuclear matrix elements

**LNV : Lepton number violation

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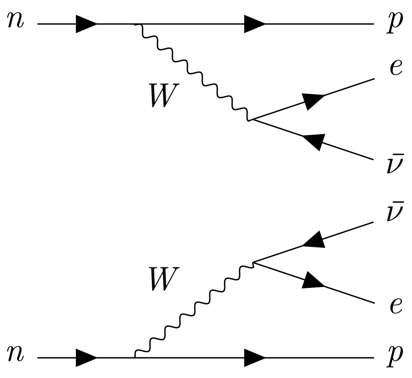
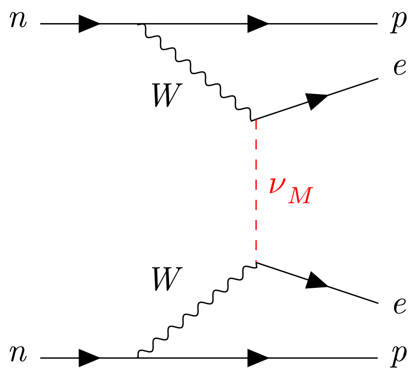
Diagram		
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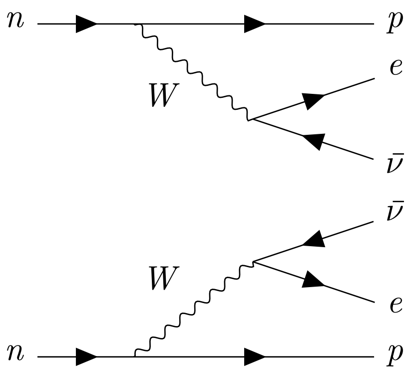
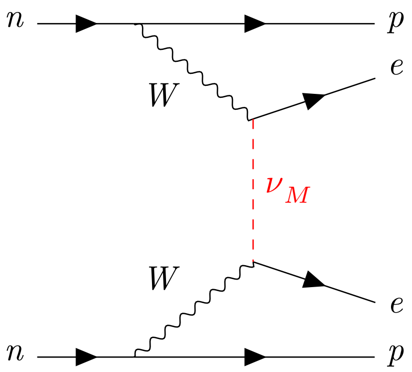
Diagram		
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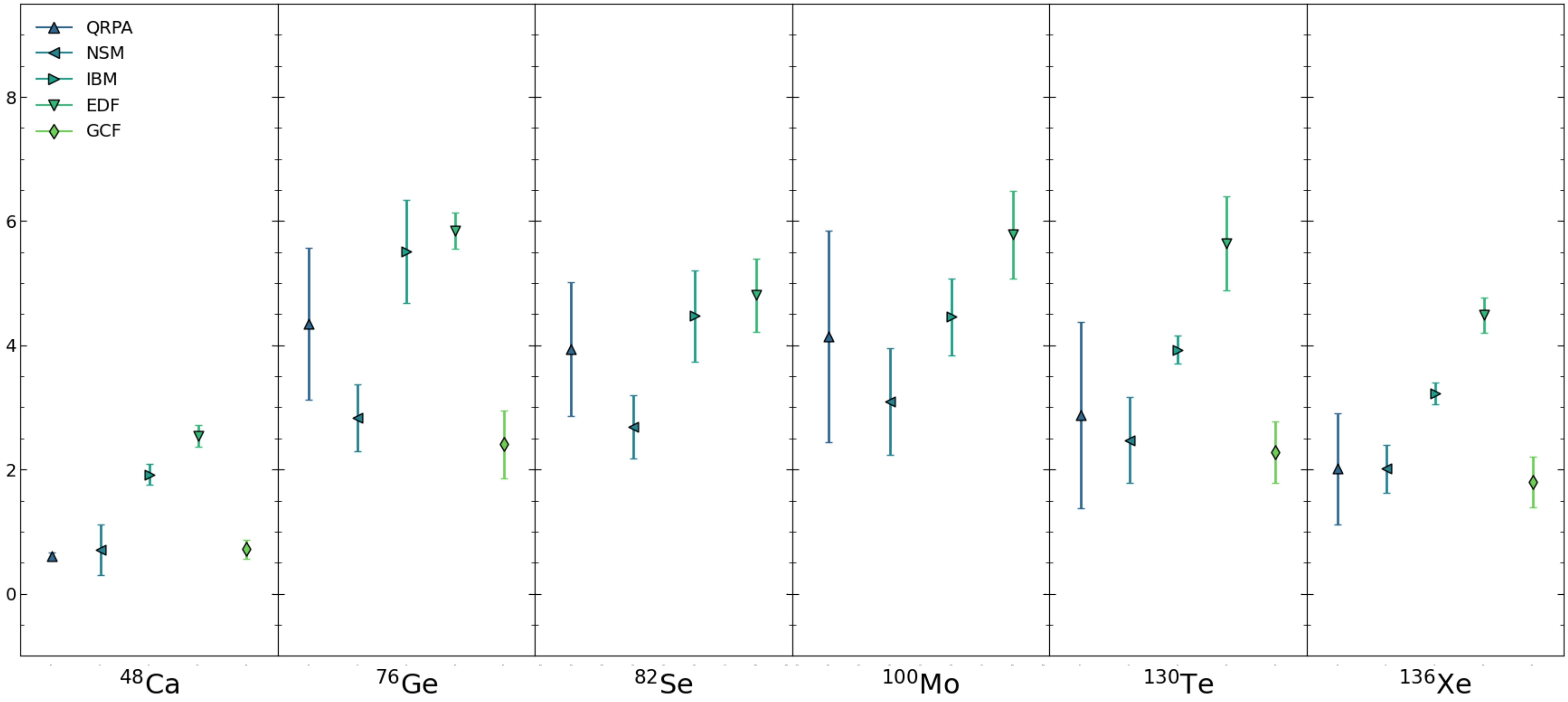
Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



Compiled values from Engel and Menéndez, Rep. Prog. Phys. 80 046301 (2017); Yao, arXiv:2008.13249 (2020); Brase et al, arXiv:2108.11805 (2021)

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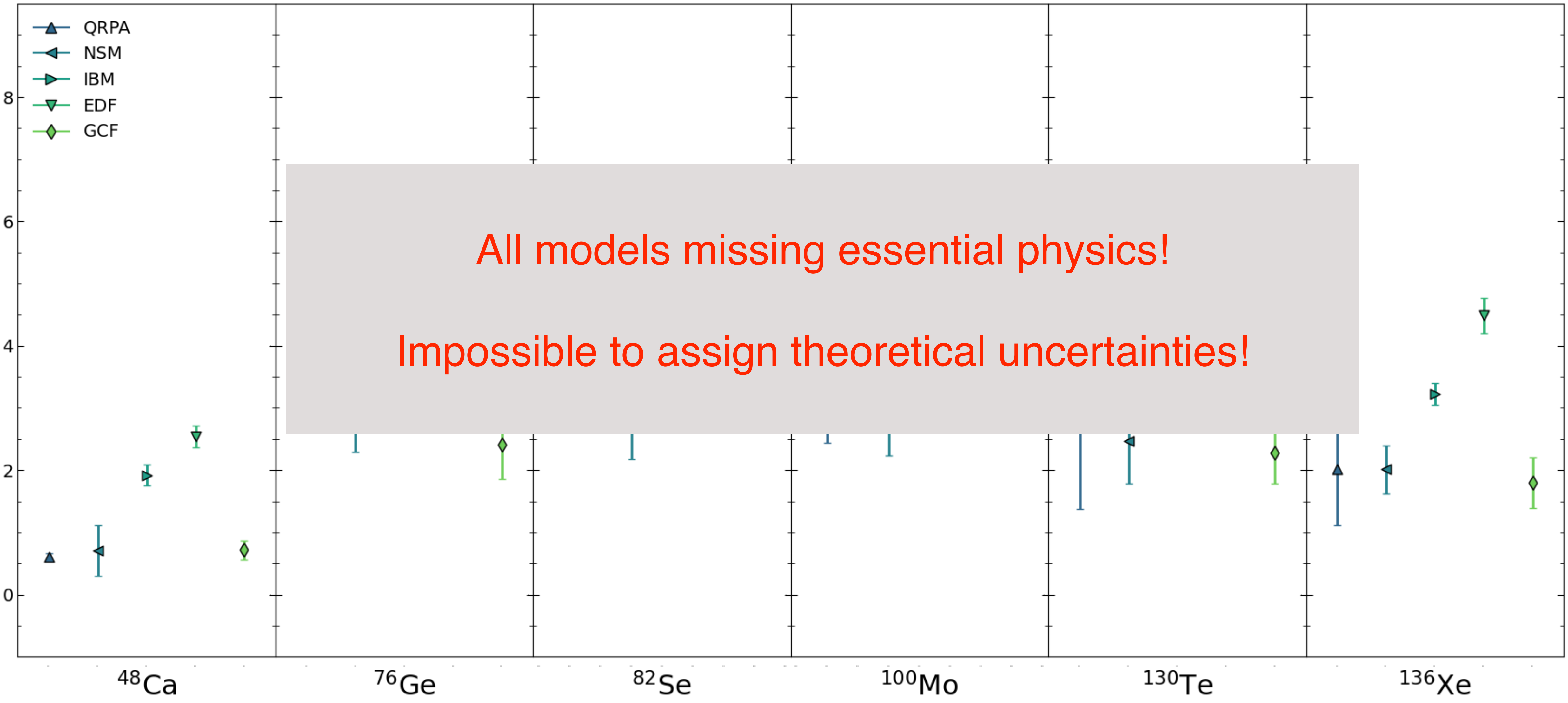

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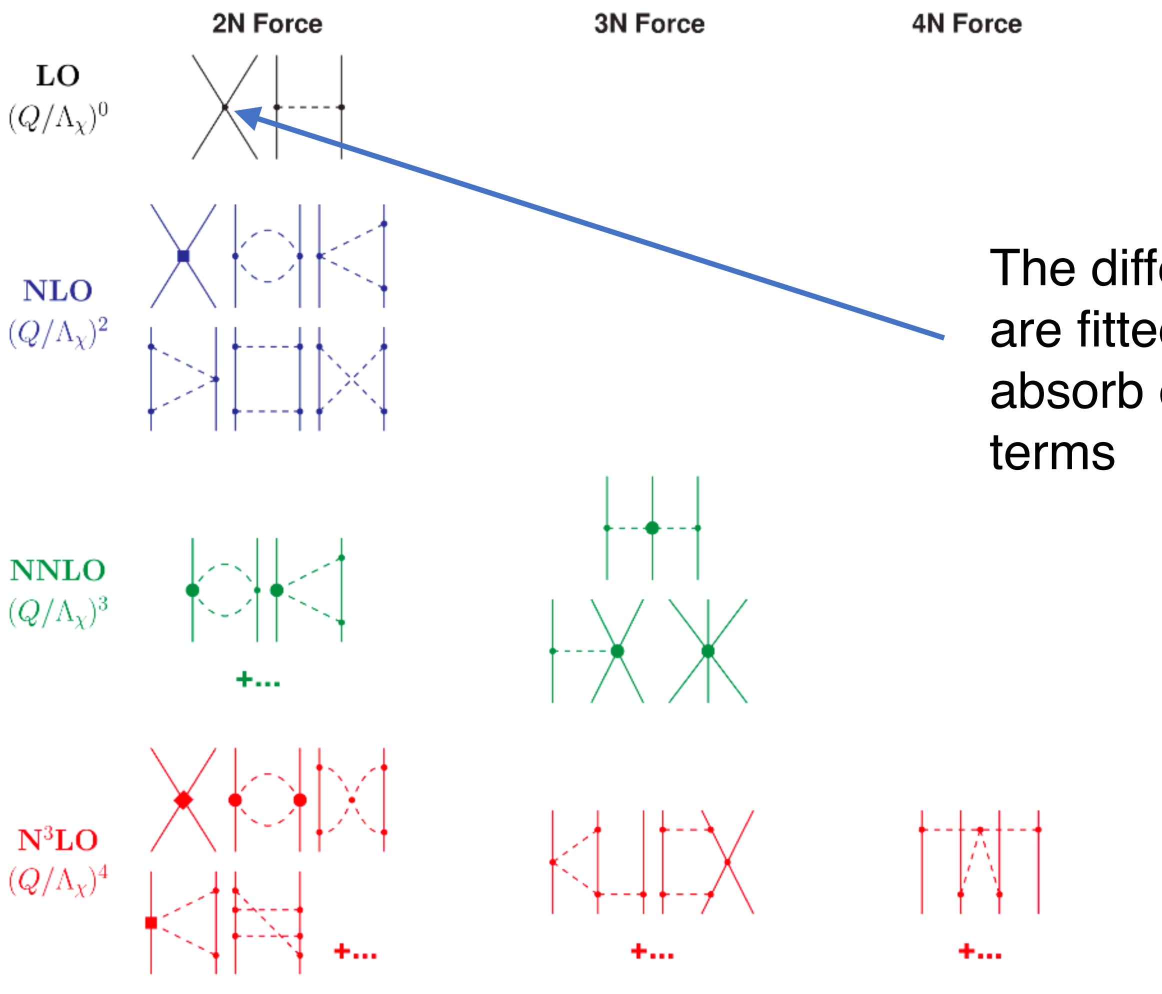
Ab initio nuclear theory

Ab initio nuclear theory: The recipe

1. Construct nuclear interaction from first principle (using chiral effective field theory (χ-EFT))
2. Solve the many-body Schrödinger equation for the nucleus with this interaction

Expansion order by order of the nuclear forces

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



The different coupling constants are fitted to few nucleons data to absorb effect of higher order terms

Machleidt and Entem, Phys. Rep., vol.503, no.1, pp.1–75 (2011)

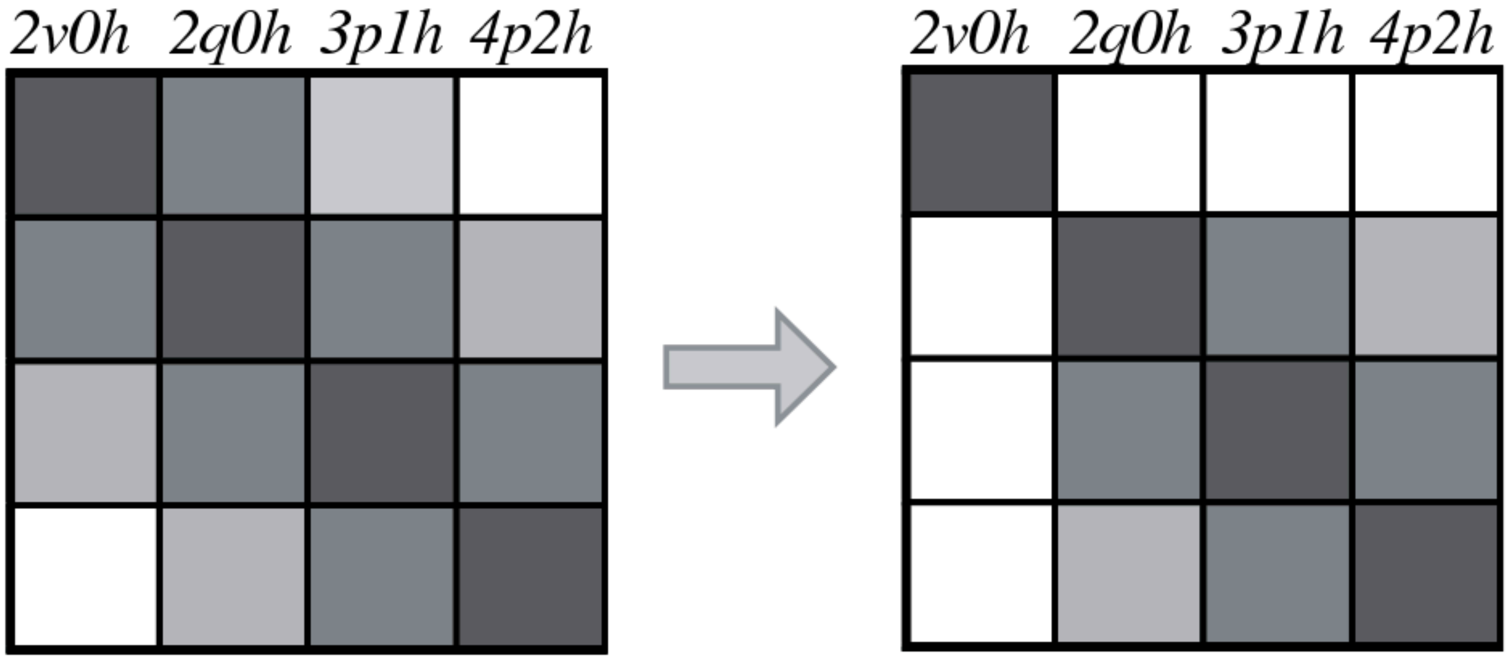
Similarity renormalization group

The general idea is to simplify the Hamiltonian by using a continuous unitary transformation:

$$\hat{H}(s) = \hat{U}(s)\hat{H}(0)\hat{U}^{\dagger}(s)$$

where s parameterized the continuous transformation, and $\hat{H}(0)$ is the starting Hamiltonian.

Valence-Space In Medium Similarity Renormalization Group



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

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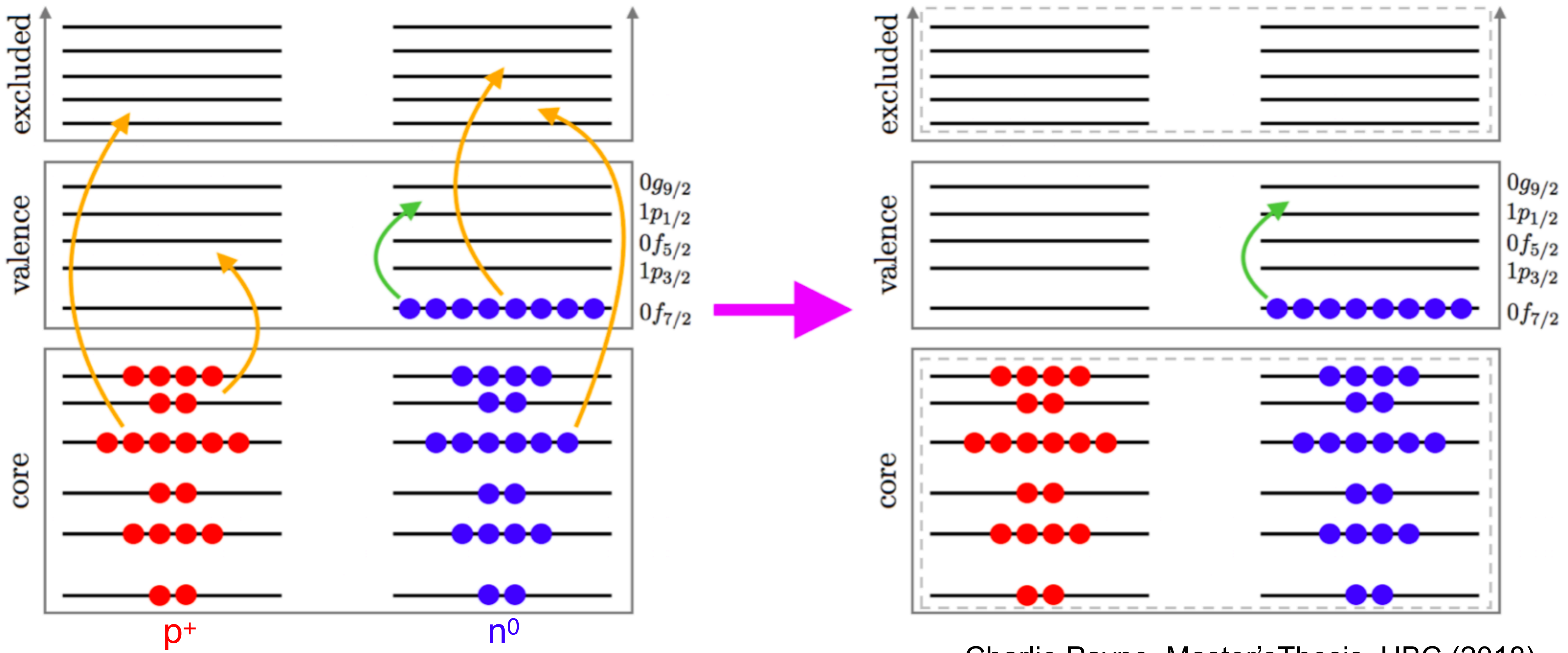

Charlie Payne, Master'sThesis, UBC (2018)

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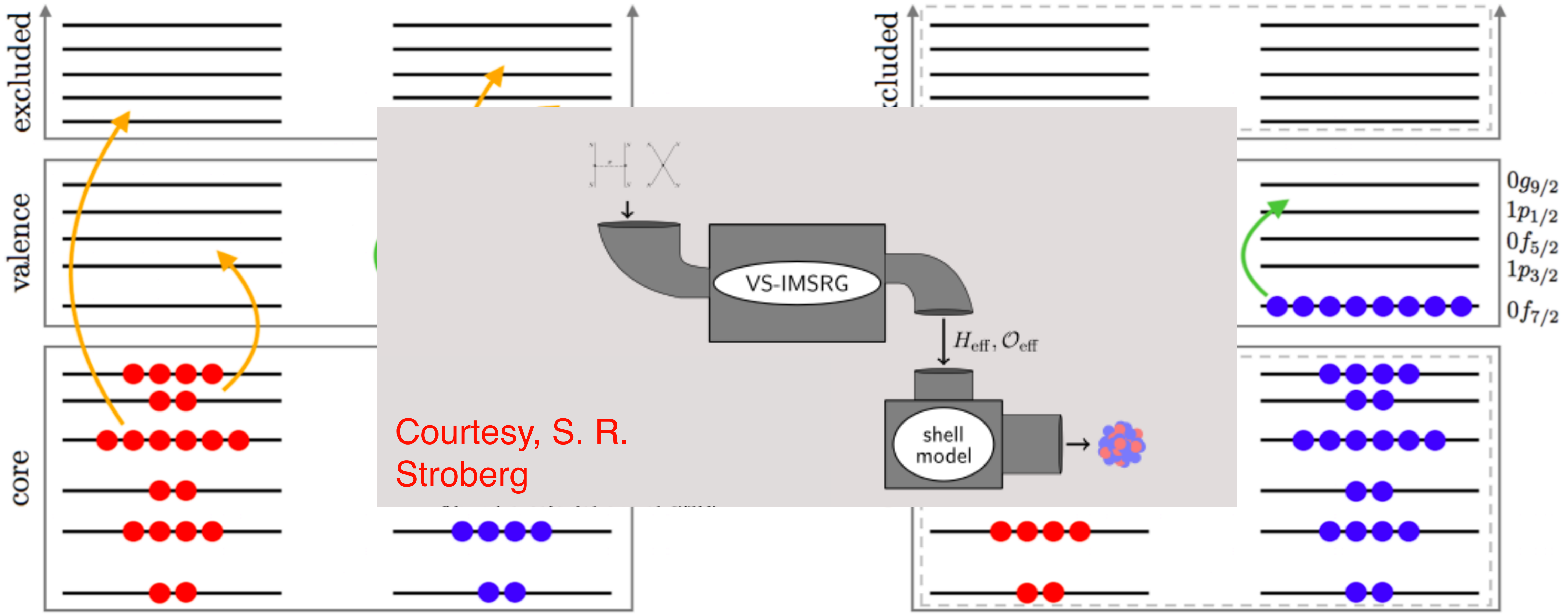

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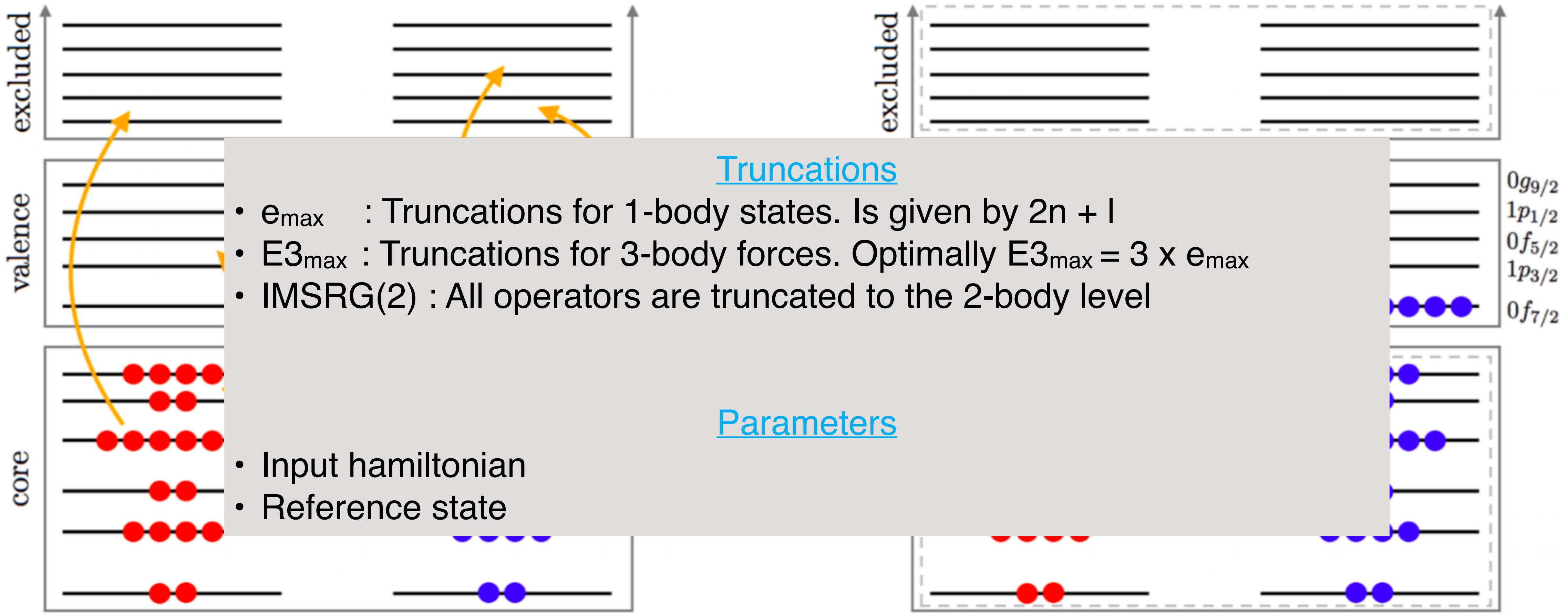


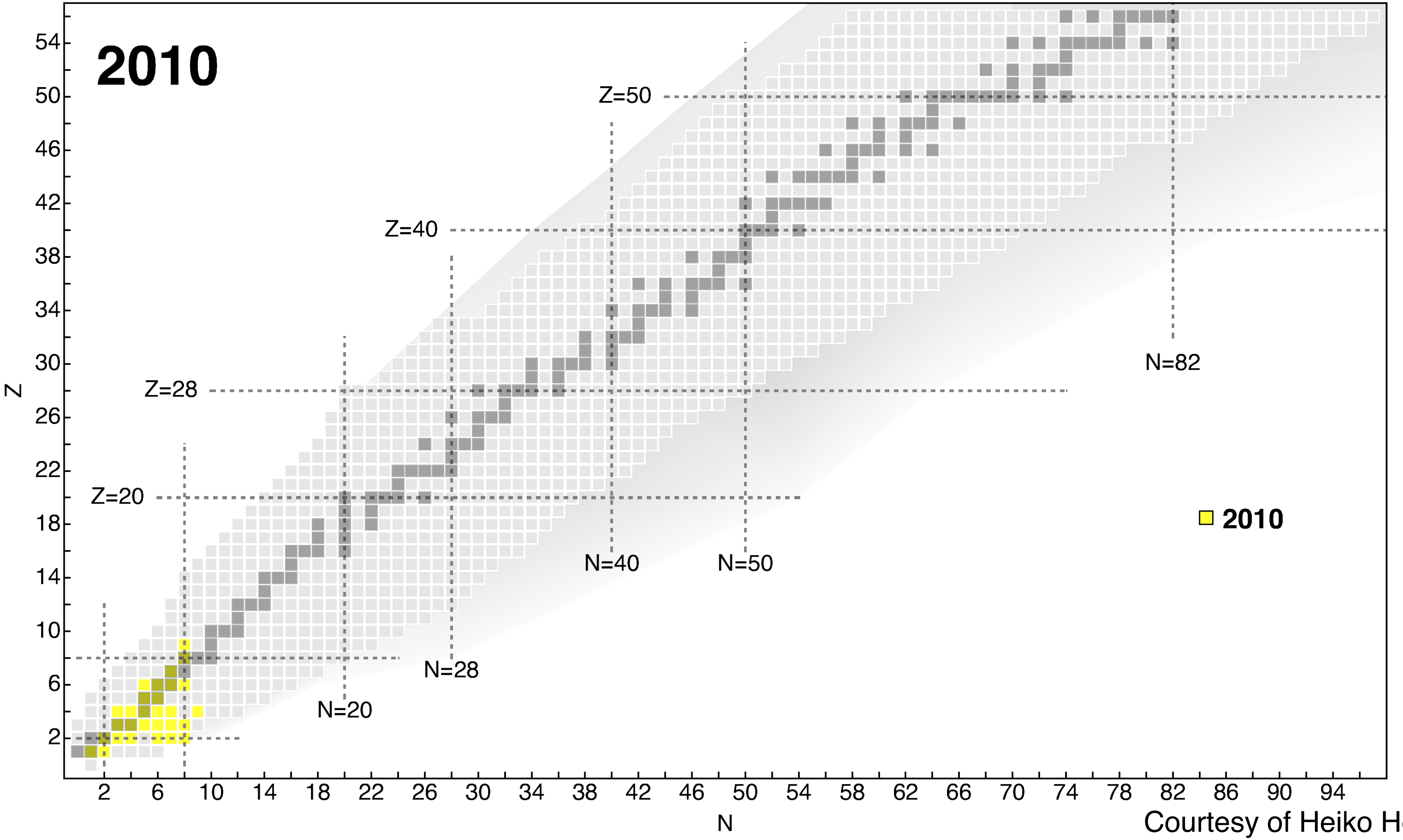
Truncations

- e_{max} : Truncations for 1-body states. Is given by 2n + l
- $E3_{max}$: Truncations for 3-body forces. Optimally $E3_{max} = 3 \times e_{max}$
- IMSRG(2) : All operators are truncated to the 2-body level

Parameters

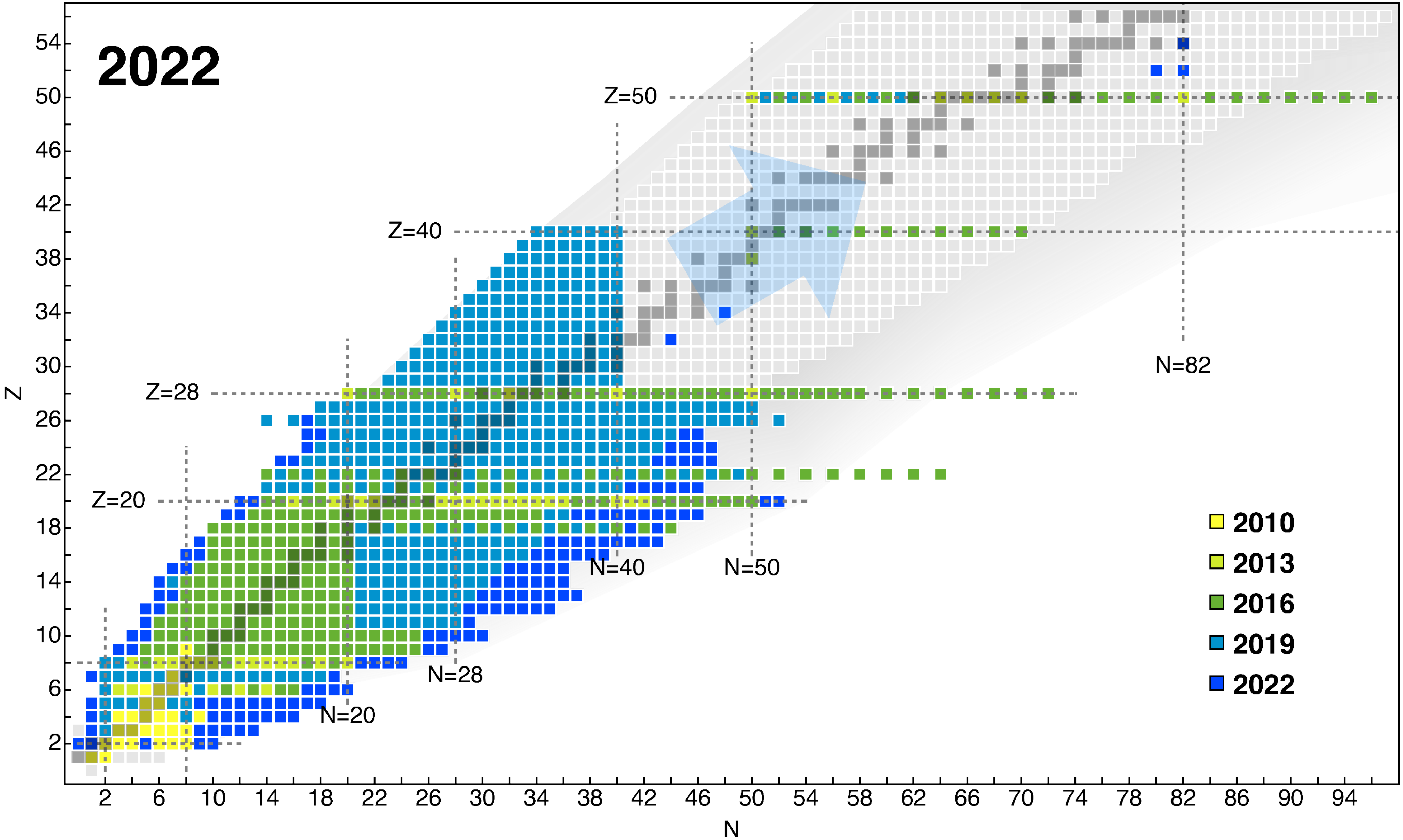
- Input hamiltonian
- Reference state

The ab initio revolution



Courtesy of Heiko Hergert

The ab initio revolution



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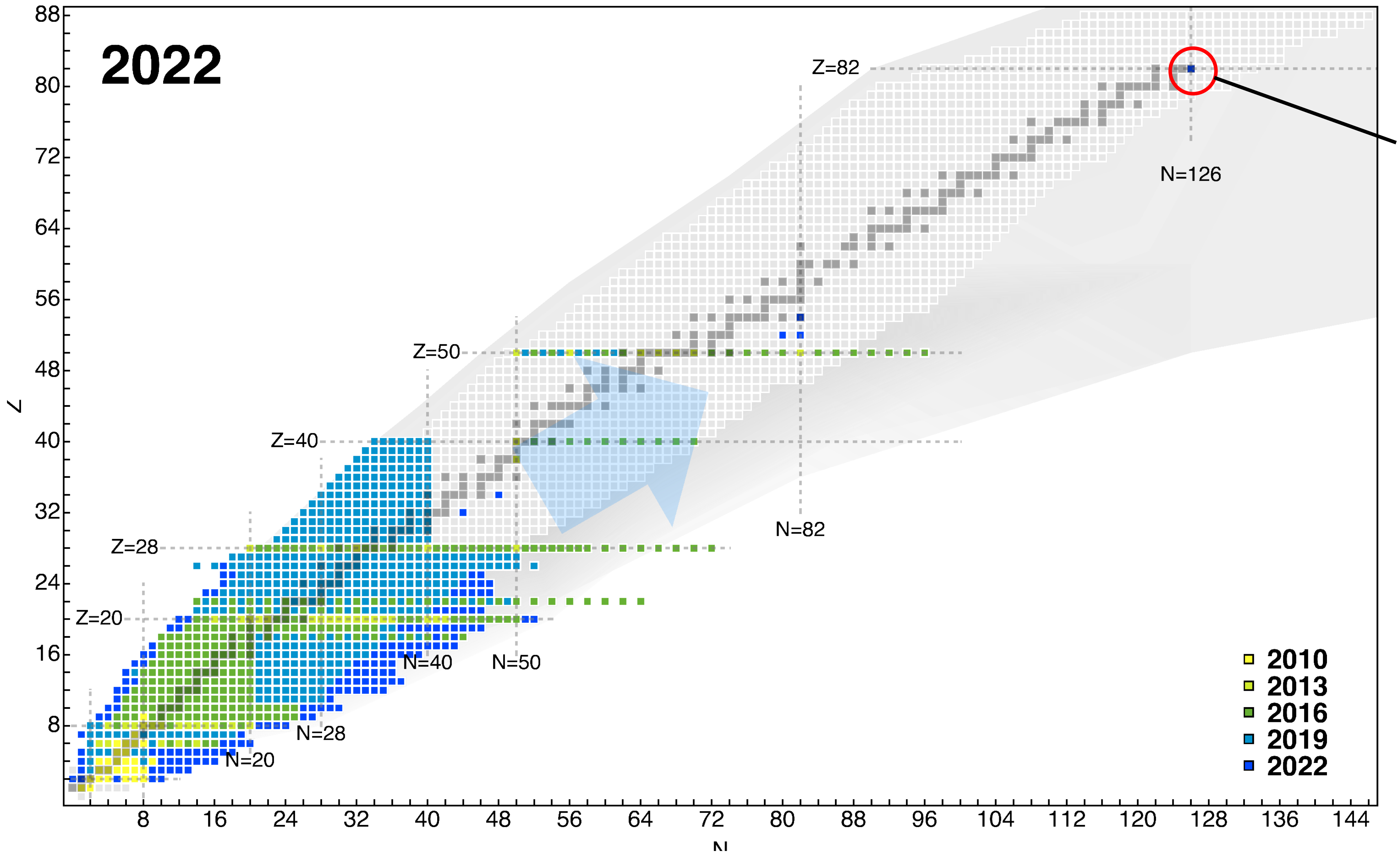
The ab initio revolution



Hu et al., Nature Physics 2022

Discovery, accelerated

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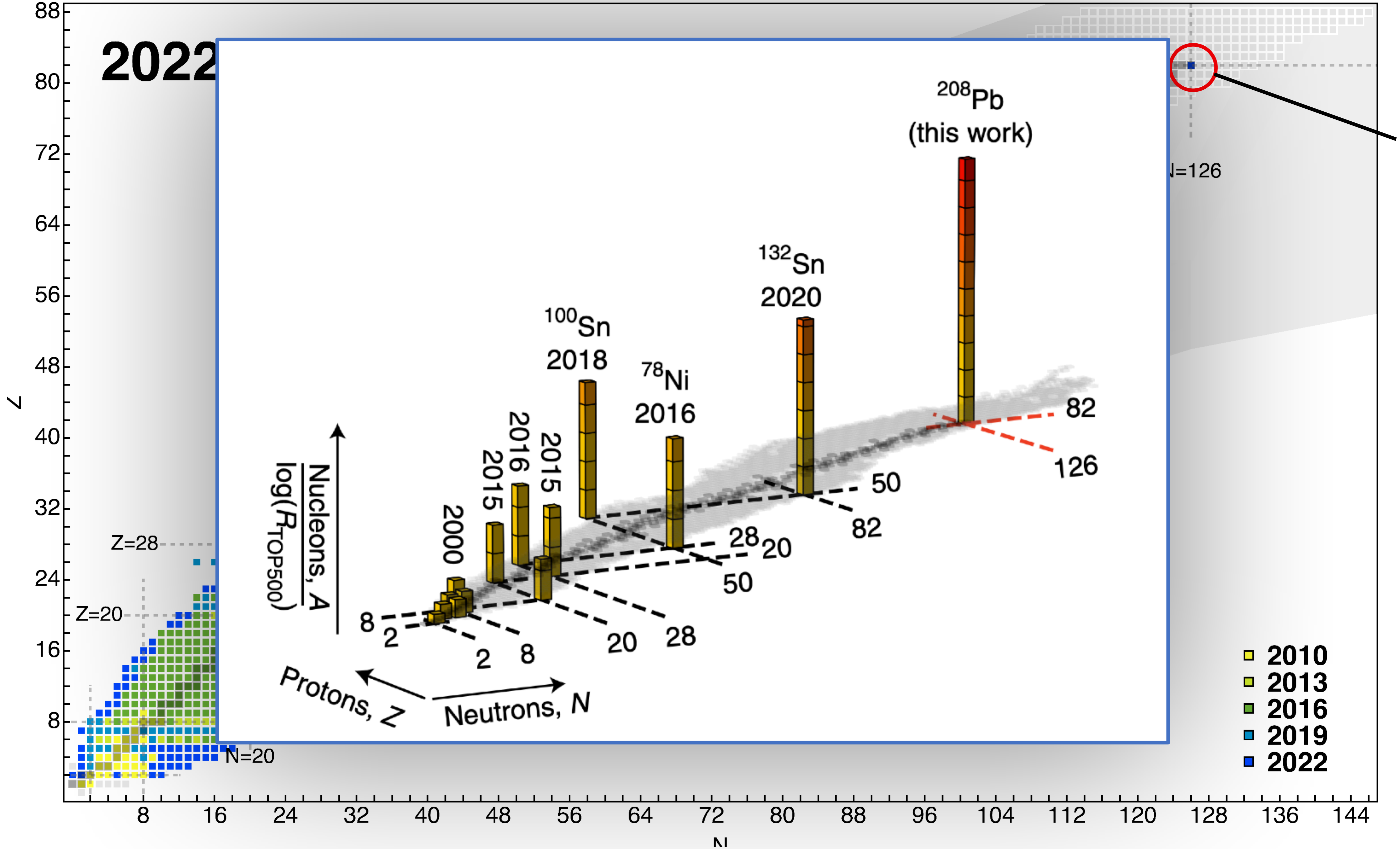

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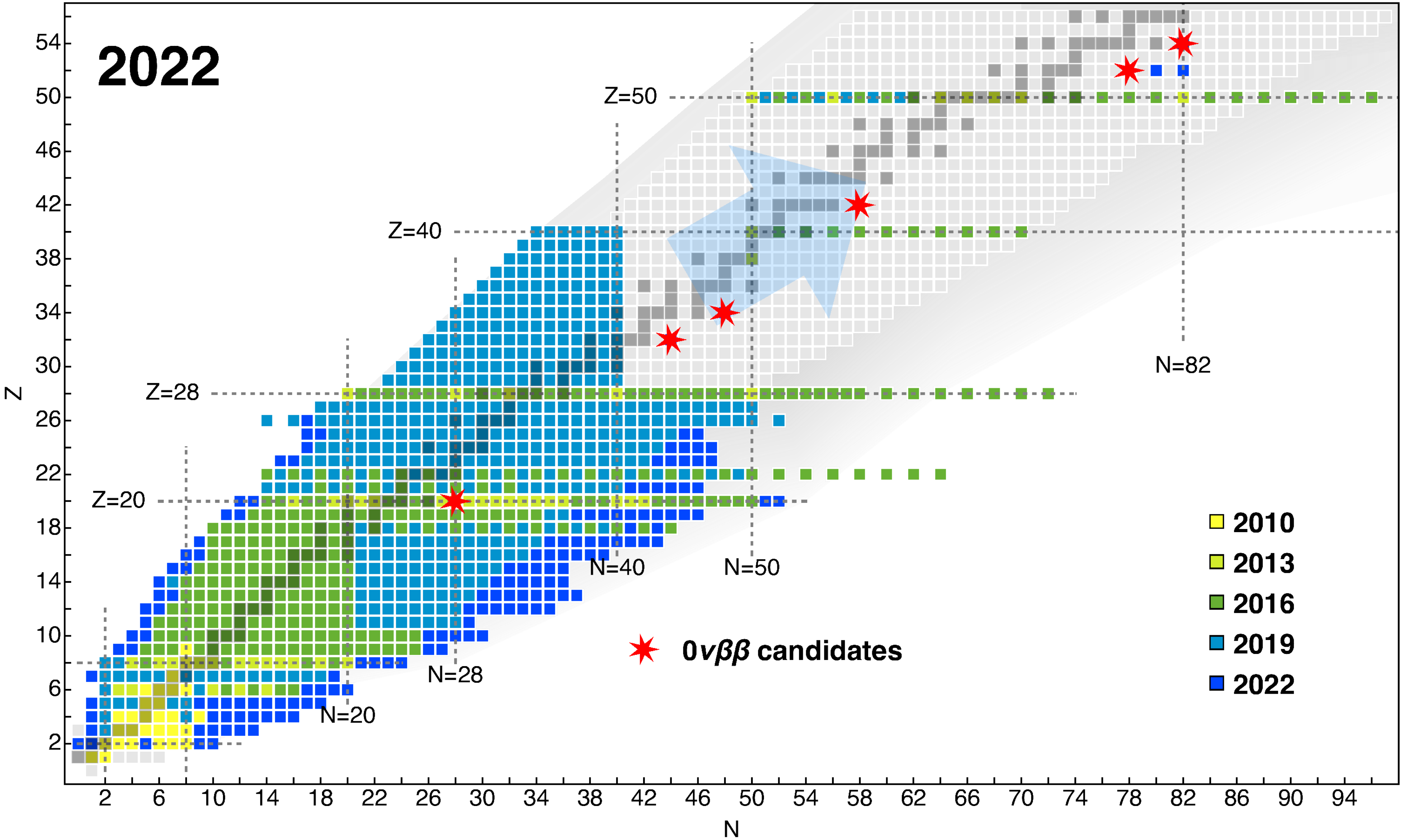

Results

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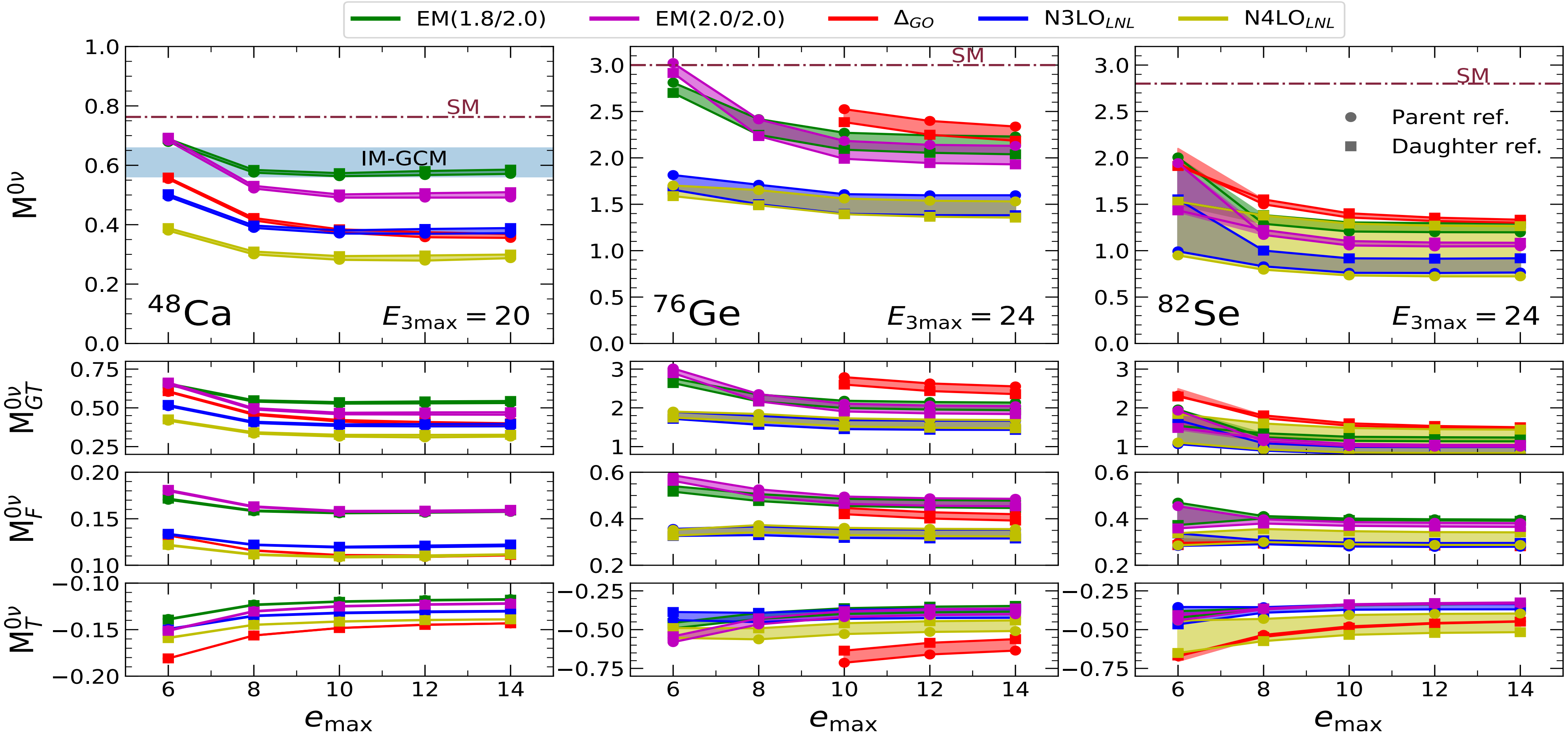
Ab Initio $0\nu\beta\beta$ Decay: ^{48}Ca, ^{76}Ge and ^{82}Se

Results with 5 different input hamiltonians to study uncertainty from interaction choice.



Things to add: valence space variation, two-body currents, IMSRG(3), …

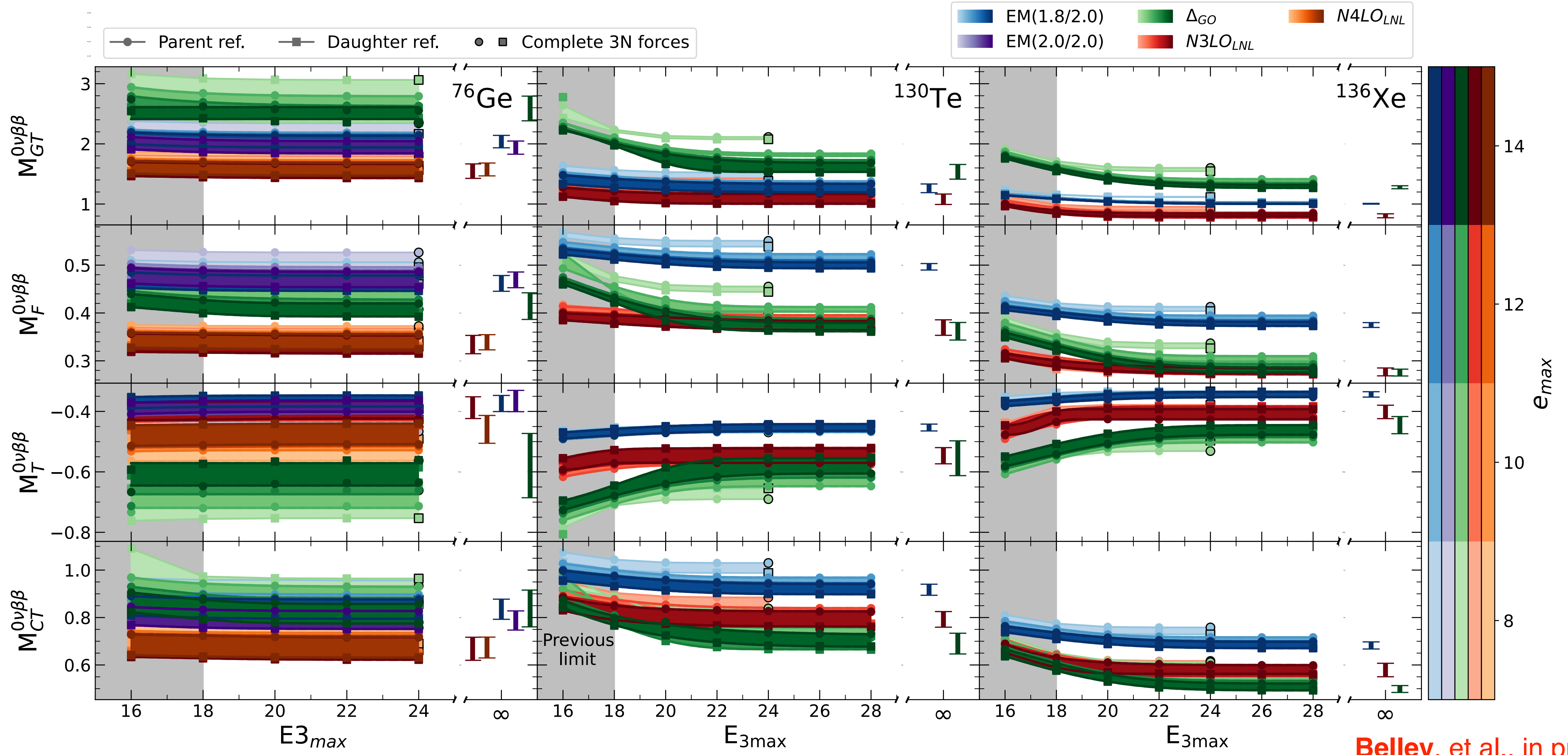
Belley, et al., PRL126.042502

Belley, et al., in prep

Ab Initio $0\nu\beta\beta$ Decay: ^{130}Te, ^{136}Xe

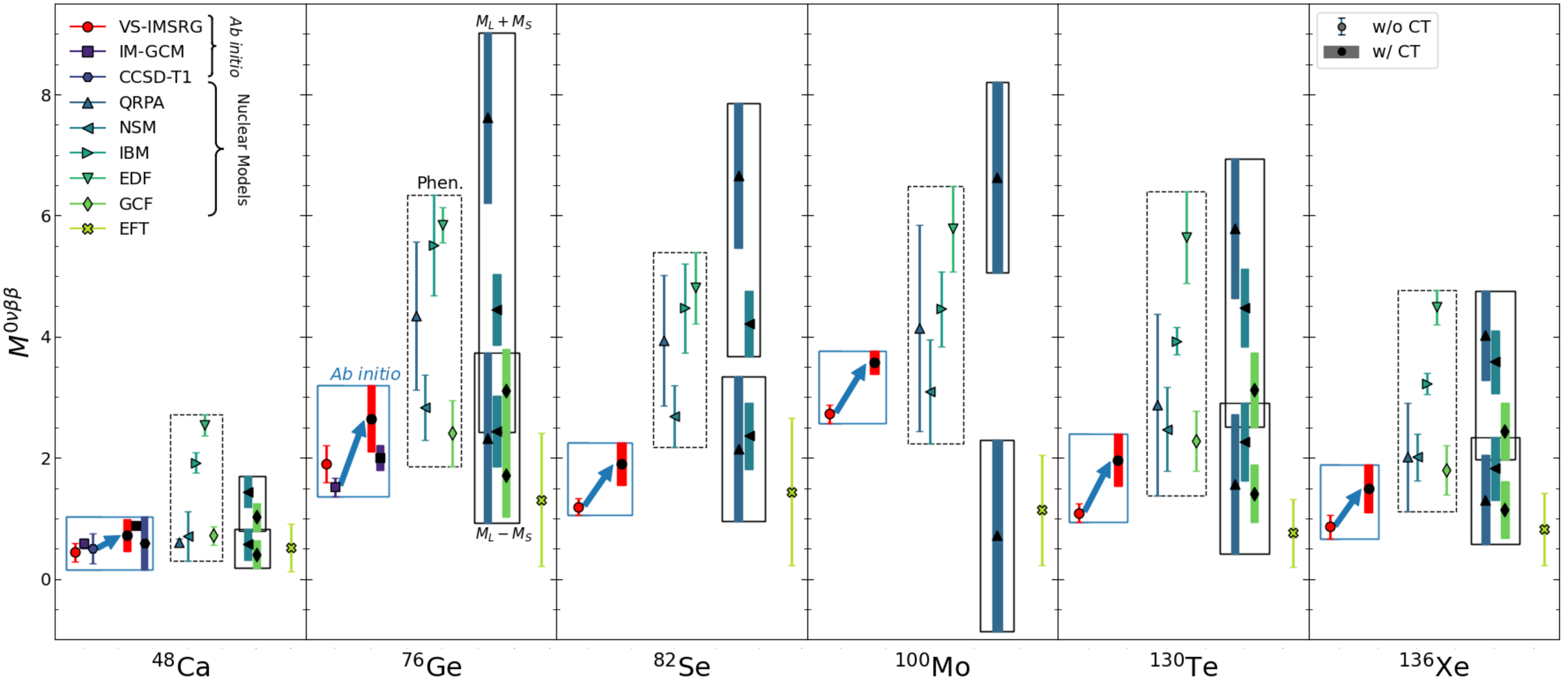
^{130}Te, ^{136}Xe major players in global searches with SNO+, CUORE and nEXO

Increased E_{3max} capabilities allow first converged ab initio calculations [EM1.8/2.0, Δ_{GO}, N3LO$_{LNL}$]



Belley, et al., in prep

0νββ-decay Matrix Elements: The new picture



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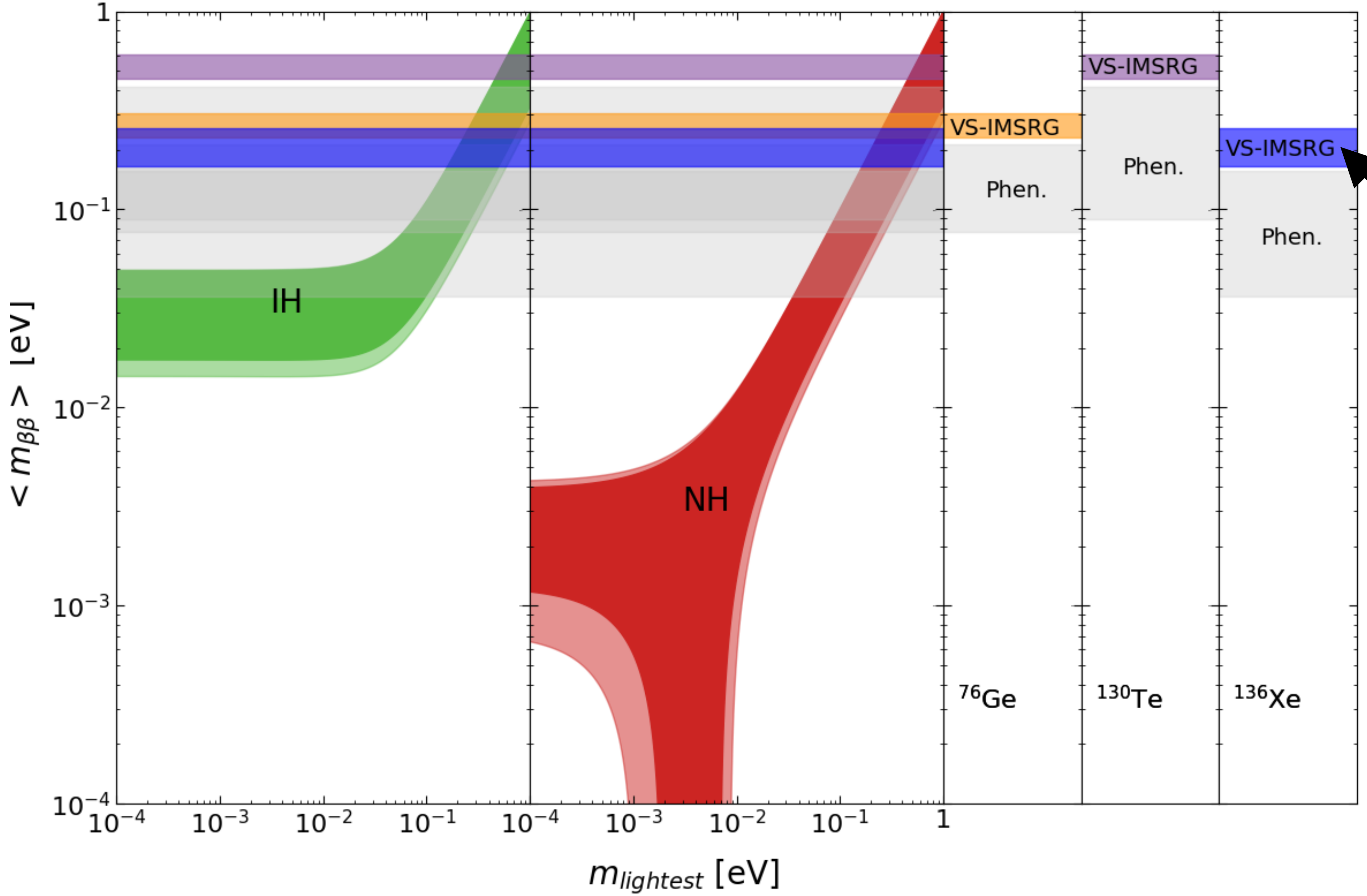
Ab Initio 0νββ Decay: Effect on experimental limits



Long range only

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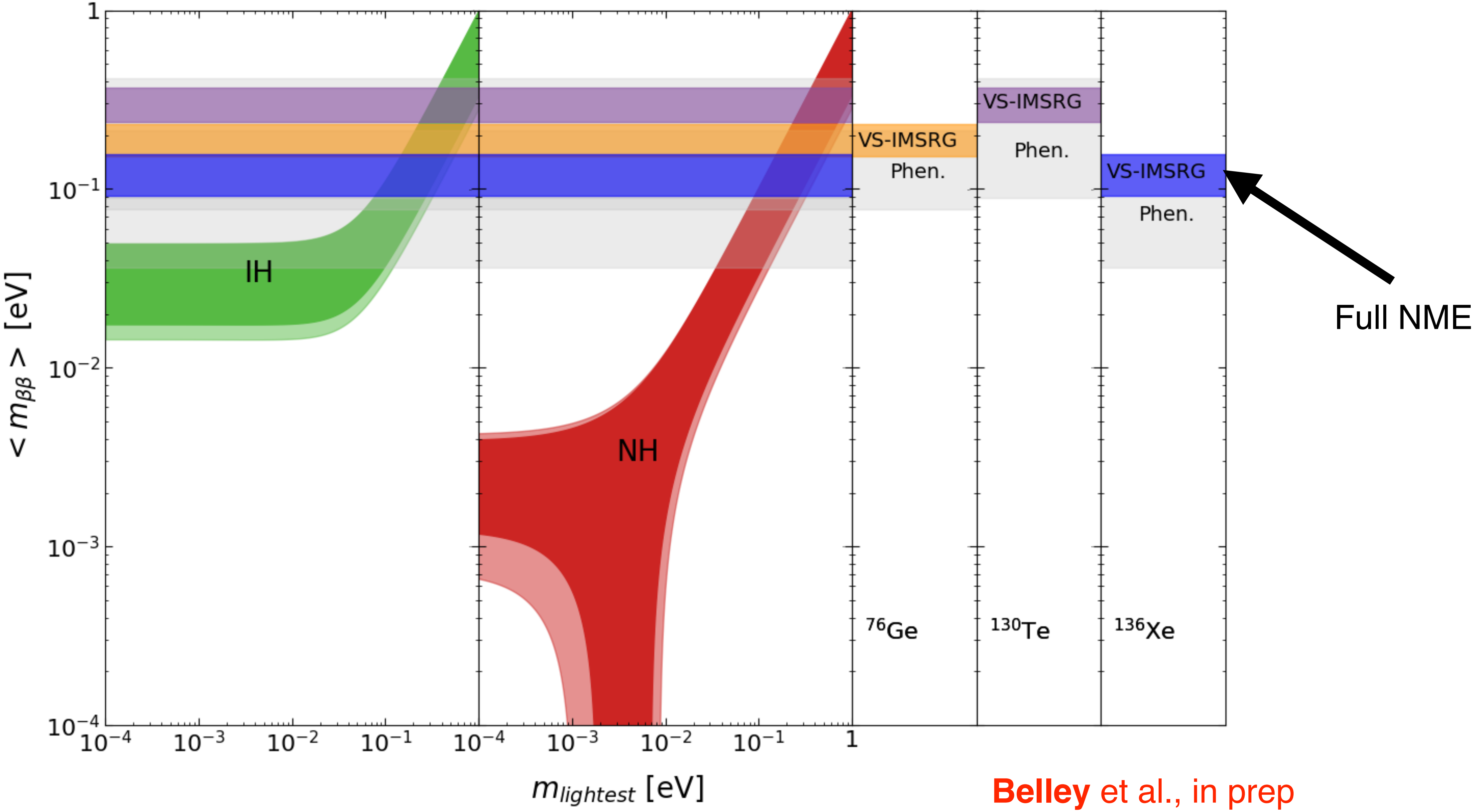

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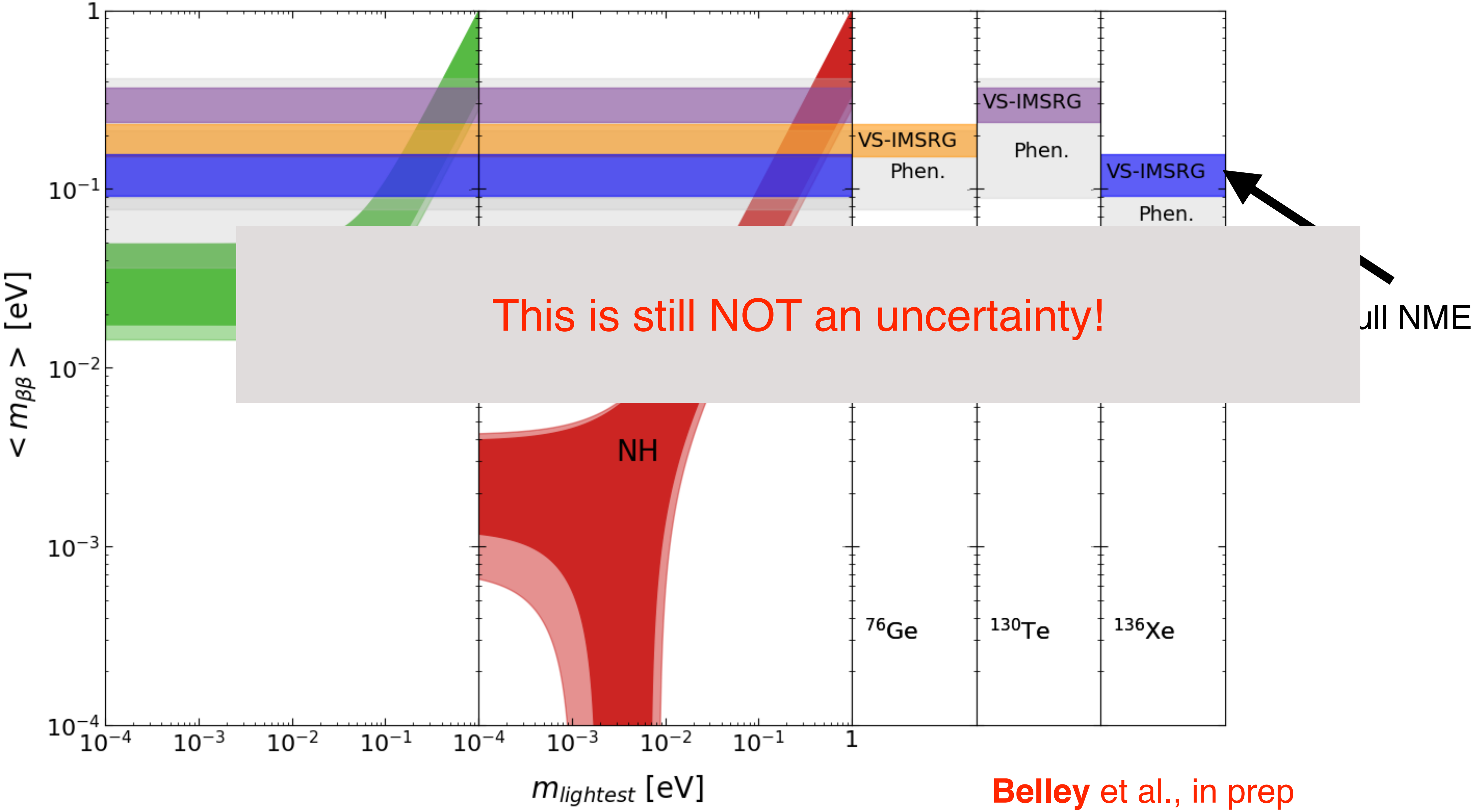

This is still NOT an uncertainty!

Belley et al., in prep

Assessing the uncertainty

Uncertainty can be split into 3 sources:

- The many-body method (VS-IMSRG)
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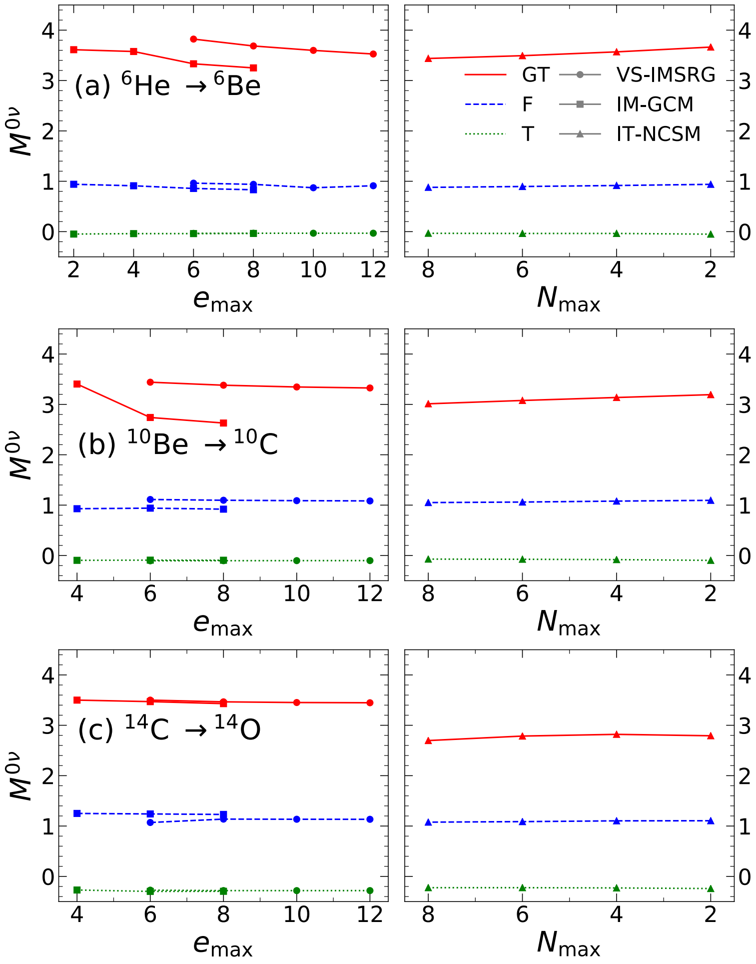
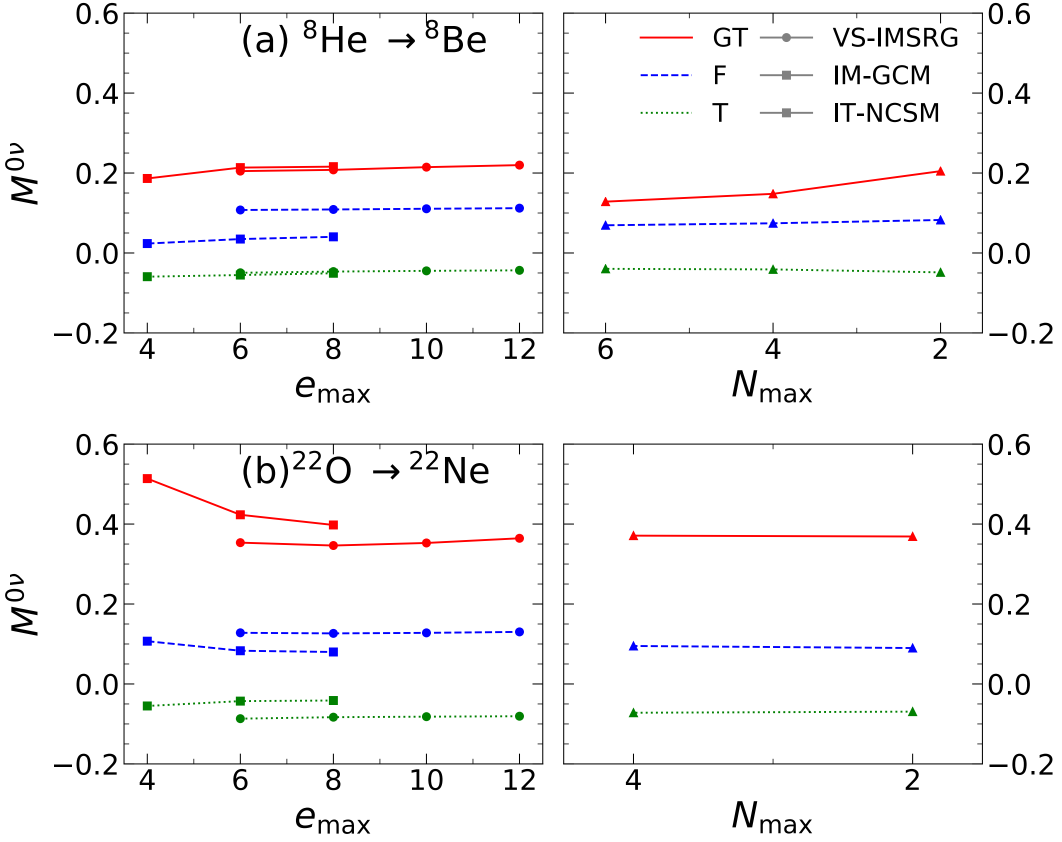
Benchmarking $0\nu\beta\beta$ Decay in Light Nuclei: Summary

Benchmark with other ab initio method for fictitious decays in light nuclei

$\Delta T = 0$





$\Delta T = 2$

Yao, **Belley**, et al., PhysRevC.103.014315

Reasonable to good agreement in all cases

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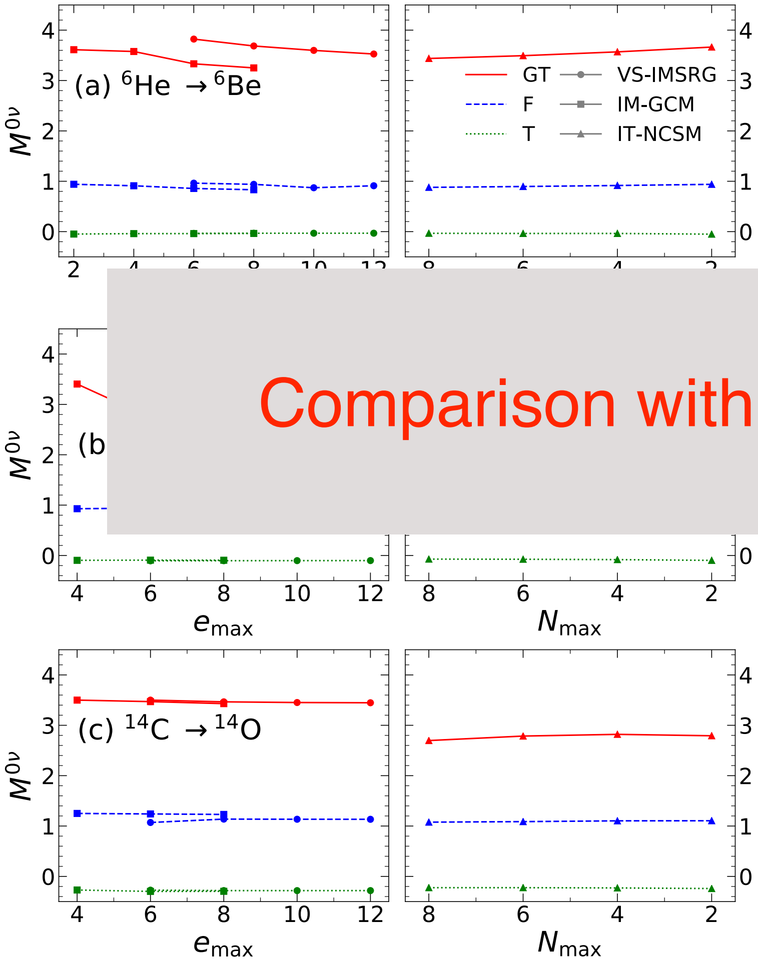
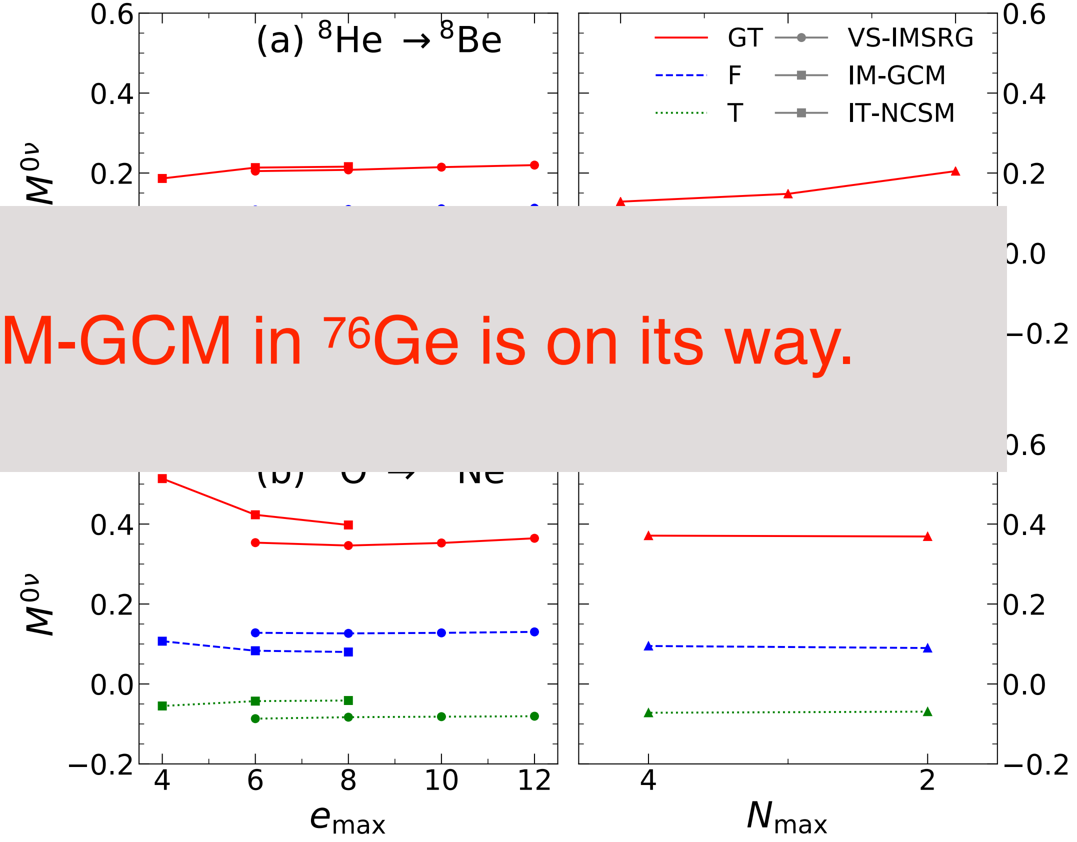


Comparison with IM-GCM in ^{76}Ge is on its way.

$\Delta T = 2$



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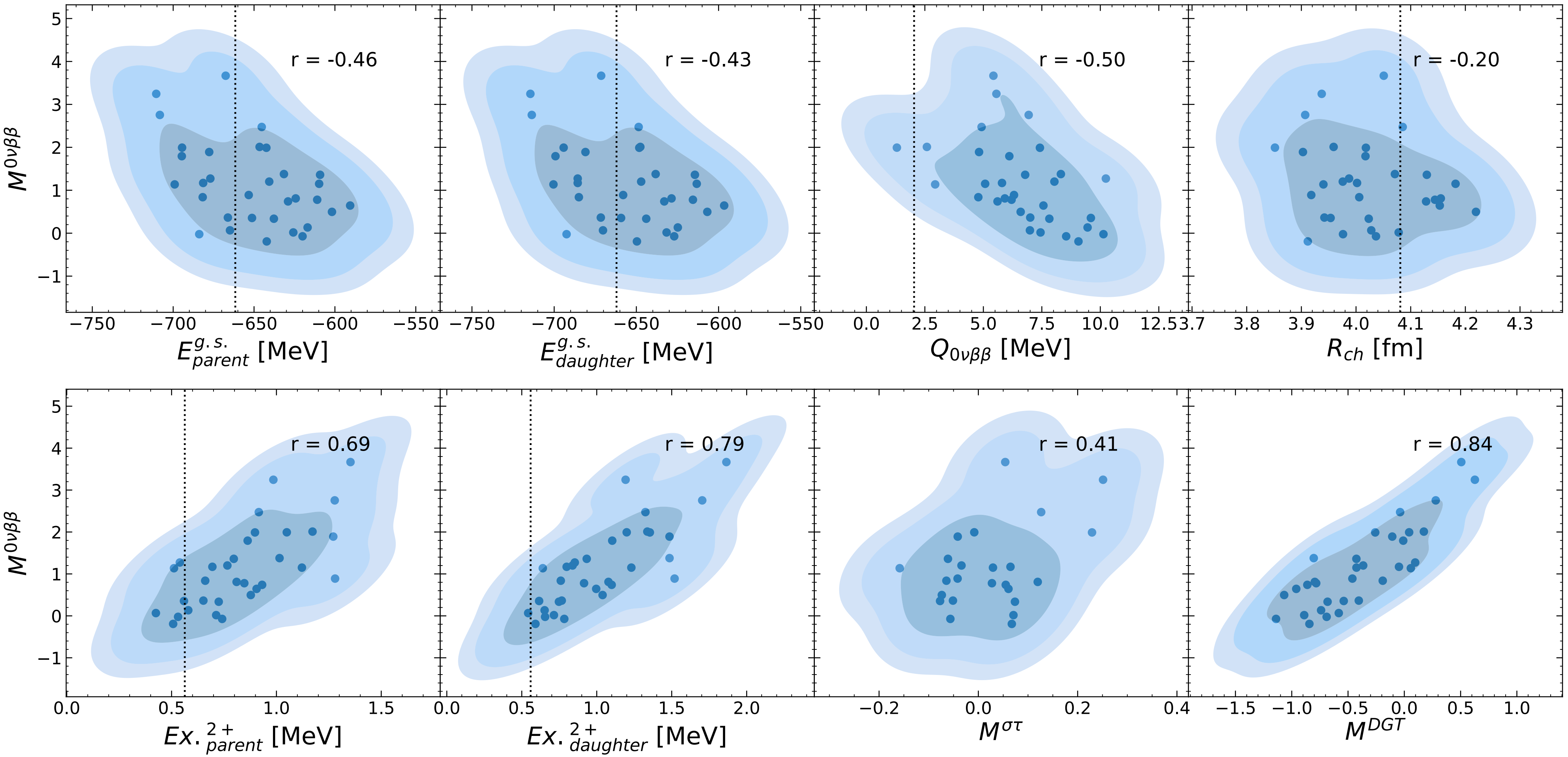
Correlation between observables

In ^{76}Ge:

Belley et al., arXiv:2210.05809



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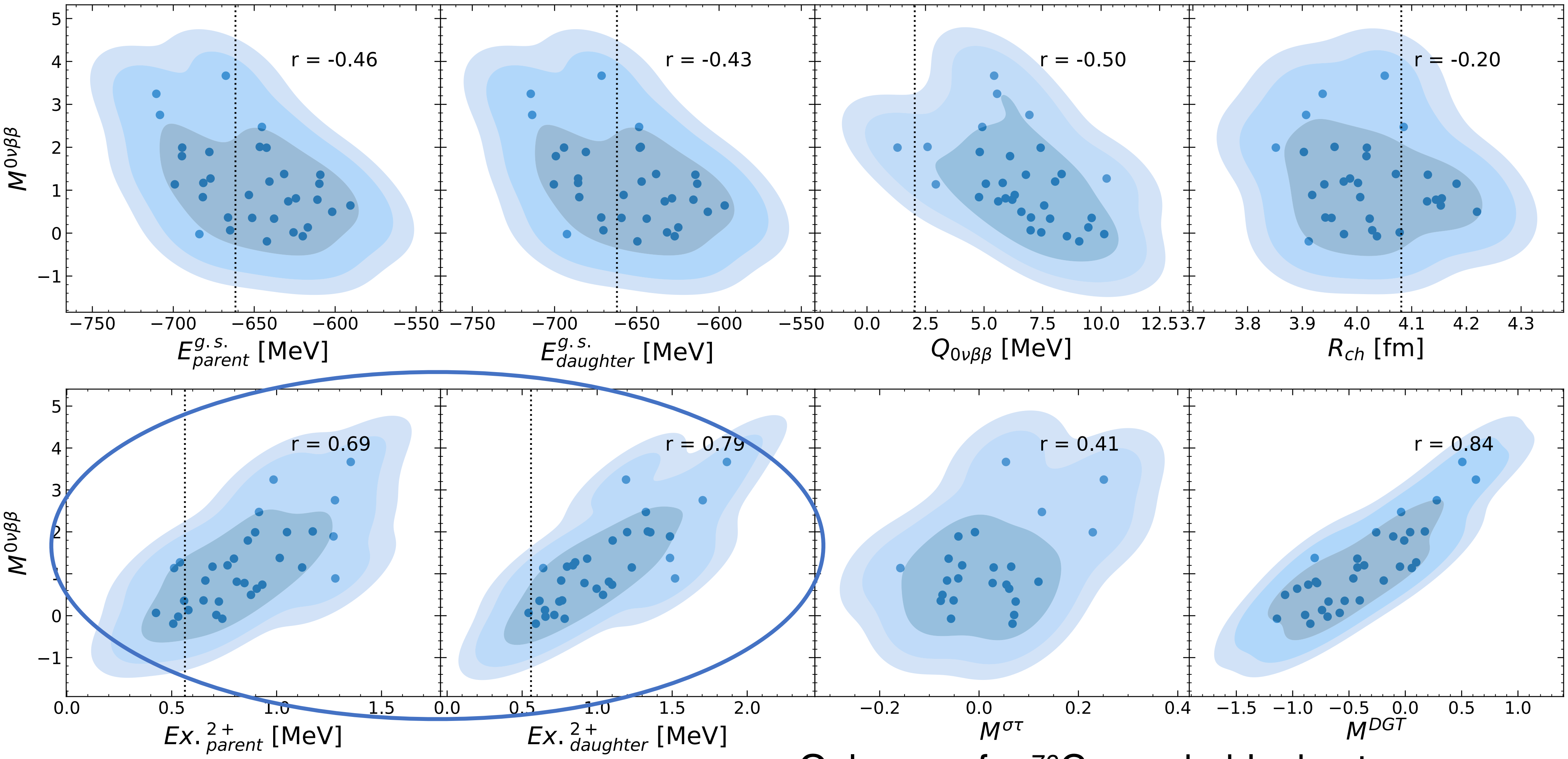

Only seen for ^{76}Ge, probably due to deformed nuclei involved.

Correlation between observables

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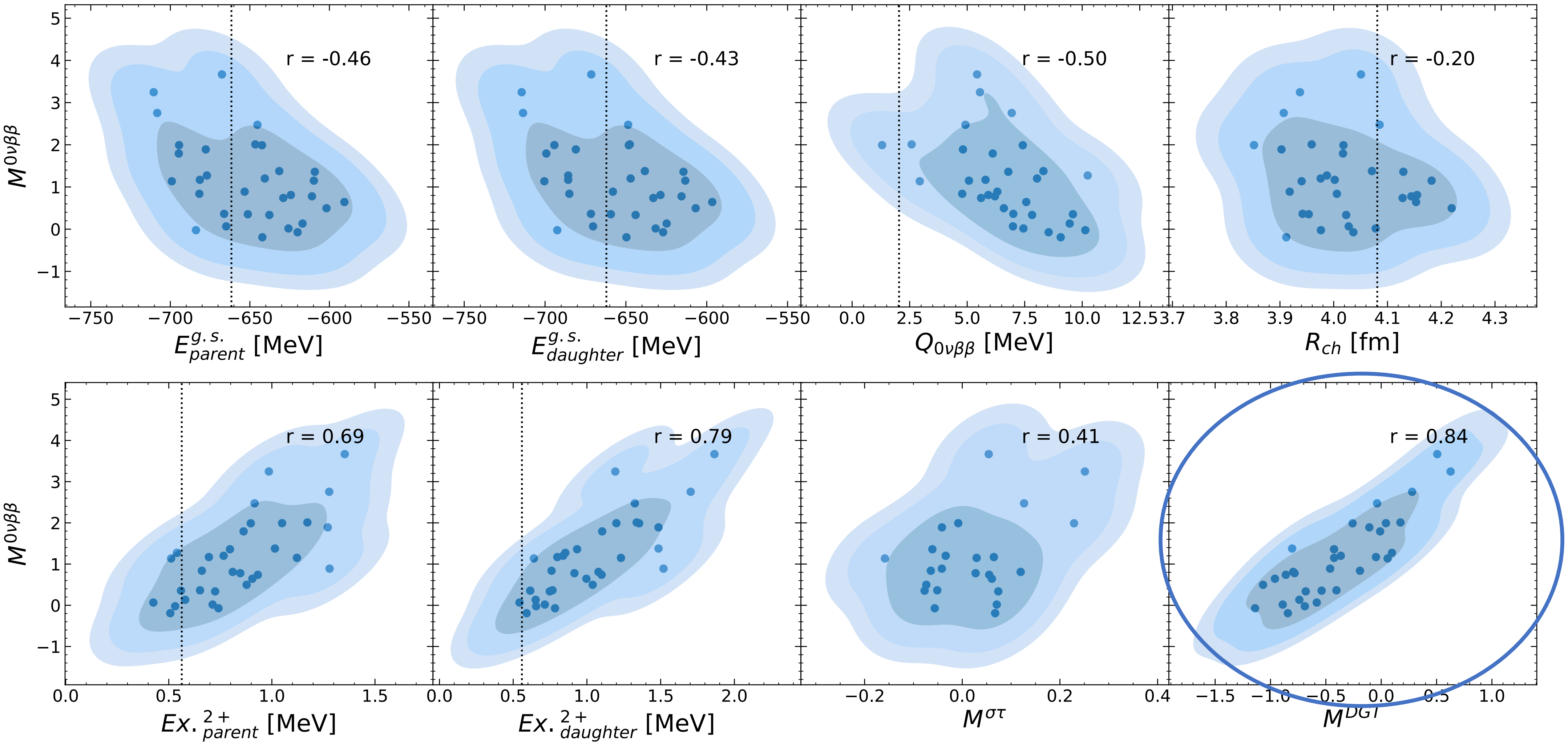
Belley et al., arXiv:2210.05809



Only correlation seen in multiple nuclei is with the unobserved double Gamow-Teller transition NME.

Global sensitivity analysis

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$$\Rightarrow$$

Need emulators to speed up calculations.

Emulators for many-body methods

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1. **Physics driven**
   - Incorporates some knowledge about the physics into the model
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Eg: Eigenvector continuation emulator for the Coupled Cluster method.

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E.g. Neural networks, Gaussian processes

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Using Gaussian Process as an emulator

- Idea behind Gaussian Processes regression is to assume that the function we want to fit can be represented as a multivariate gaussian, i.e.

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

  where μ is a mean function and $K(\mathbf{x}, \mathbf{x})$ is the covariance matrix between the inputs. By optimizing the hyperparameters of the covariance function, we can obtain a good representation of our function.

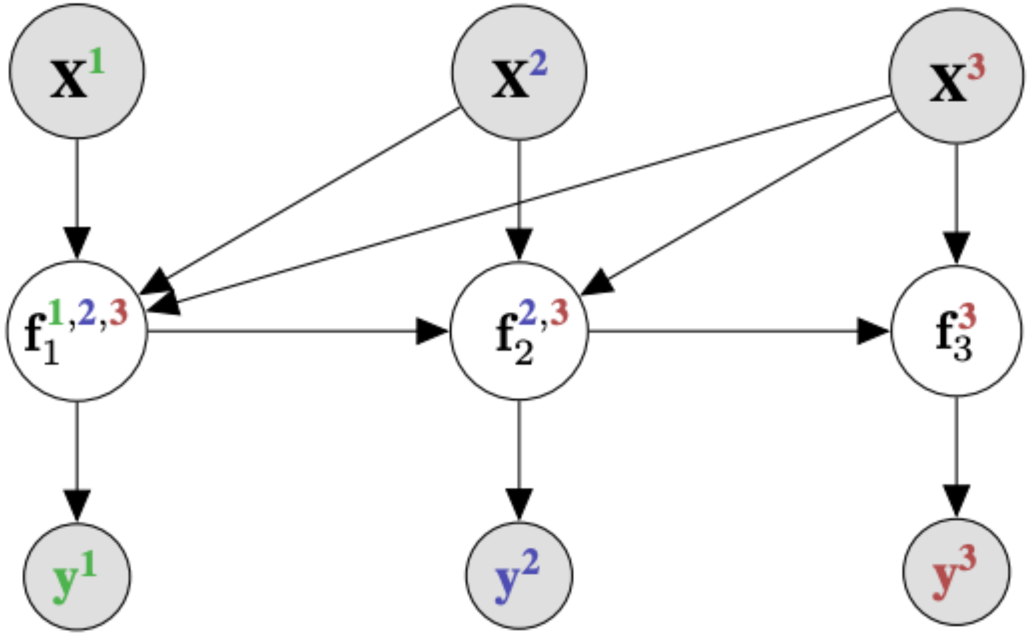
- Gaussian Processes regression usually do better than neural networks for small datasets. They also have the advantage to come with an uncertainty on the result at each data point.

- Multi-Tasks Gaussian Process: Uses multiple correlated outputs from same inputs by defining the kernel as $K_{inputs} \otimes K_{outputs}$. This allows us to increase the number of data points without needing to do more expansive calculations.

- Multi-Fidelity Gaussian Process: Uses few data points of high fidelity (full IMSRG calculations) and many data points of low fidelity (e.g. Hartree-Fock results, lower e_{max}). The difference function is fitted by a Gaussian process in order to predict the value of full calculations using the low fidelity data points. This assumes a linear scaling for between the low- and high-fidelity calculations.

The MM-DGP algorithm

- When the relation between low-fidelity and high-fidelity data is complicated, the simple multi-fidelity approach does not produce good results.
- Deep gaussian processes [1] link multiple gaussian processes inside a neural network to improve results.
- This can be used to model the difference function between the low-fidelity and high-fidelity by including outputs of the previous fidelity as an input of higher fidelity by taking a kernel of the form: $K(\mathbf{x}, \mathbf{x}) = k(\mathbf{x}, \mathbf{x}) \cdot k(f_{prev}(\mathbf{x}), f_{prev}(\mathbf{x})) + k_{bias}(\mathbf{x}, \mathbf{x})$
- This was developed for single-output gaussian processes and we have adapted it for multi-output case, creating the MM-DGP: Multi-output Multi-fidelity Deep Gaussian Process.



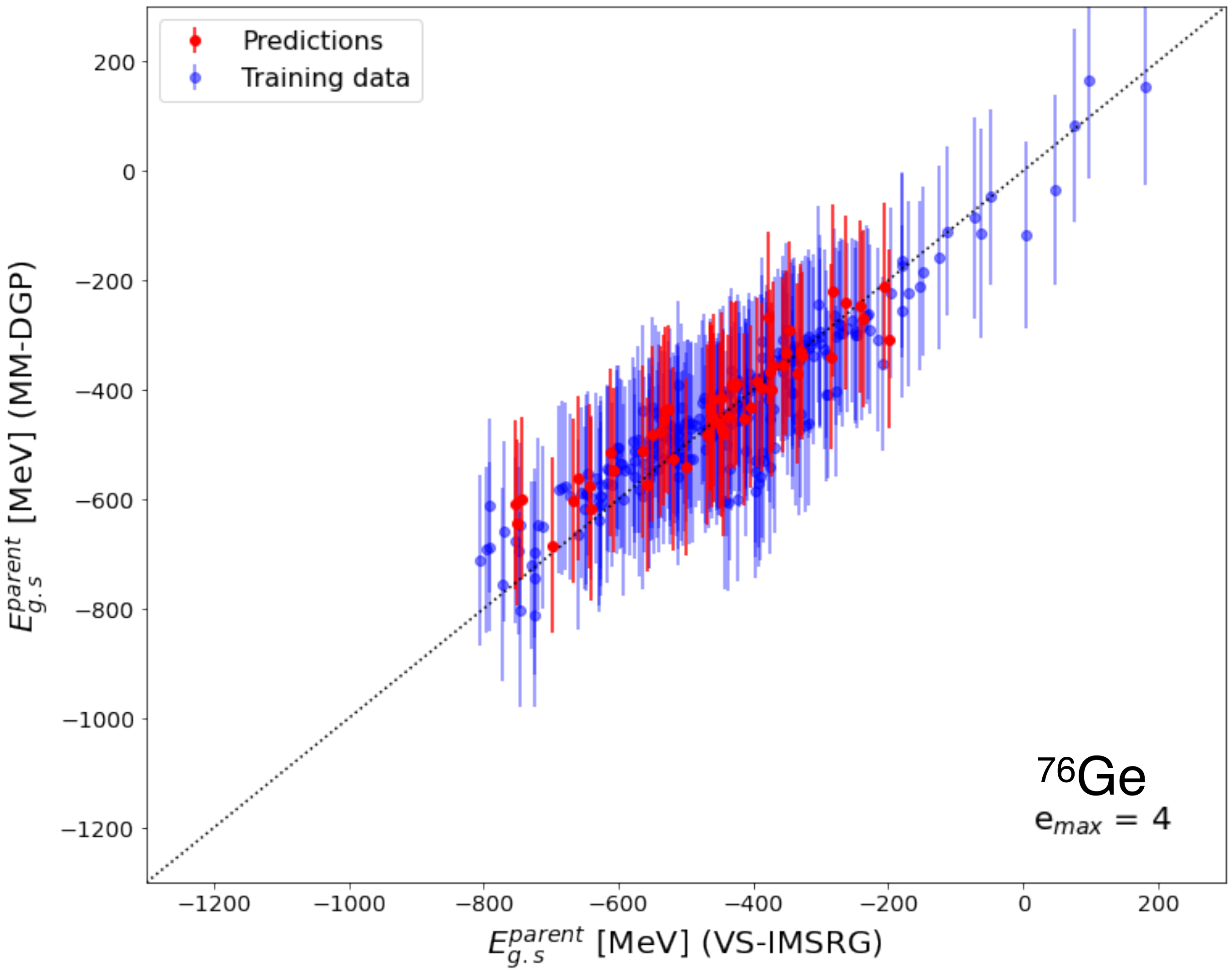
Taken from [1].

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

The MM-DGP algorithm: Energies

Using Δ-full chiral EFT interactions at N2LO:

250 training points



Belley, Pitcher et al. in prep.

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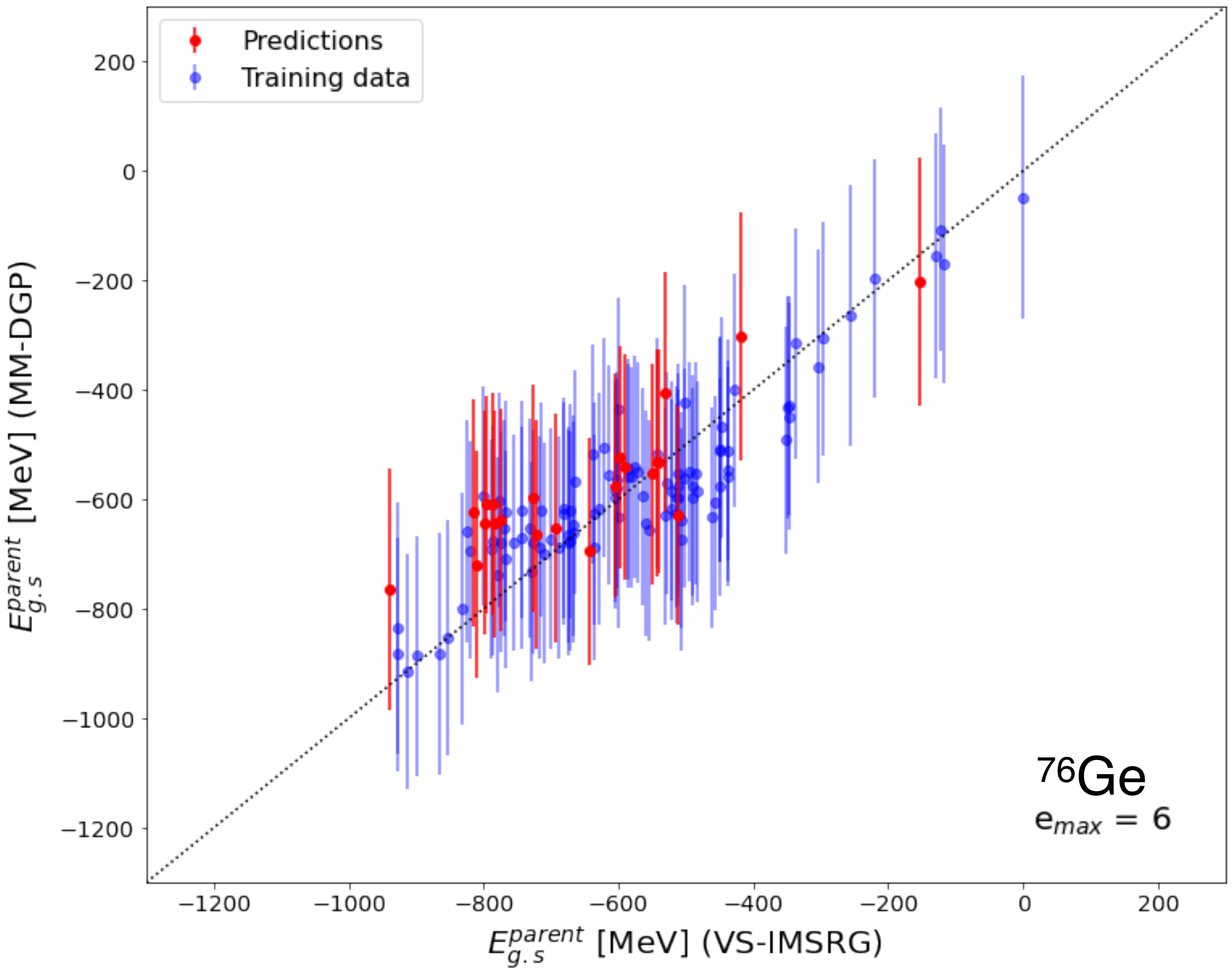

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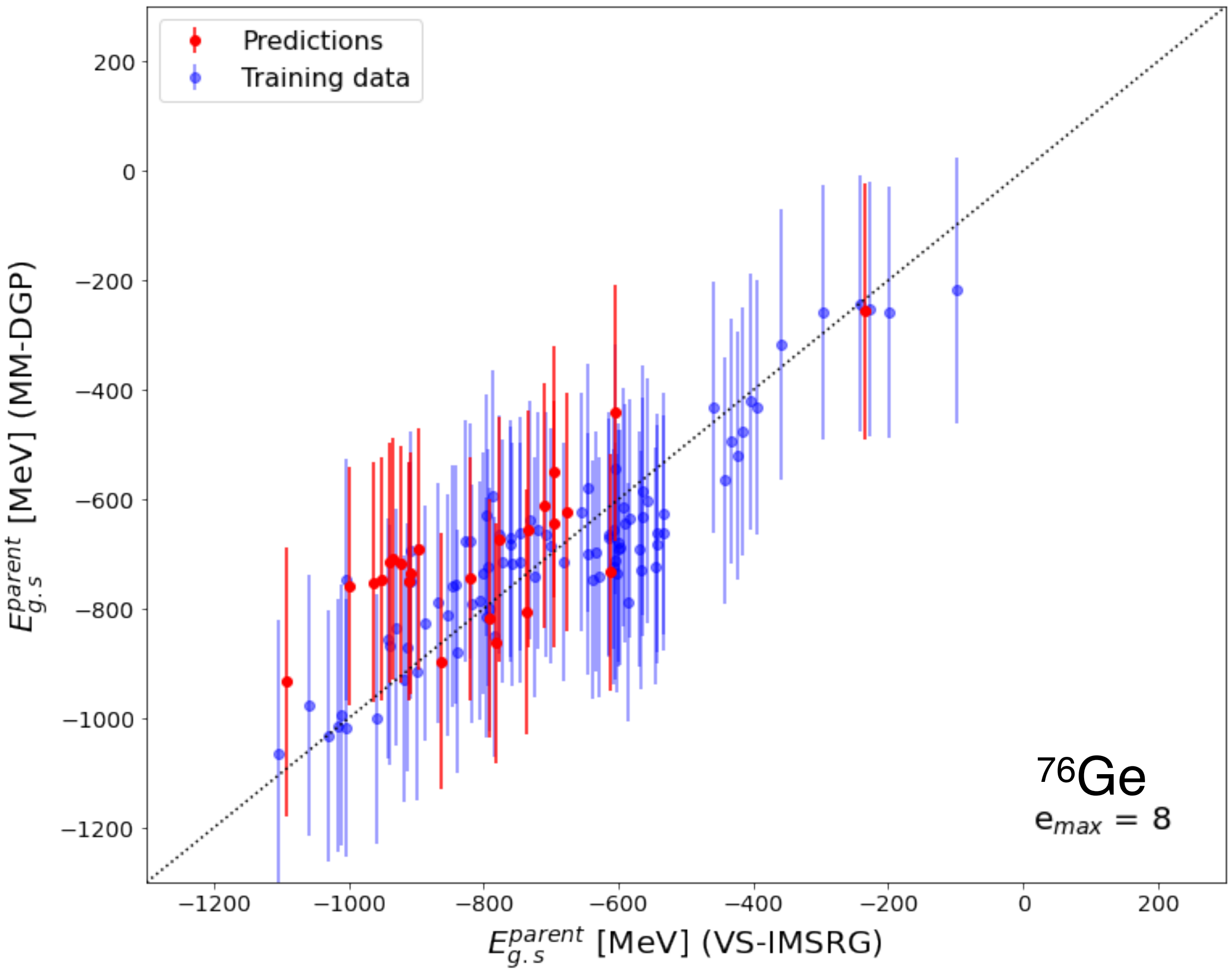
The MM-DGP algorithm: Energies

Using Δ-full chiral EFT interactions at N2LO:

90 training points



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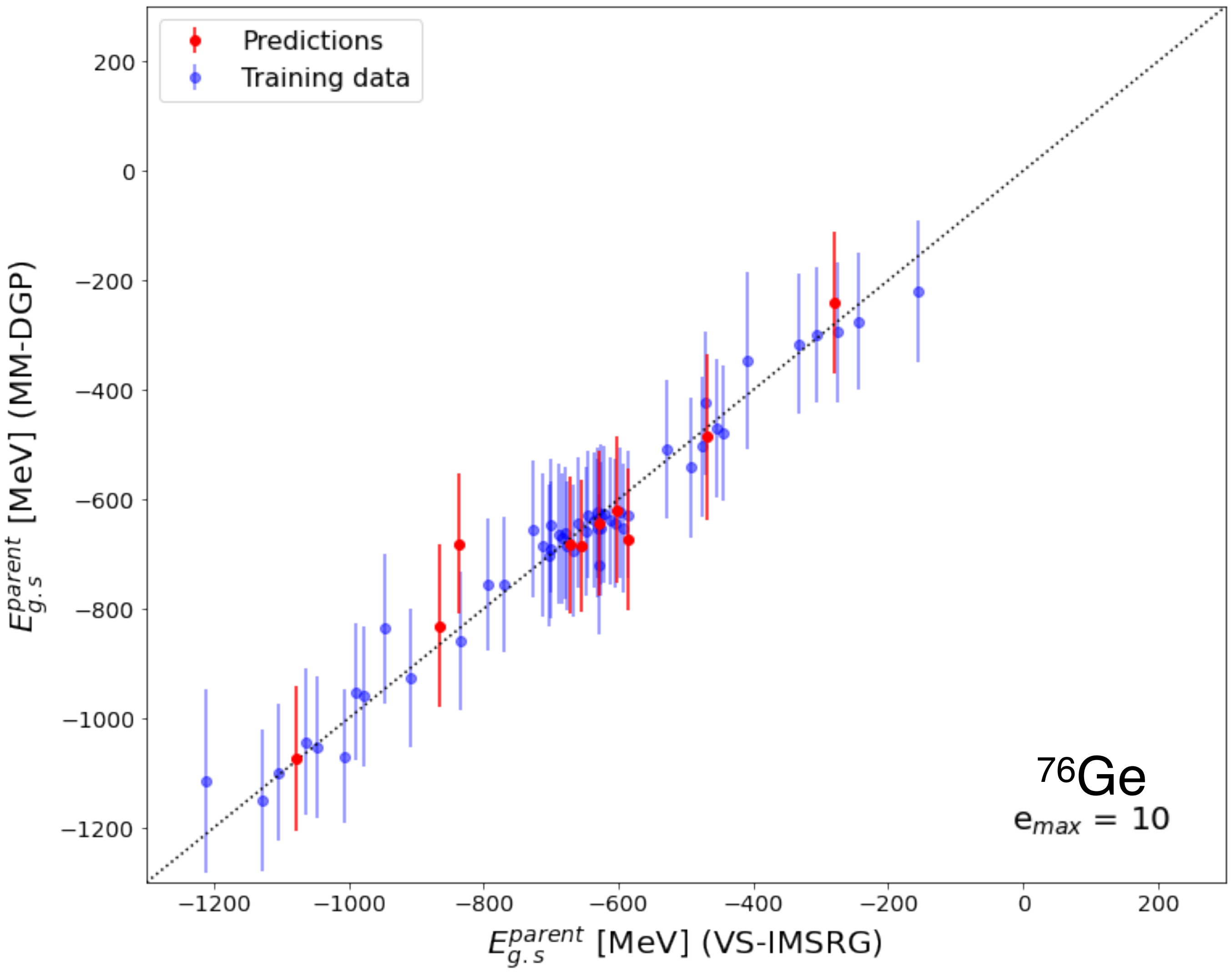

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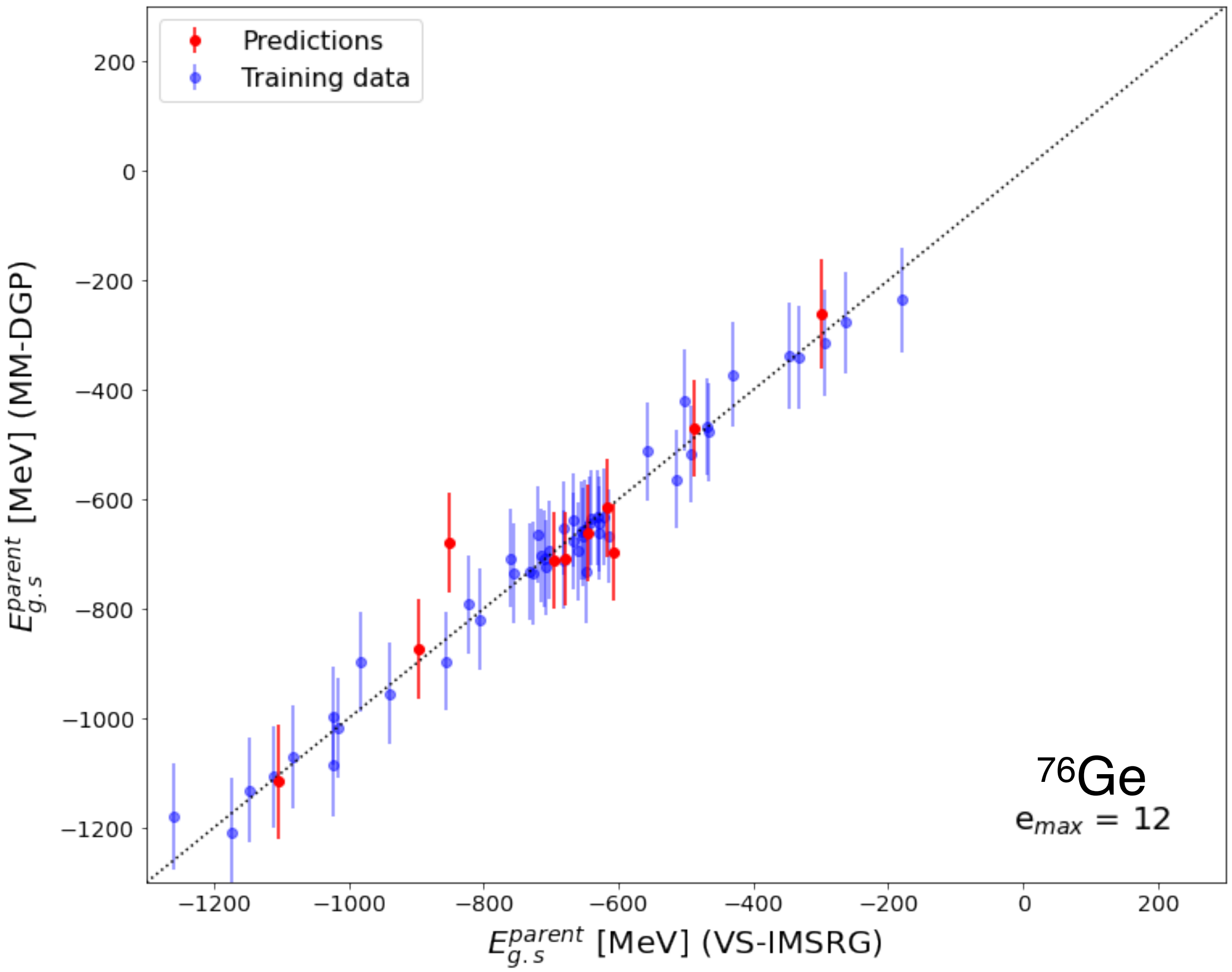

Root Mean Square Error = 29 MeV

Belley, Pitcher et al. in prep.

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The MM-DGP algorithm: $0\nu\beta\beta$ NMEs

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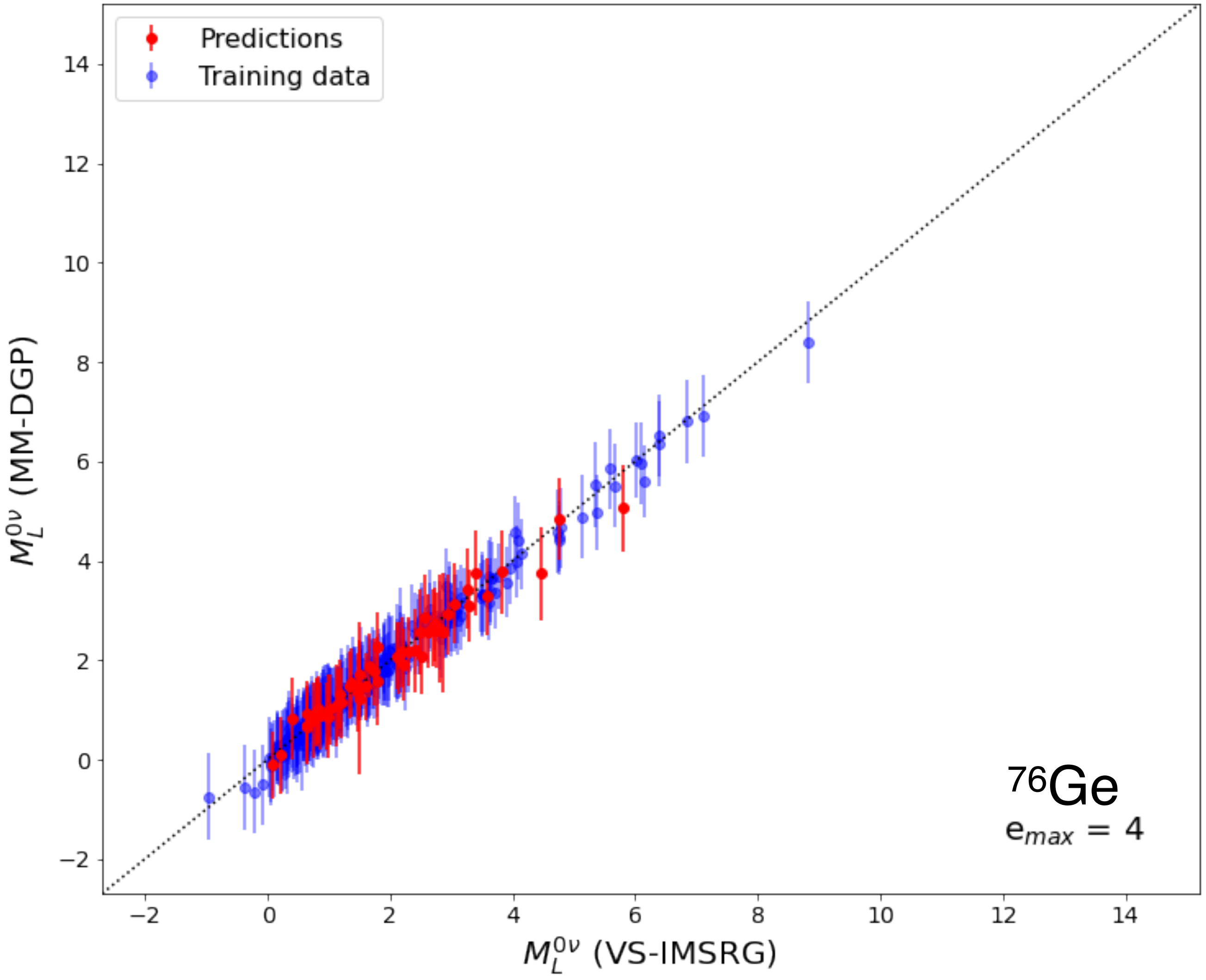

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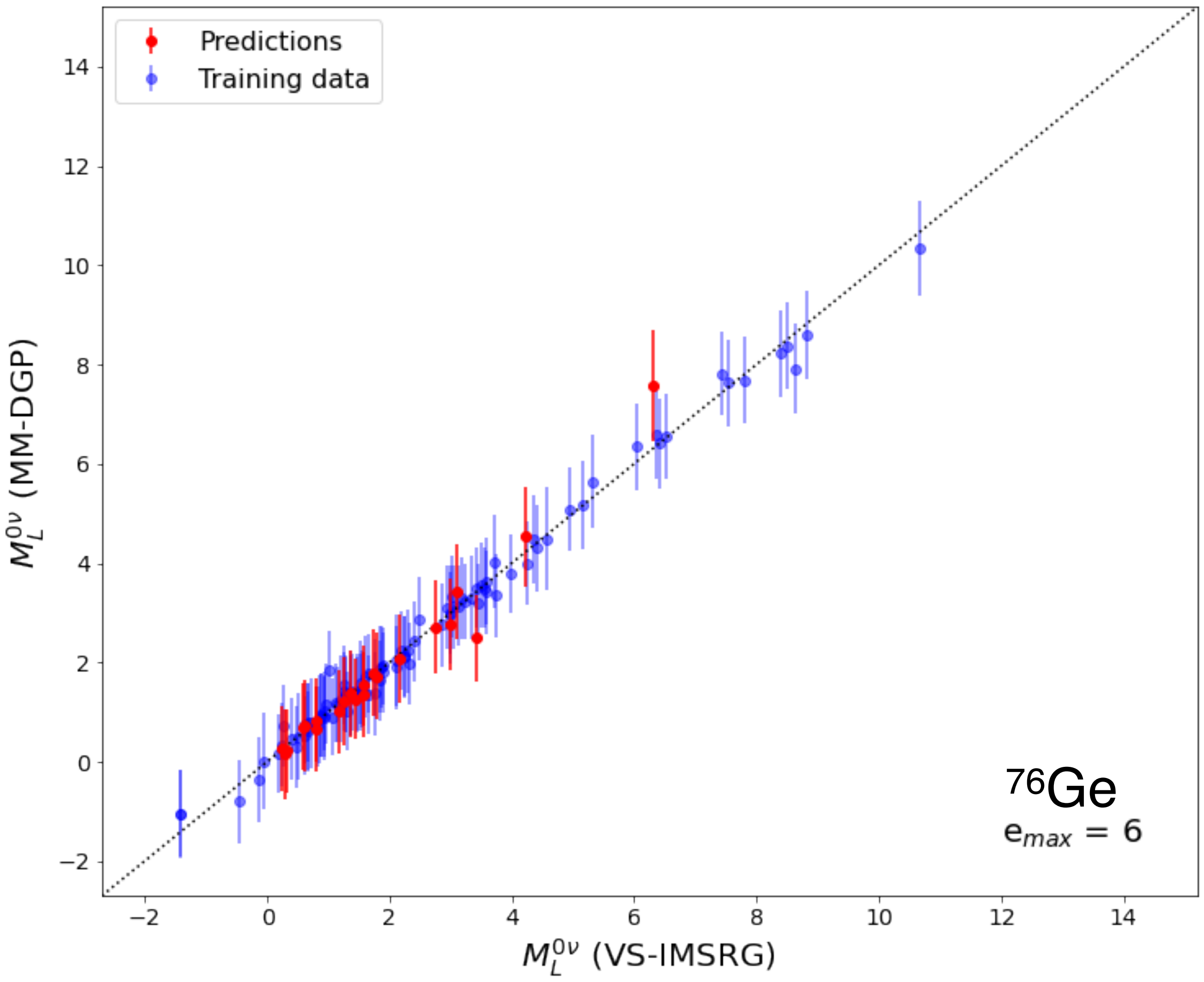

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Using Δ-full chiral EFT interactions at N2LO:

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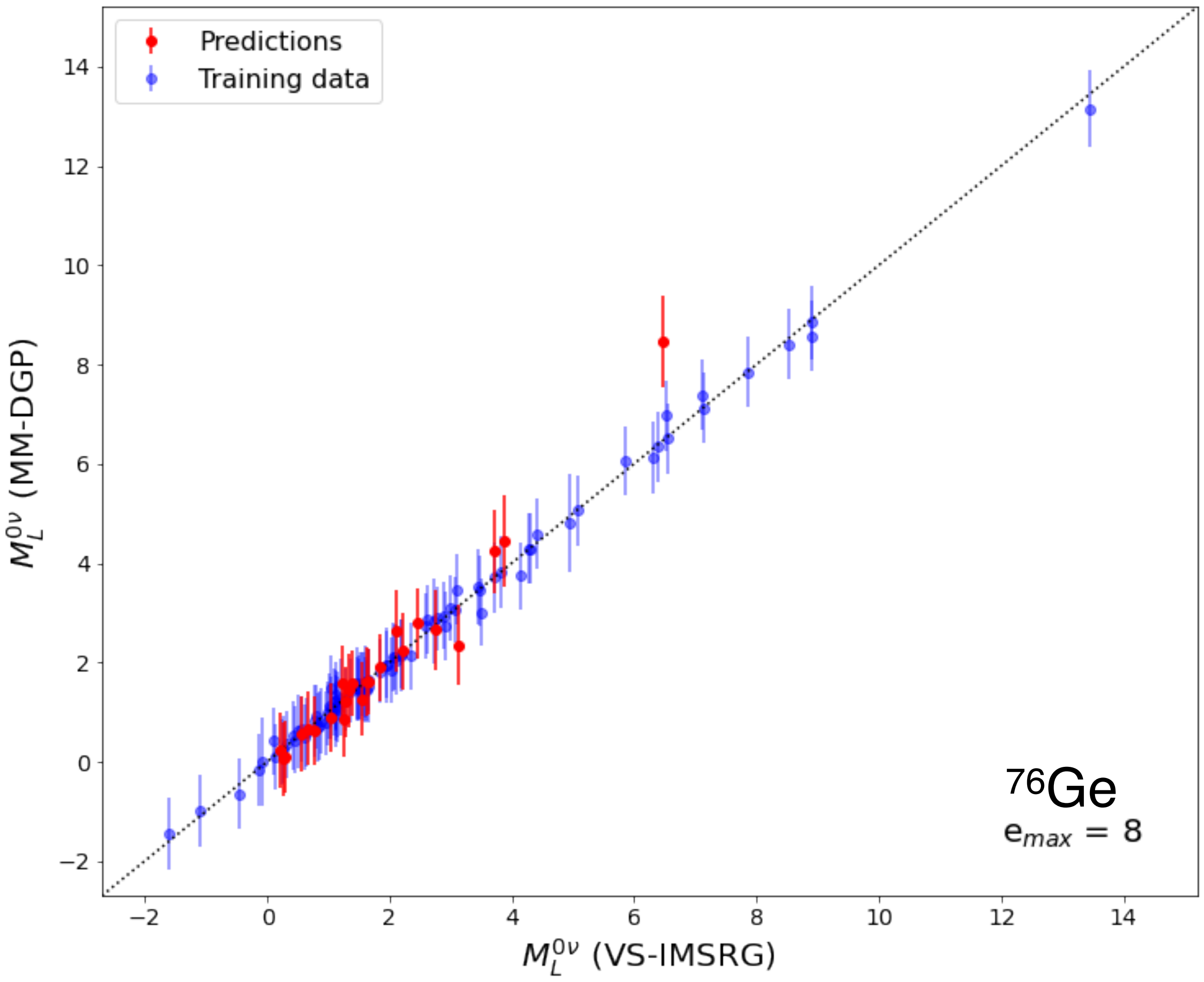
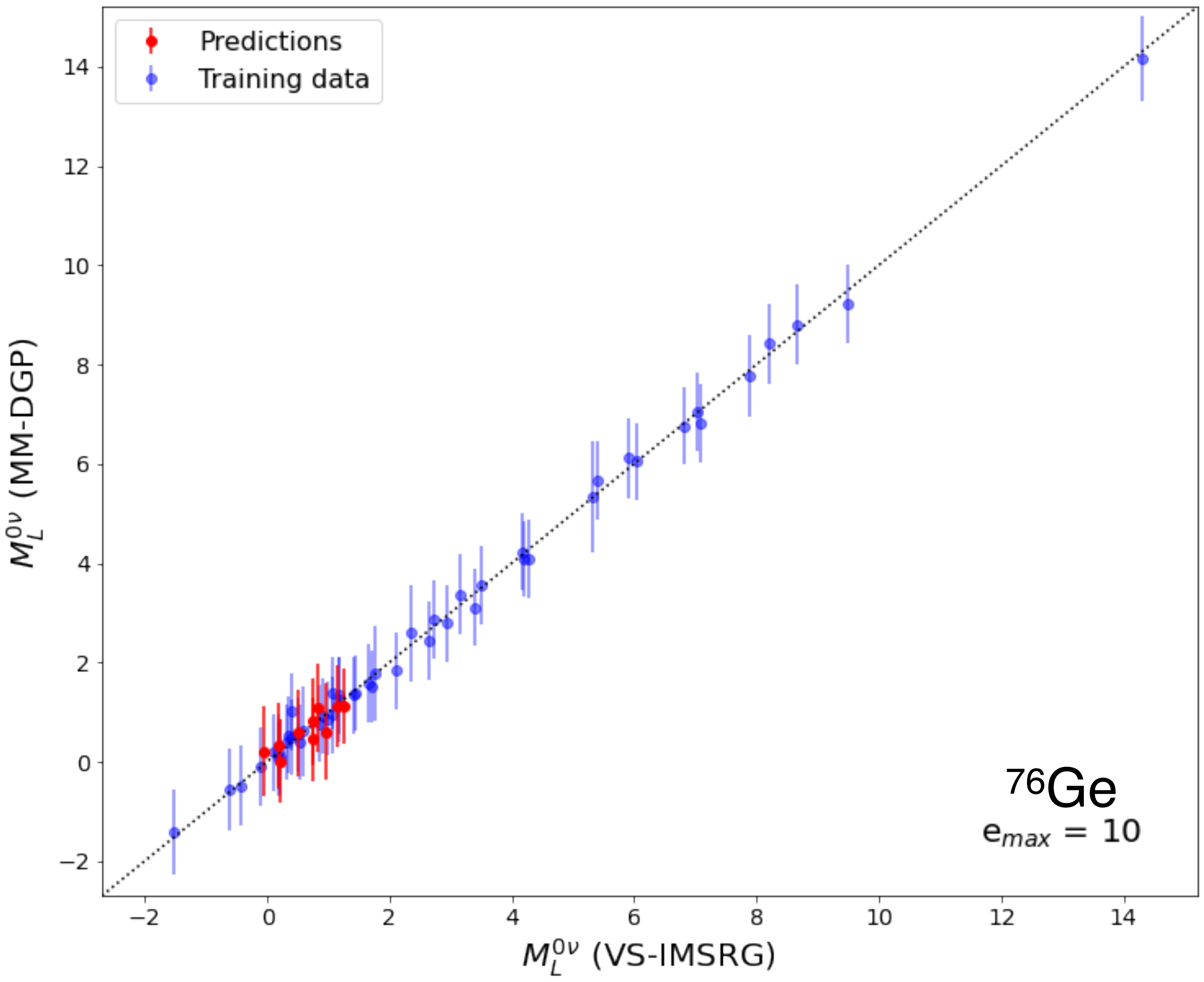


Belley, Pitcher et al. in prep.

The MM-DGP algorithm: 0νββ NMEs

Using Δ-full chiral EFT interactions at N2LO:

50 training points



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The MM-DGP algorithm: $0\nu\beta\beta$ NMEs

Using Δ-full chiral EFT interactions at N2LO:

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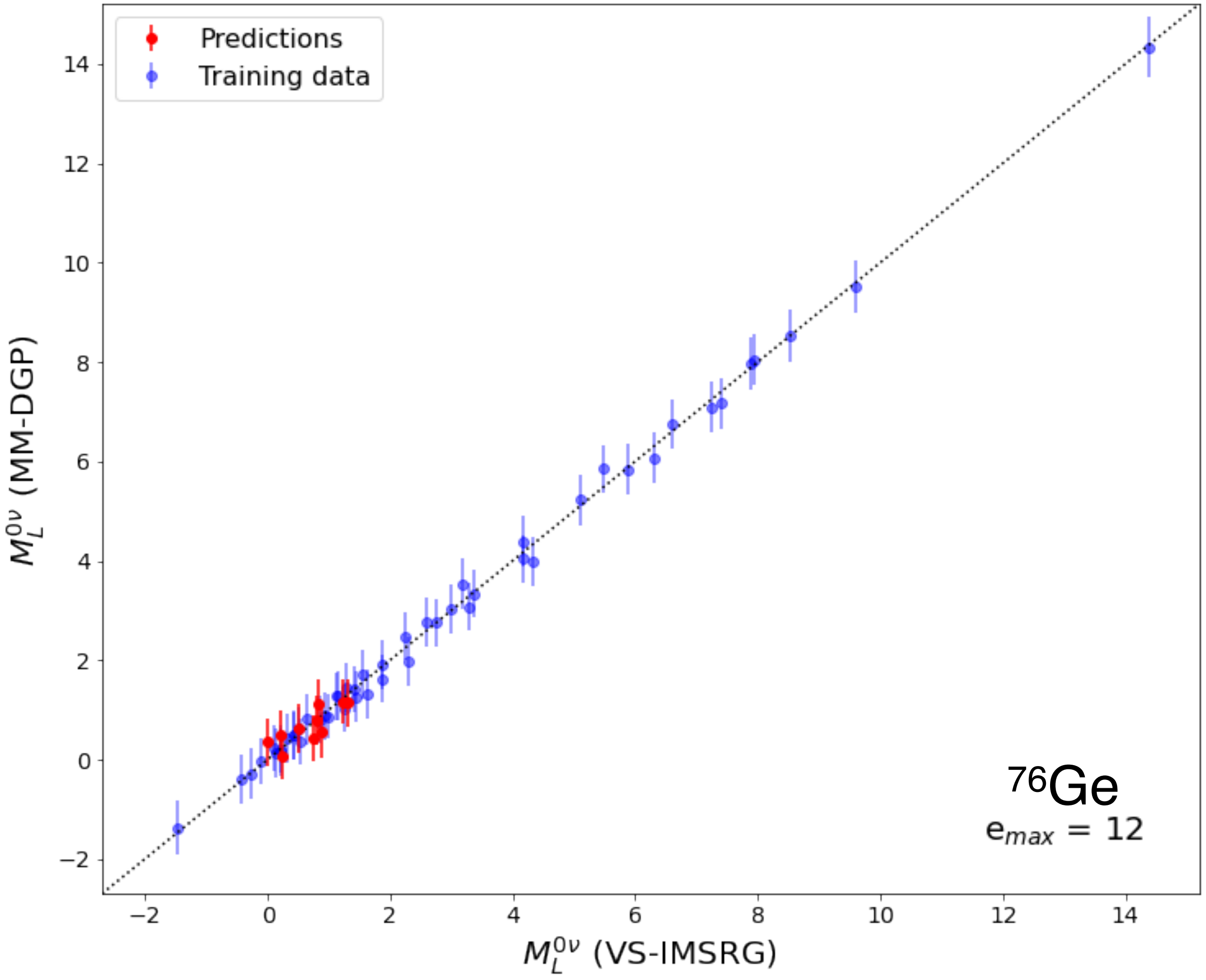
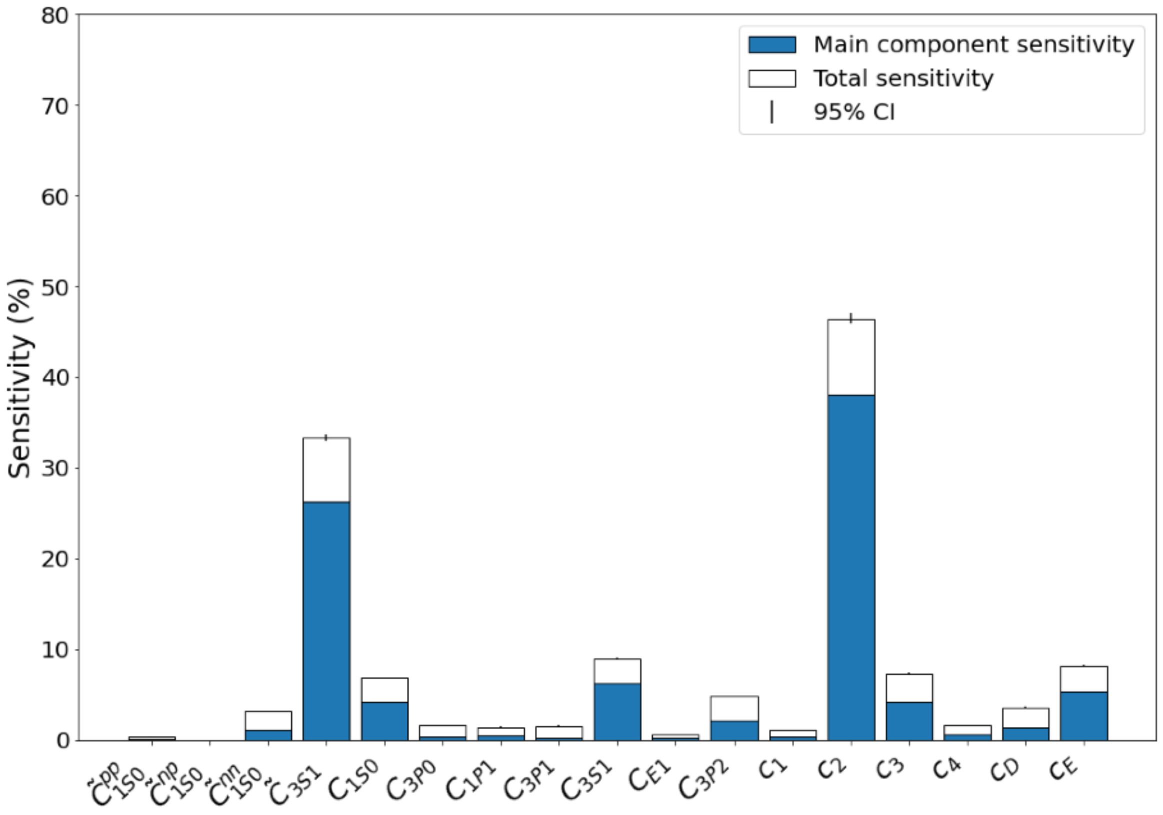


Root Mean Square Error = 0.001

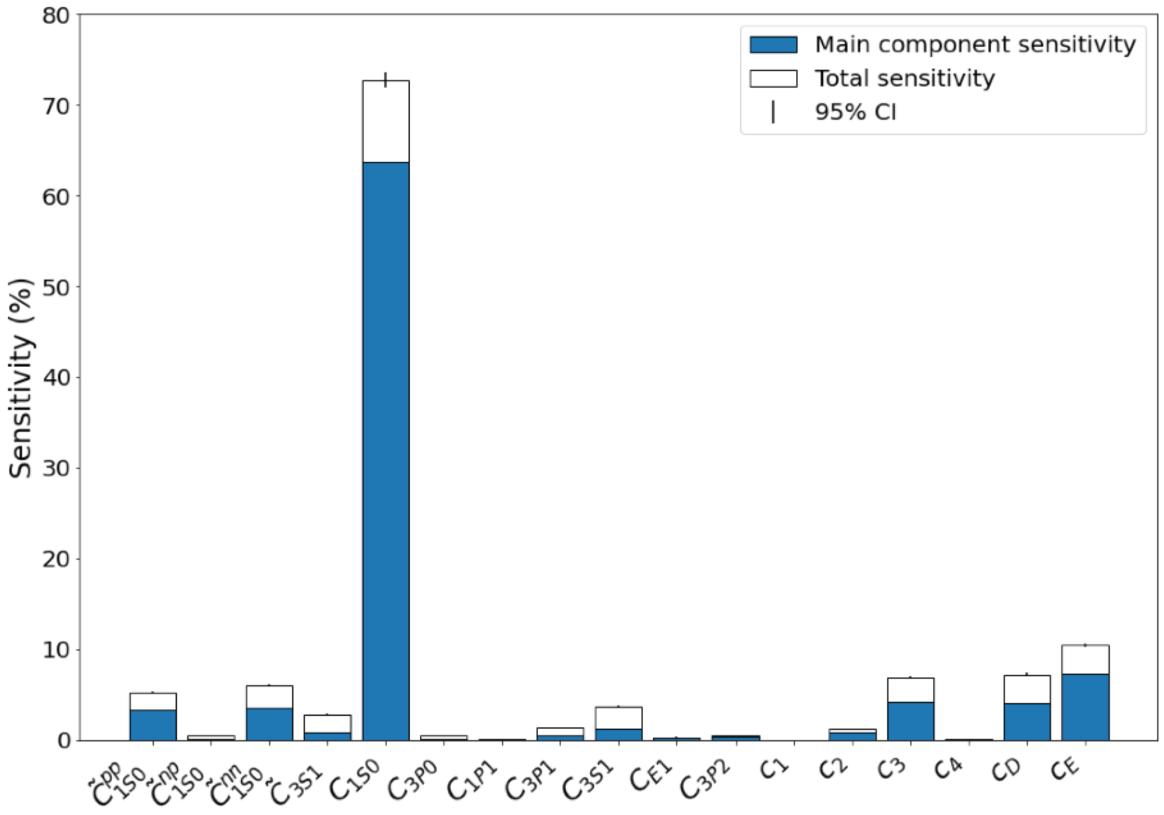
Belley, Pitcher et al. in prep.

The MM-DGP algorithm: GSA

Ground state energies



$M_L^{0\nu}$



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The MM-DGP algorithm: GSA

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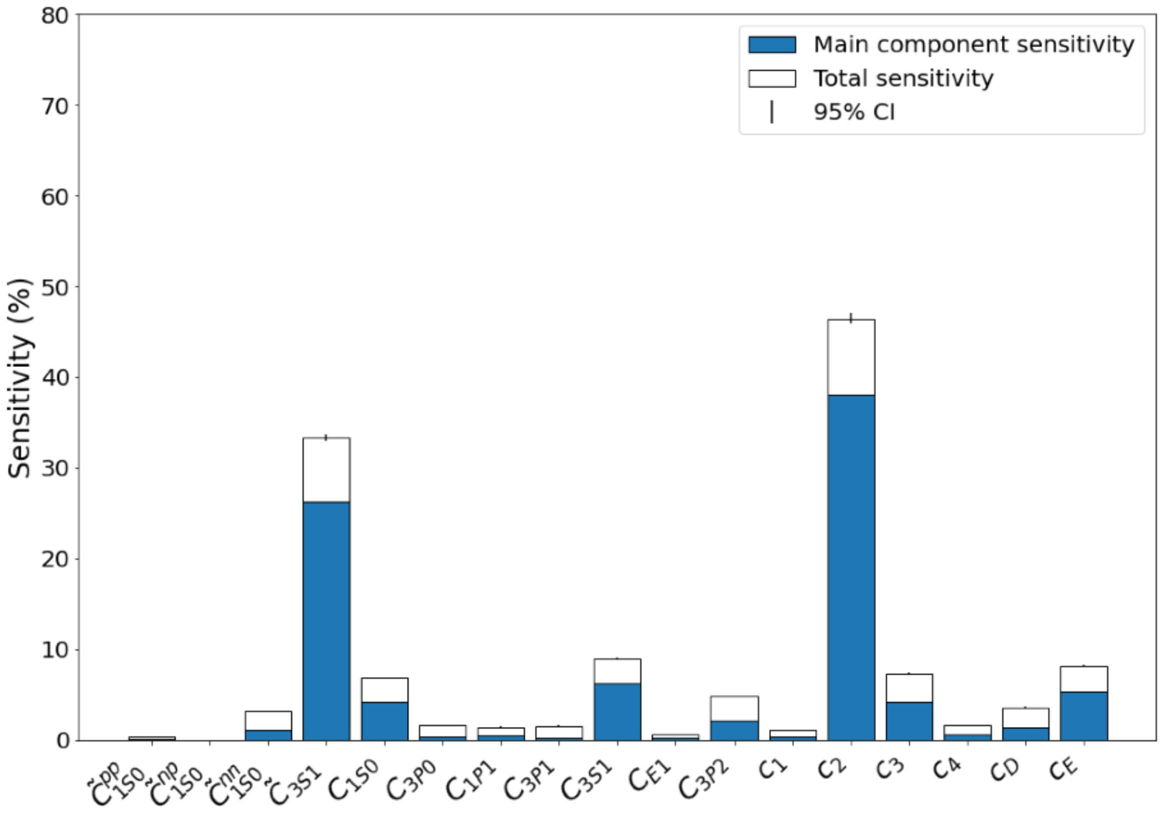

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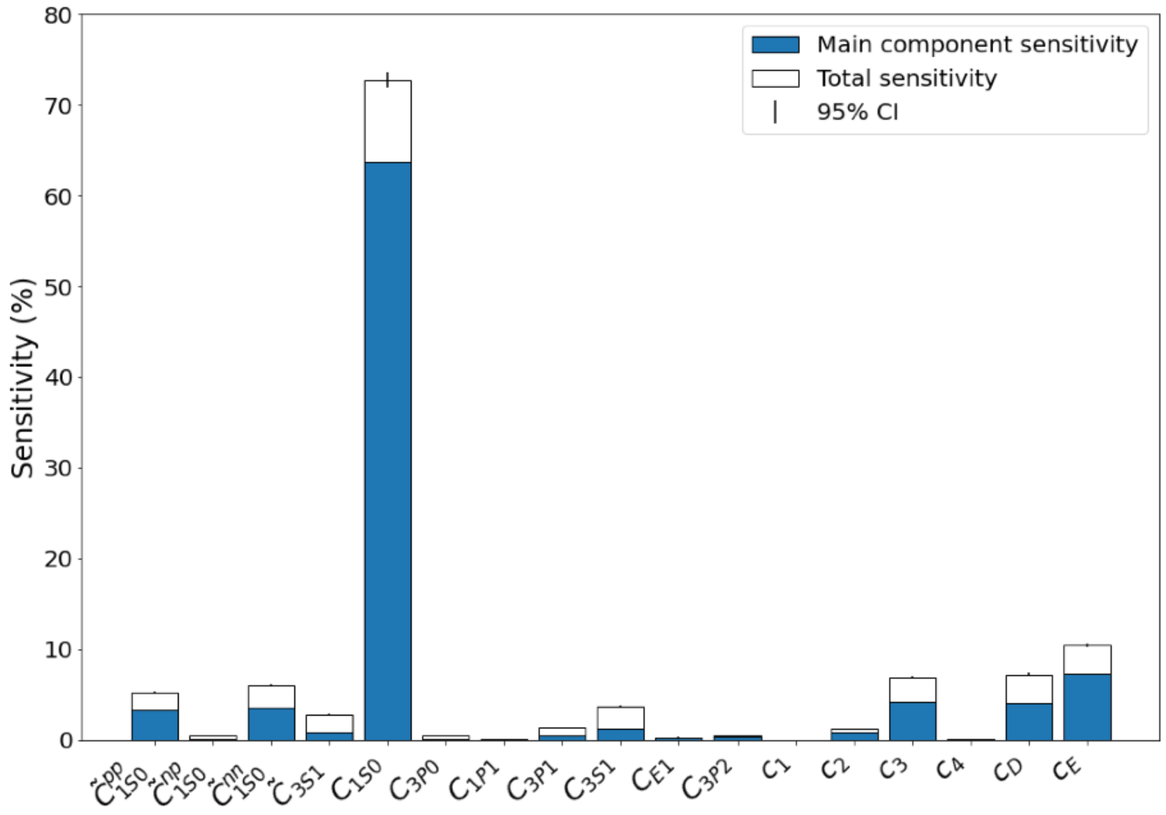


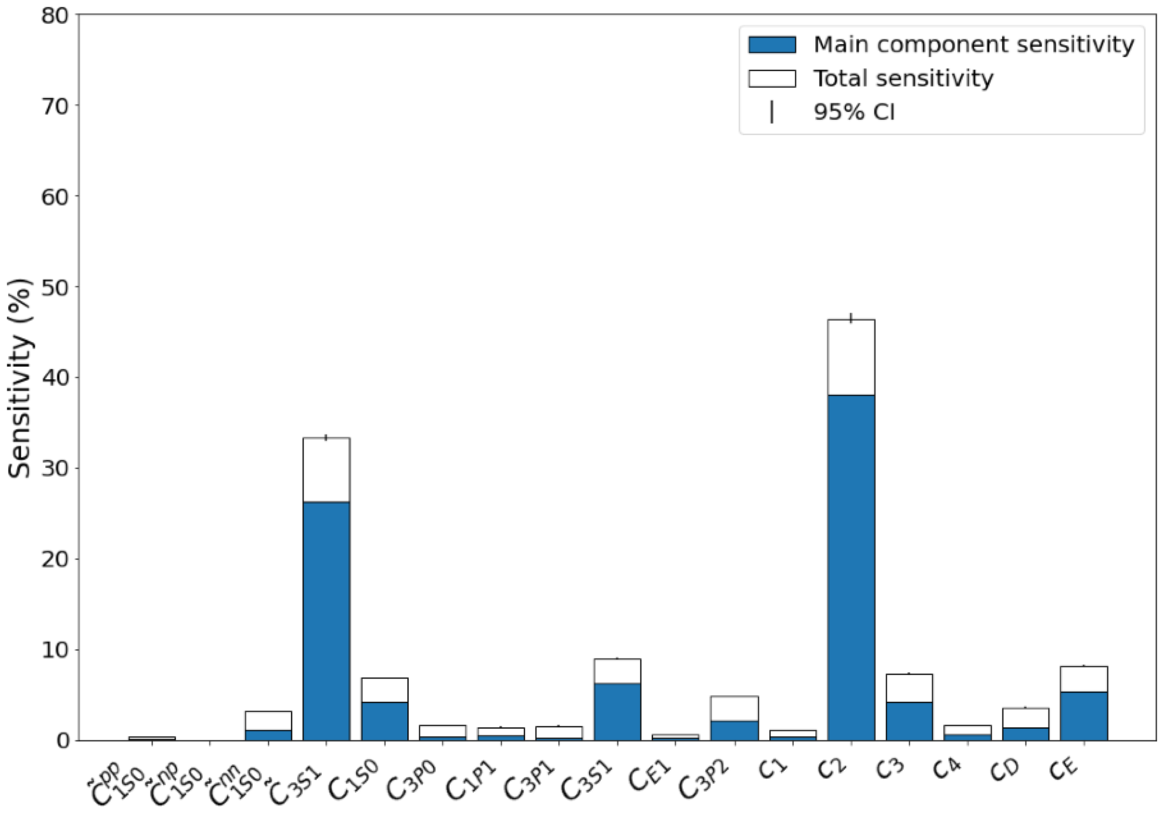
Consistent with results of Coupled Cluster and physics based emulator

Belley, Pitcher et al. in prep.

TRIUMF

The MM-DGP algorithm: GSA

Ground state energies



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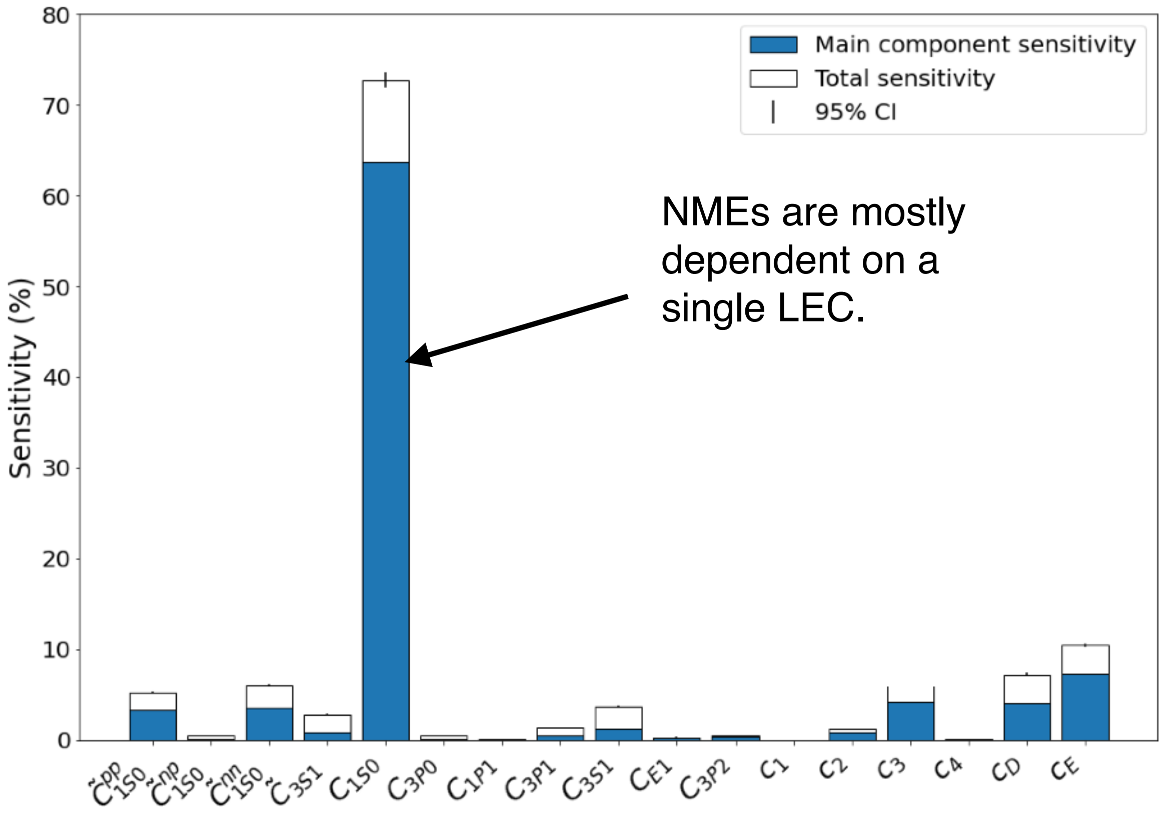

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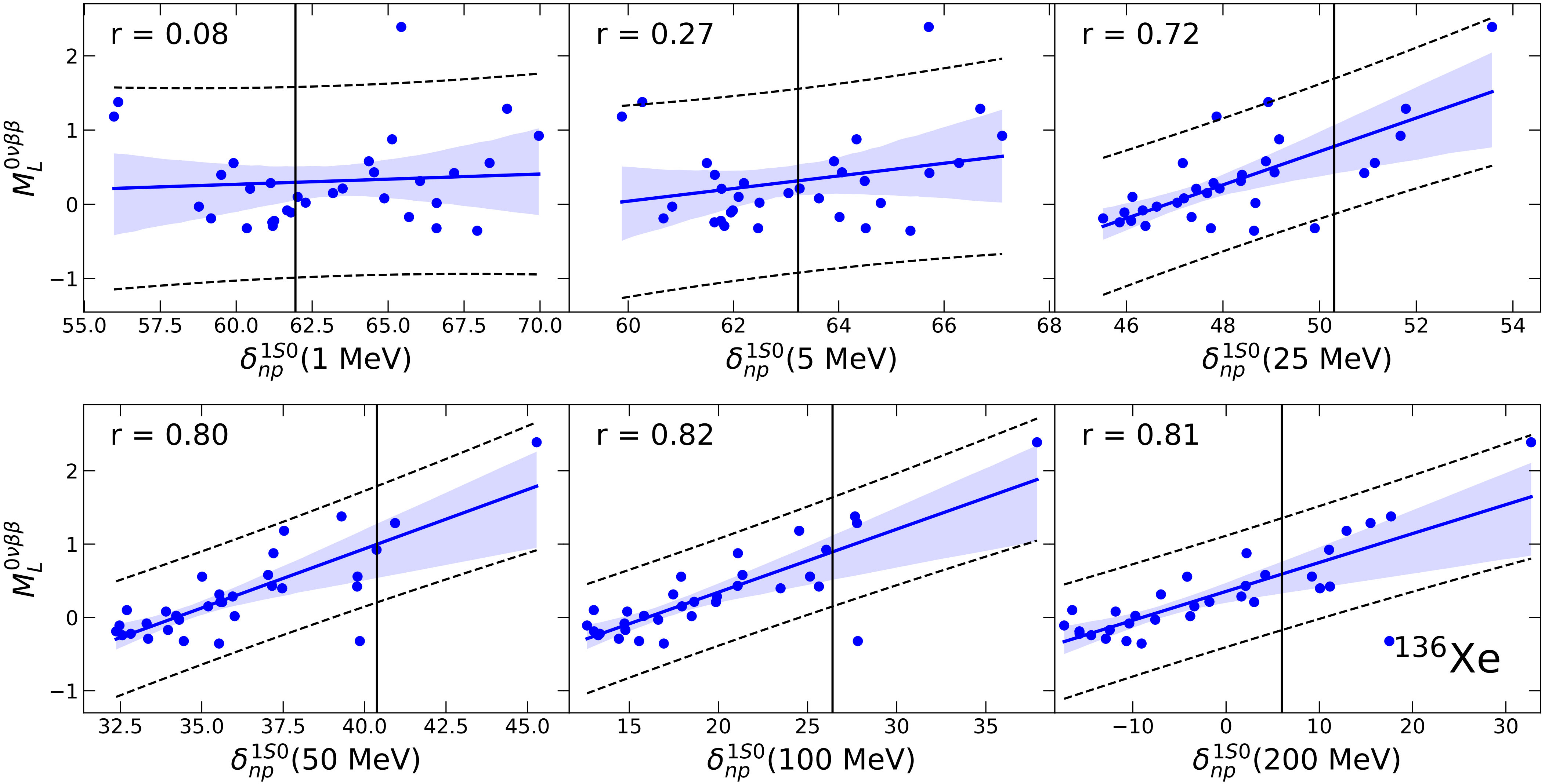
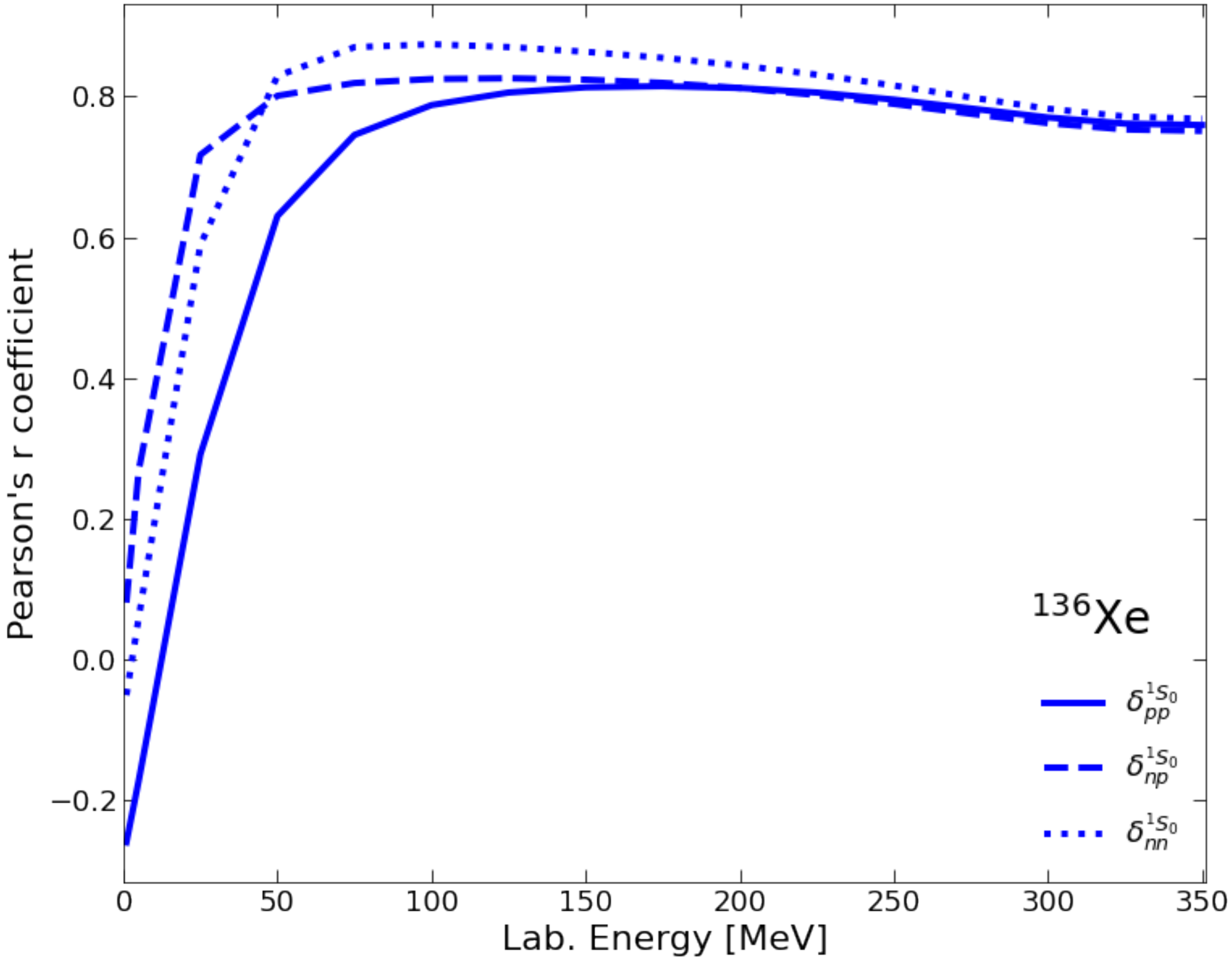
Belley, Pitcher et al. in prep.

Correlation with phase shifts



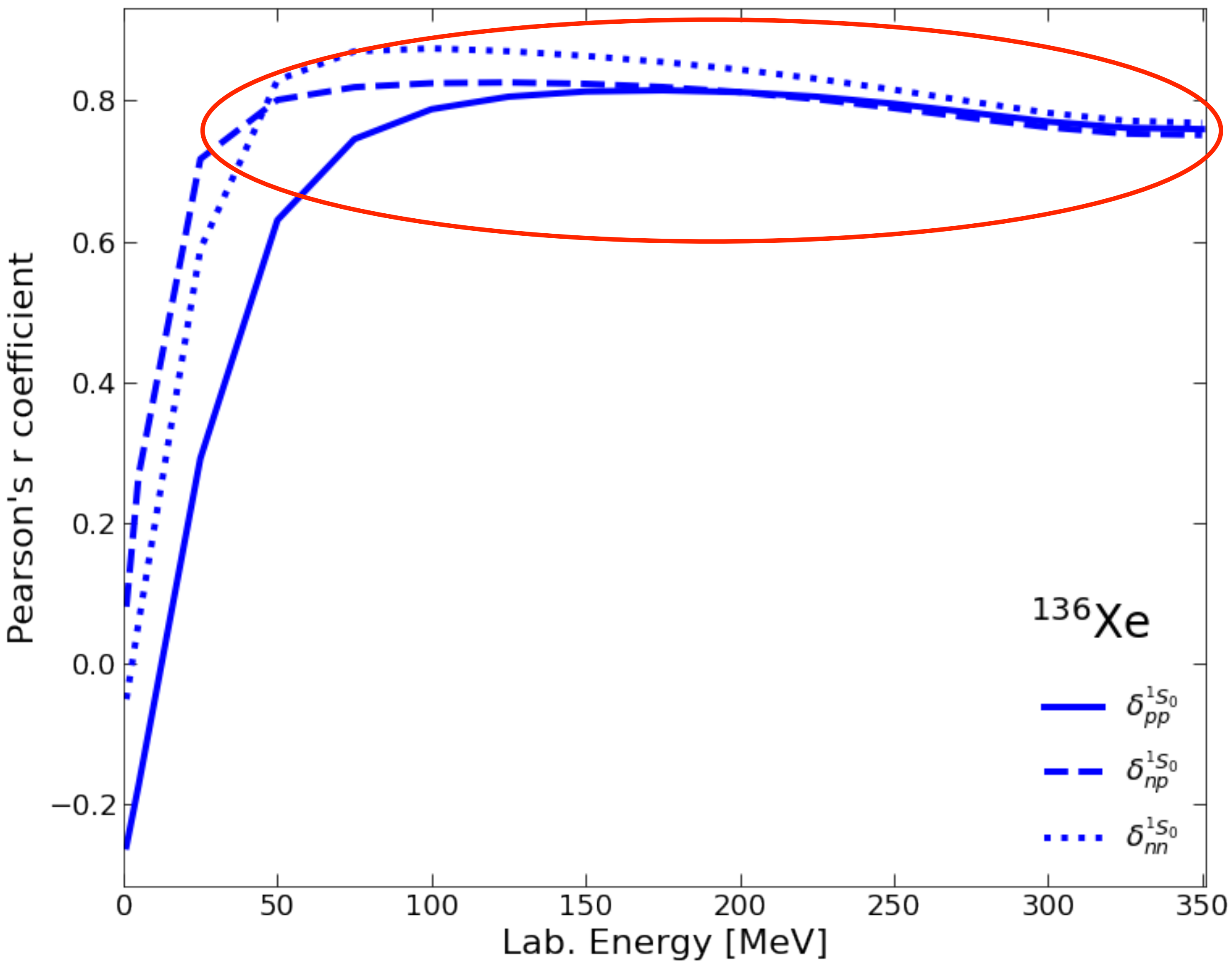
Belley, Pitcher et al. in prep.

Correlation with phase shifts



Belley, Pitcher et al. in prep.

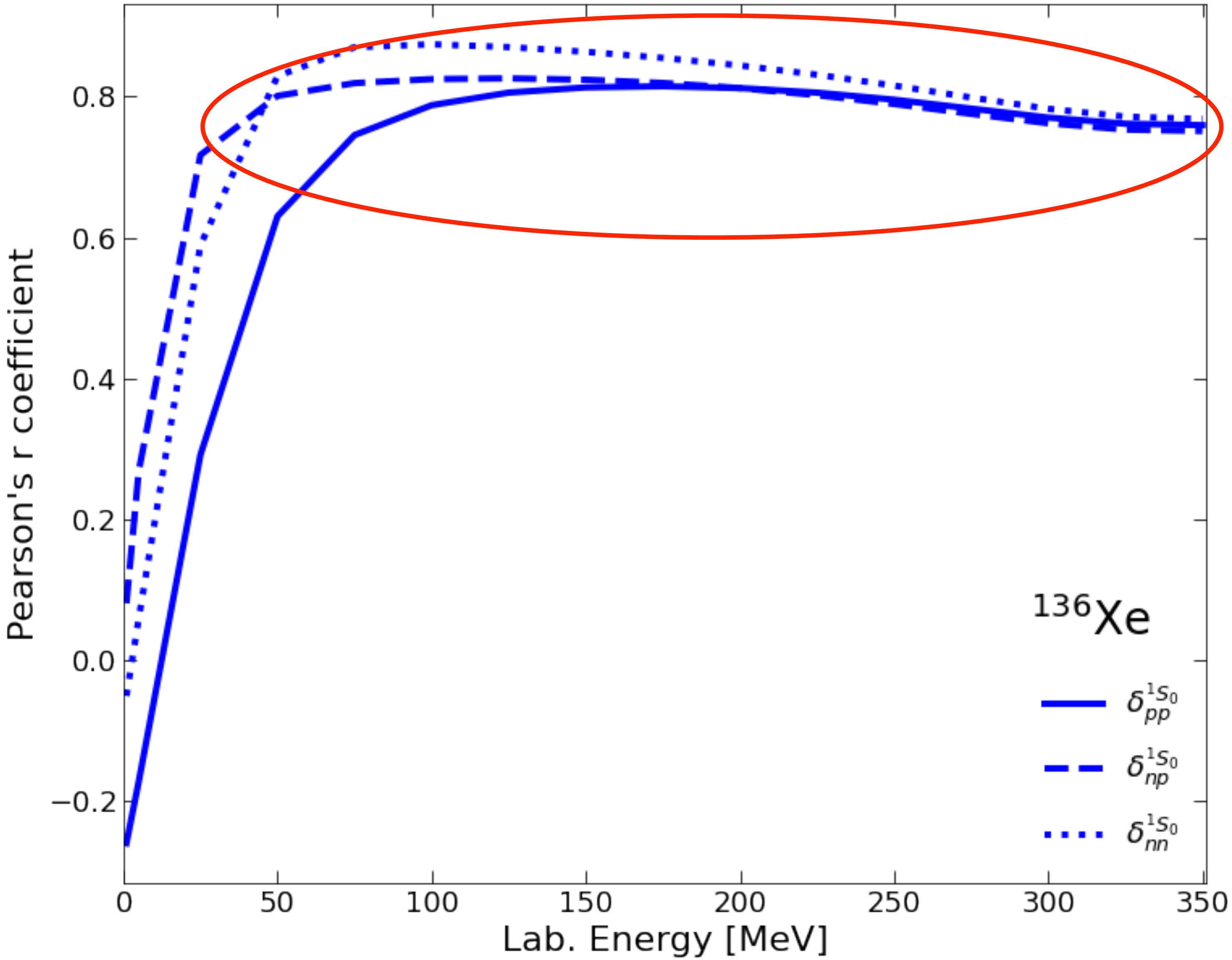
Correlation with phase shifts



Strong correlation for energies > 50 MeV

Belley, Pitcher et al. in prep.

Correlation with phase shifts



Strong correlation for energies > 50 MeV

⇛

The size matrix elements is mostly constrained by the interaction between the two nucleons that undergo the decay, given they are close enough from each others.

Belley, Pitcher et al. in prep.

Bayesian approach

Value of the nuclear matrix elements (what we are interested in)

Different values obtain with different interactions/ methods

Any other relevant information we have before hand

$$prob(y\,|\,y_k, I) \propto prob(y_k\,|\,y, I) \times prob(y\,|\,I)$$

We read $prob(A\,|\,B)$ as probability of A given B

Bayesian approach

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$$prob(y \mid y_k, I) \propto prob(y_k \mid y, I) \times \underbrace{prob(y \mid I)}$$

We read $prob(A \mid B)$ as probability of A given B

Prior
Assume a uniform prior for low energy constants of natural size. Then use history matching to remove implausible samples from the set. Assume each of the remaining samples to be as likely as the others.

Bayesian approach

Value of the nuclear matrix elements (what we are interested in)

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$$prob(y \mid y_k, I) \propto \underbrace{prob(y_k \mid y, I)} \times \underbrace{prob(y \mid I)}$$

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Likelihood
Probability that this sample give a results that is representative of experimental values.

Chosen to be a multivariate normal centred at the experimental value for few observables we have data on (calibrating observables).

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$$prob(y \mid y_k, I) \propto prob(y_k \mid y, I) \times prob(y \mid I)$$

We read $prob(A \mid B)$ as probability of A given B

Posterior distribution
Probability distribution for the final value given the data and our previous knowledge (what we want to obtain).

For finite samples, we use sampling/importance resampling to obtain the final PDF.

Likelihood
Probability that this sample give a results that is representative of experimental values.

Chosen to be a multivariate normal centred at the experimental value for few observables we have data on (calibrating observables).

Prior
Assume a uniform prior for low energy constants of natural size. Then use history matching to remove implausible samples from the set. Assume each of the remaining samples to be as likely as the others.

Posterior distribution of the NMEs

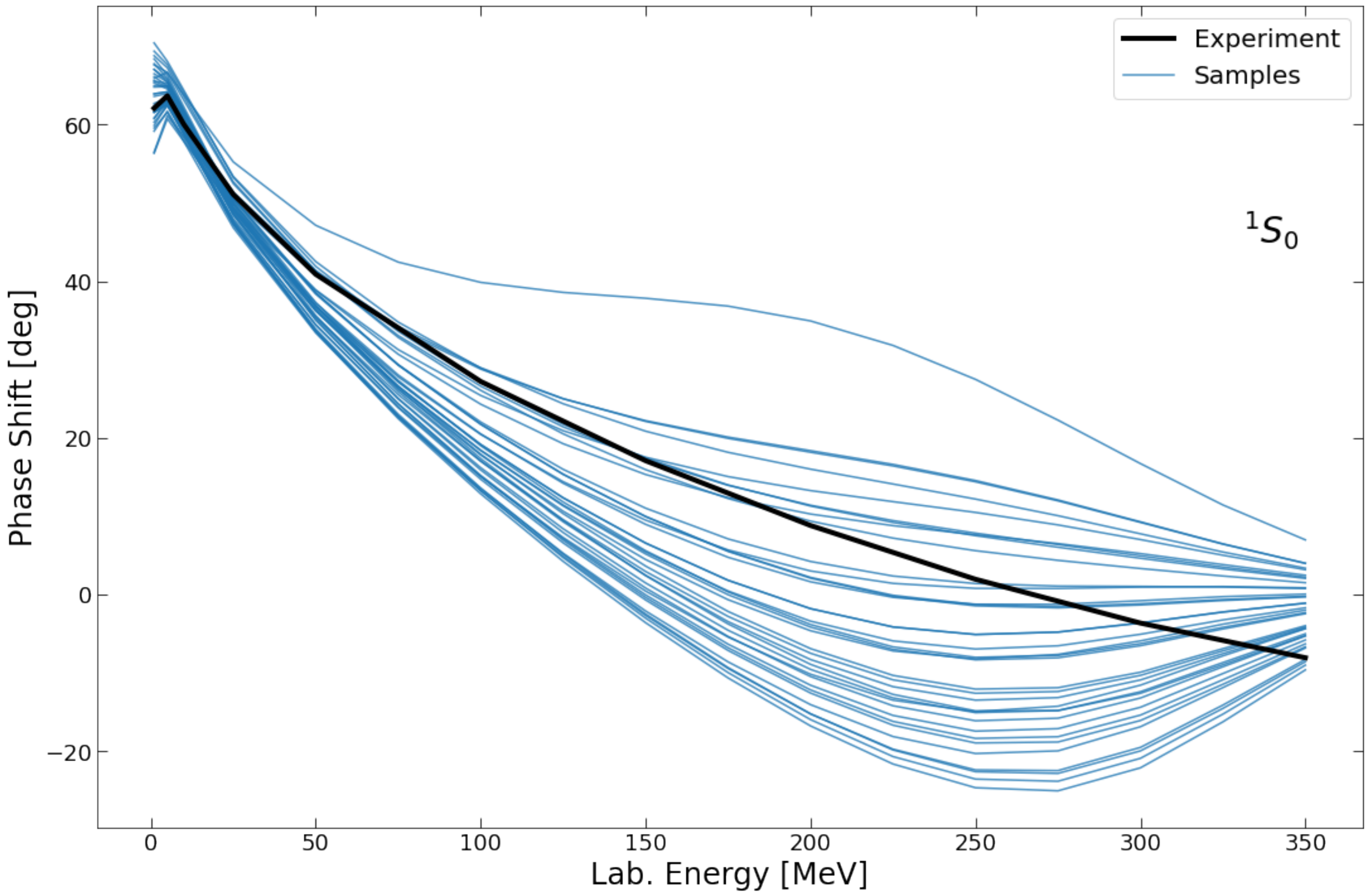
- Use 8188 “non-implausible” samples obtain by Jiang, W. G. et al. (arXiv:2212.13216)
- Many-body problem is “solved” with the MM-DGP.
- Considers all sources of uncertainties by taking:

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

where the ϵ’s are the errors coming from different sources and are assumed to be normally distributed and independent.

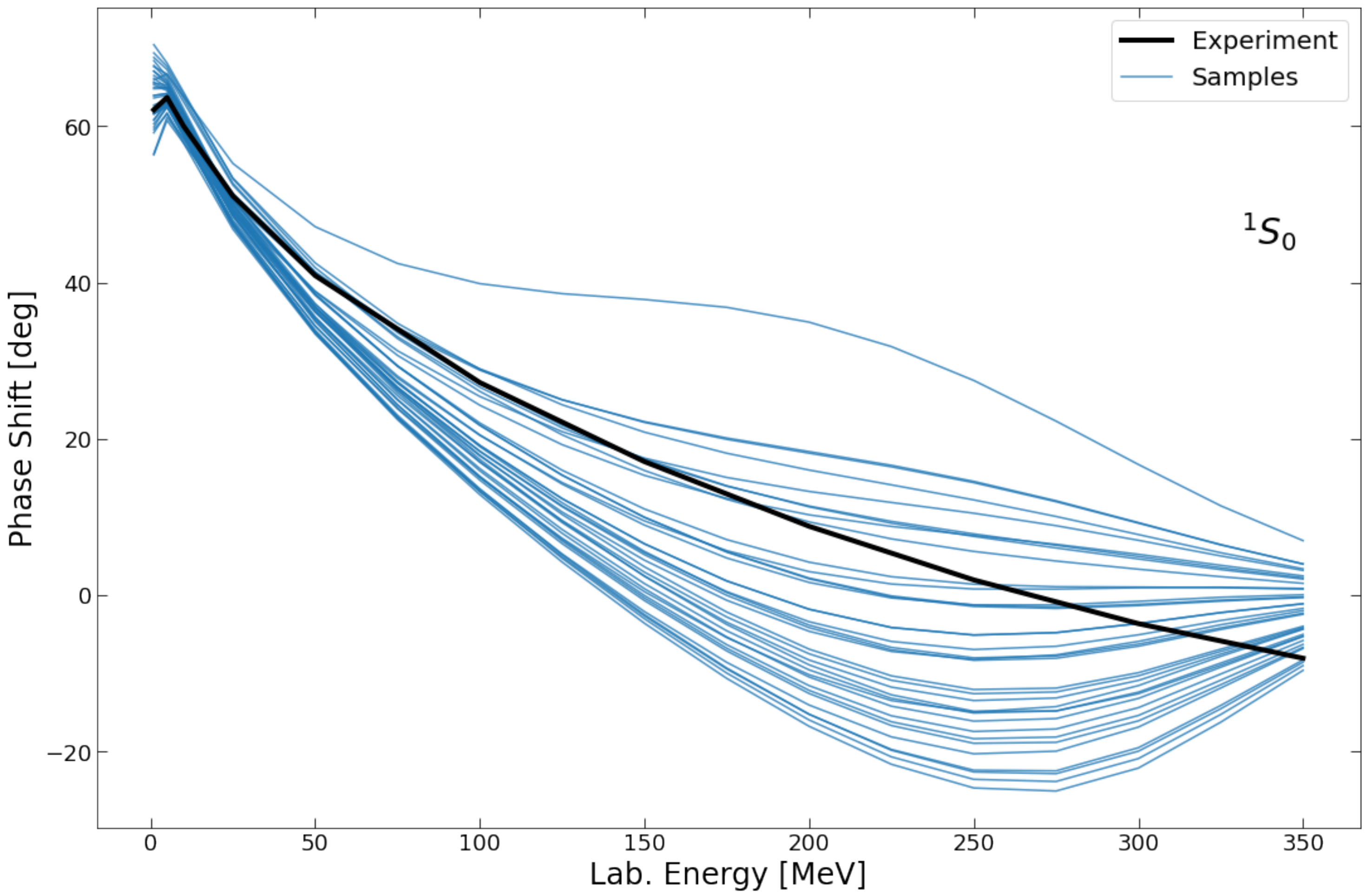
- Interaction are weighted by the $^1S_0$ neutron-proton phase shifts at 50, 100 and 200 MeV.

Choice of calibration observables



Belley, Pitcher et al. in prep.

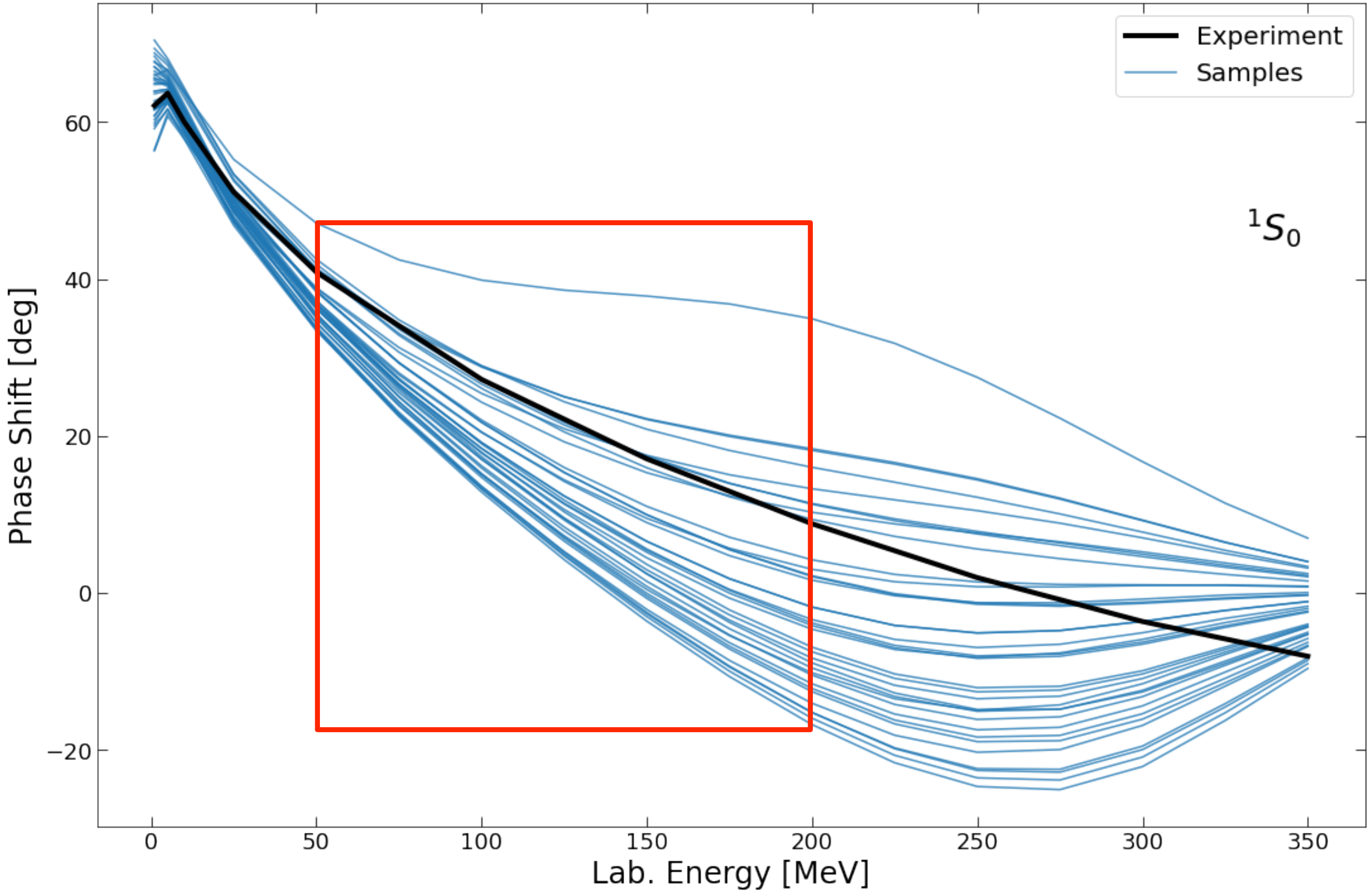
Choice of calibration observables



- Choose np phase shift because it shows correlations at lower energies than pp phase shift and there is little data for the nn phase shift.

Belley, Pitcher et al. in prep.

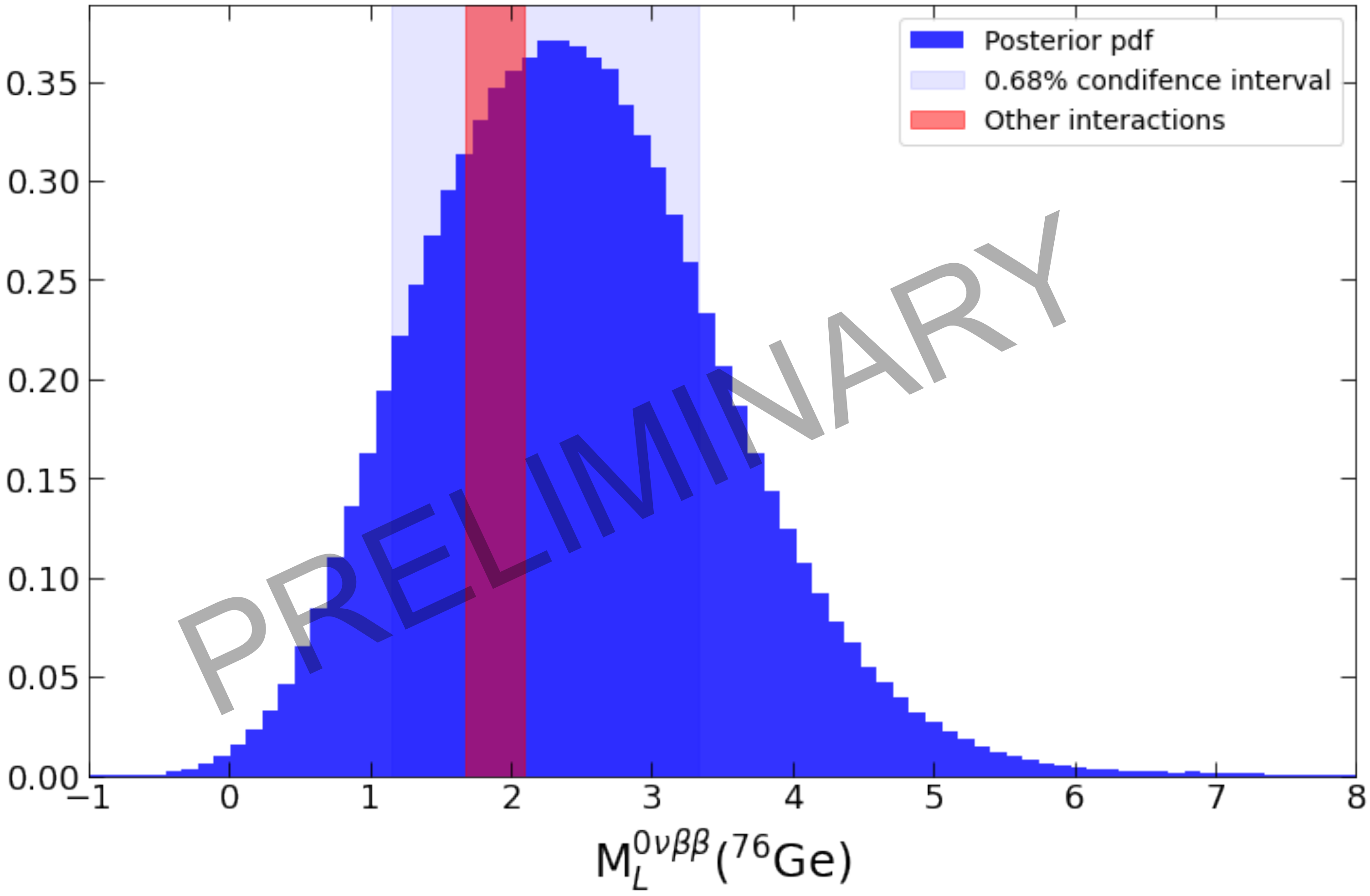
Choice of calibration observables



- Choose np phase shift because it shows correlations at lower energies than pp phase shift and there is little data for the nn phase shift.
- Consider values at 50, 100 and 200 MeV to balance between having a strong correlation with the NMEs and a good description of experimental data.

Belley, Pitcher et al. in prep.

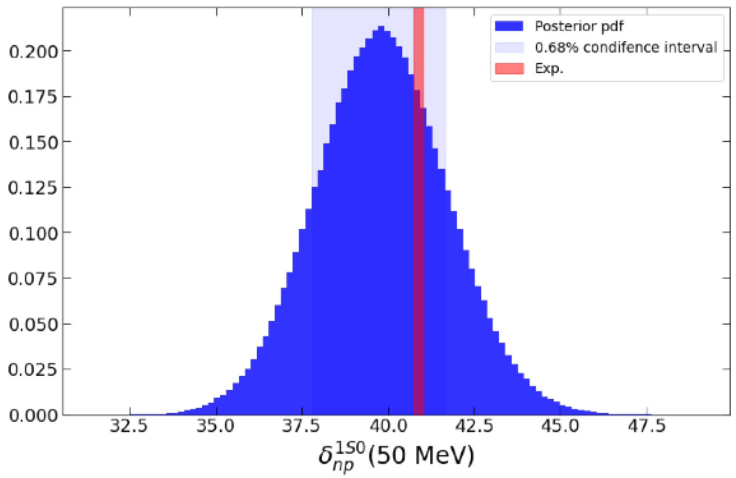
Posterior distribution of the NMEs

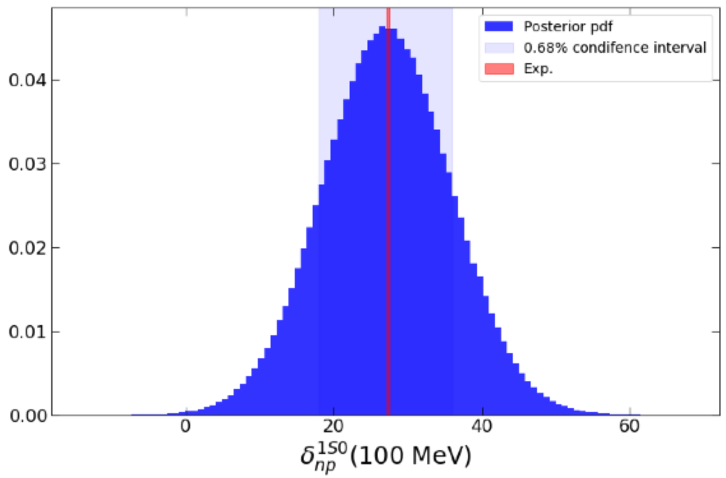


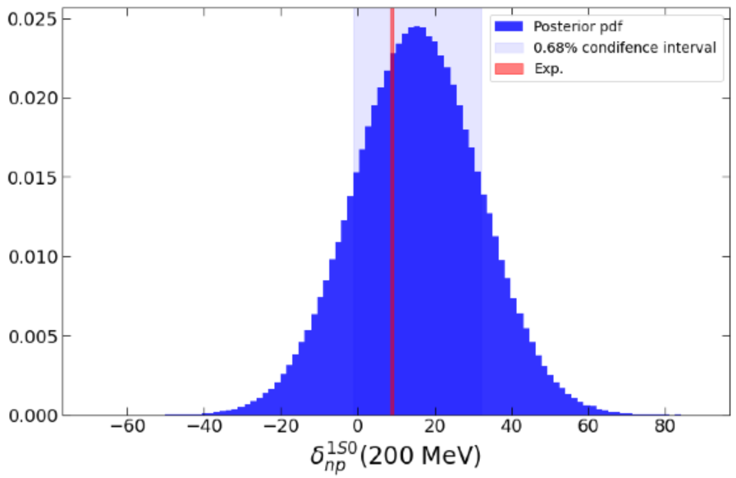
Disclaimer: Some of the uncertainty terms are currently estimated and still need to be more carefully looked into.

Posterior distribution of other observables

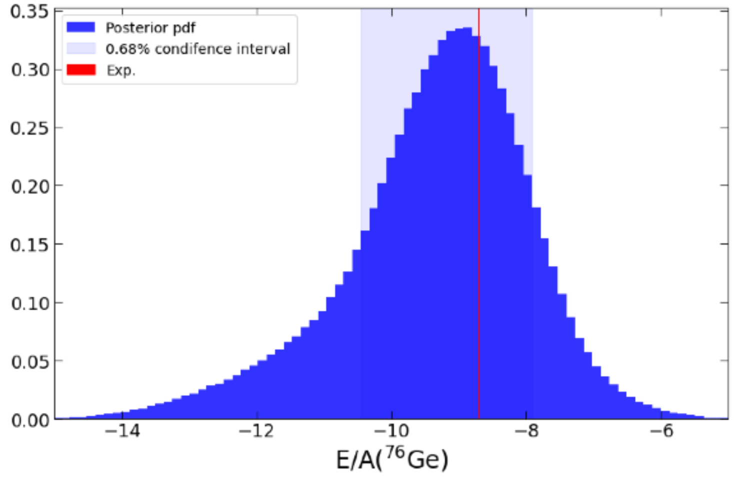
Calibration observables:

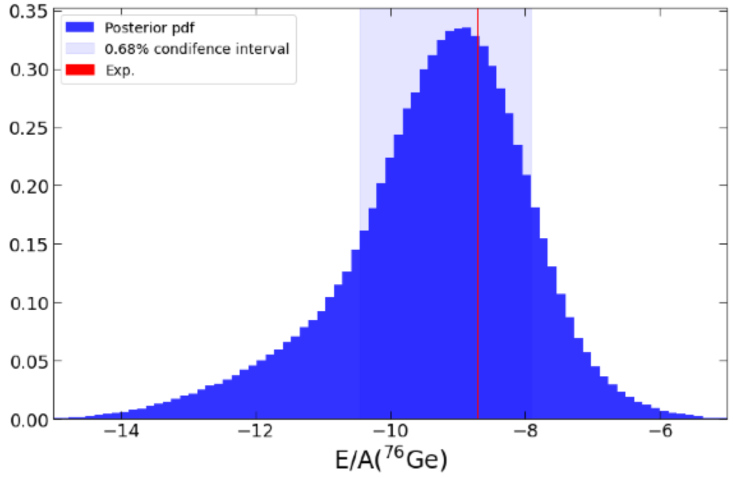






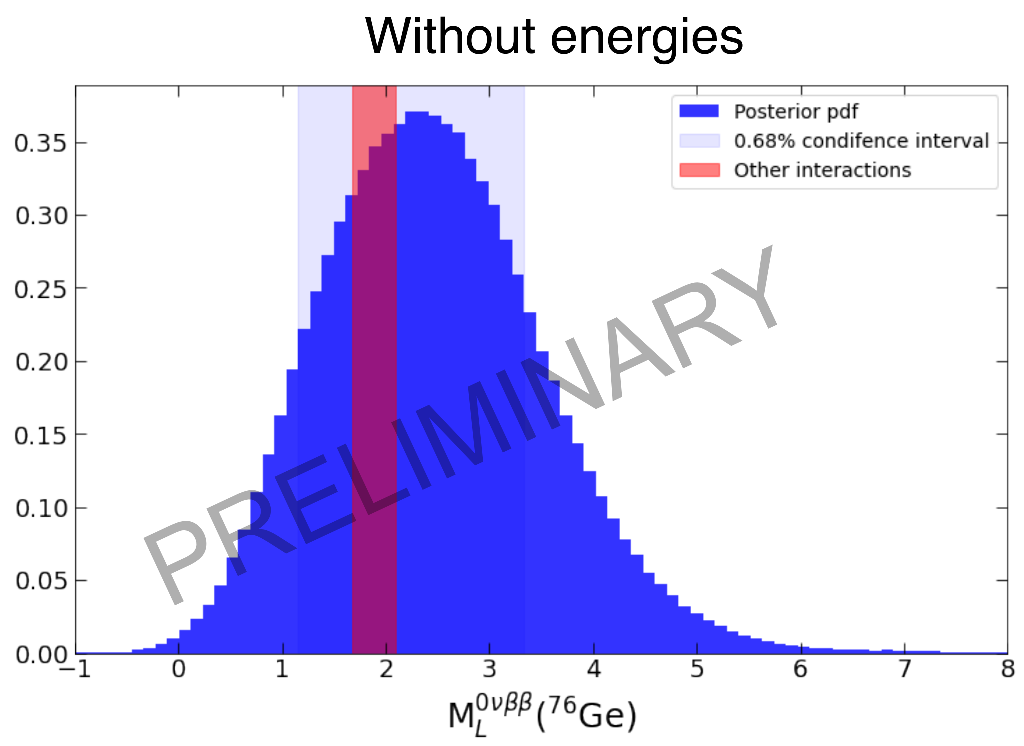
Validation observables:





Changing the calibration

We can verify that the energies are indeed uncorrelated to the NMEs by adding them to the calibration observables.



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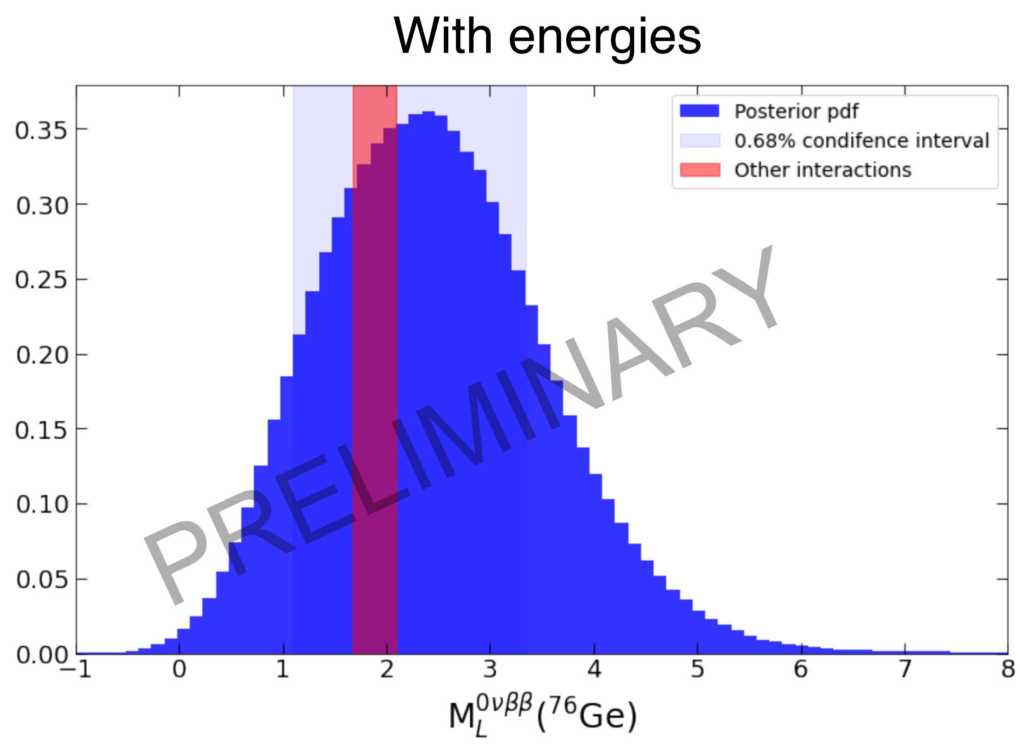
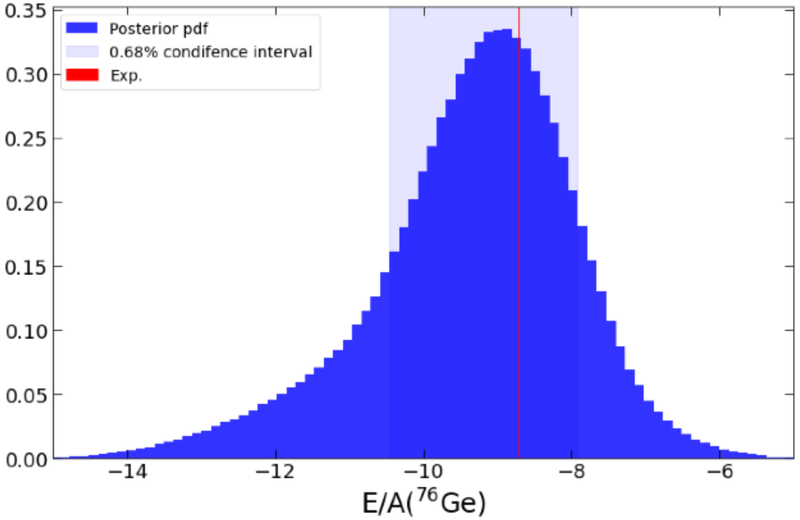


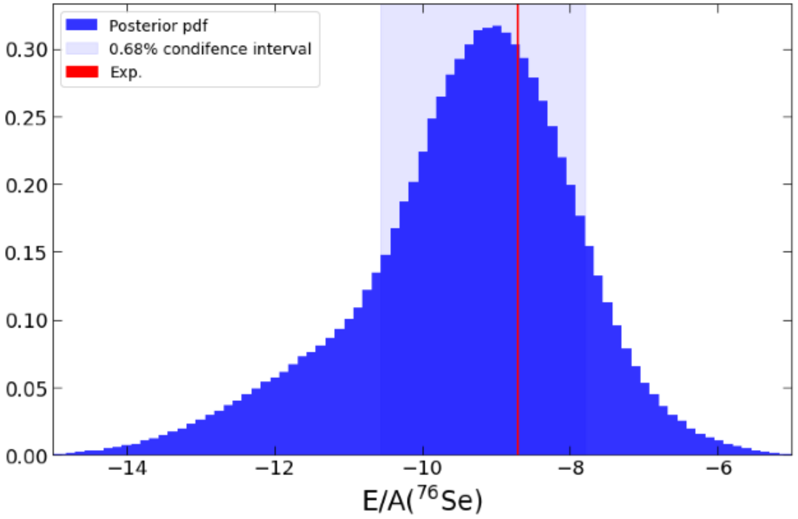
Final values change by less the 0.01!

Changing the calibration

Only noticeable change is seen in the PDF for the energies:

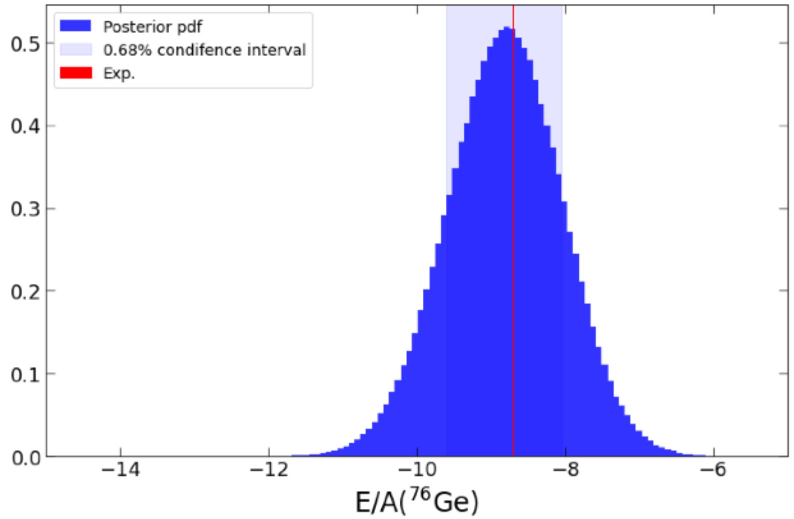
Without energies

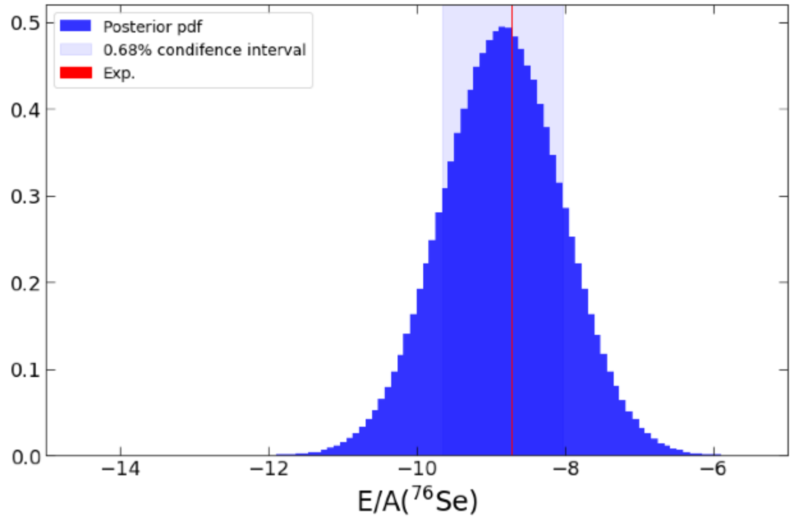




$\Rightarrow$

With energies





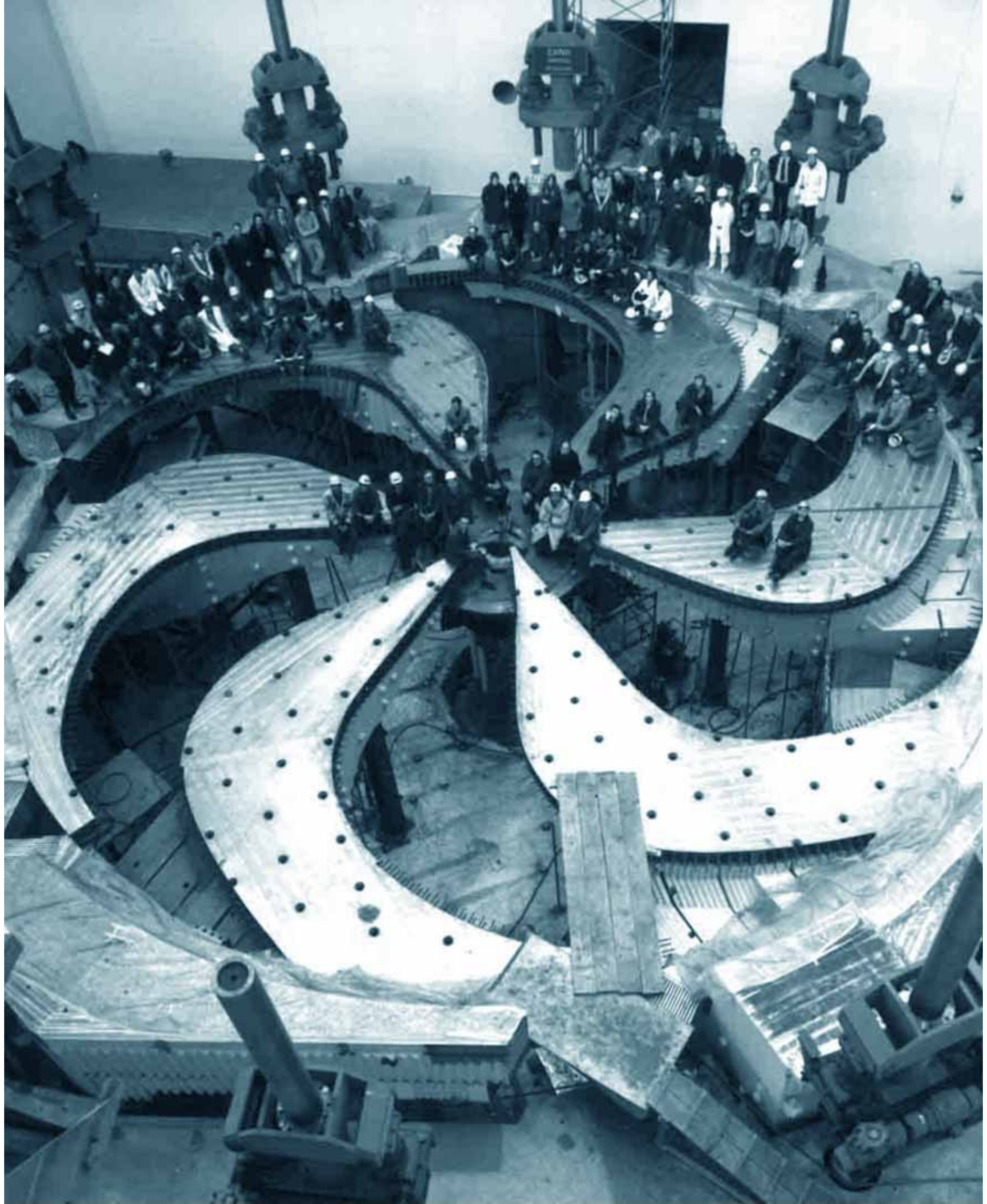
TRIUMF

Summary…

1. Computed first ever ab initio NMEs of isotopes of experimental interest, which is a first step towards computing NME with reliable theoretical uncertainties.
2. Computed NME with multiple interactions for ^{48}Ca, ^{76}Ge, ^{82}Se, ^{100}Mo ,^{130}Te and ^{136}Xe.
3. Study of effect of the contact term on the NMEs.
4. Studied correlations between multiple operators using a wide range of interactions.
5. Developed an emulator for the VS-IMSRG based on Gaussian processes and obtain first statistical uncertainty.

… and outlook

1. Include finite momentum 2-body currents and other higher order effects.
2. Large scale ab initio uncertainty analysis with other methods for "final" NMEs.
3. Include contact term to the statistical uncertainty.
4. Study other exotic mechanism proposed for $0\nu\beta\beta$.



Discovery, accelerated

Questions?

abelley@triumf.ca