Nuclear mass tables from energy density functionals

Tomás R. Rodríguez

Bundesministerium für Bildung und Forschung
TECHNISCHE UNIVERSITÄT DARMSTADT
NAVI Nuclear Astrophysics Virtual Institute
HIC for FAIR Helmholtz International Center

Outline

1. Introduction

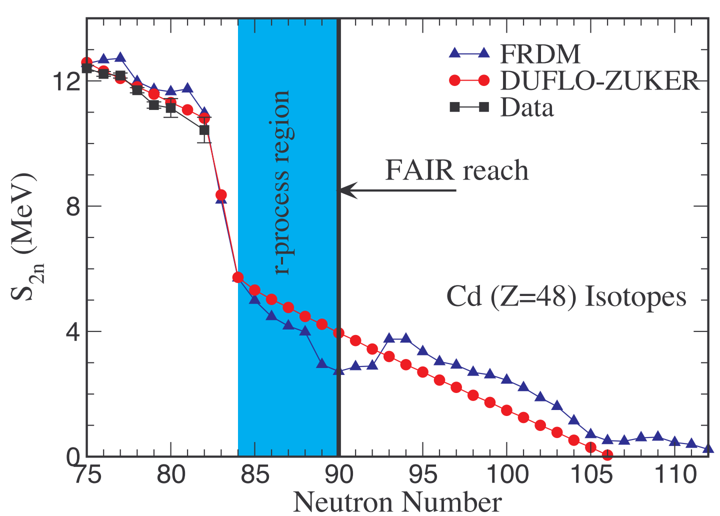
2. Convergence and numerical noise

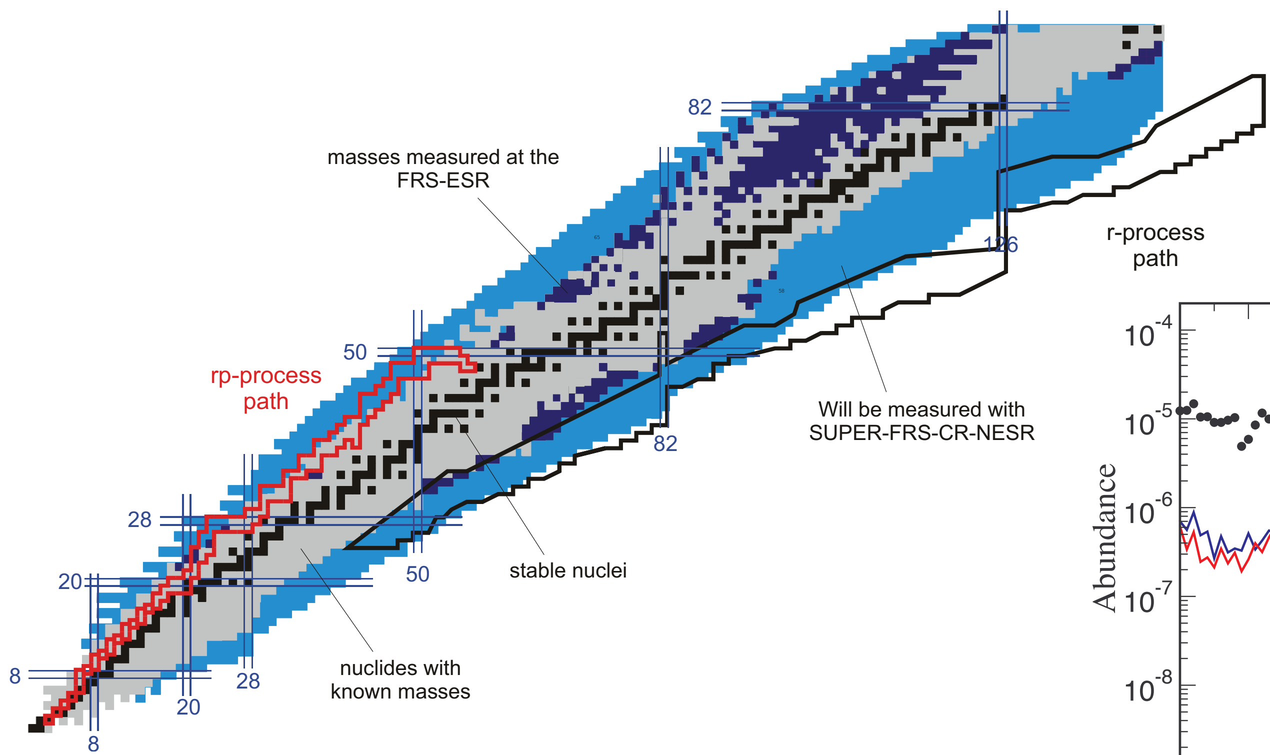
3. Beyond mean field effects

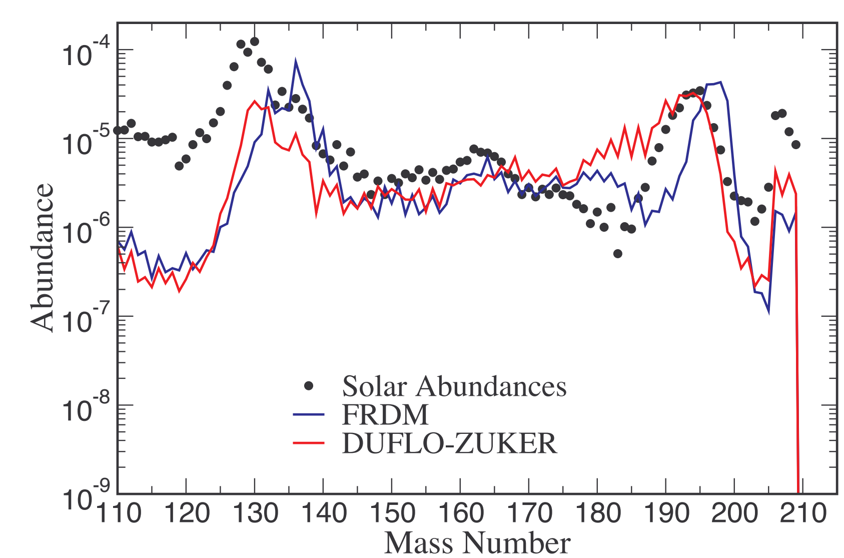
4. Summary and outlook

Motivation

- Nuclear masses are one of the most relevant input for nucleosynthesis calculations, in particular for the r-process.
- Masses (separation energies) affect significantly (n,γ) capture rates, (γ,n) photodissociation reactions and Q-values for β-decay.
- Only few nuclei are/will be experimentally explored in the relevant region for r-process nucleosynthesis ⇒ <u>we require theoretical predictions.</u>







Courtesy: J. Mendoza-Temis

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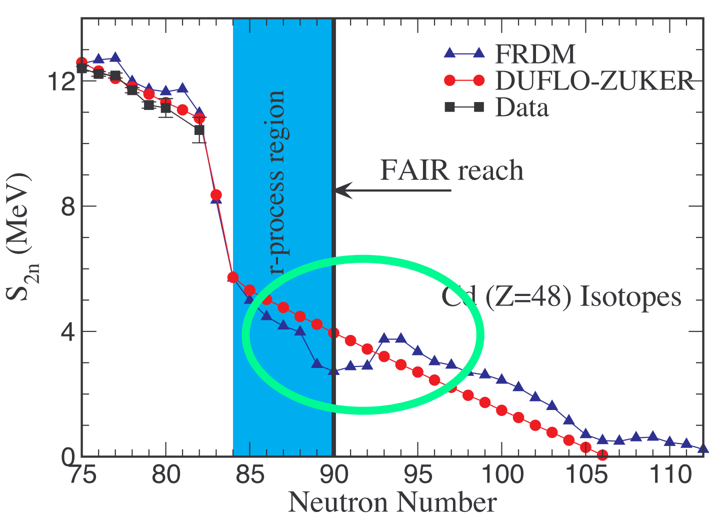

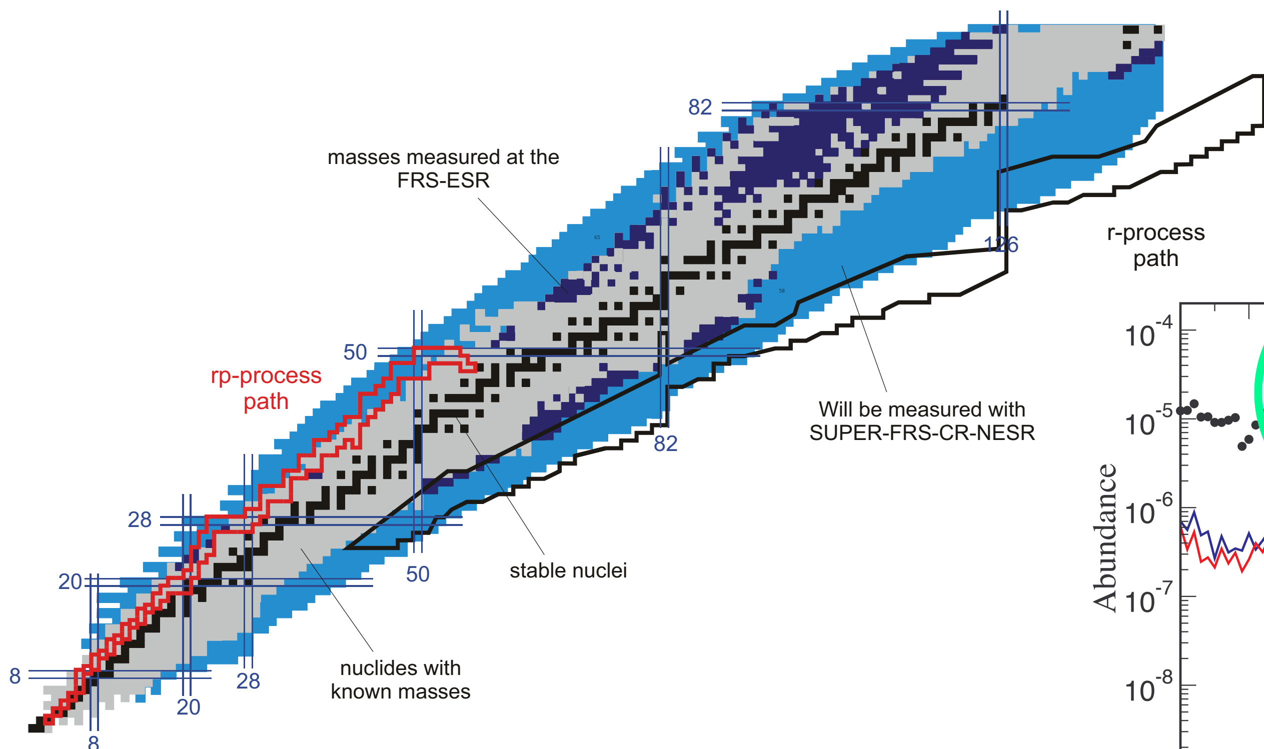

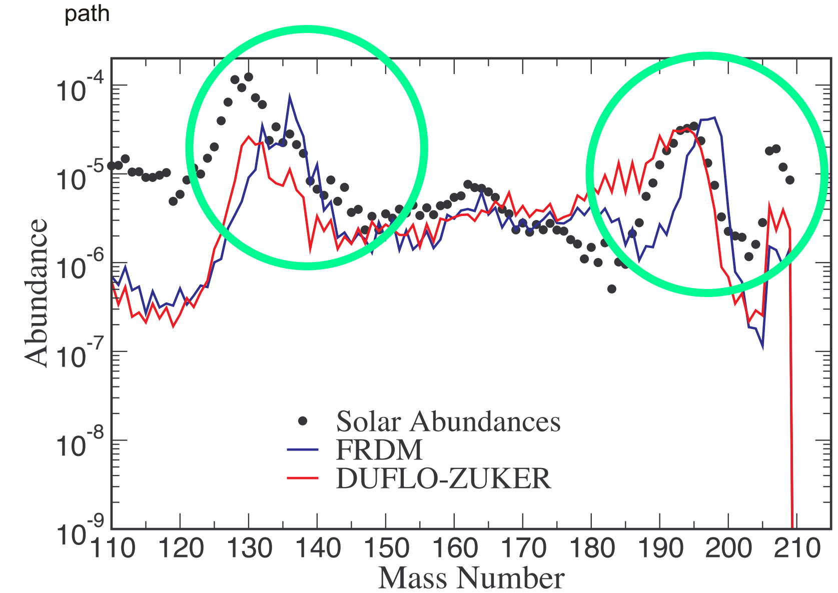

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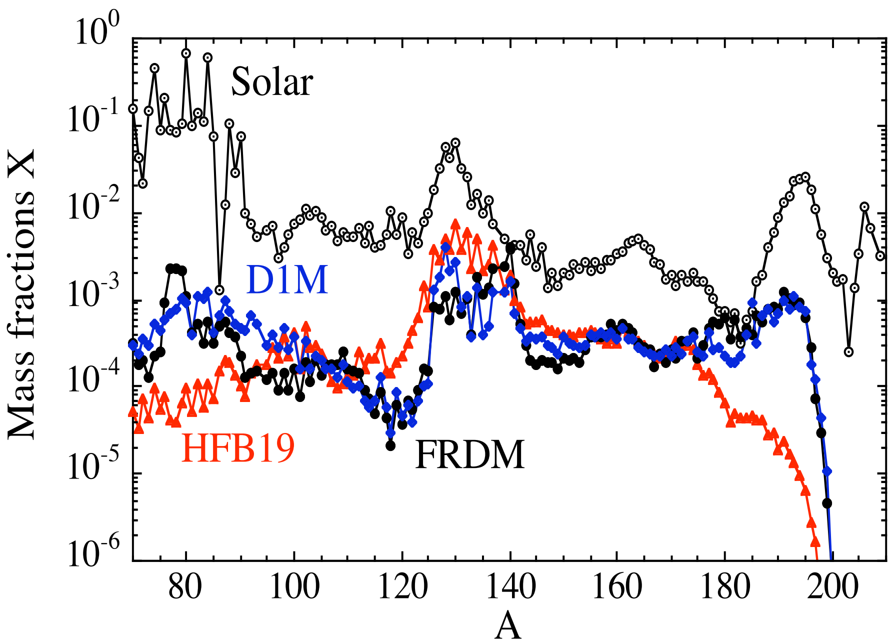
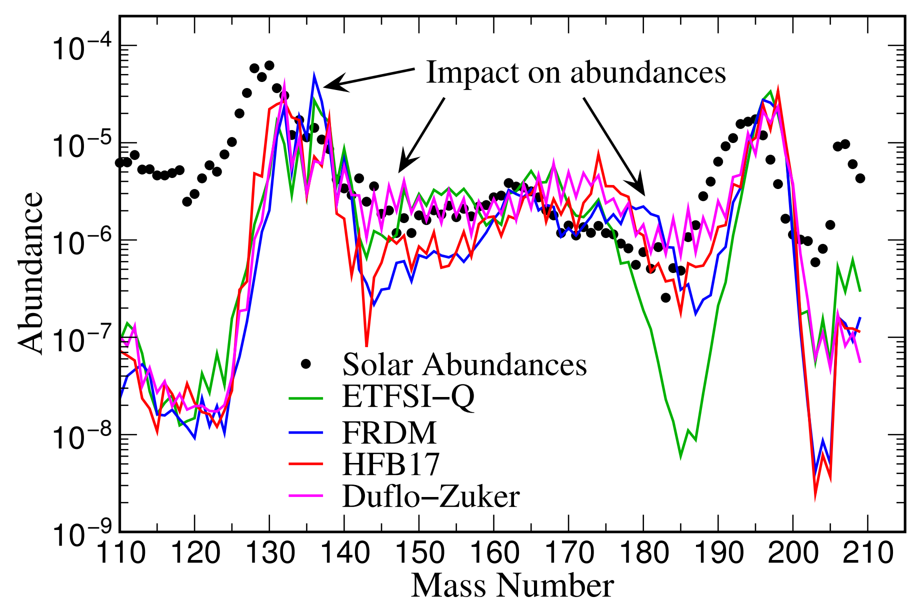
Motivation

- Impact of the nuclear mass model on r-process nucleosynthesis calculations:

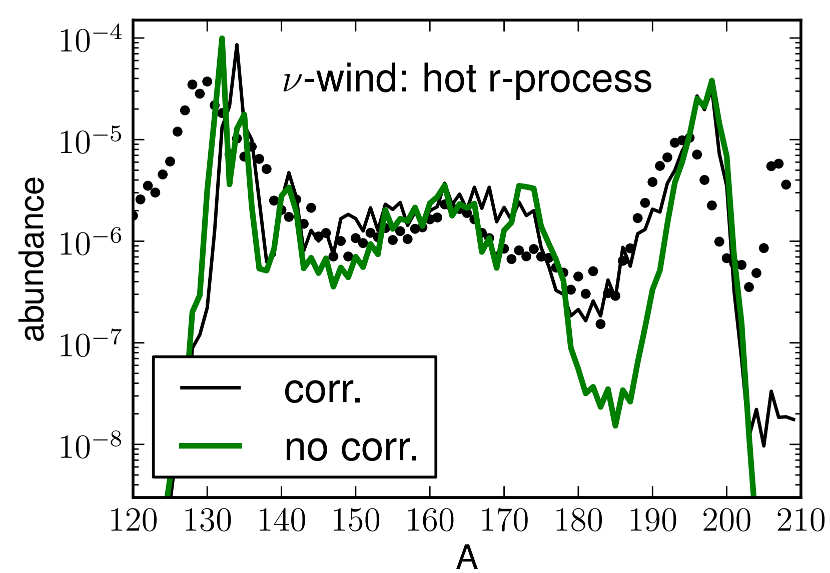
Final abundances depend on the mass model used (for the same astrophysical conditions)



Goriely et al.



Arcones and Martínez-Pinedo, PRC 83, 045809 (2011)



Arcones and Bertsch, PRL 108, 151101(2012)

Mass models

• Experimental masses where available: ~2149 (Audi *et al.* 2003).

• Theoretical global nuclear mass models widely used in nucleosynthesis calculations:

➡ Finite Range Droplet Model (FRDM). (Möller et. al 1995)

➡ Extended Thomas-Fermi plus Strutinsky Integral (ETFSI). (Aboussir et al. 1995)

➡ Duflo-Zuker (DZ) functional based on Shell Model. (Duflo and Zuker 1995)

➡ Self-consistent mean field models based on Hartree-Fock-Bogoliubov approximations:

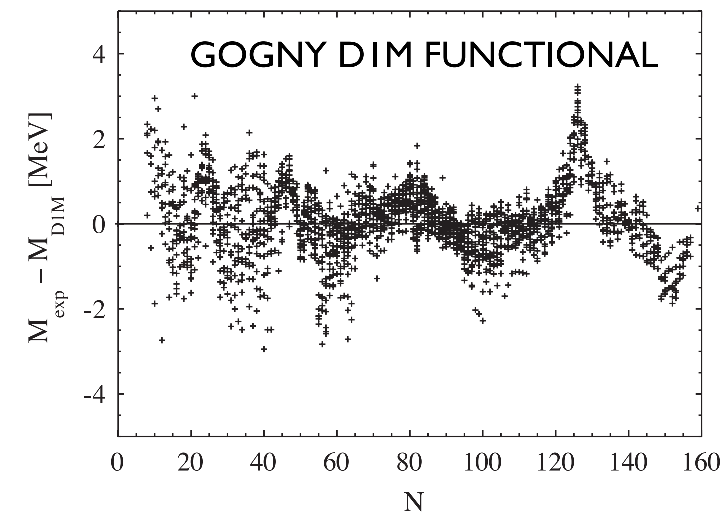
- Skyrme HFB-* (Goriely et al 2009)
- Gogny D1M (Goriely et al. 2009)
- UNEDF (J. Erler et al. 2012)

Typical r.m.s. deviation from the experimental data ~0.6 MeV

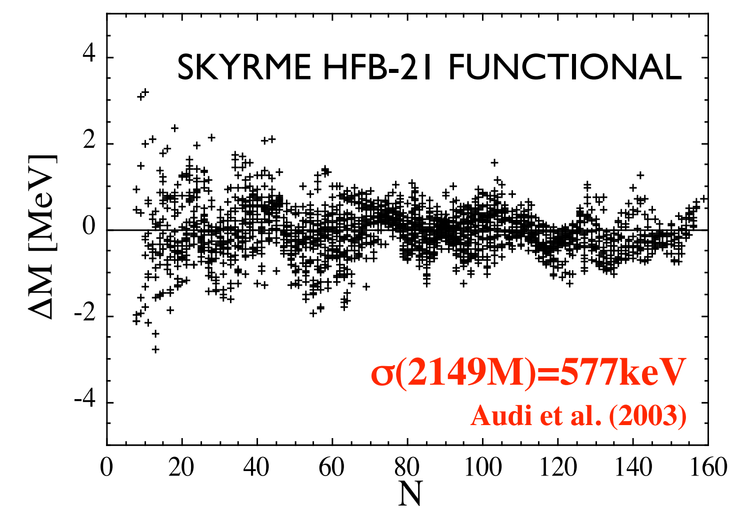
Microscopic mass models

- Self-consistent mean field approximations provide a very good description of known data.

- There are still some problems in transitional regions and local uncertainties:
  - Numerical noise.
  - Some physics missing: Restoration of broken symmetries and configuration mixing.
  - Nuclei with odd number of protons/neutrons are not treated in equal footing as the even-even ones



Goriely et al., PRL 102, 242501 (2009)



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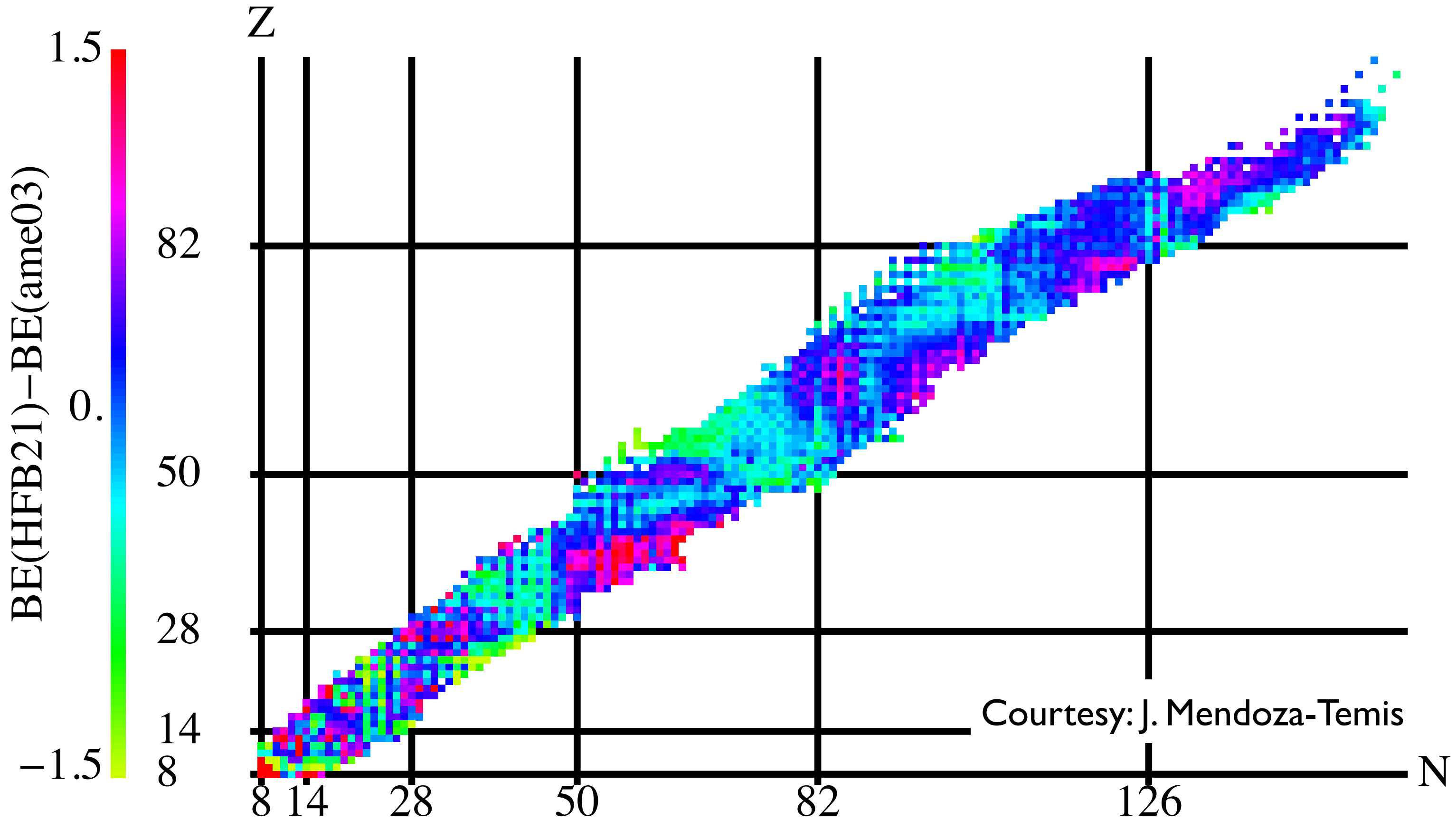

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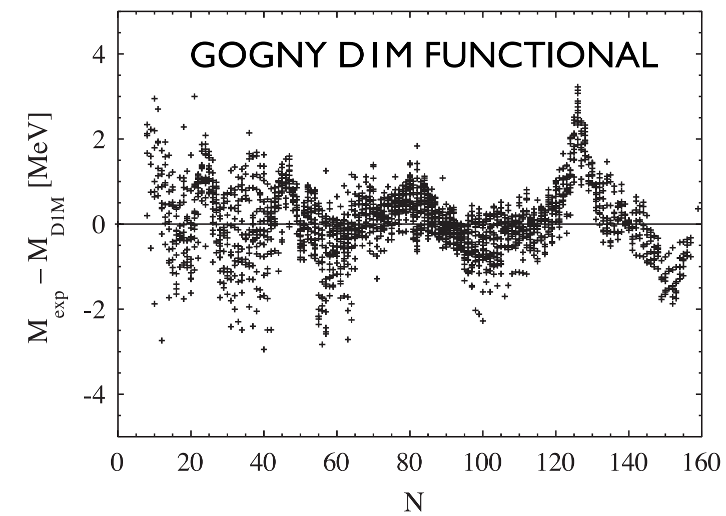

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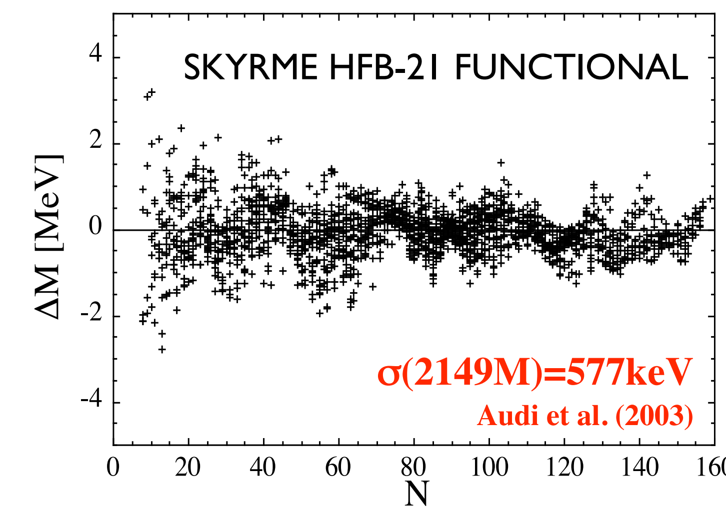

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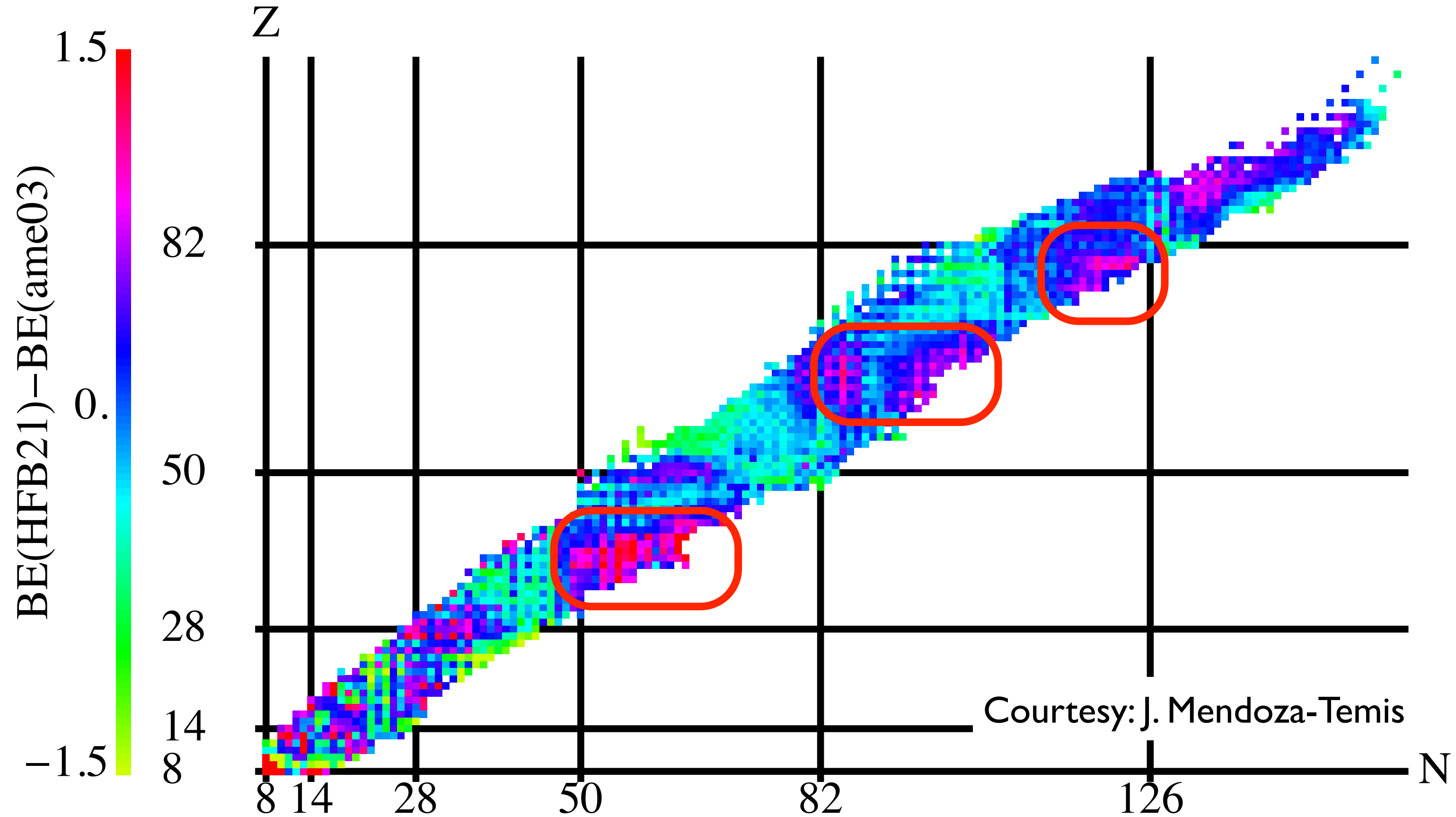

Self-consistent (beyond) mean field description

- **Effective nucleon-nucleon interaction:**

Gogny force (D1S-D1M) that is able to describe properly many phenomena along the whole nuclear chart.

$$V(1,2) = \sum_{i=1}^{2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2}\left(W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau\right)$$
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spin-orbit term

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- **Methods of solving the many-body problem: Variational approaches**

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Coulomb term: $$+V_{\text{Coulomb}}(\vec{r}_1,\vec{r}_2)$$

- **Methods of solving the many-body problem: Variational approaches**

➡**Parameters of the effective interaction are fitted to reproduce experimental data solving the many-body problem at certain level of approximation (mean field normally).**

Hartree-Fock-Bogoliubov (HFB)

Variational space: $\{|\Phi(\vec{q})\rangle\}$ set of **product-type** wave functions which fulfill:

- Quasiparticle vacua: $$\alpha_k(\vec{q})|\Phi(\vec{q})\rangle = 0$$
- Most general linear combination of the arbitrary single particle basis: $$\alpha_k^\dagger(\vec{q}) = \sum_l U_{lk}(\vec{q})c_l^\dagger + V_{lk}(\vec{q})c_l$$
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1. finite basis!! convergence?

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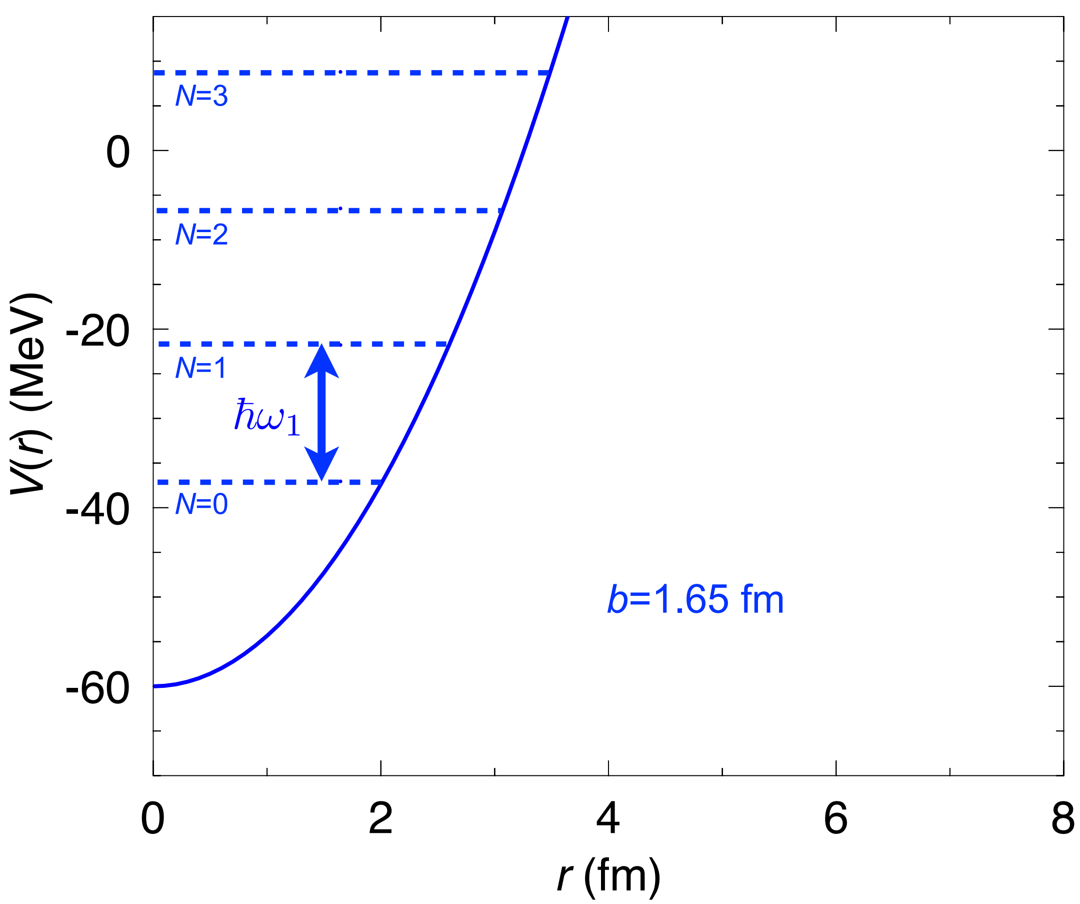
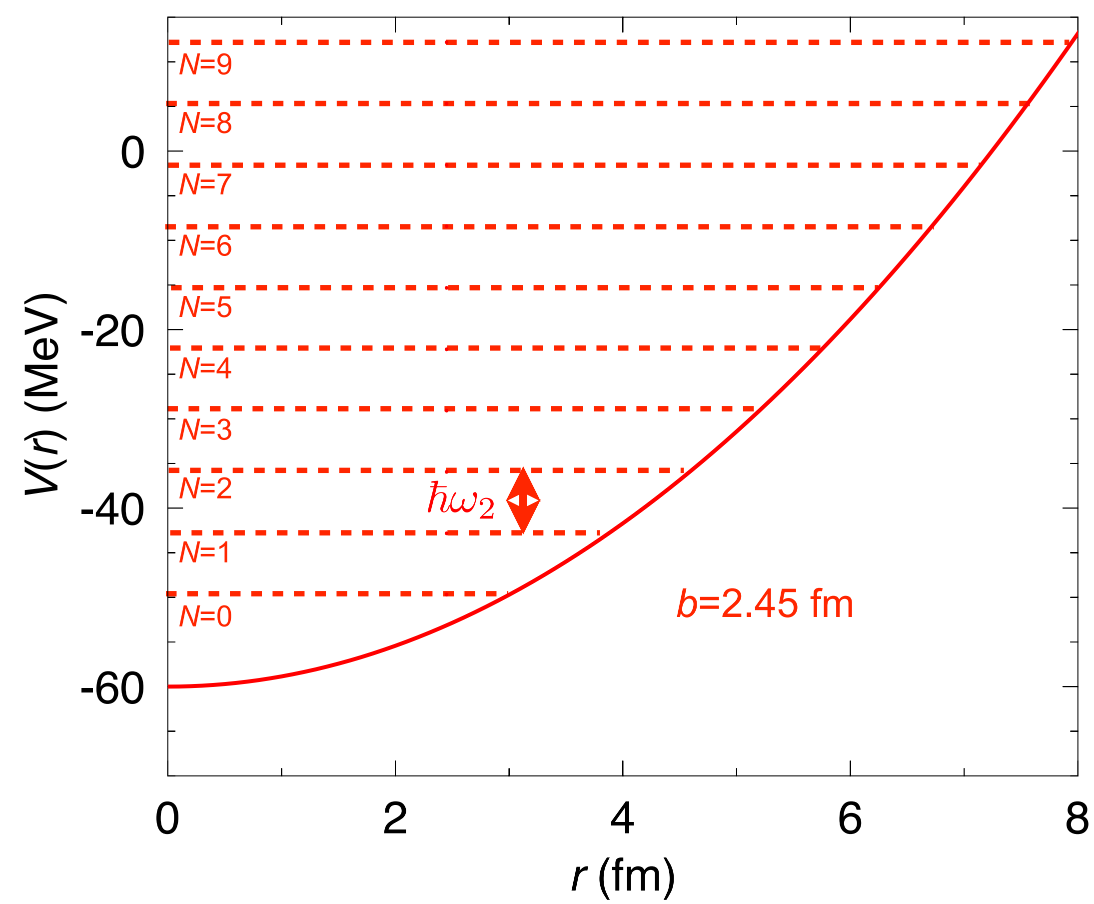
- **Results must not depend on the choice of the arbitrary single particle basis if it is complete.**





Self-consistent mean field

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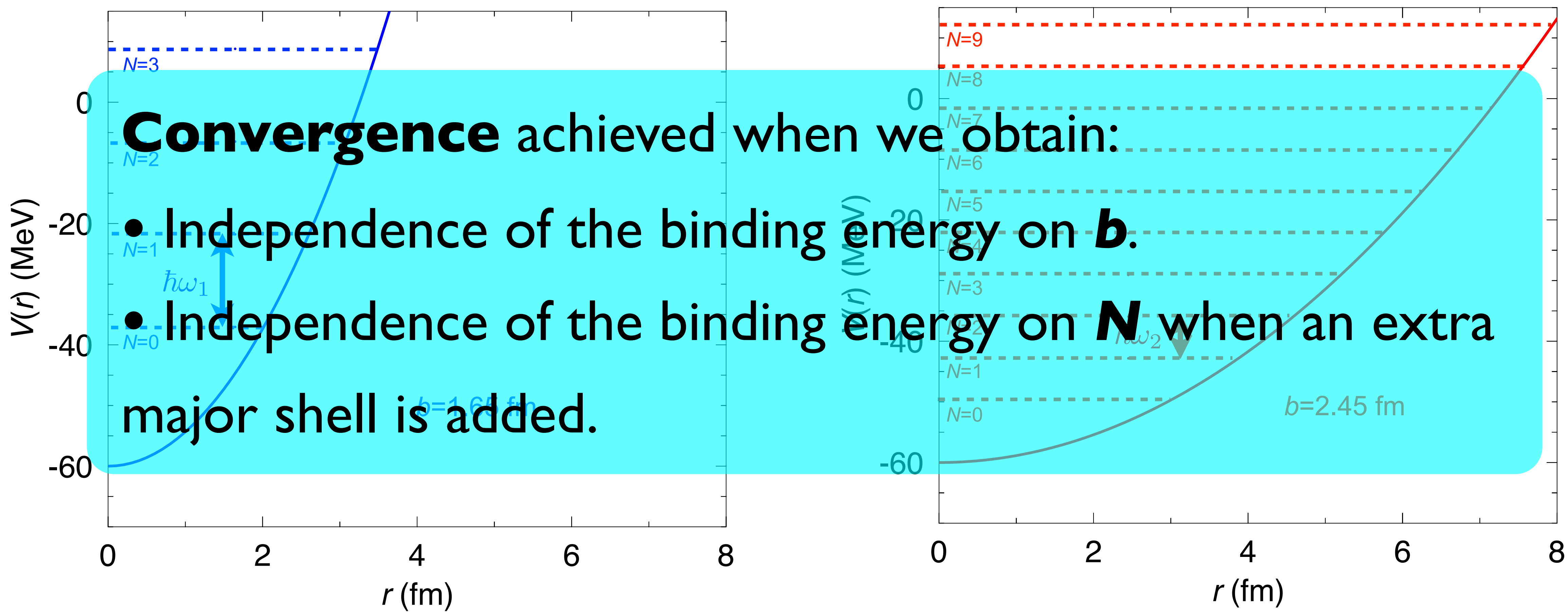


Convergence achieved when we obtain:

- Independence of the binding energy on ***b***.
- Independence of the binding energy on ***N*** when an extra major shell is added.

Examples in *ab-initio* calculations

P. Maris et *al.*, Phys. Rev C 79 (2009)

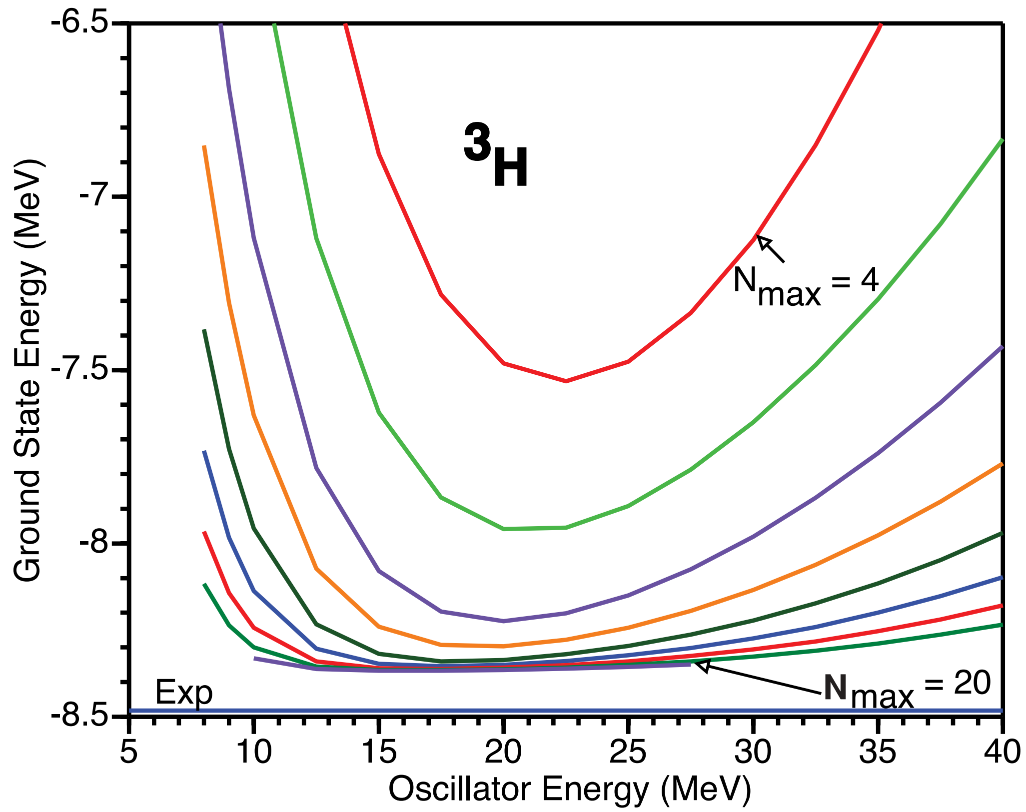


FIG. 10. (Color online) Calculated ground-state energy of ^{3}H as a function of the oscillator energy, $\hbar\Omega$, for selected values of $N_{\max}$. The curve closest to experiment corresponds to the value $N_{\max} = 20$ and successively higher curves are obtained with $N_{\max}$ decreased by two units for each curve.

R. Roth, Phys. Rev C 79 (2009)

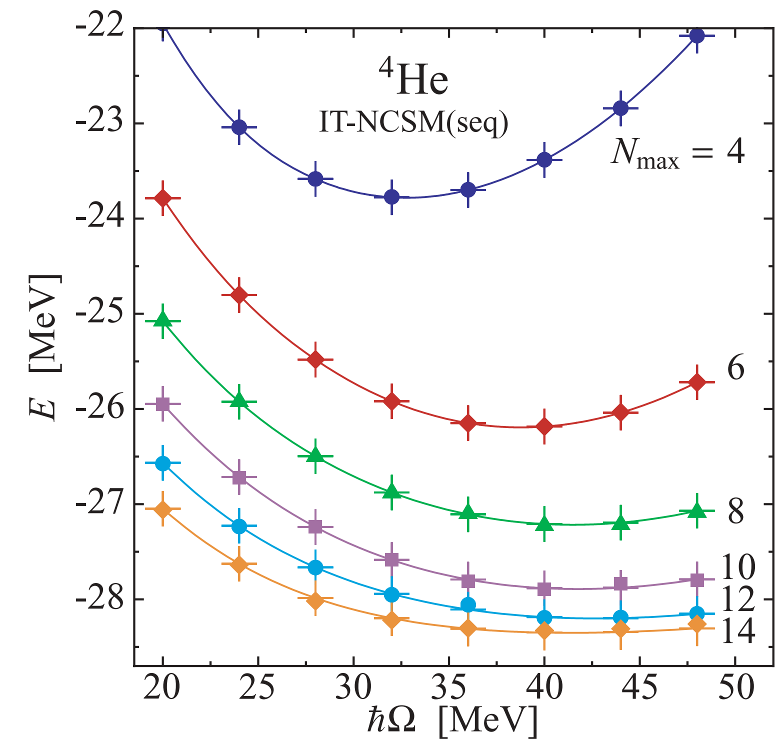
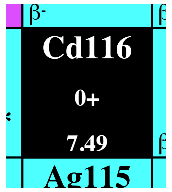
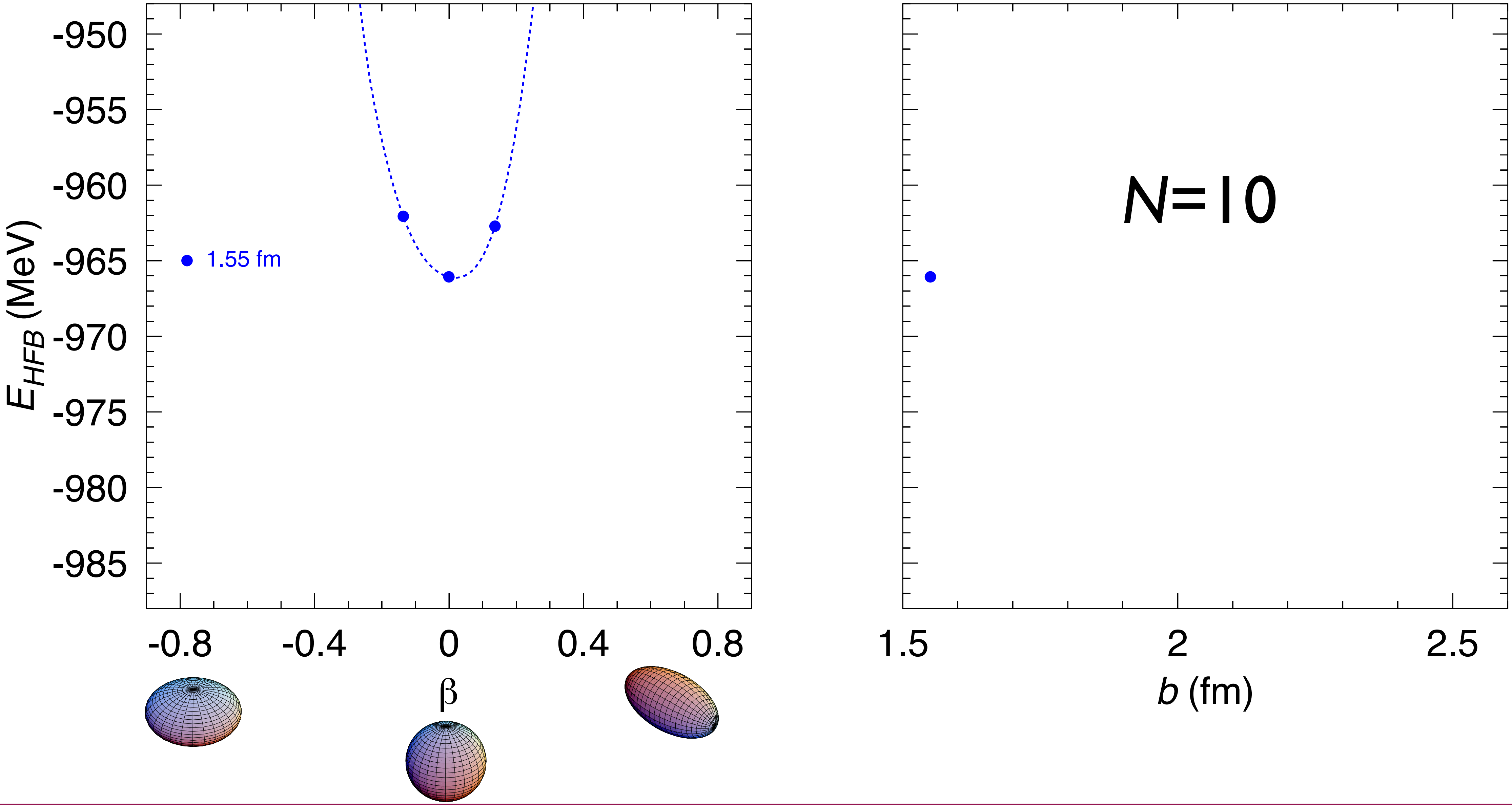


FIG. 7. (Color online) Ground-state energies of ^{4}He obtained for the V_{UCOM} interaction as function of the oscillator frequency $\hbar\Omega$ for different $N_{\max}\hbar\Omega$ model spaces. Results of IT-NCSM(seq) calculations (solid symbols) are compared with full NCSM calculations (crosses).

Effects of deformation on the convergence

Example: 



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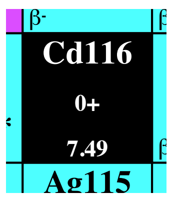
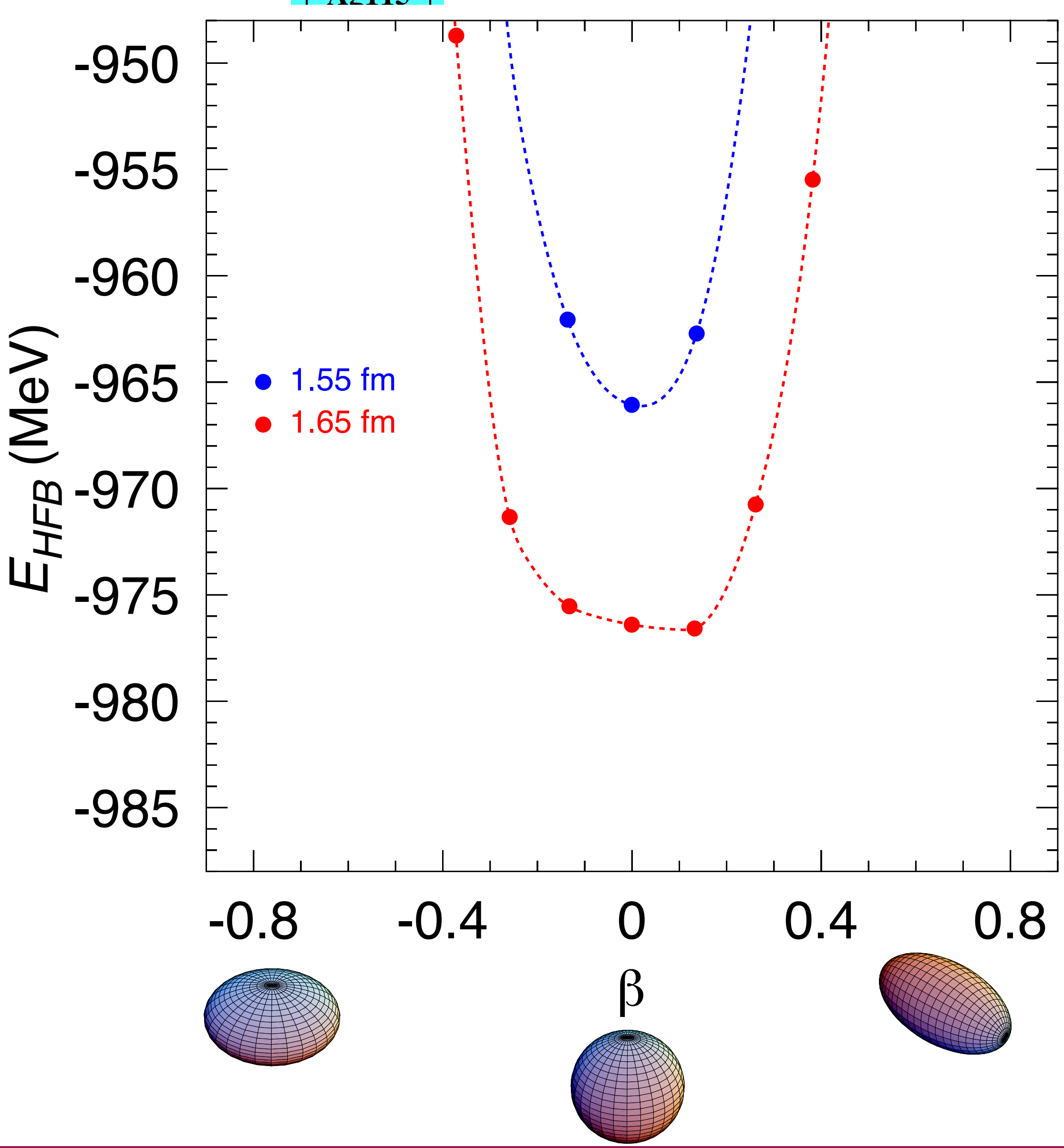
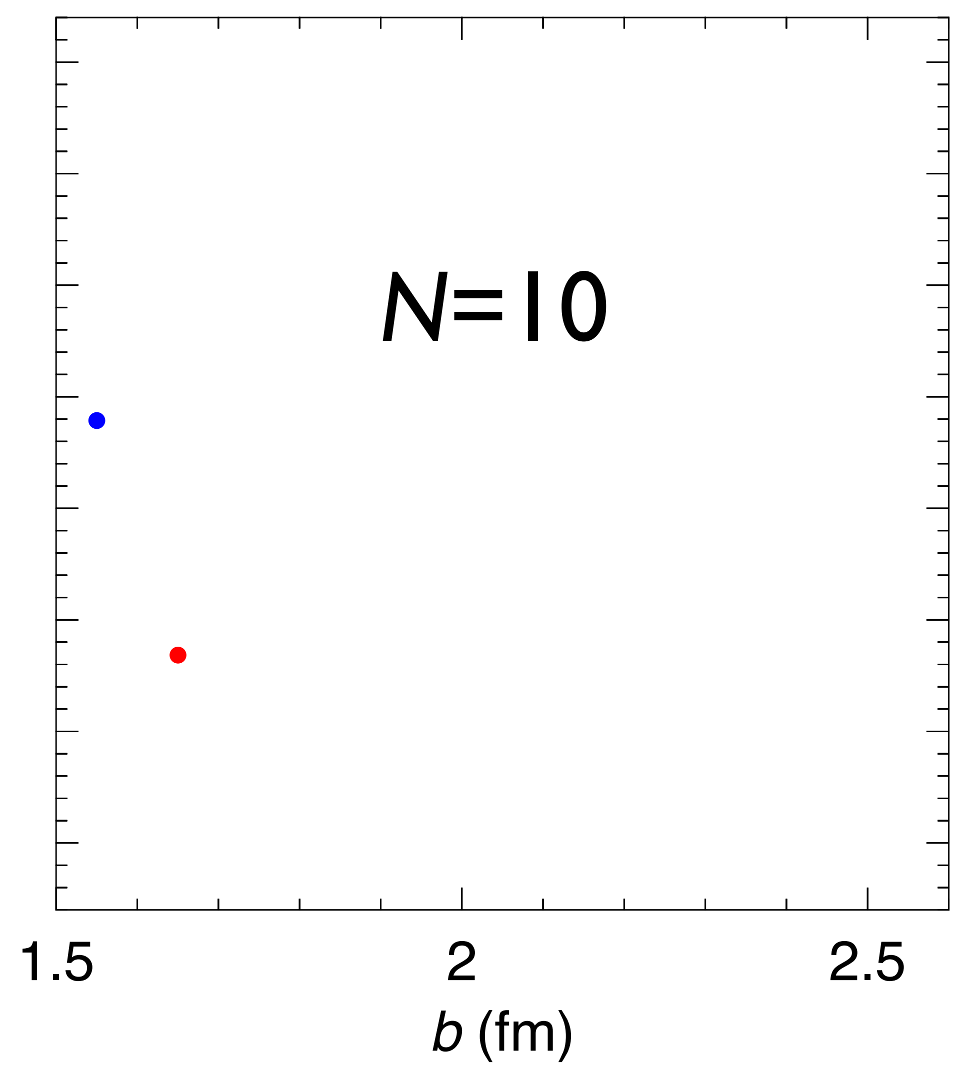
Example: 





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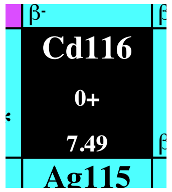
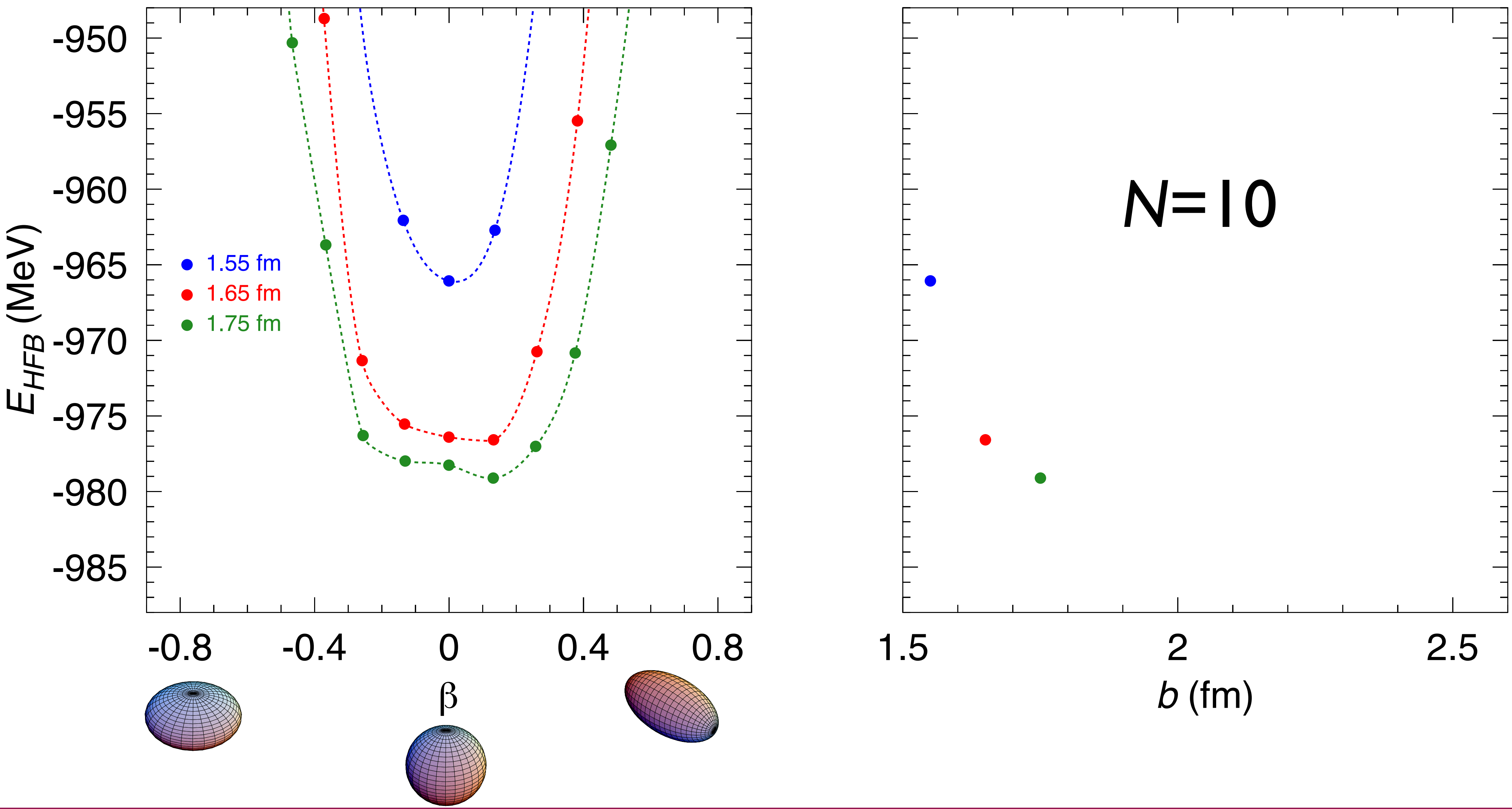
Example: 



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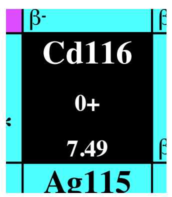
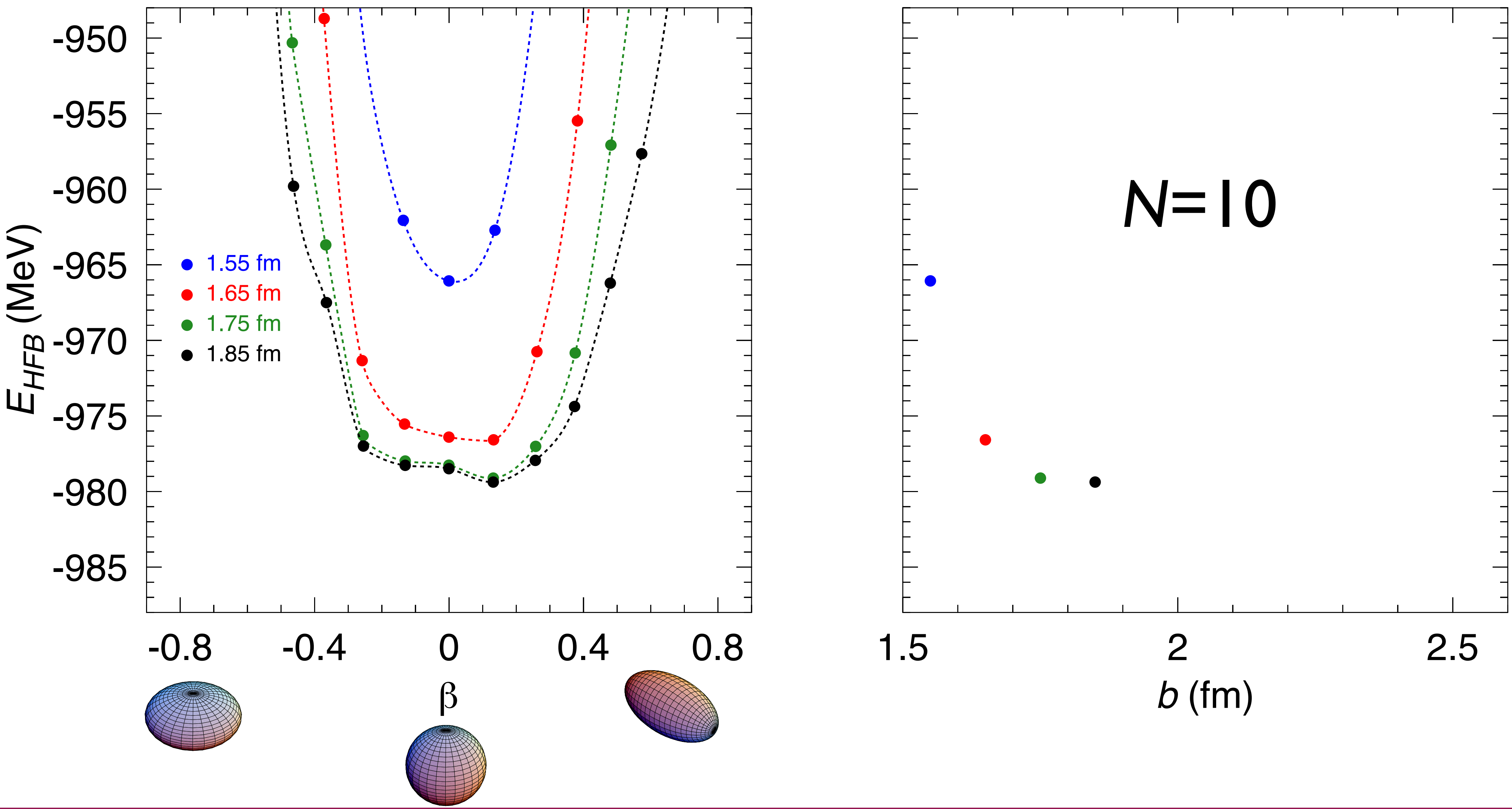
Example: 



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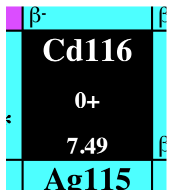
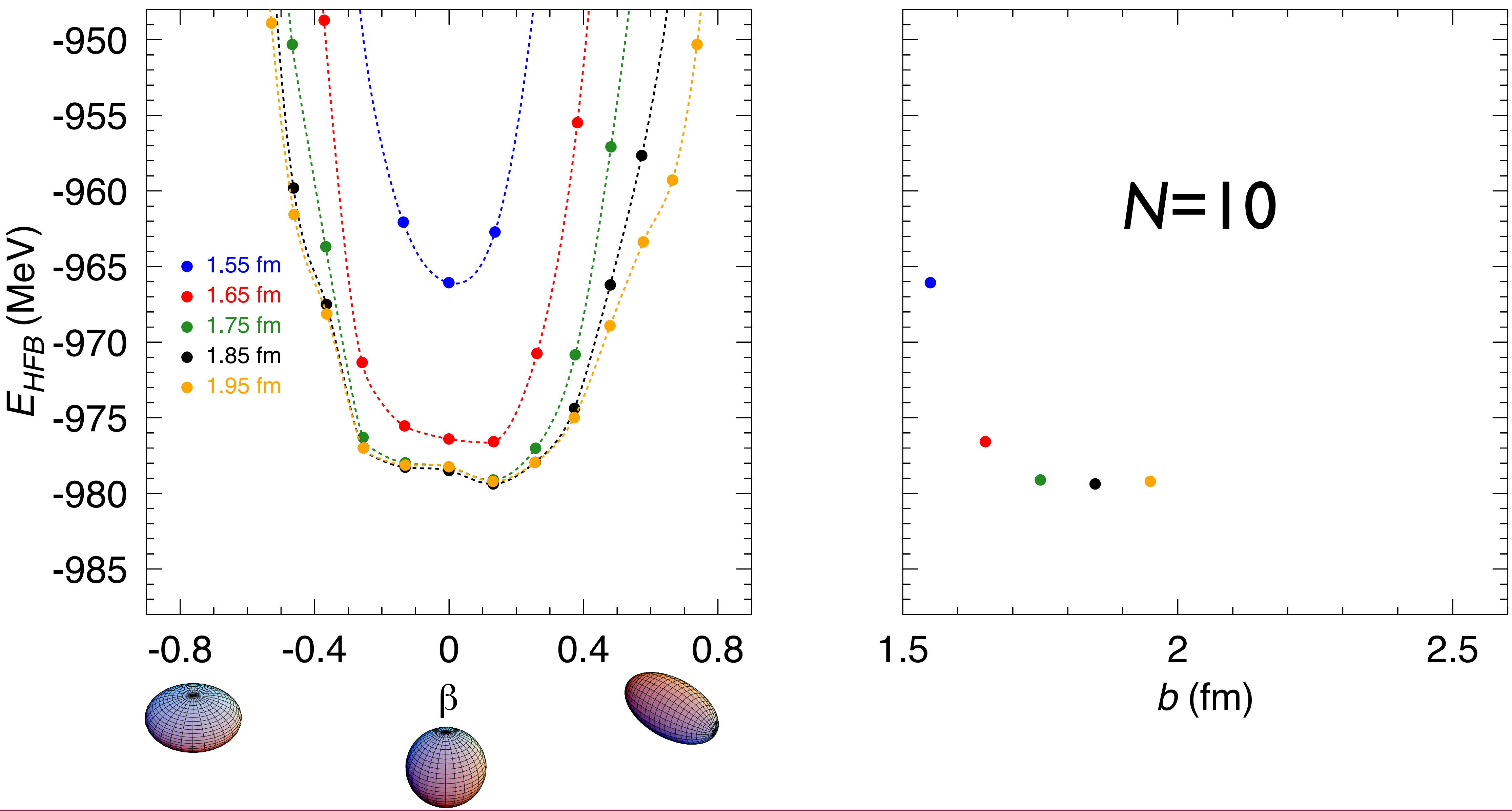
Example: 



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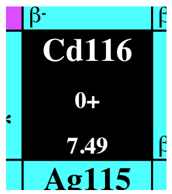
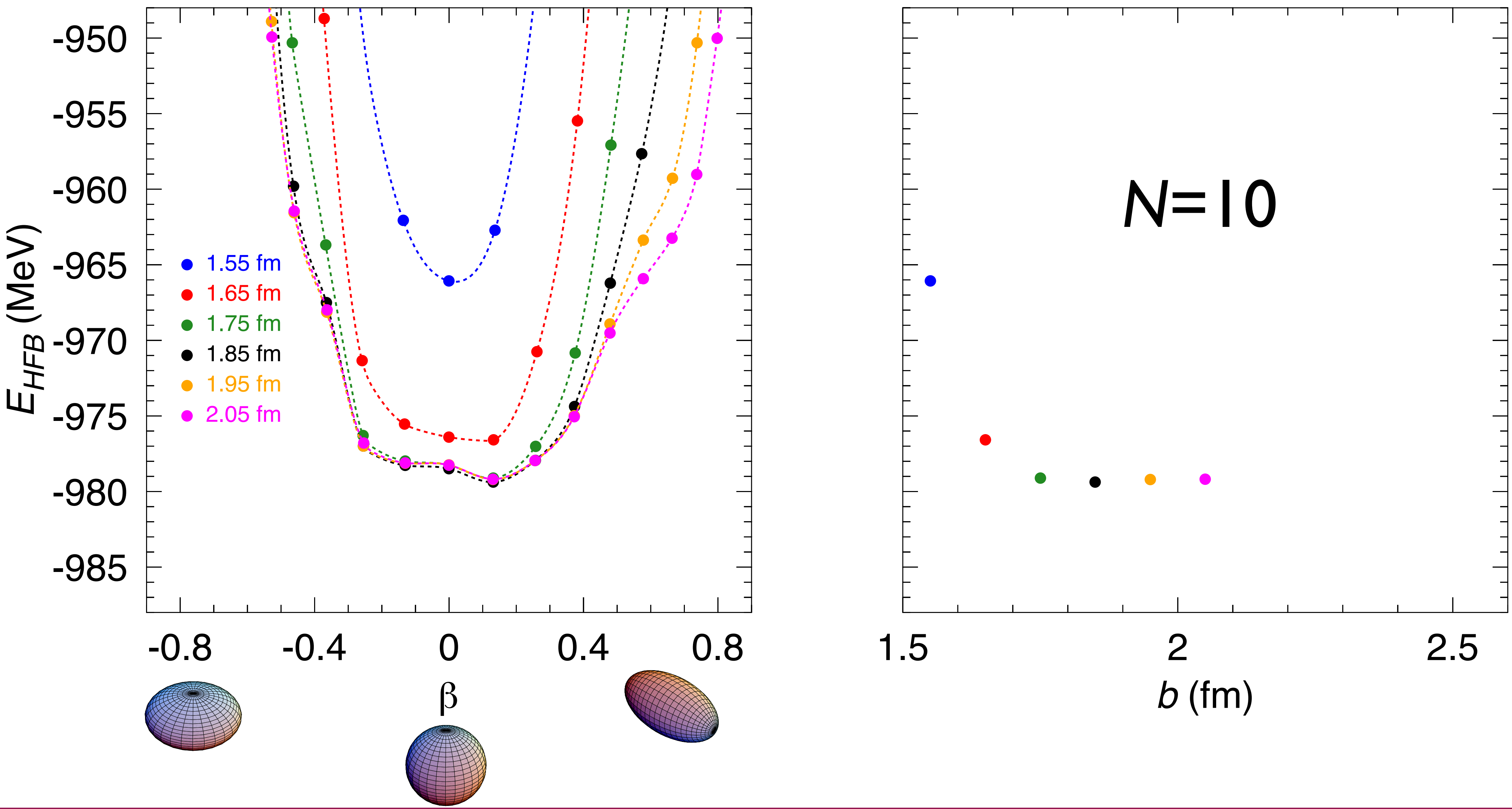
Example: 



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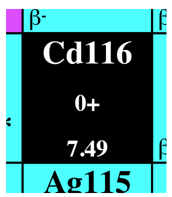
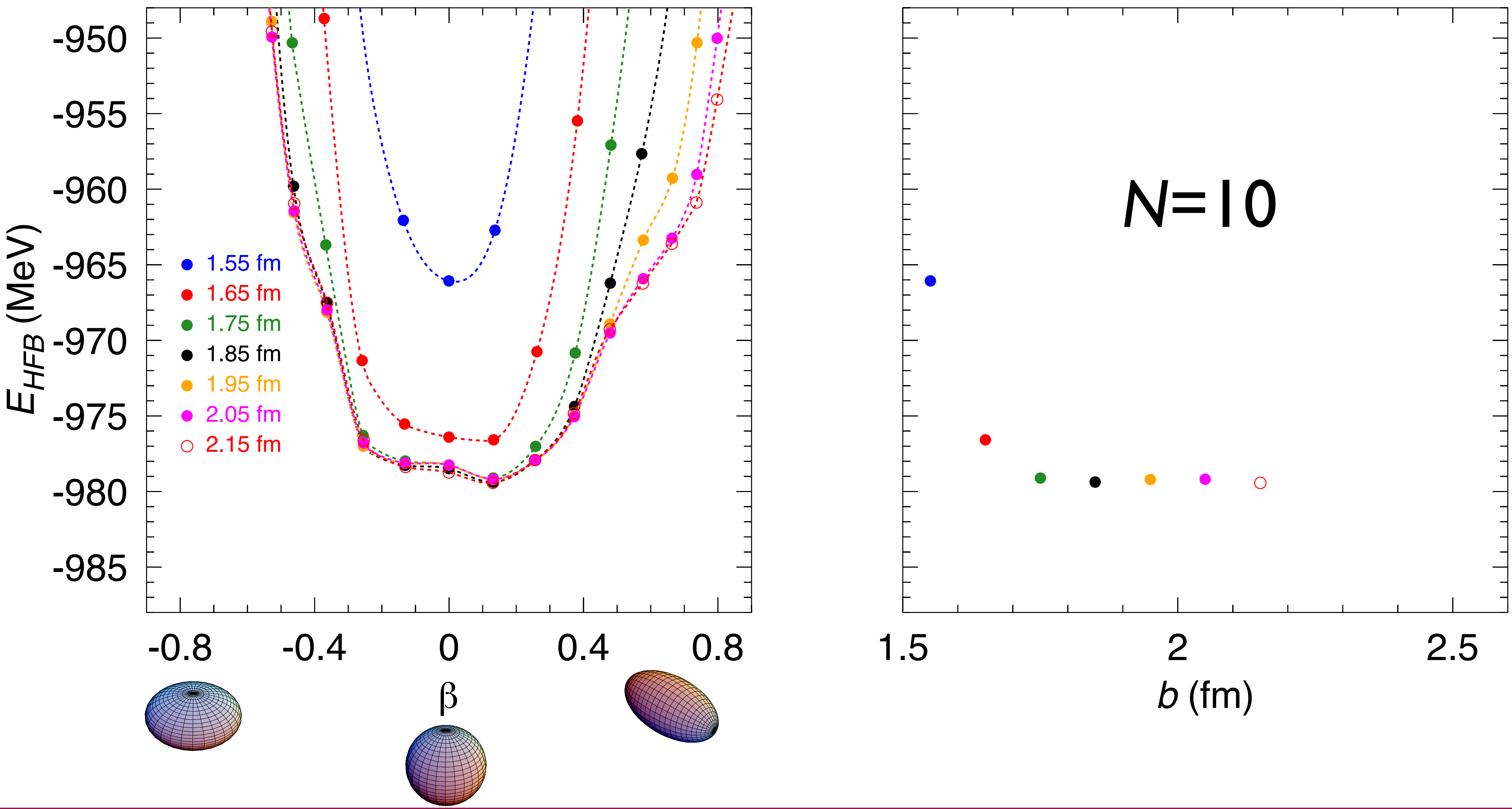
Example: 



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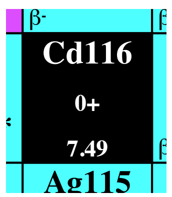
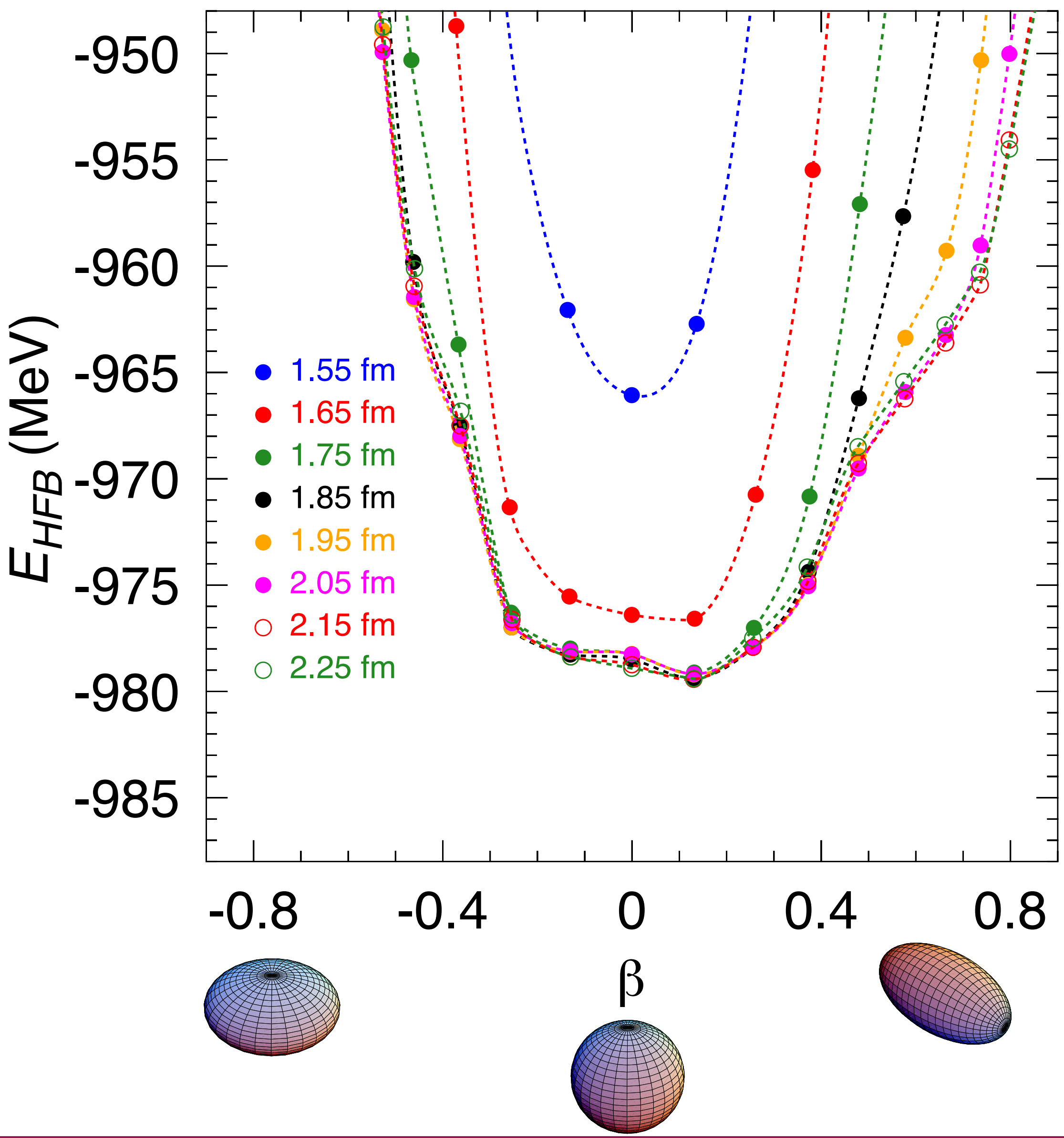
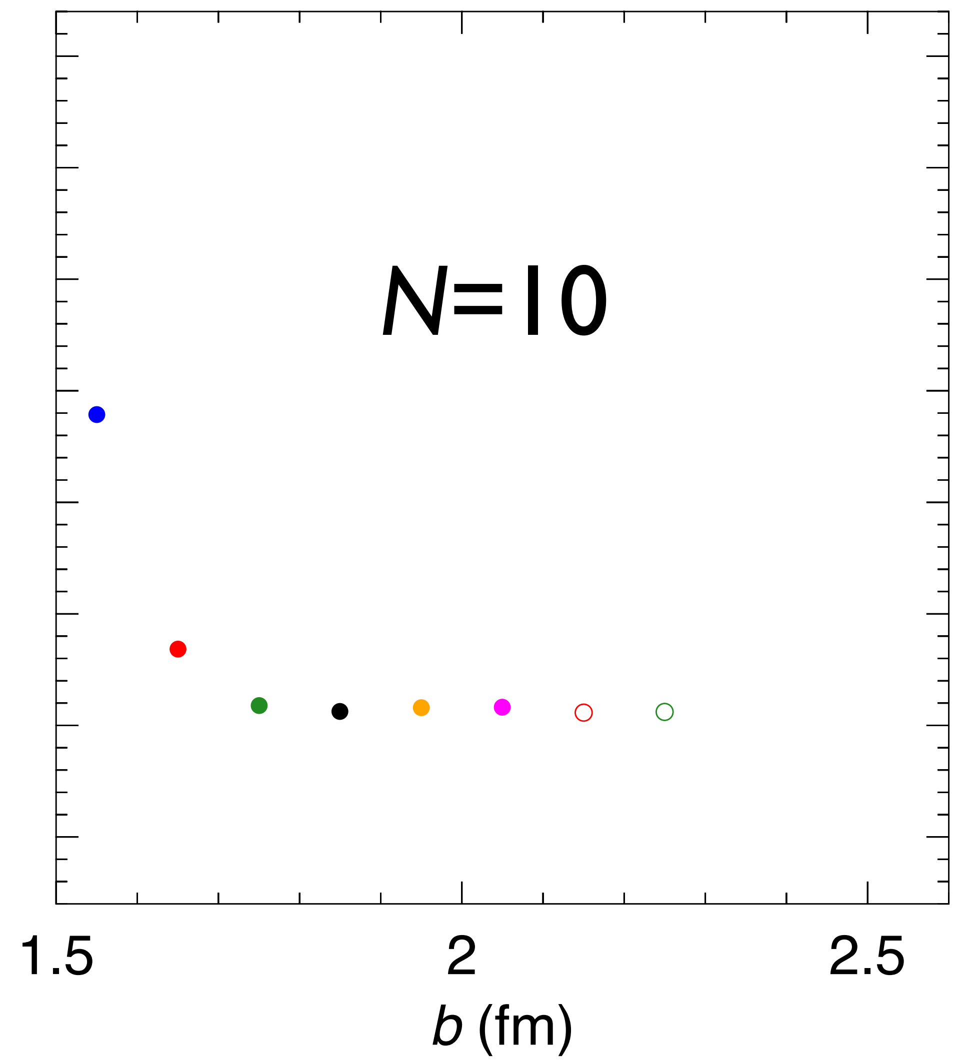
Example: 





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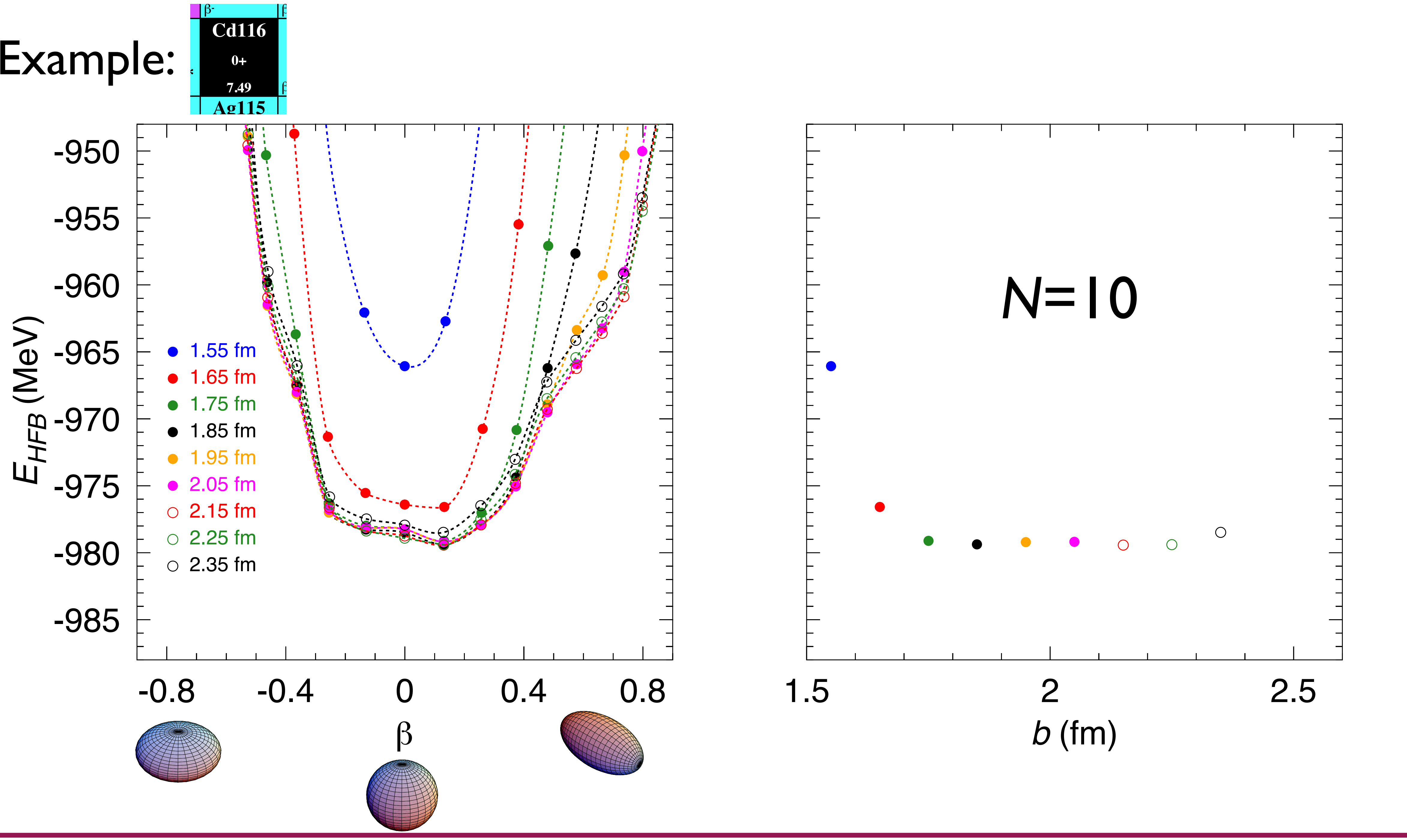

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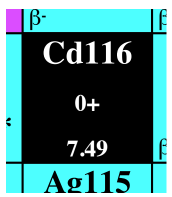
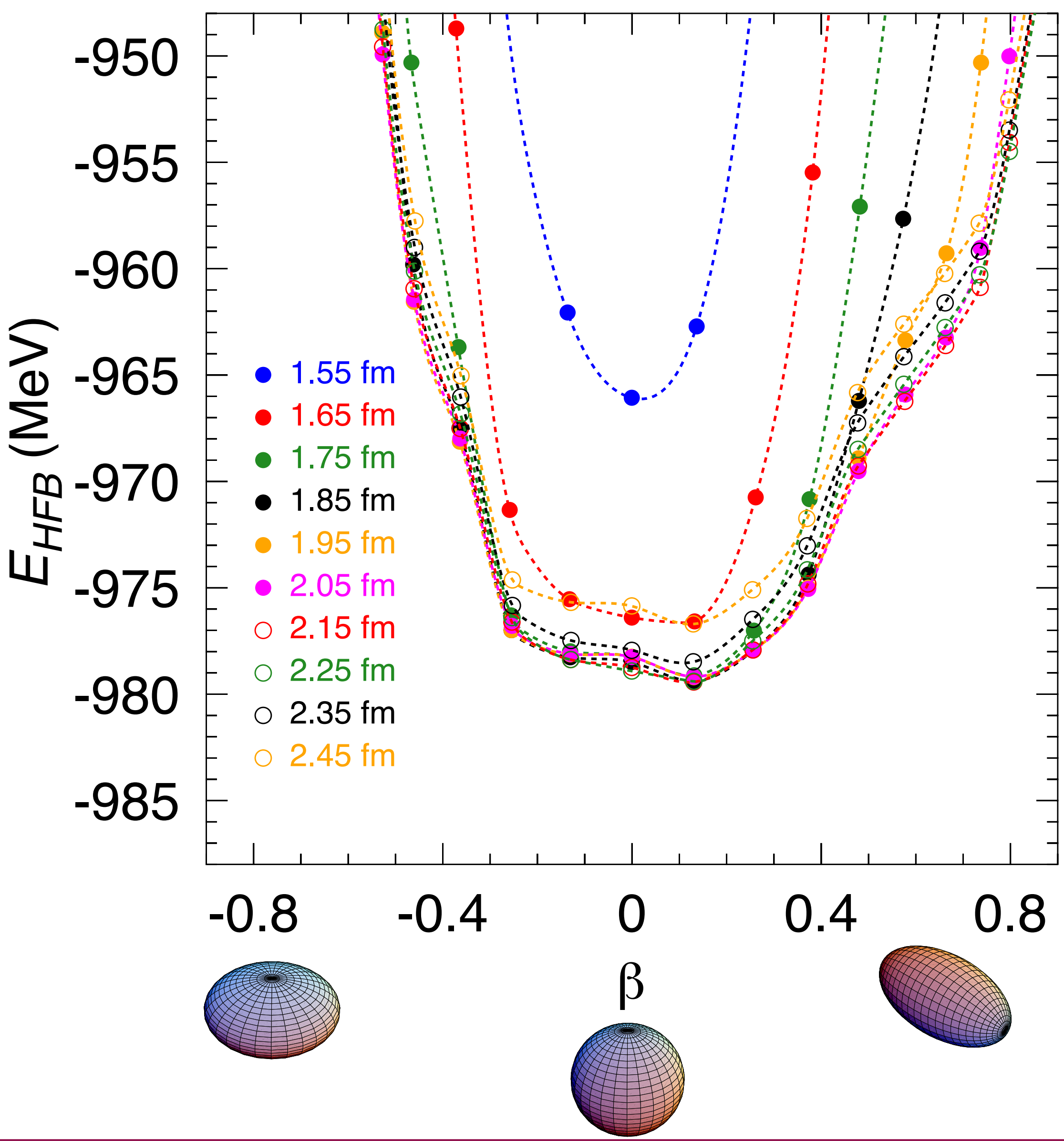
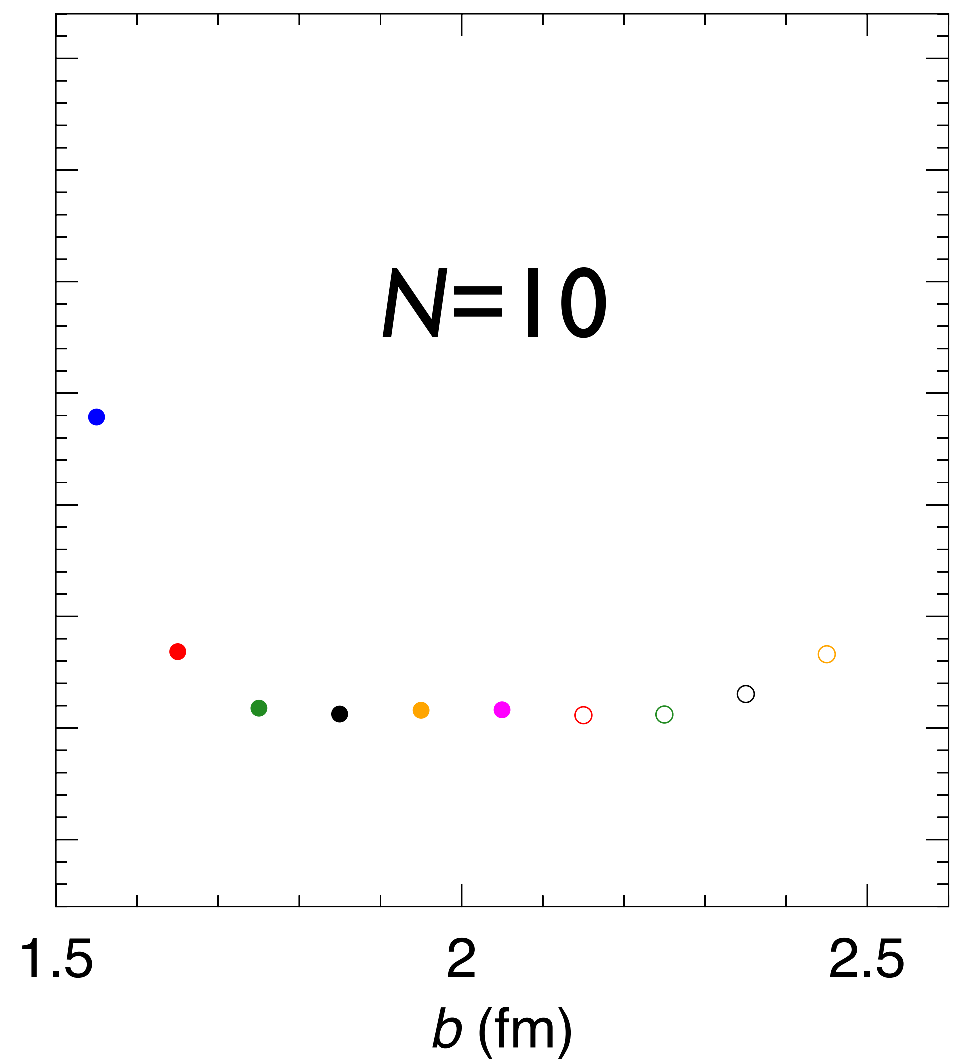
Example: 





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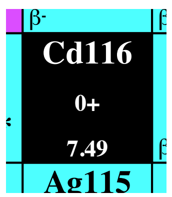
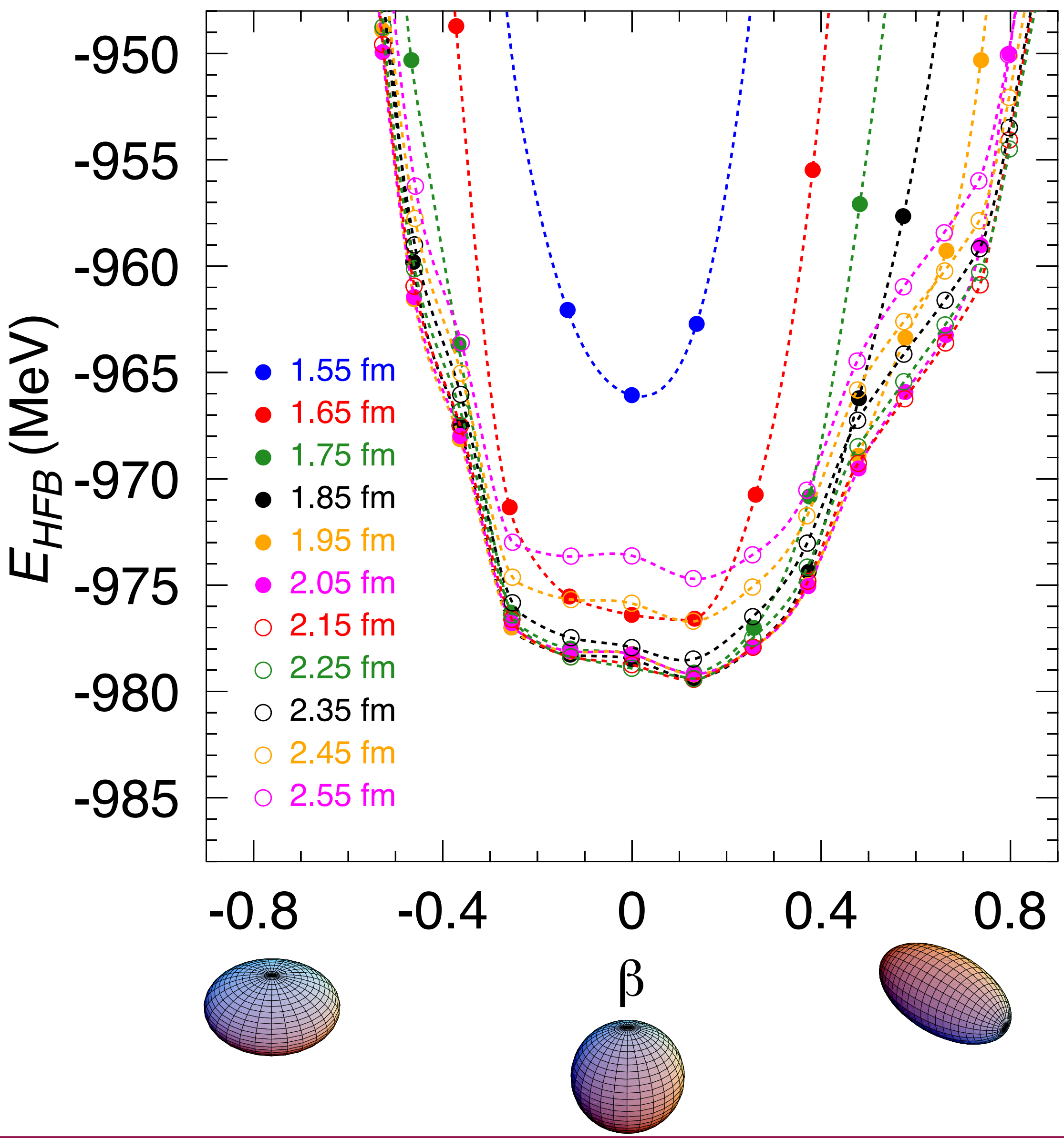
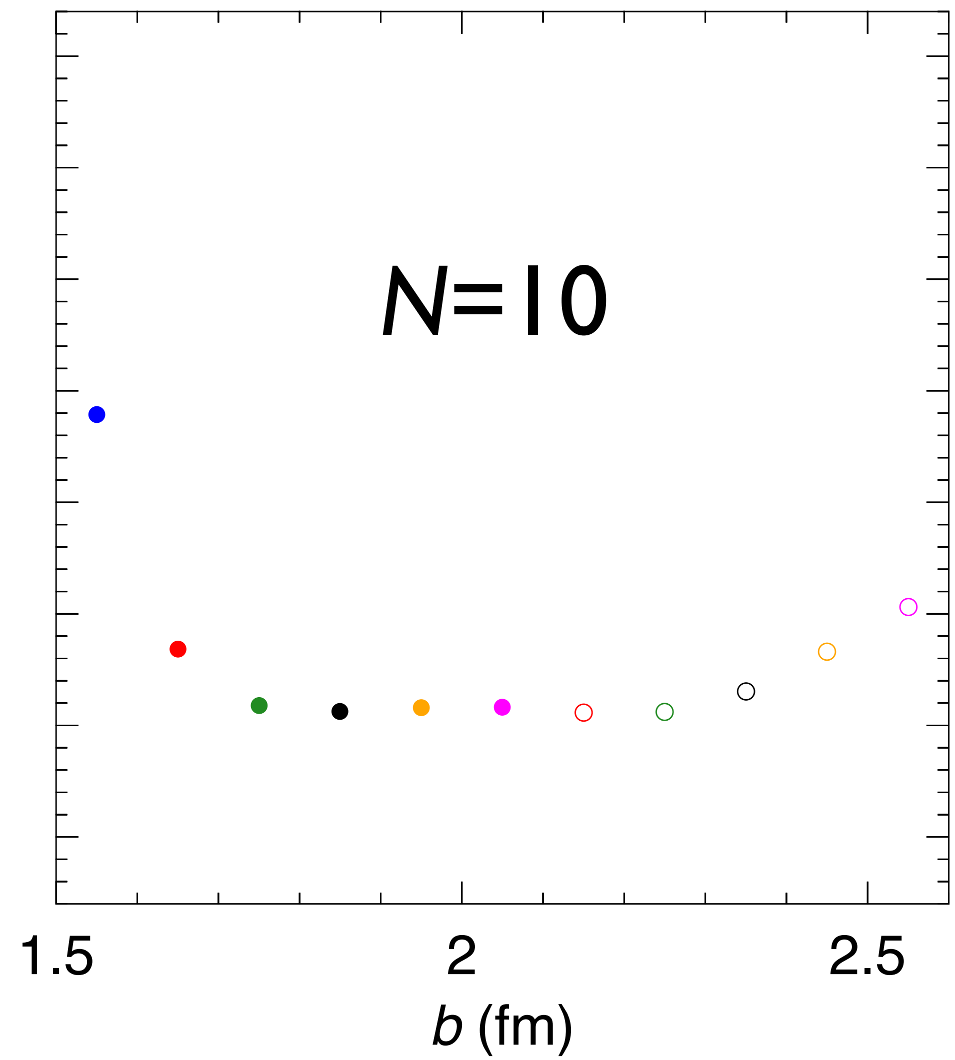
Example: 





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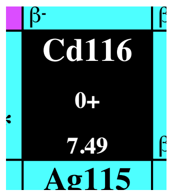
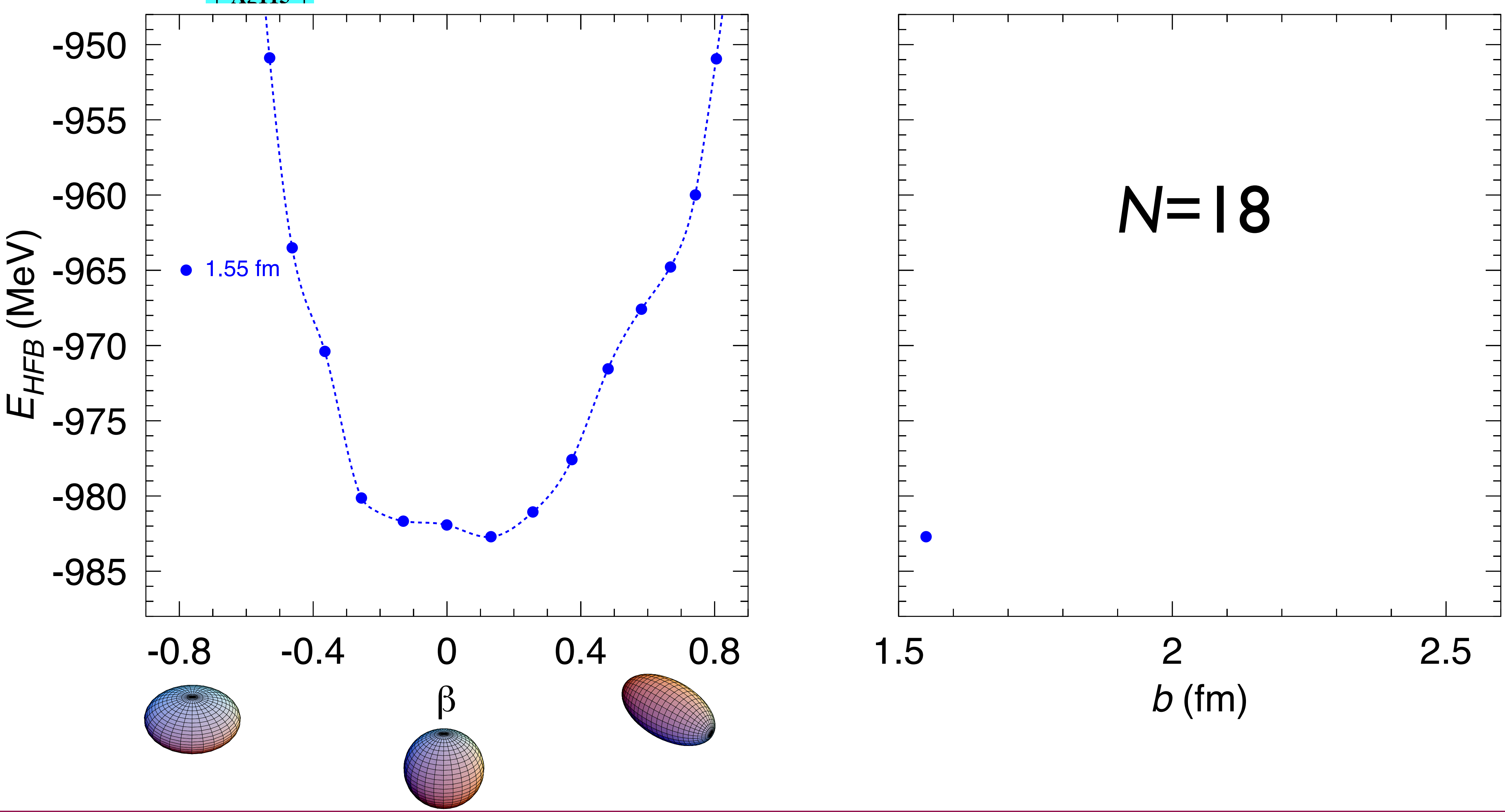
Example: 



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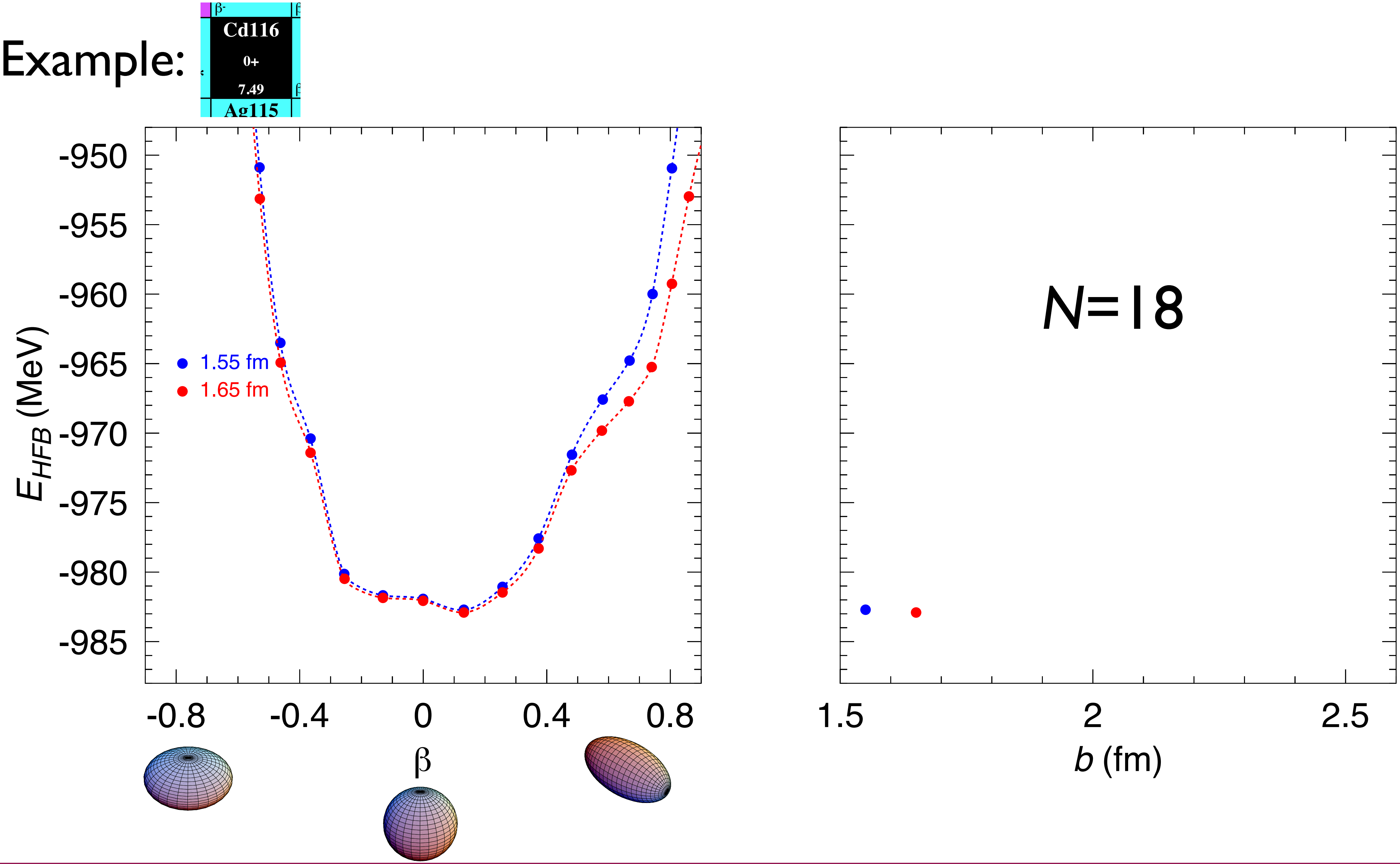

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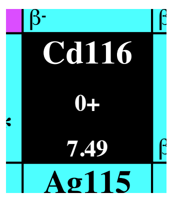
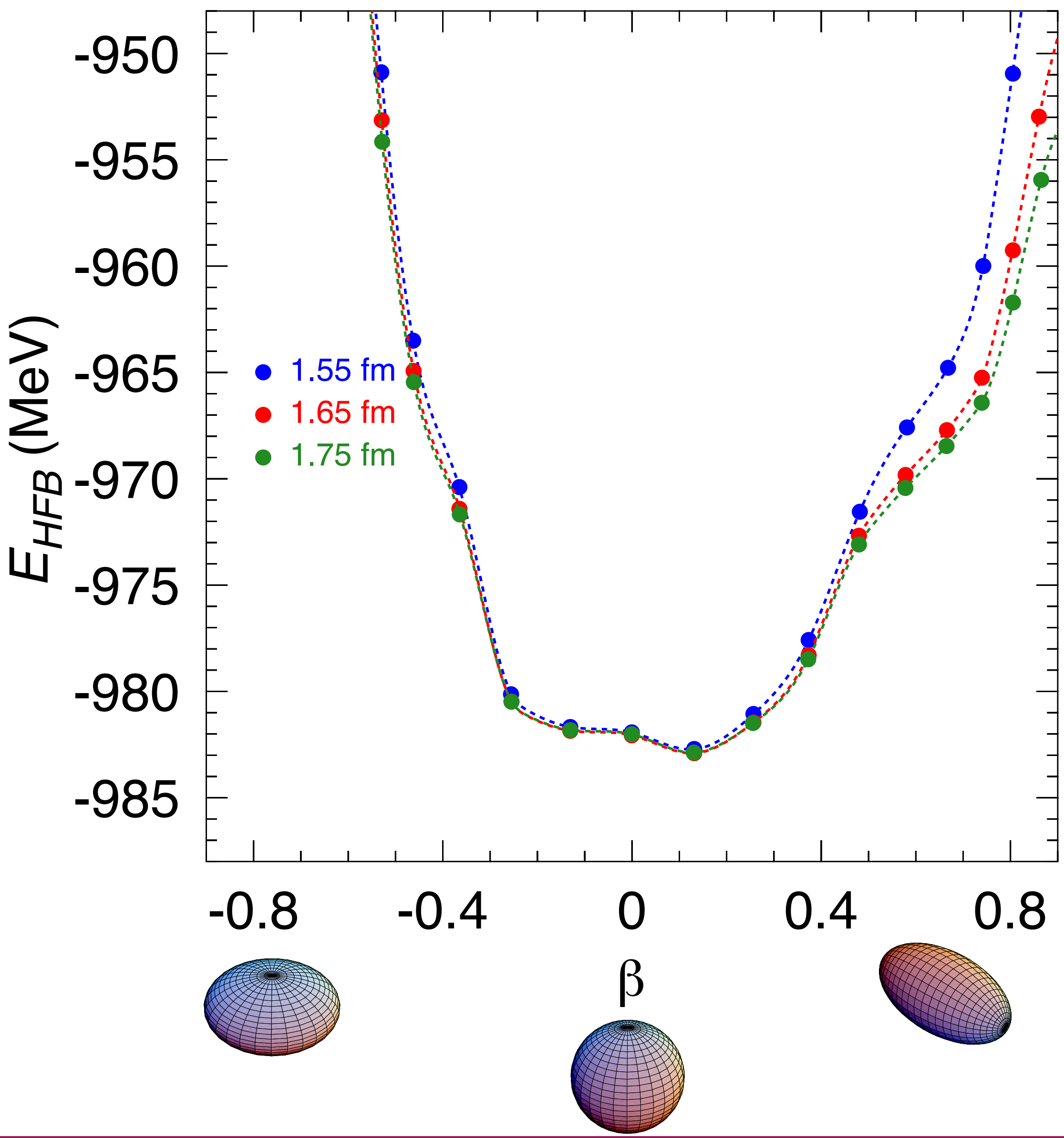
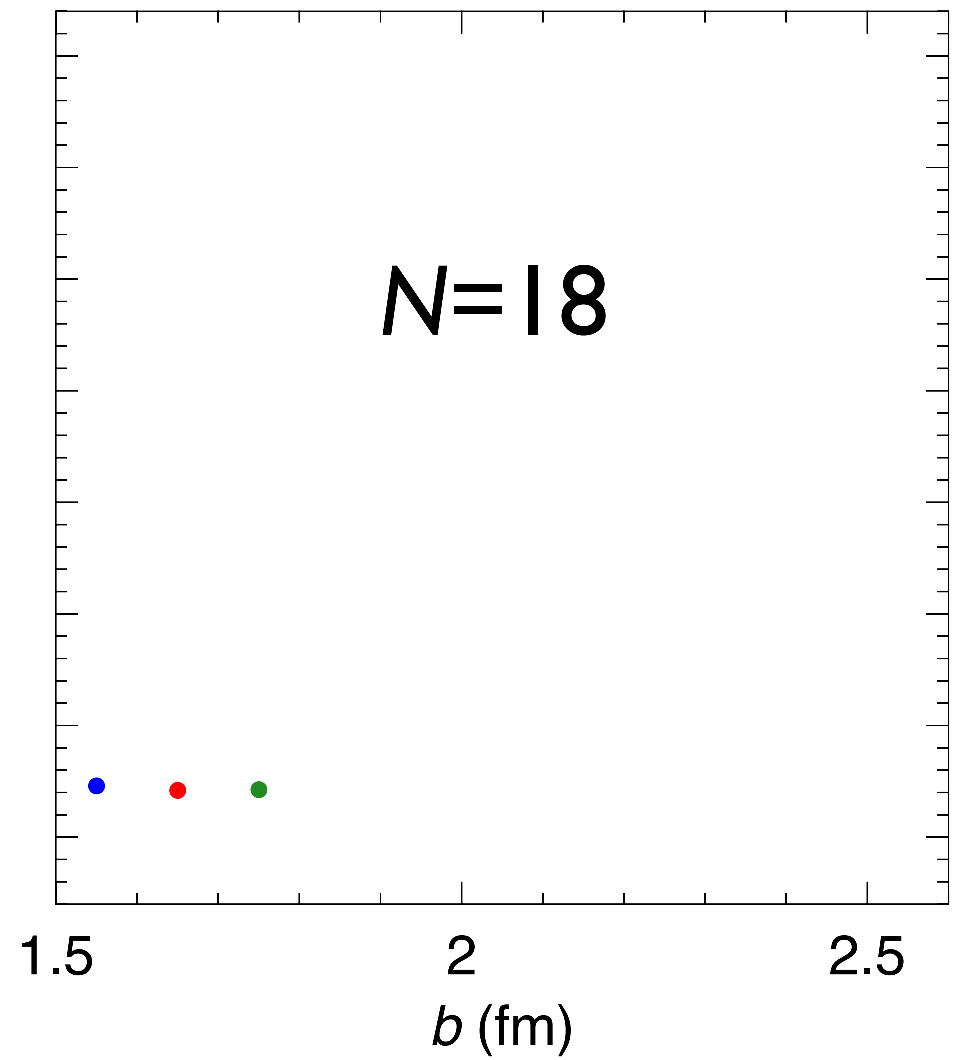
Example: 





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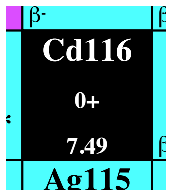
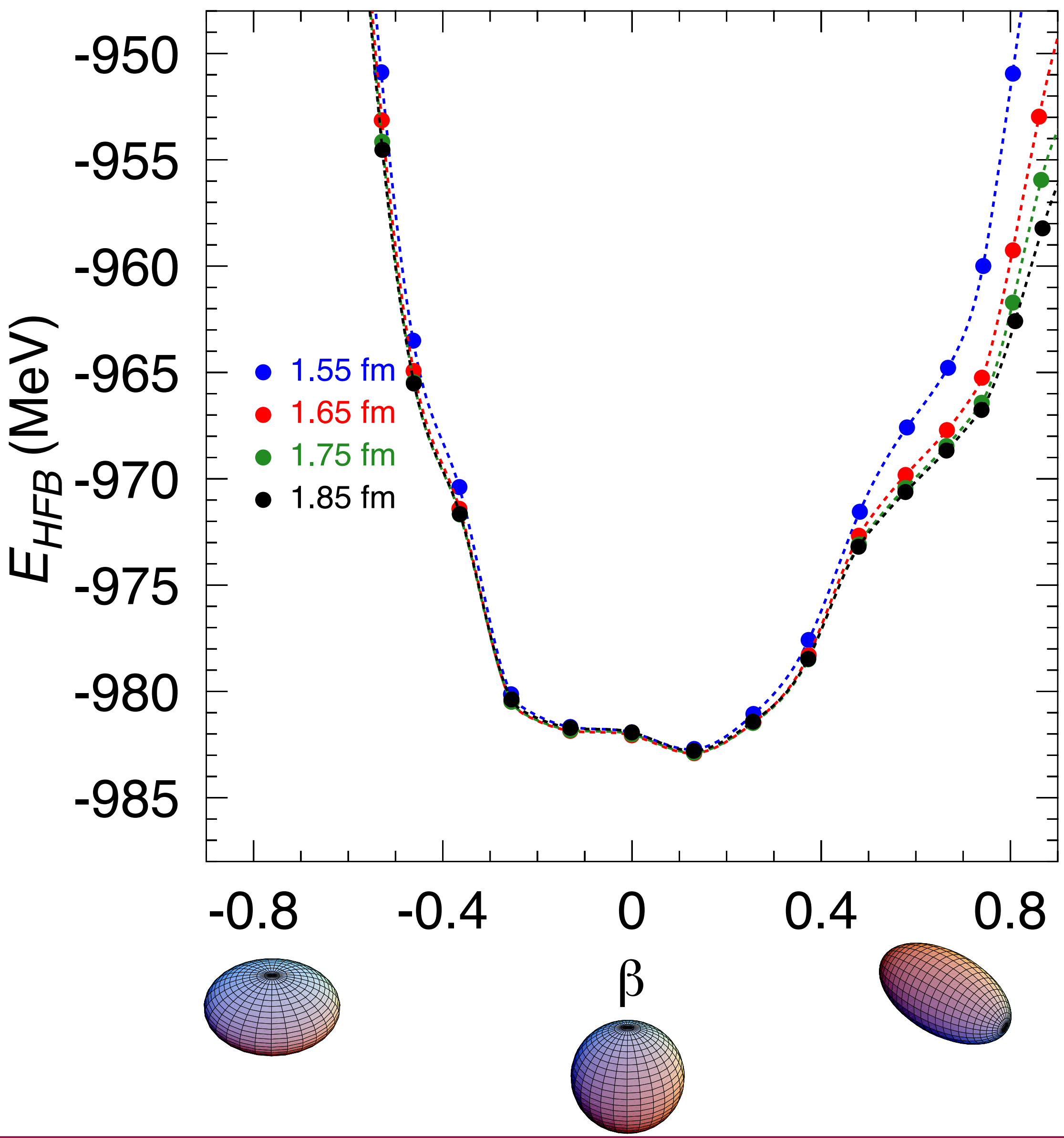
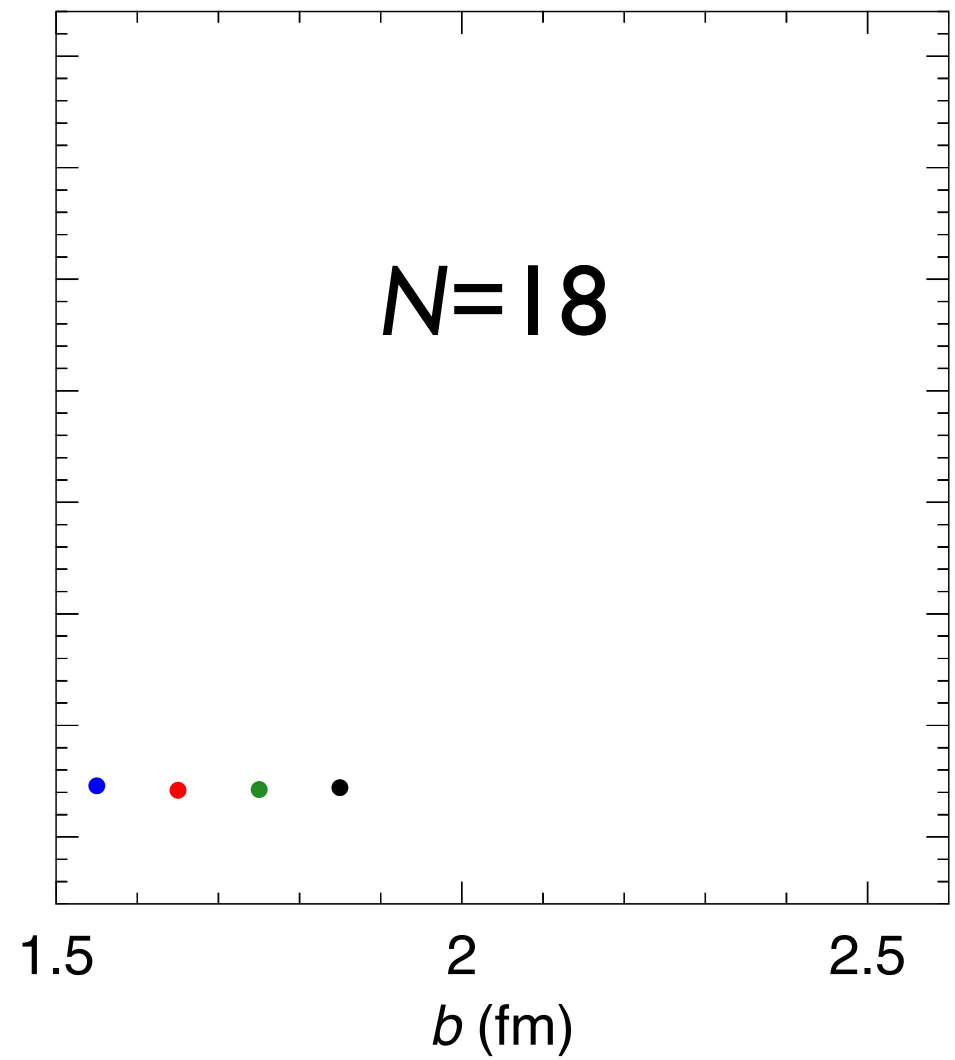
Example: 





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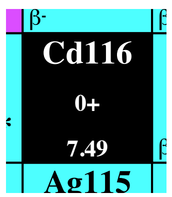
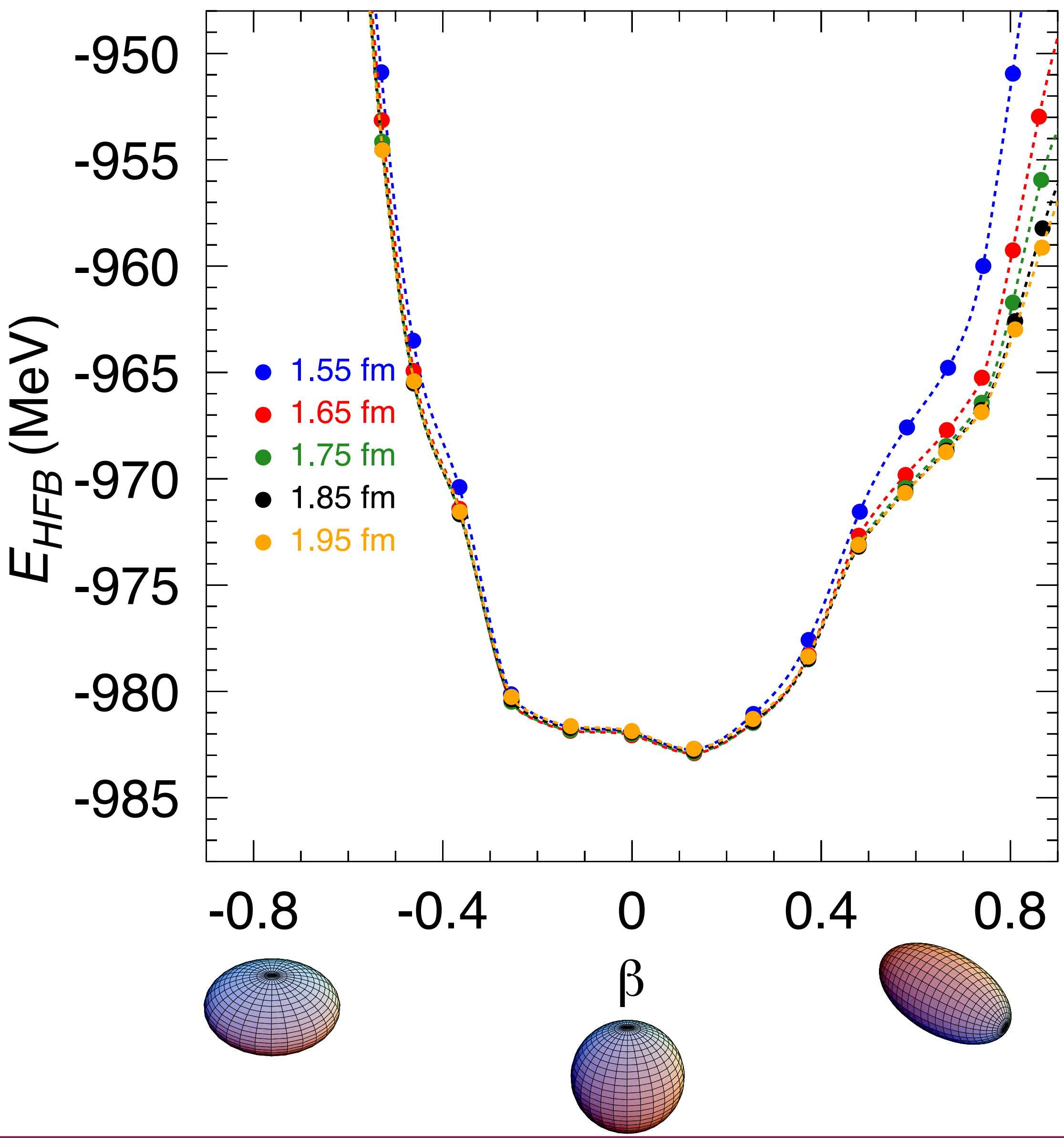
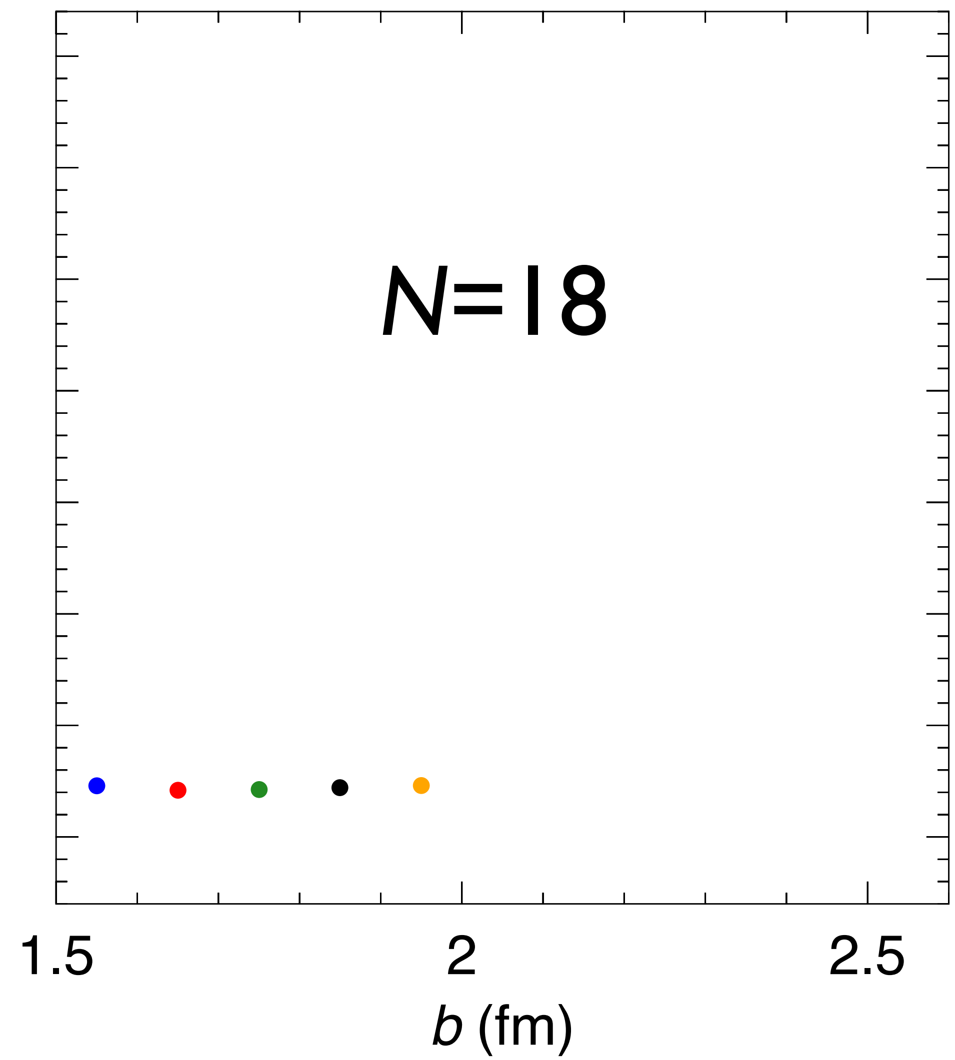
Example: 





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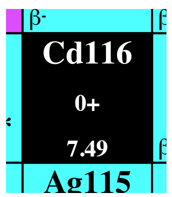
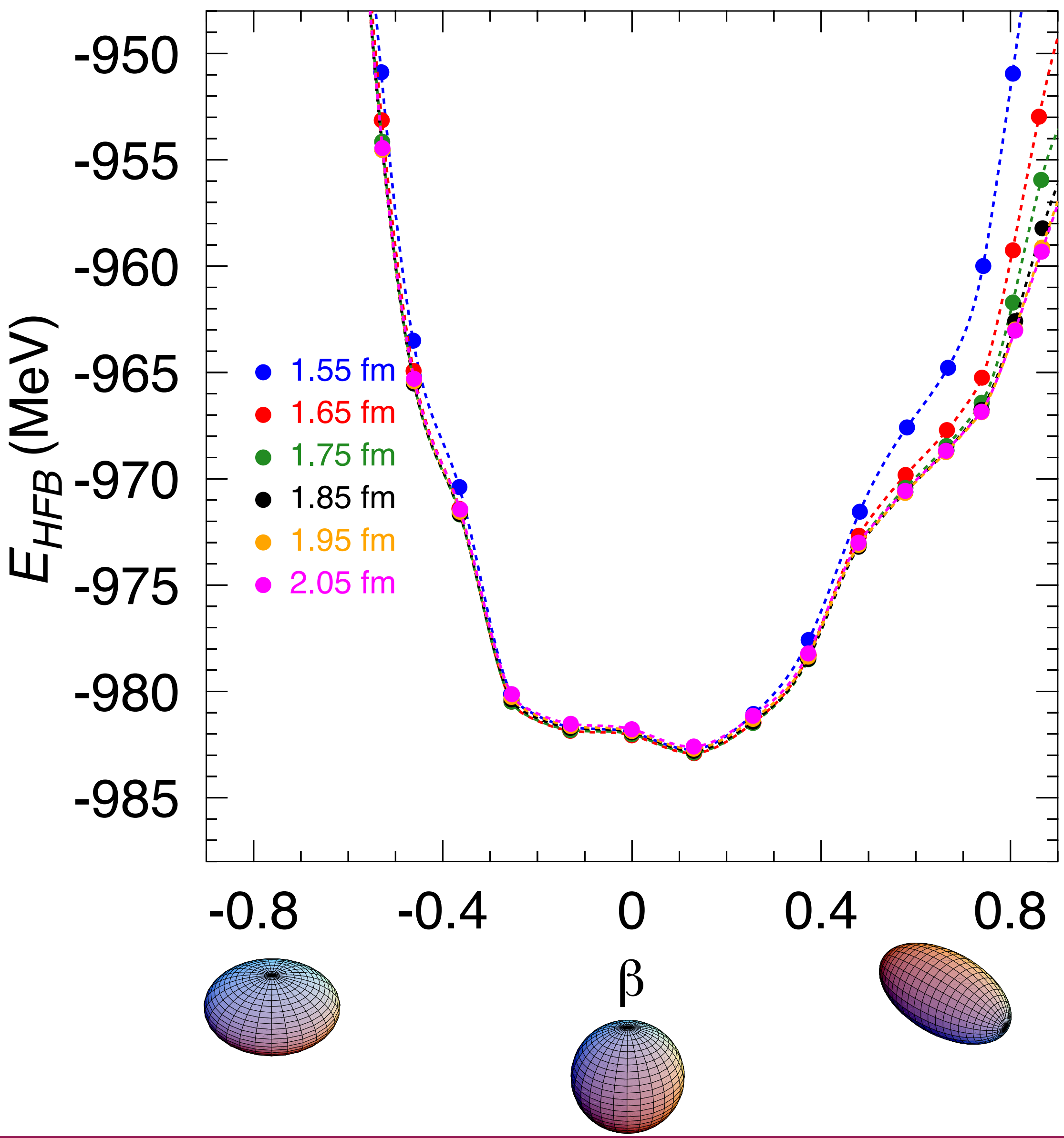
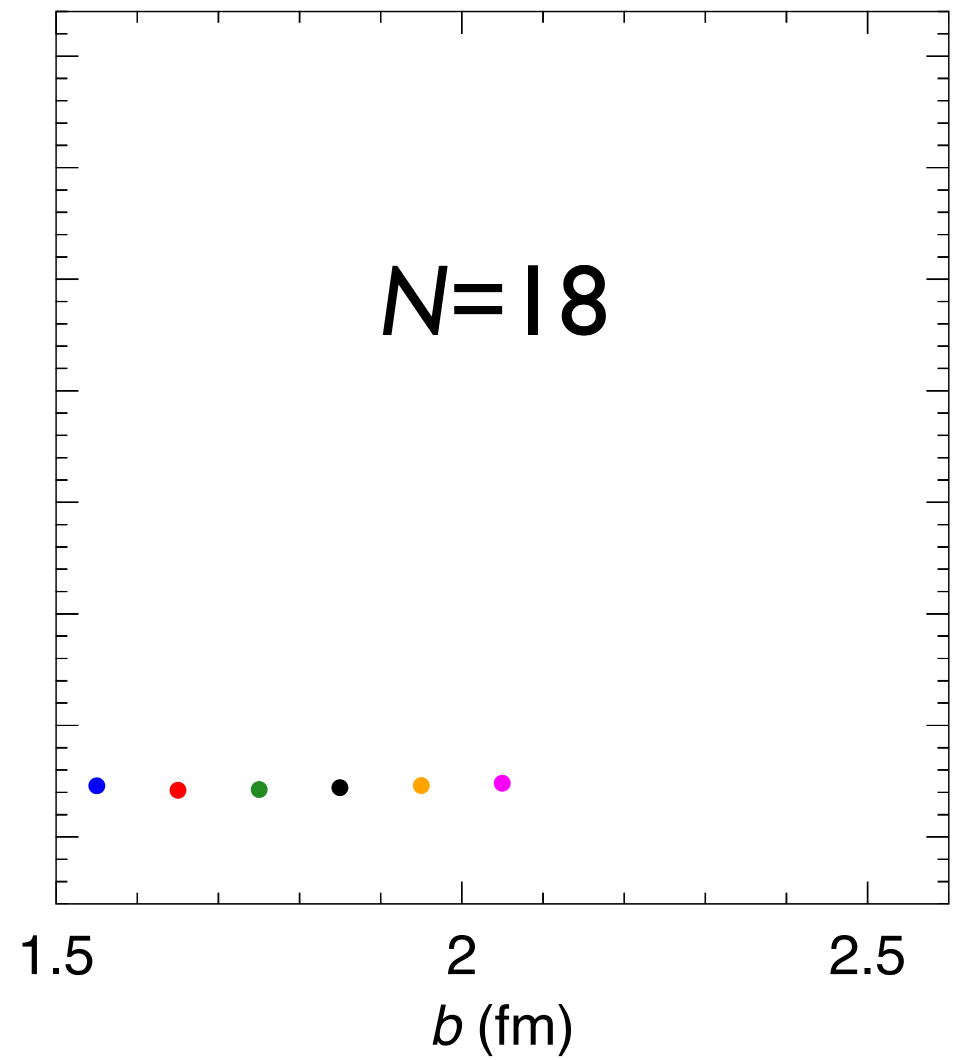
Example: 





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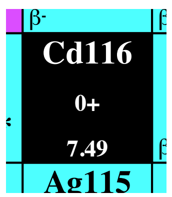
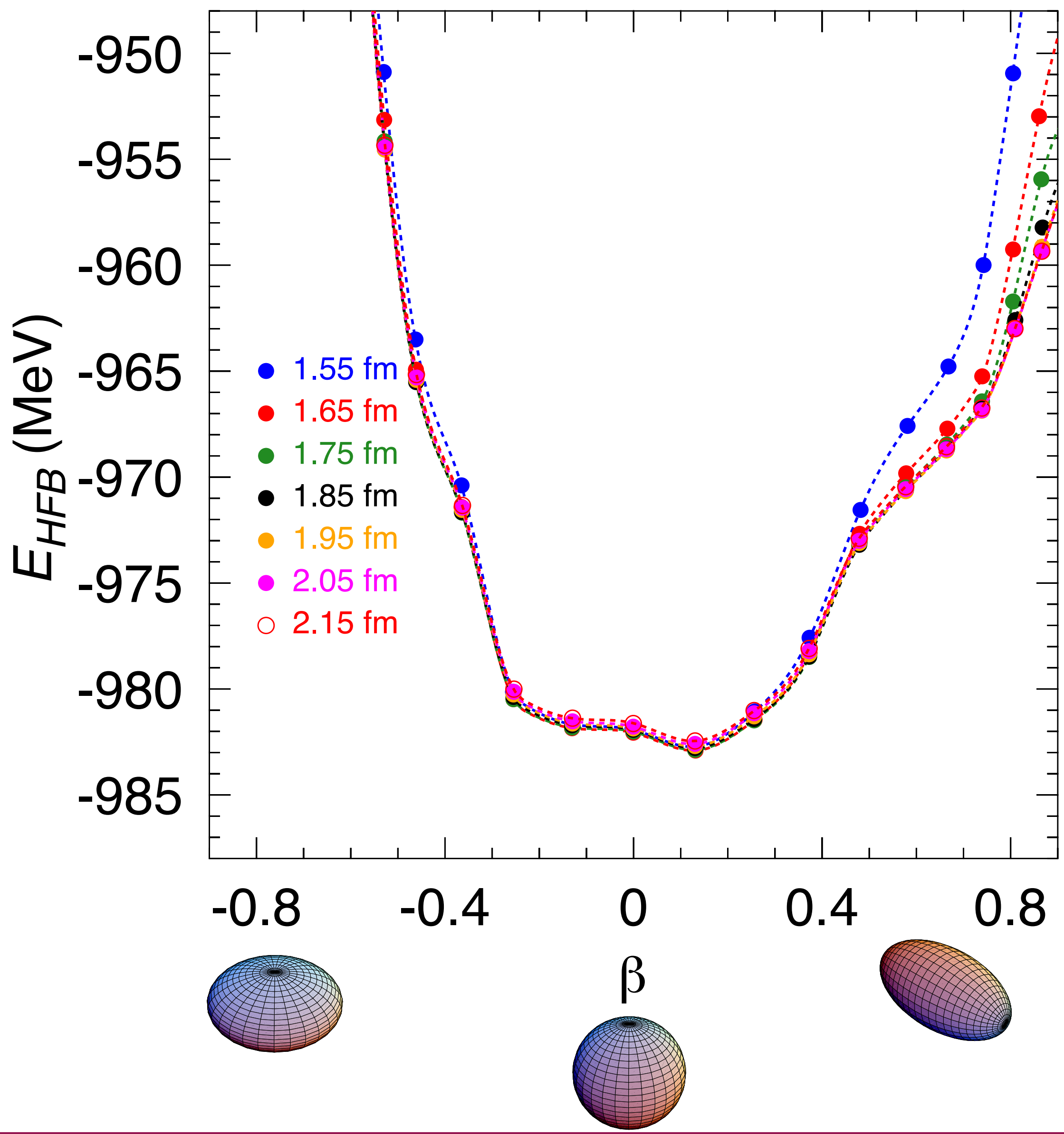
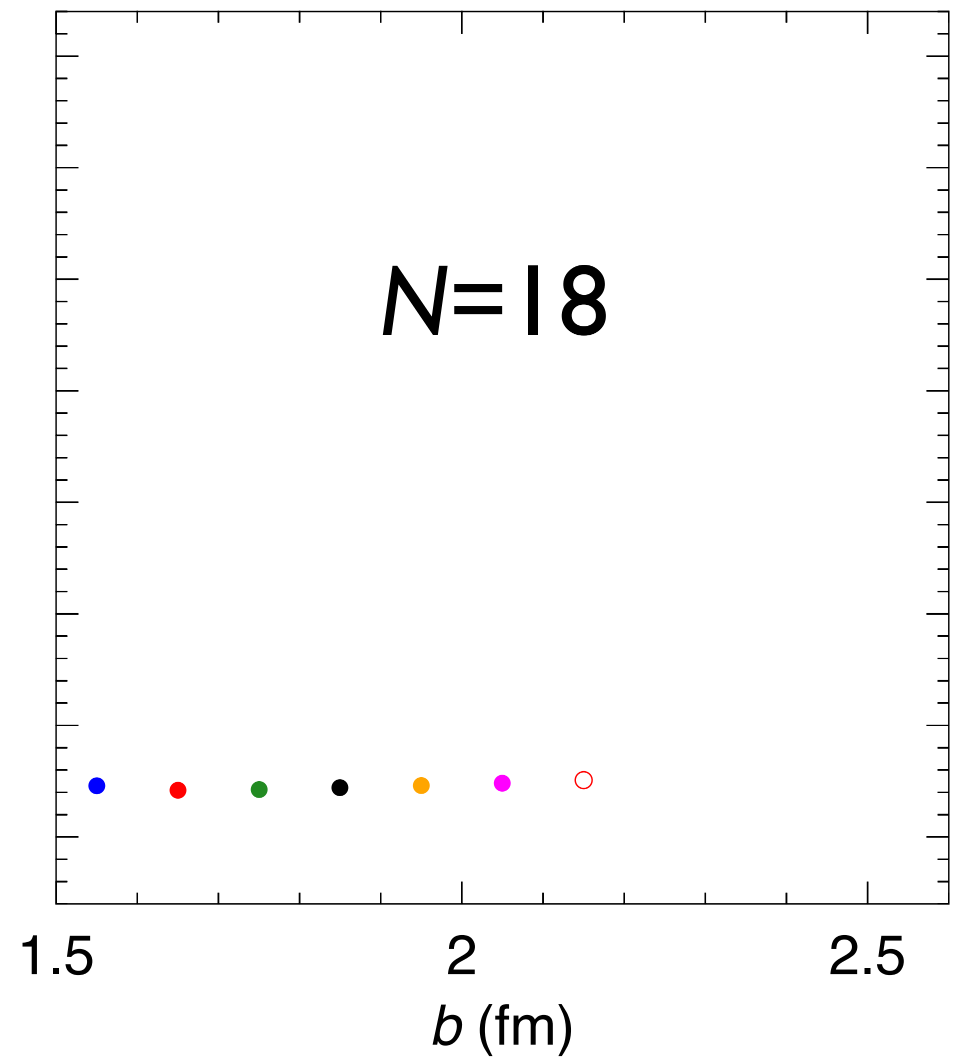
Example: 





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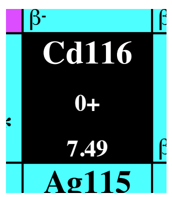
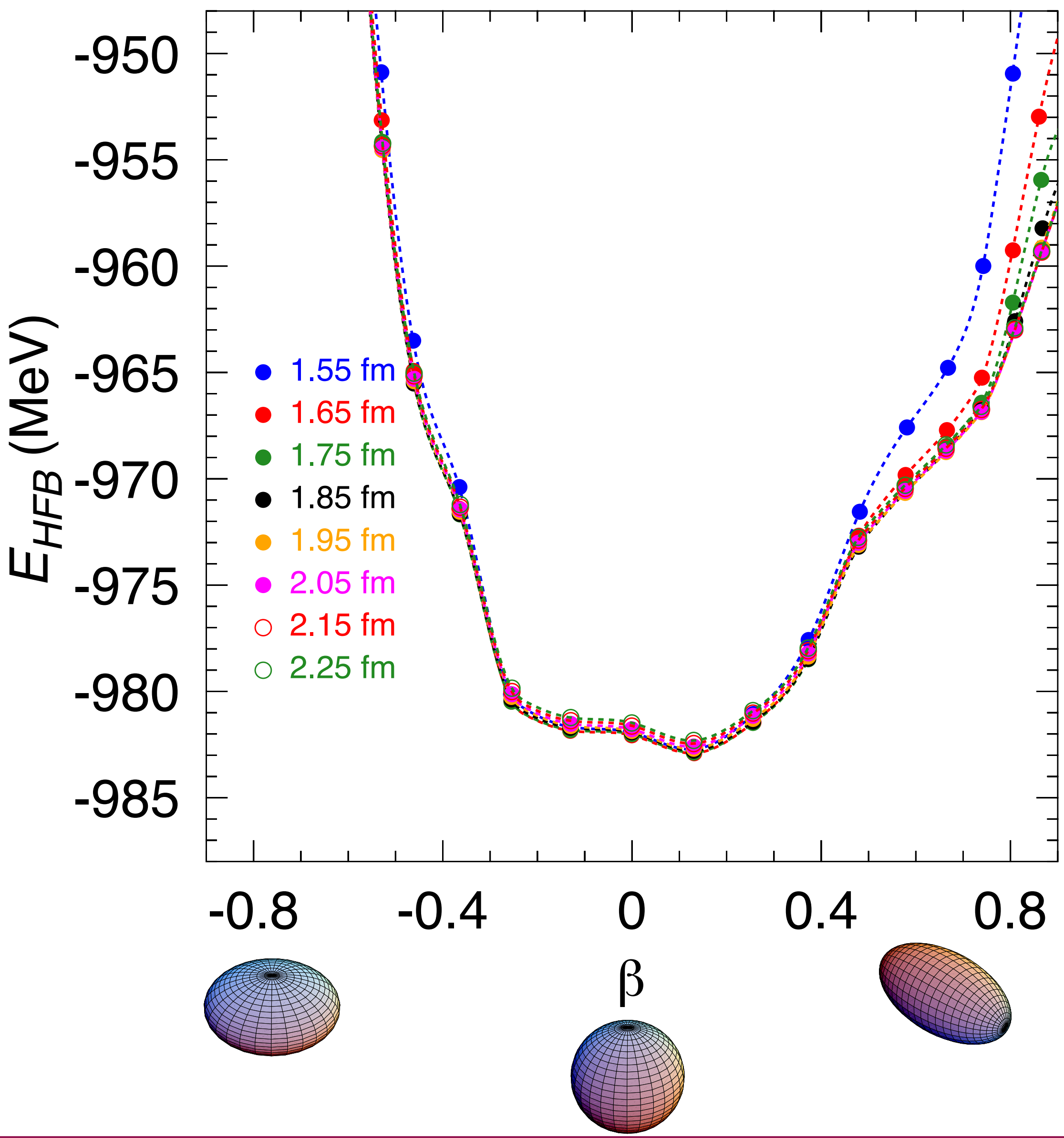
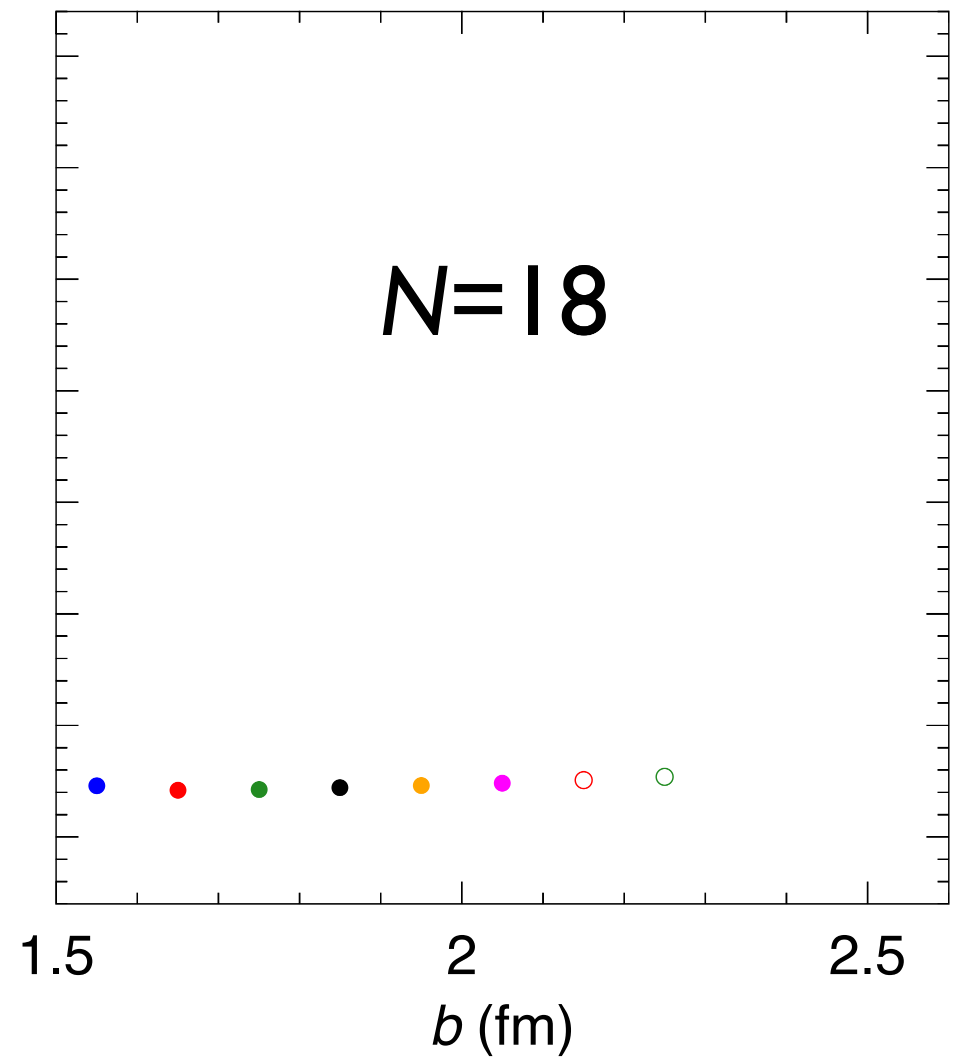
Example: 





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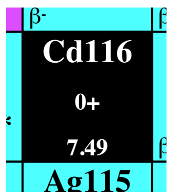
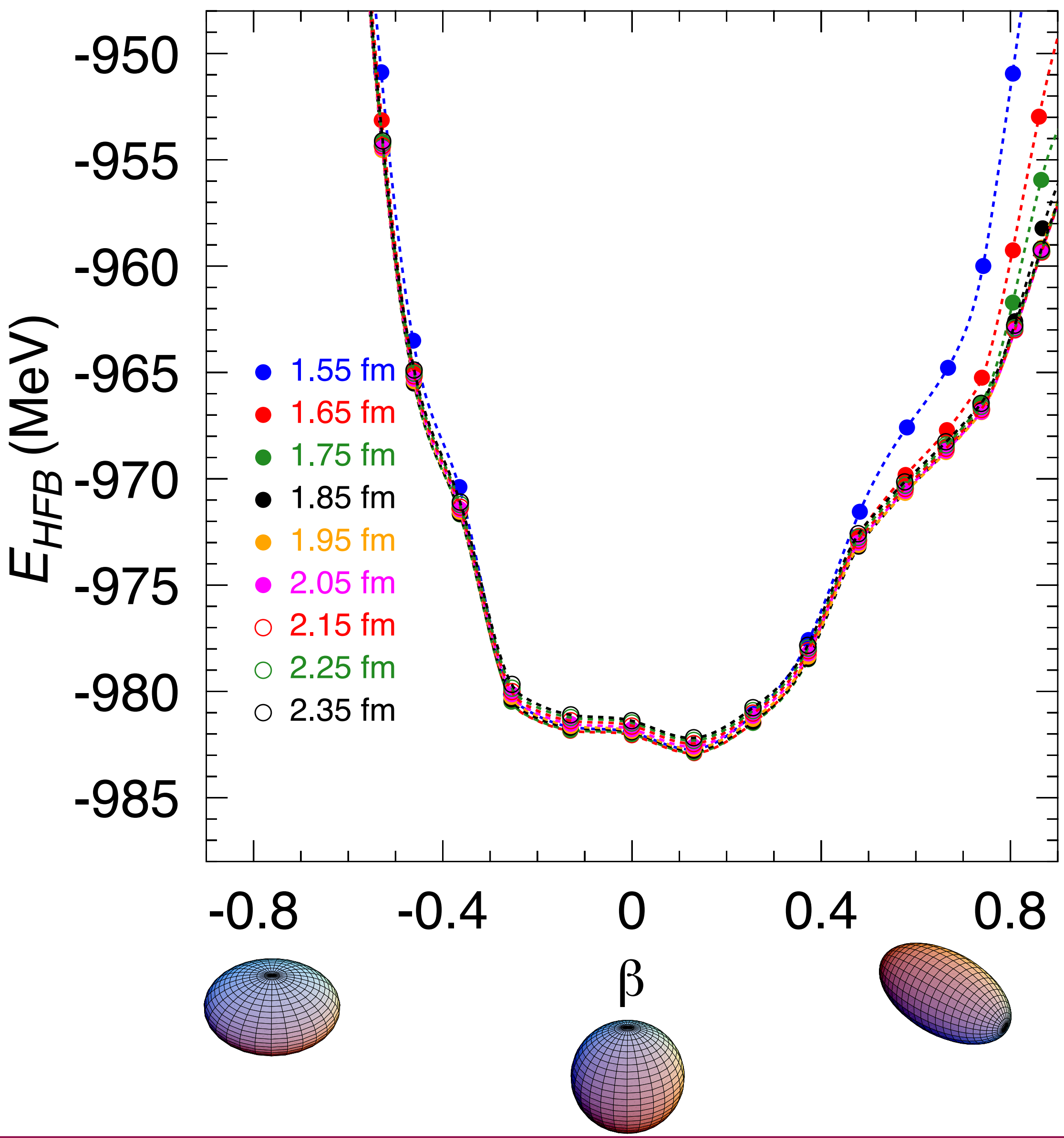
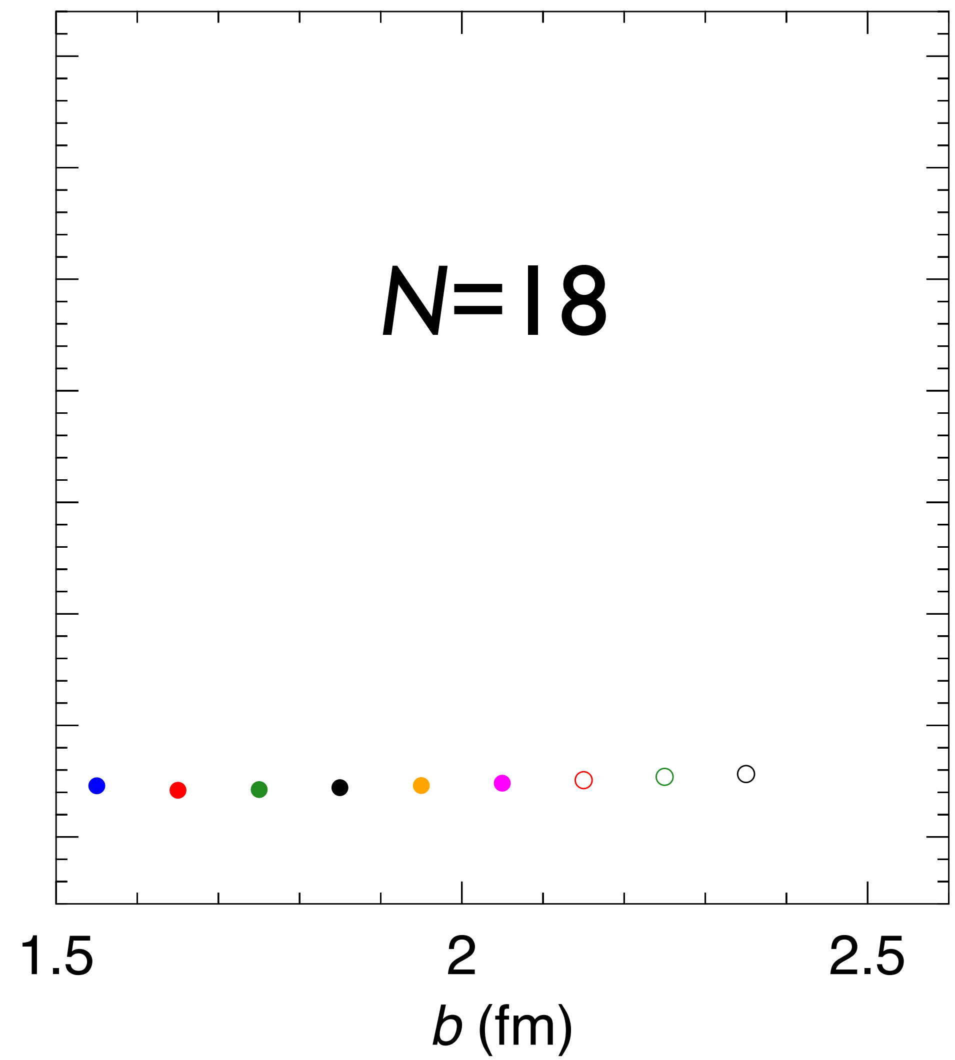
Example: 





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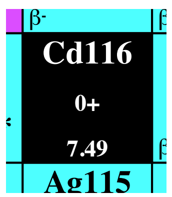
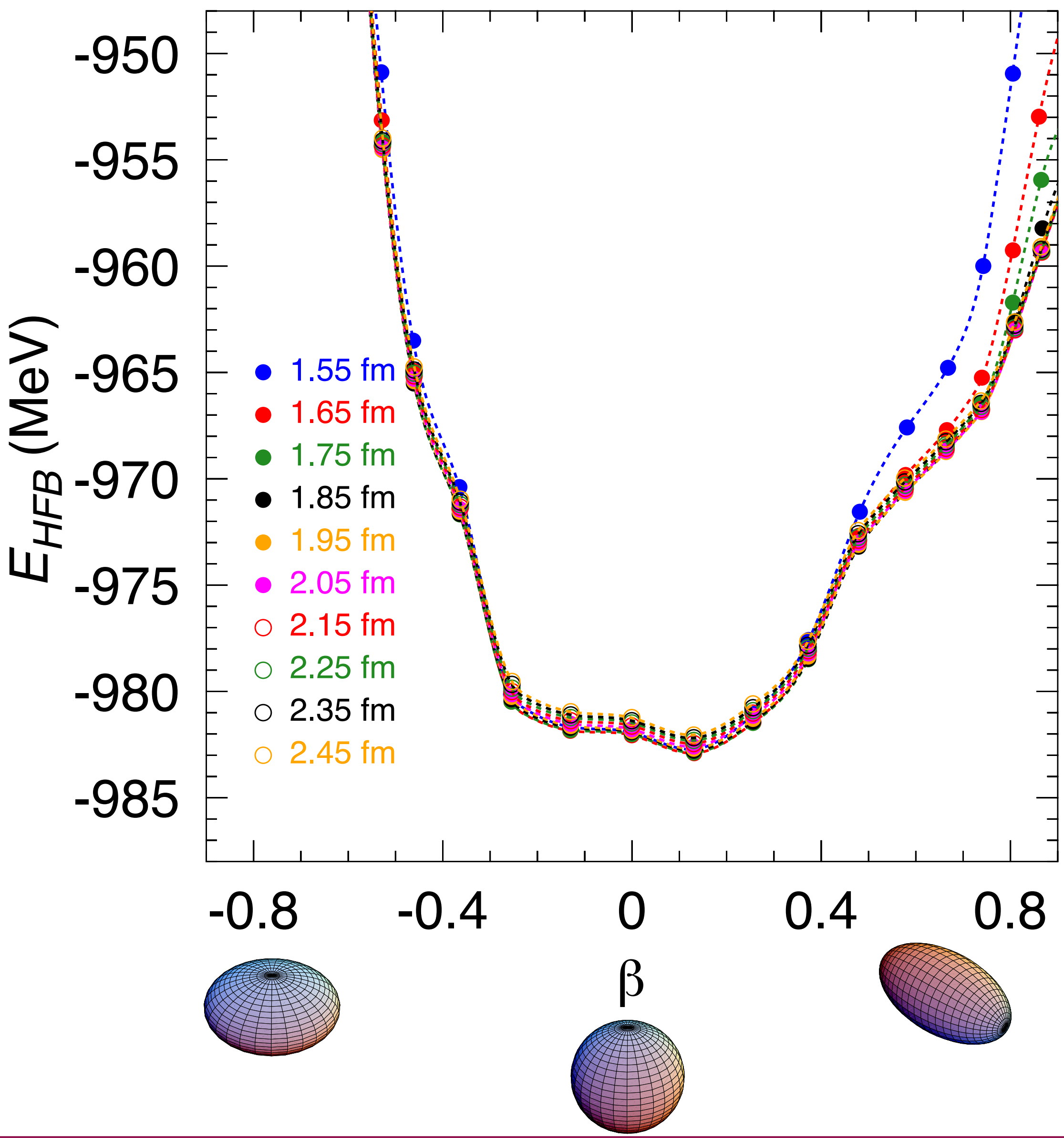
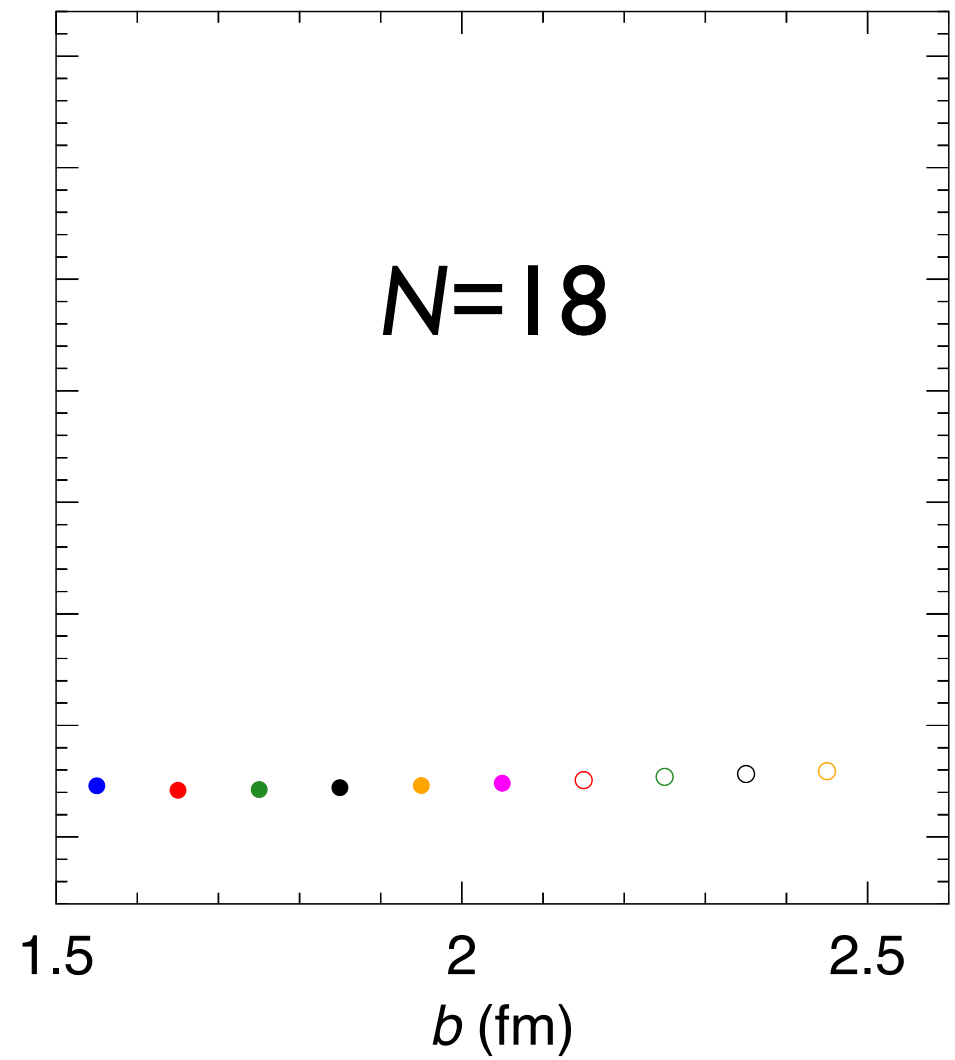
Example: 





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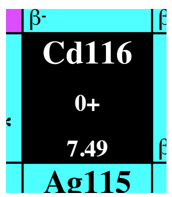
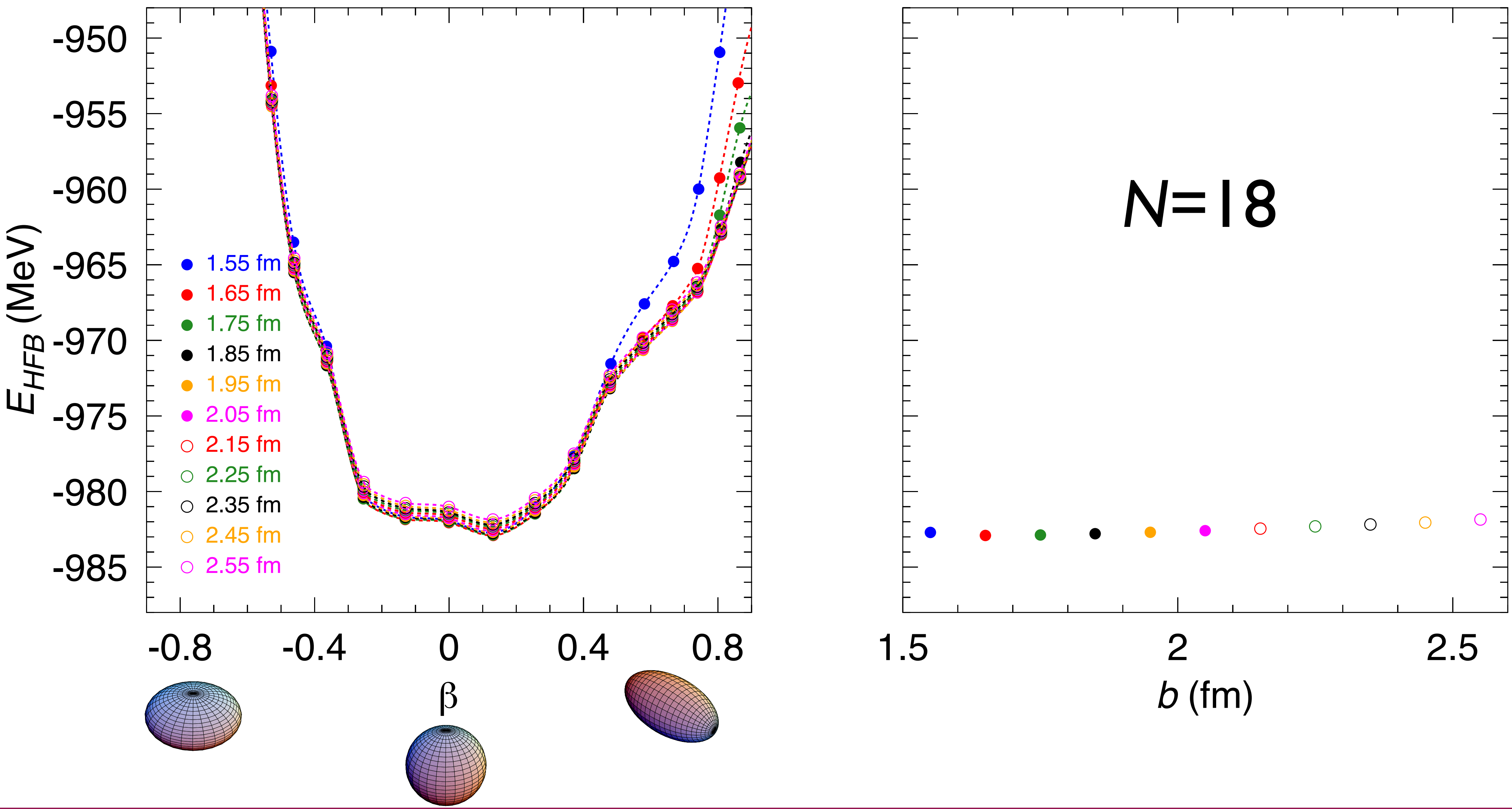
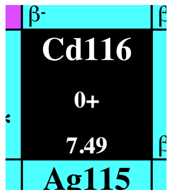
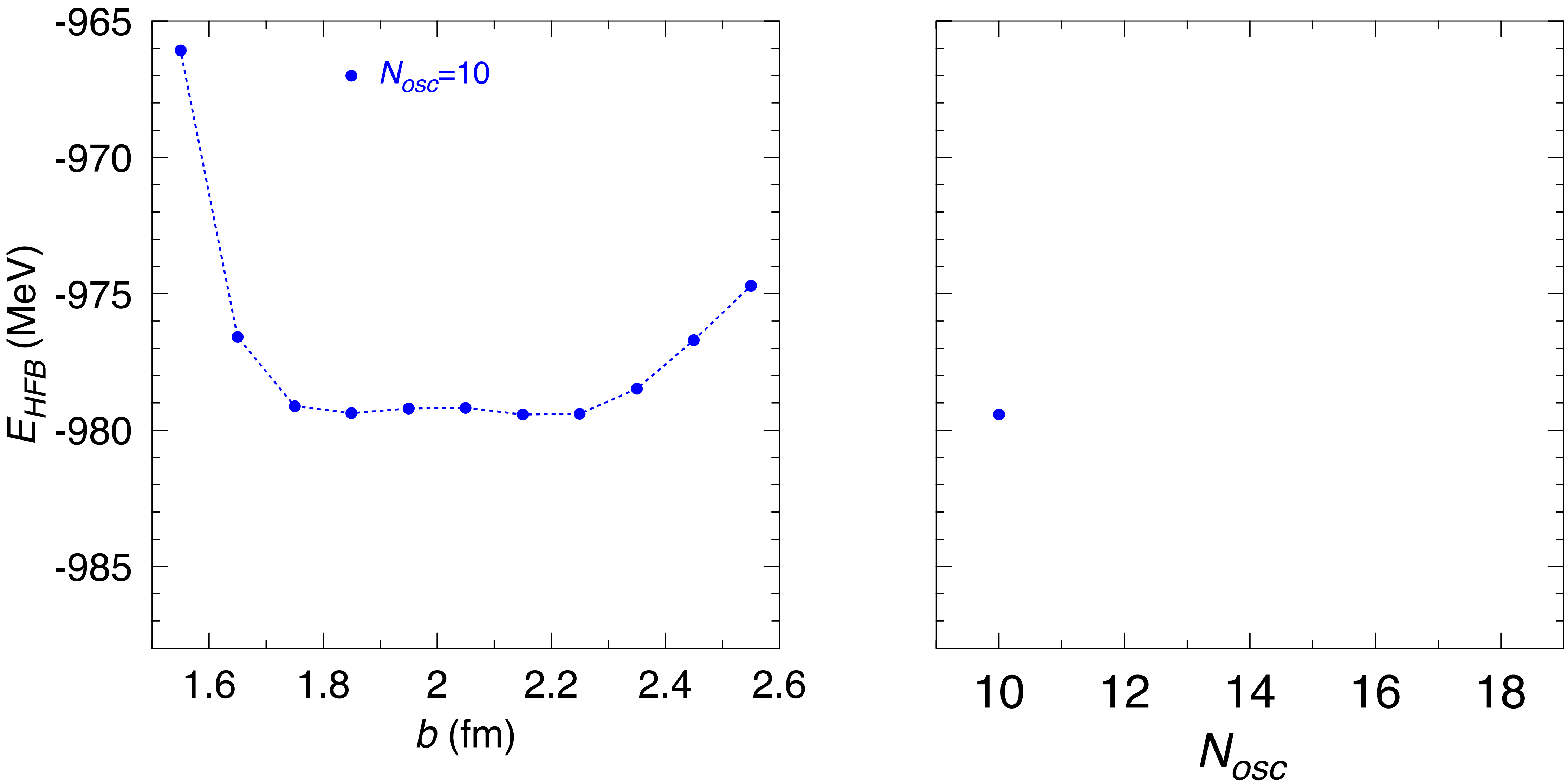
Example: 



Final convergence

Example: 



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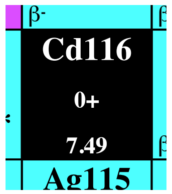
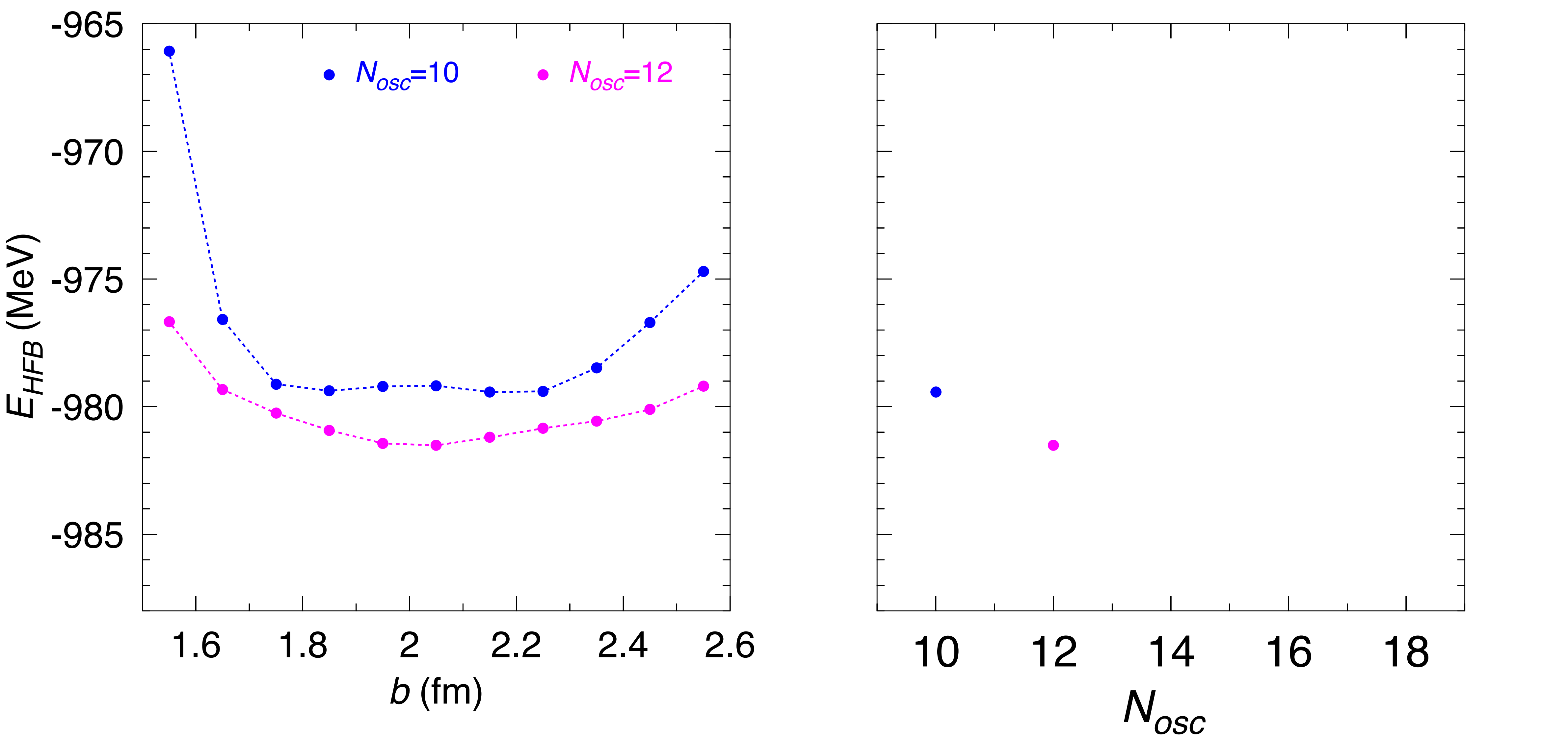
Example: 



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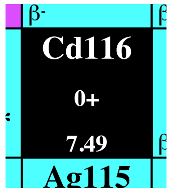

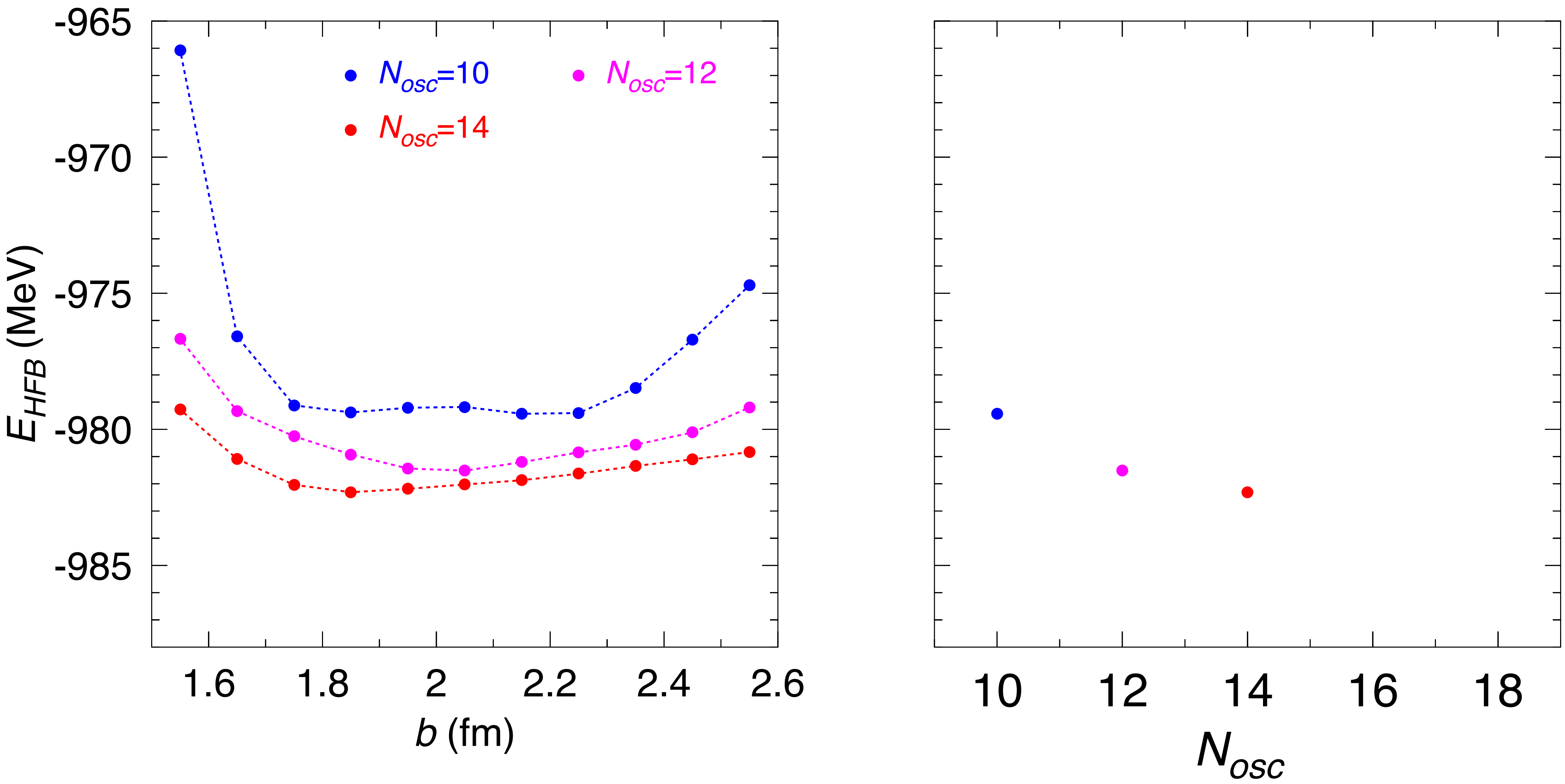

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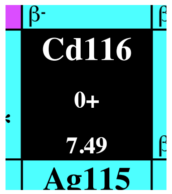
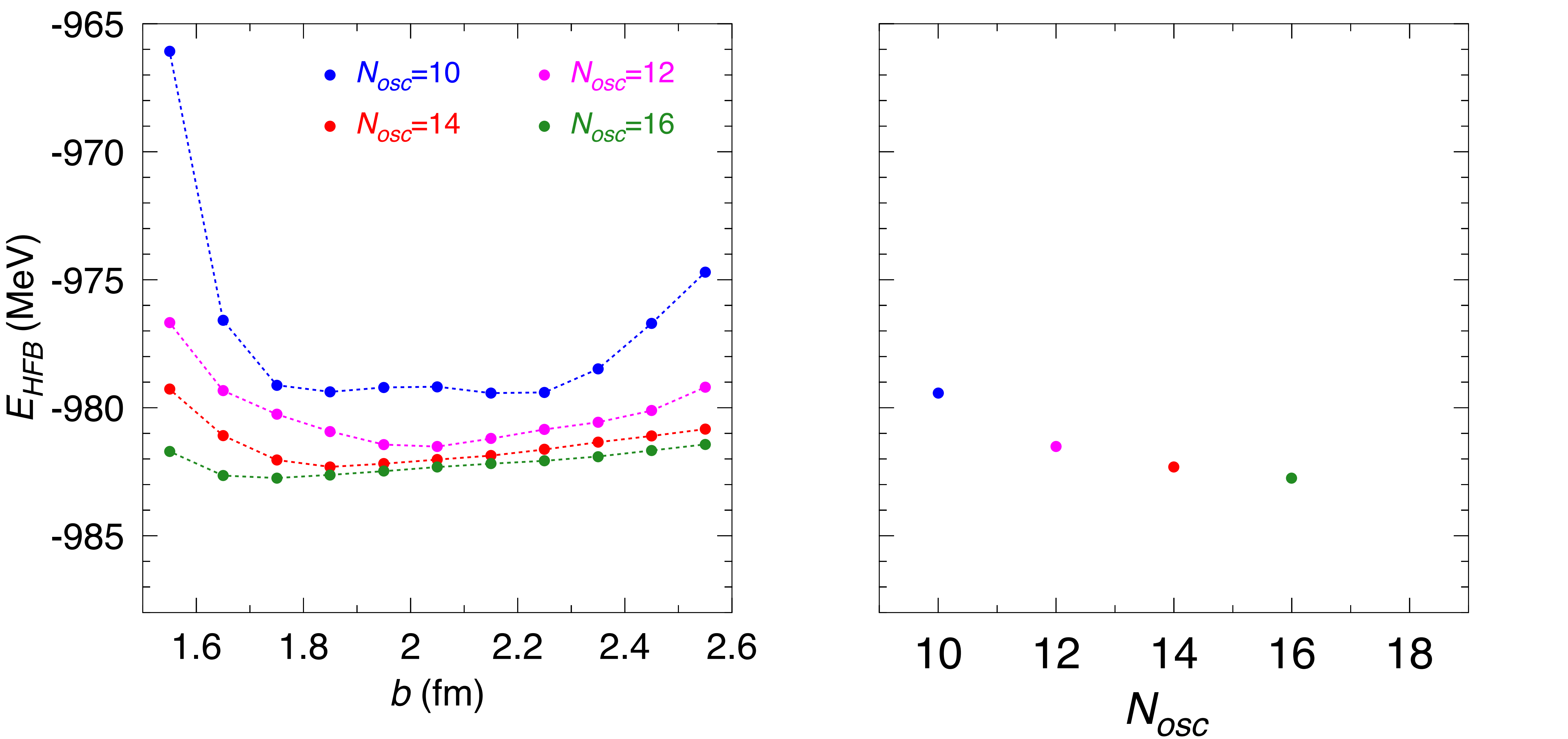
Example: 



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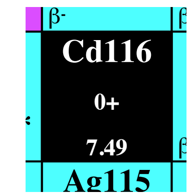
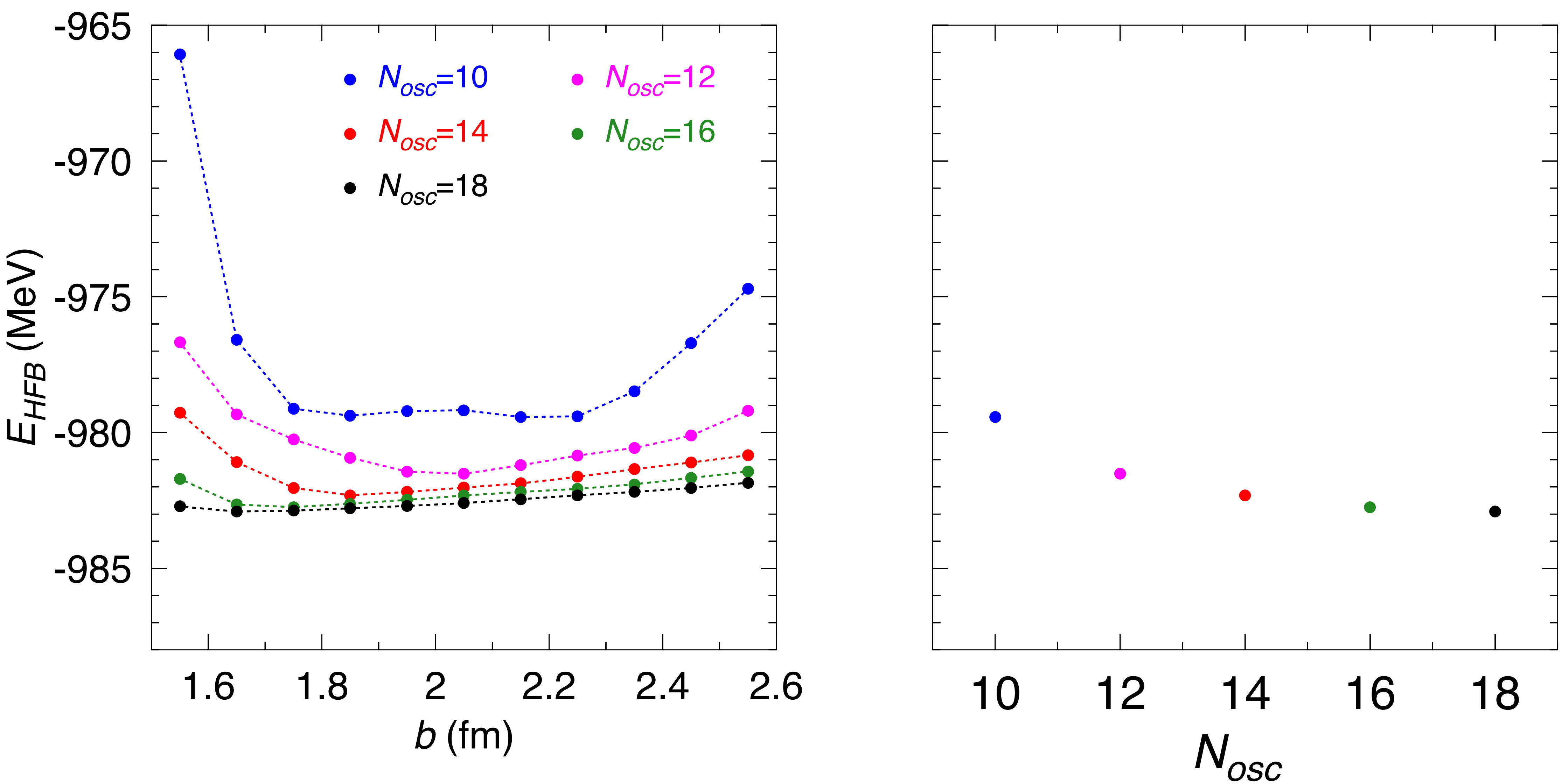
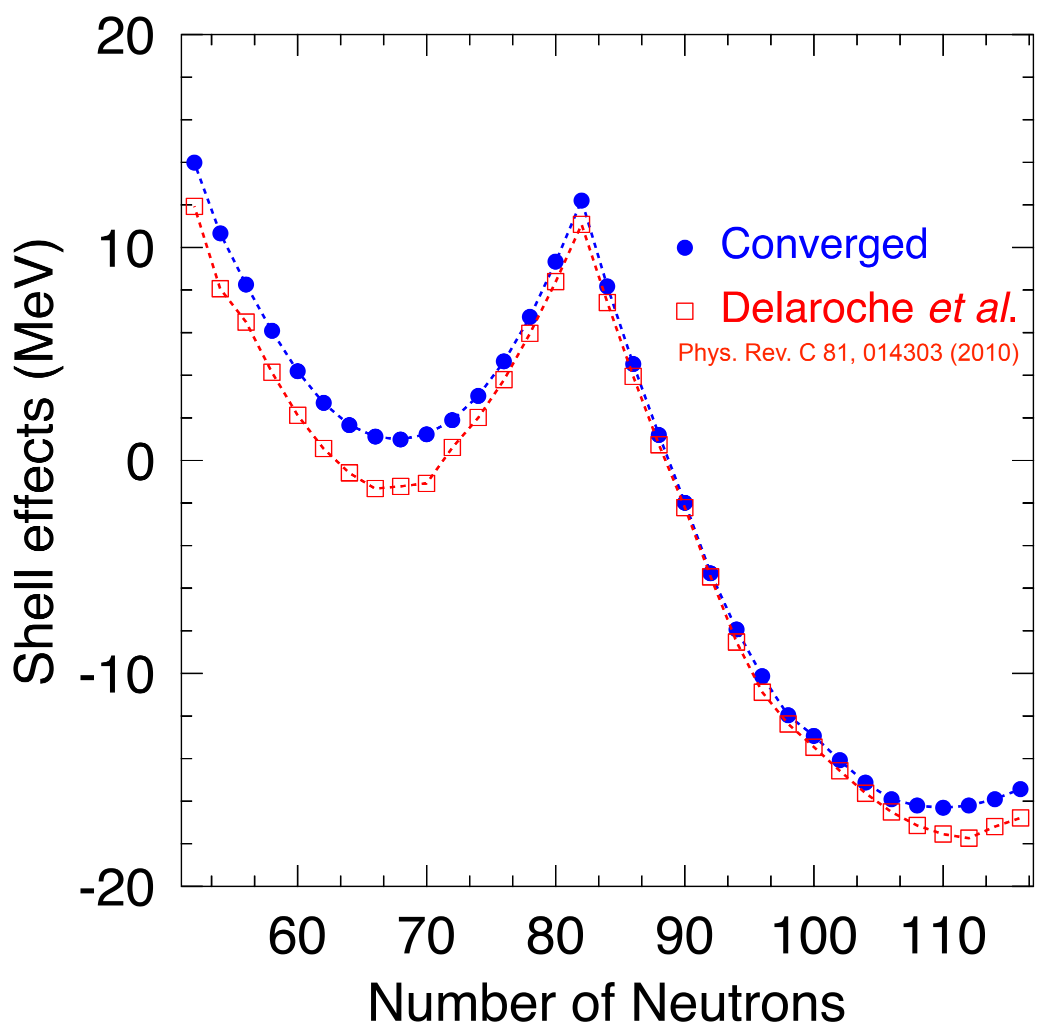
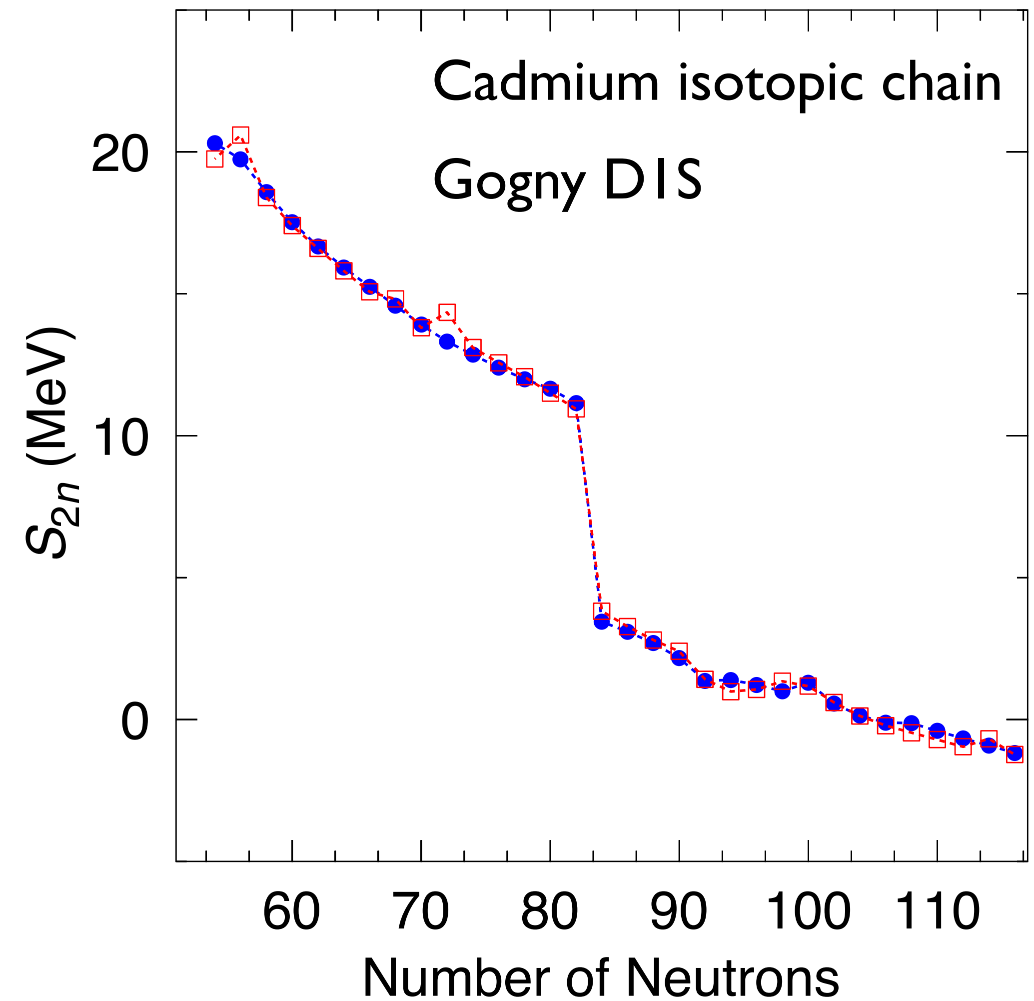
Example: 



Convergence

- Published tables could contain some lack of convergence in the total binding energy.
- Two neutron separation energies are better converged.
- Artificial 'jumps' or 'noise' could appear in the S_{2n} due to lack of convergence.





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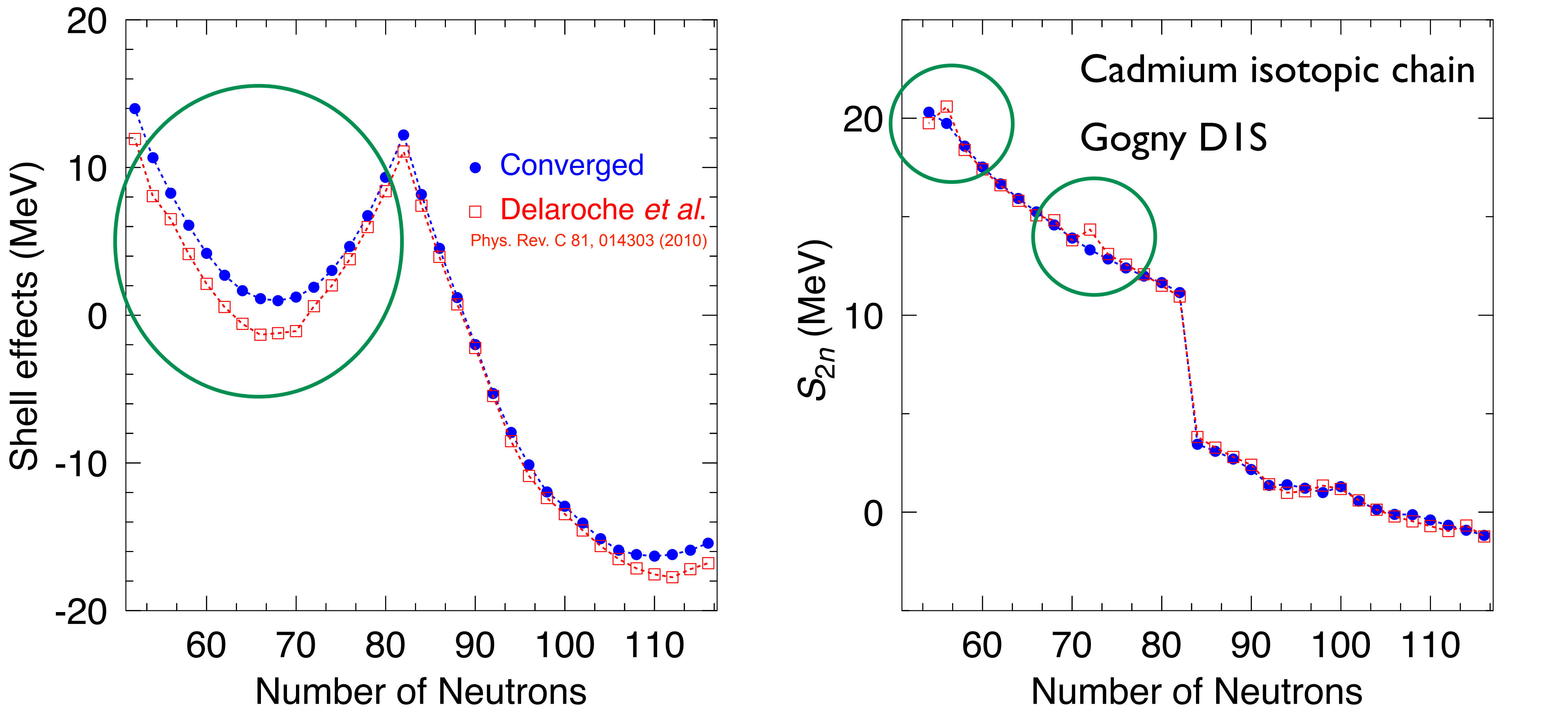

Self-consistent beyond mean field description

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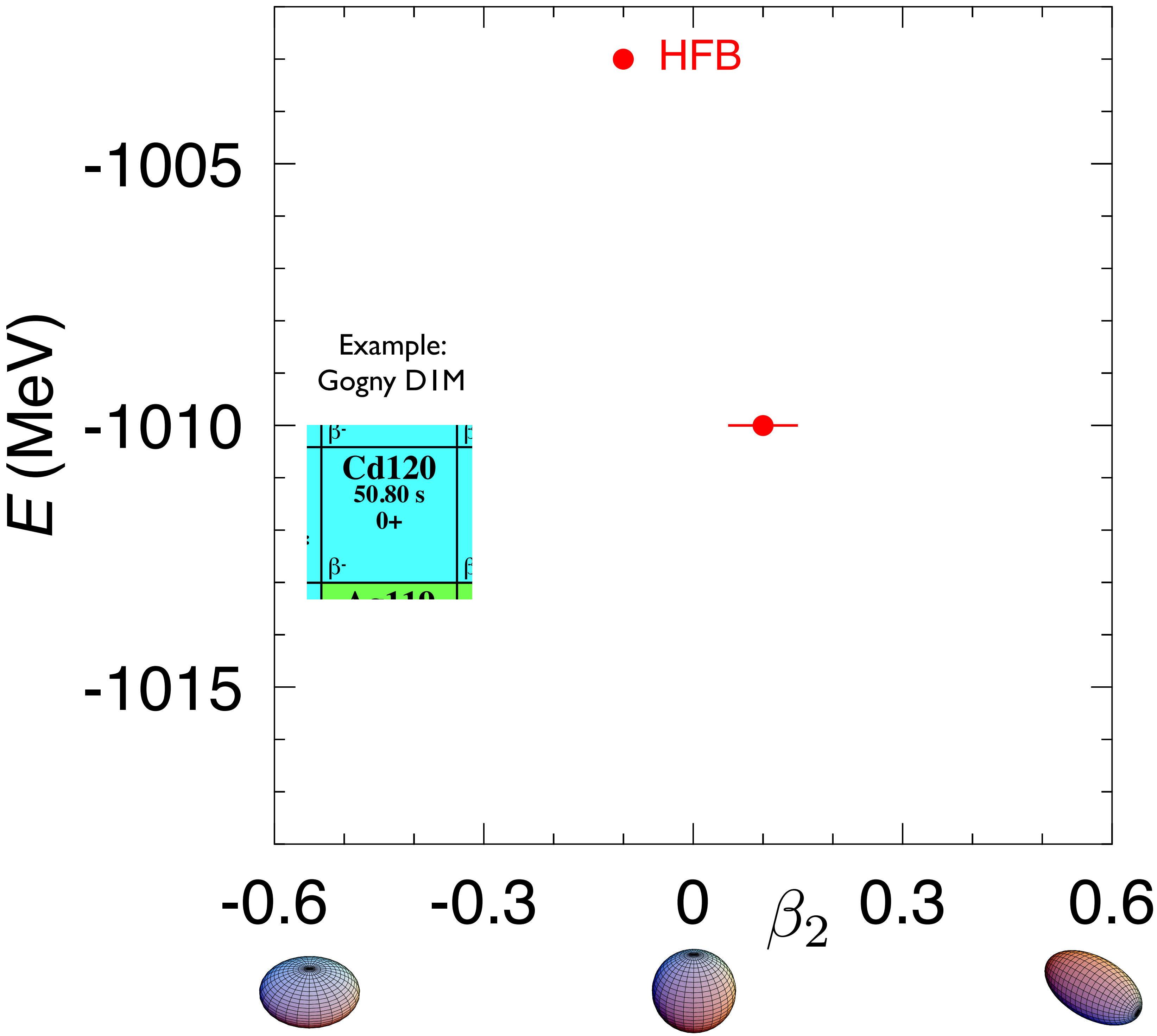

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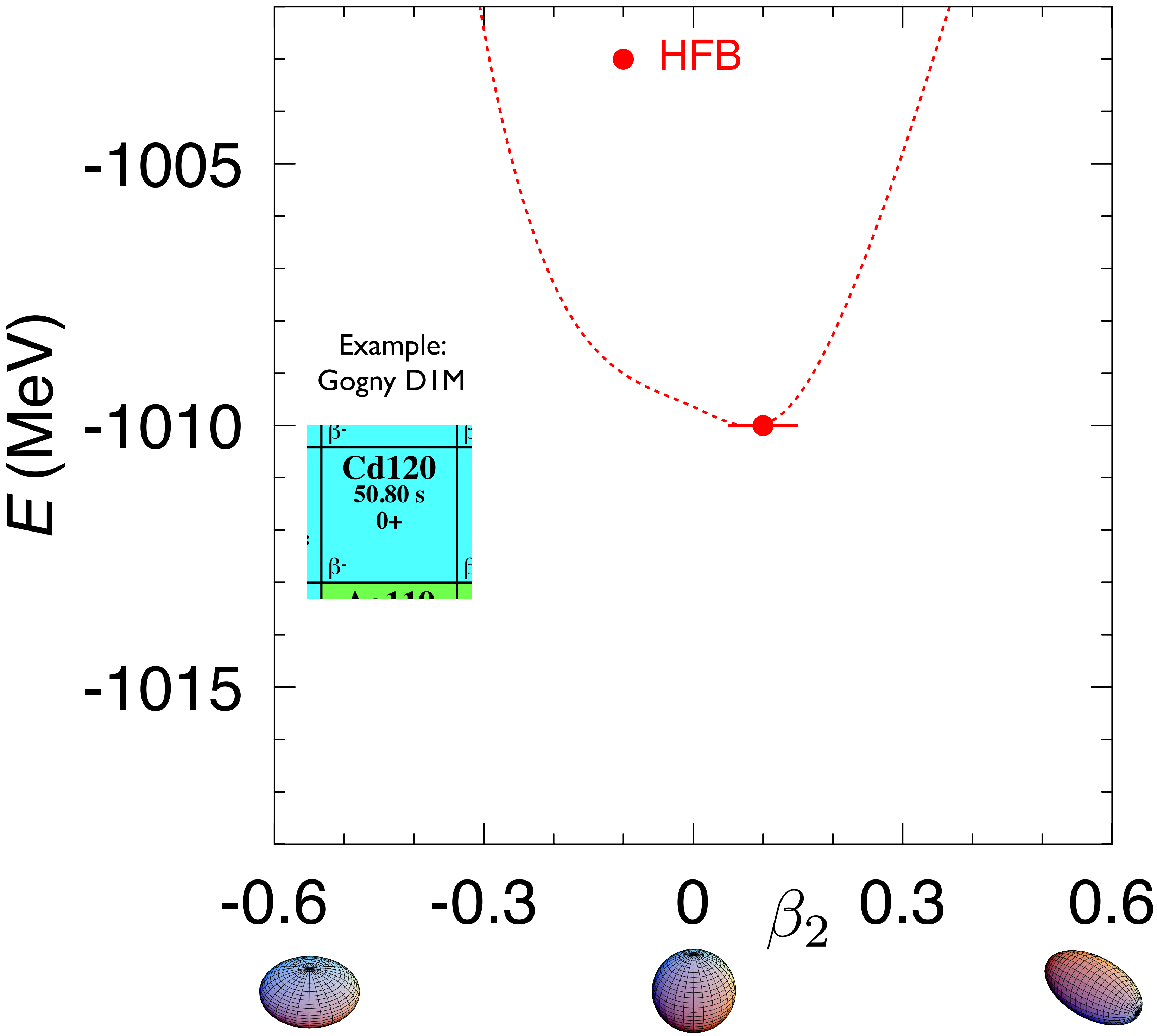

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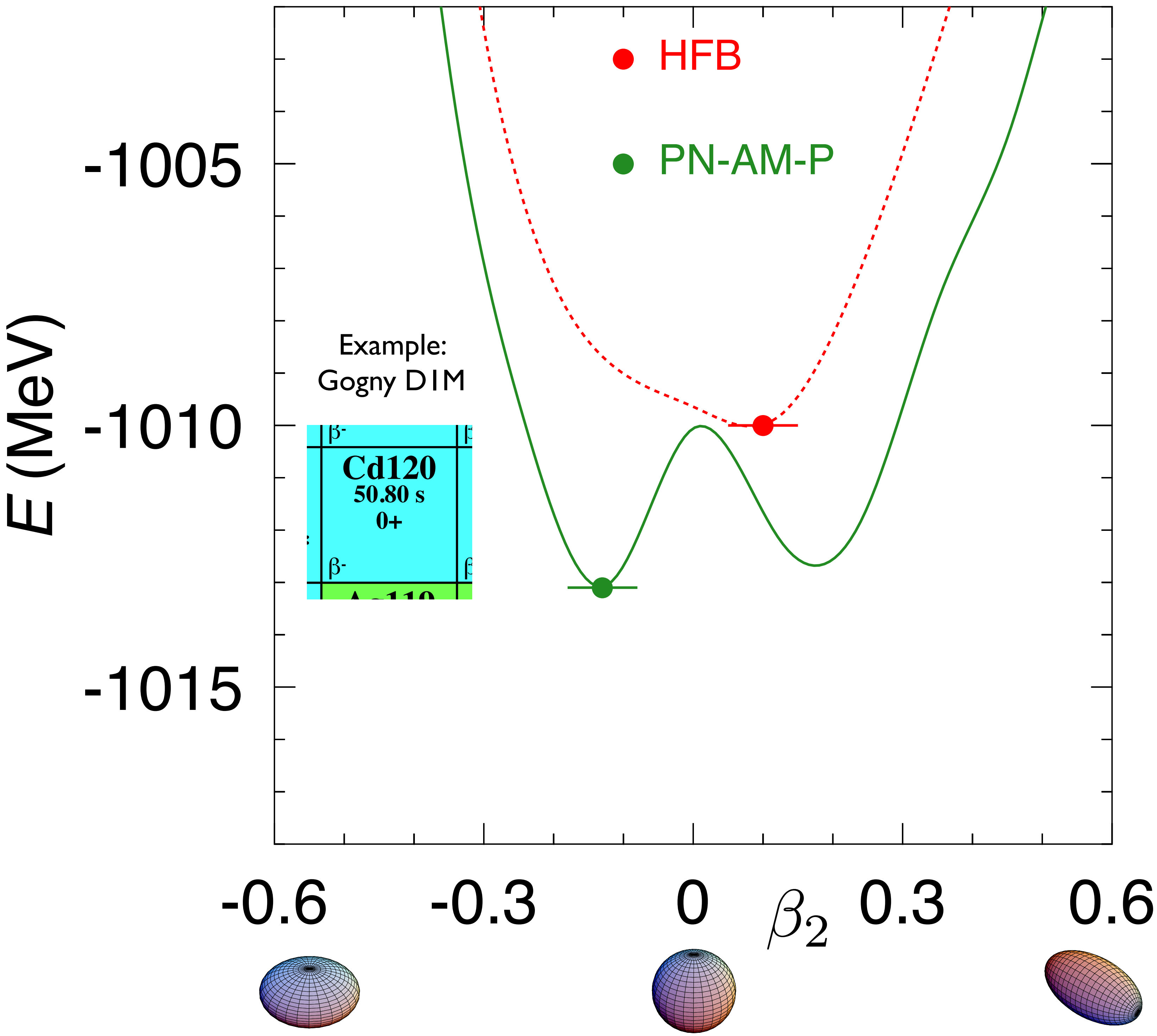

- Mean field: Hartree-Fock-Bogoliubov (HFB). No symmetry conservation and no configuration mixing.

- Beyond mean field (I): Exact projection on particle number and angular momentum J=0. (~3-4 MeV correlation energy)

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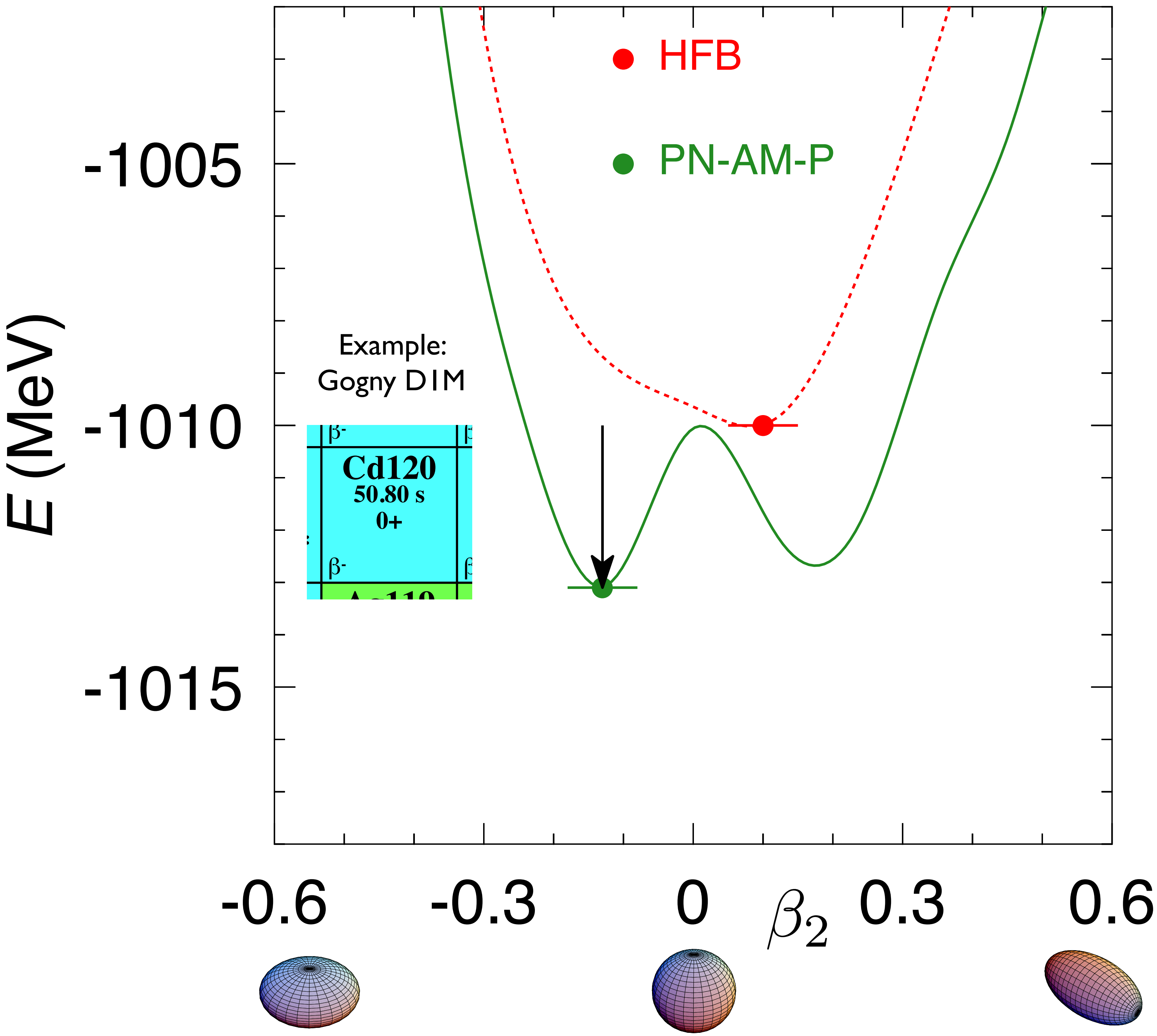

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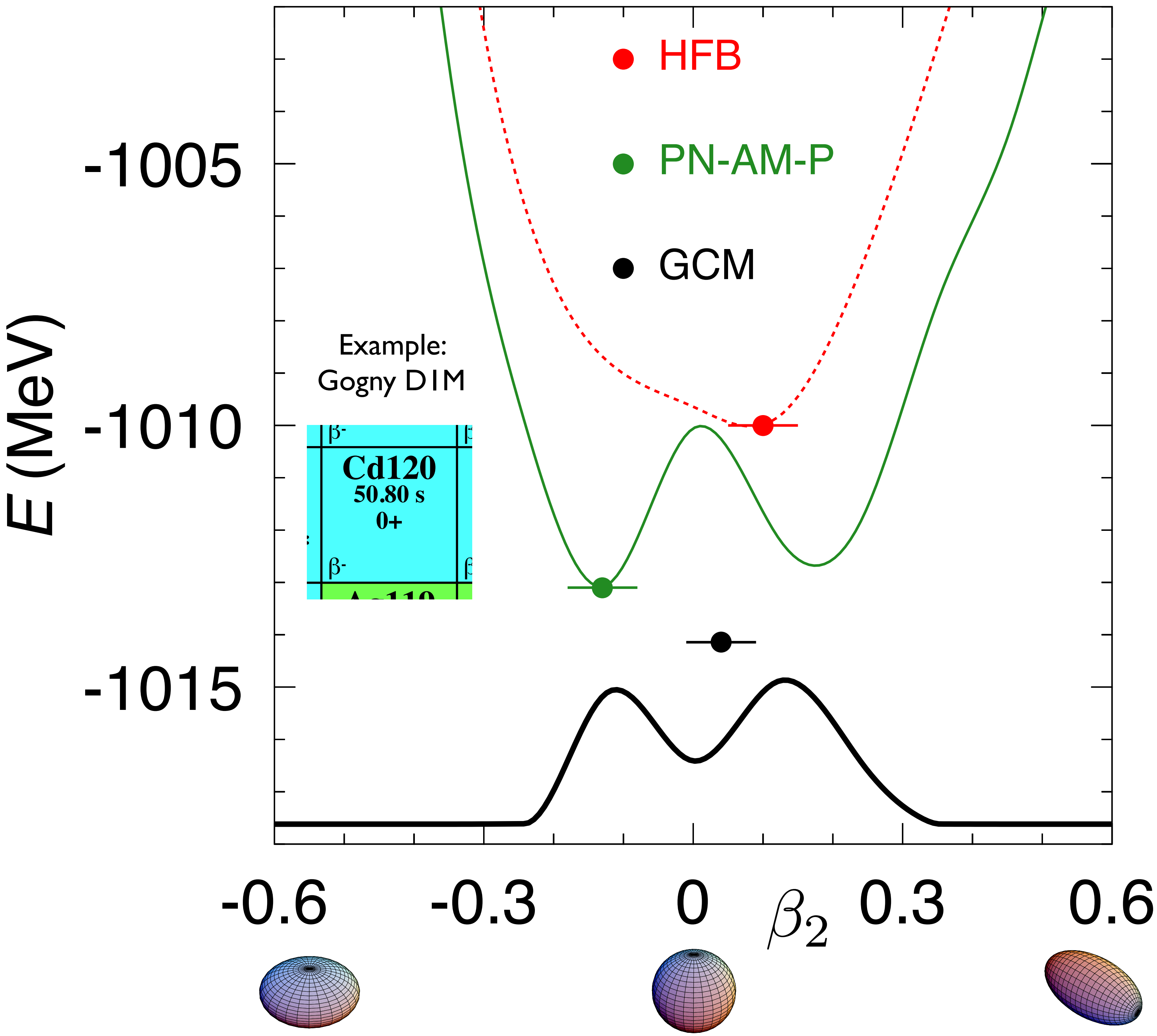

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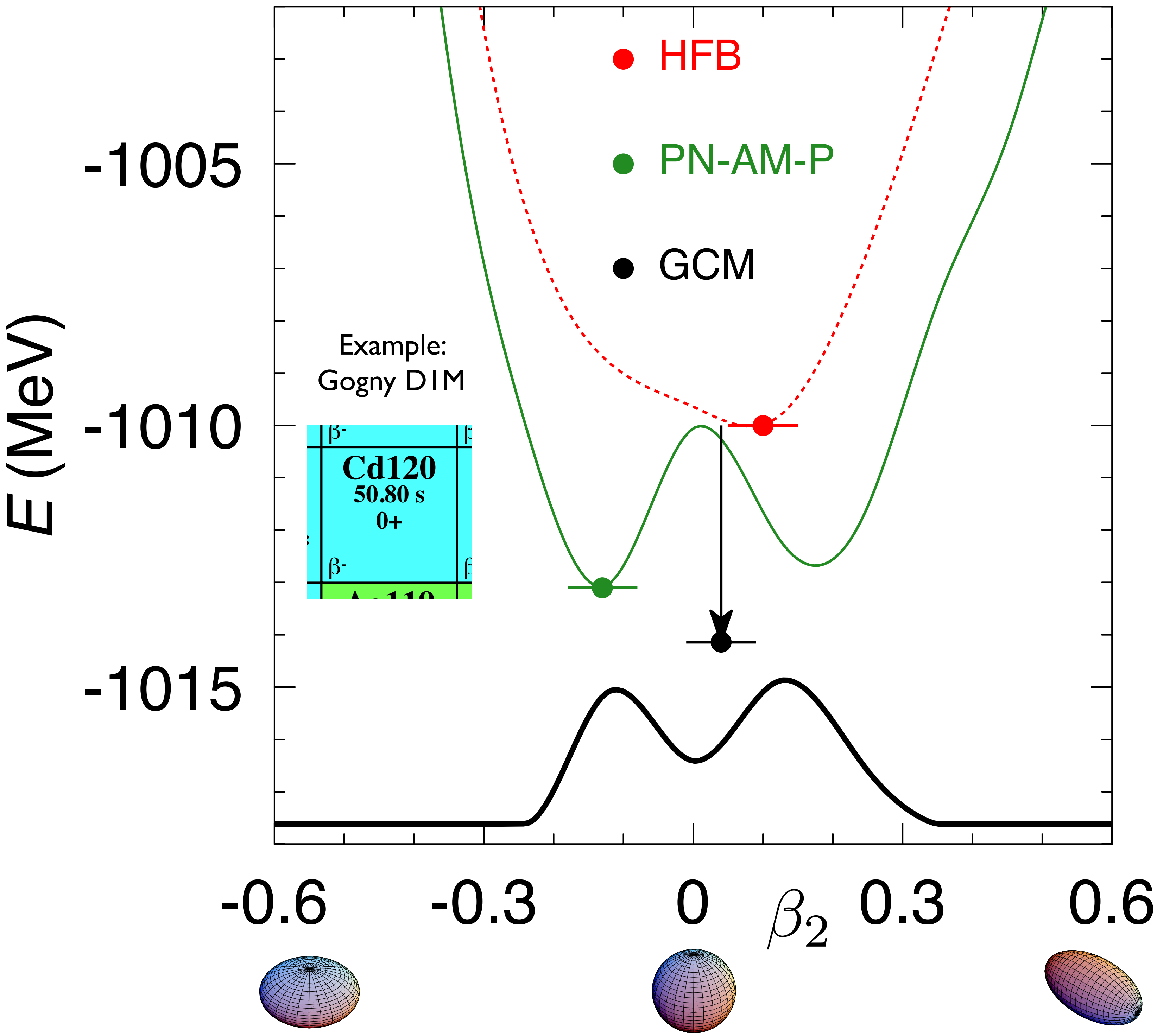

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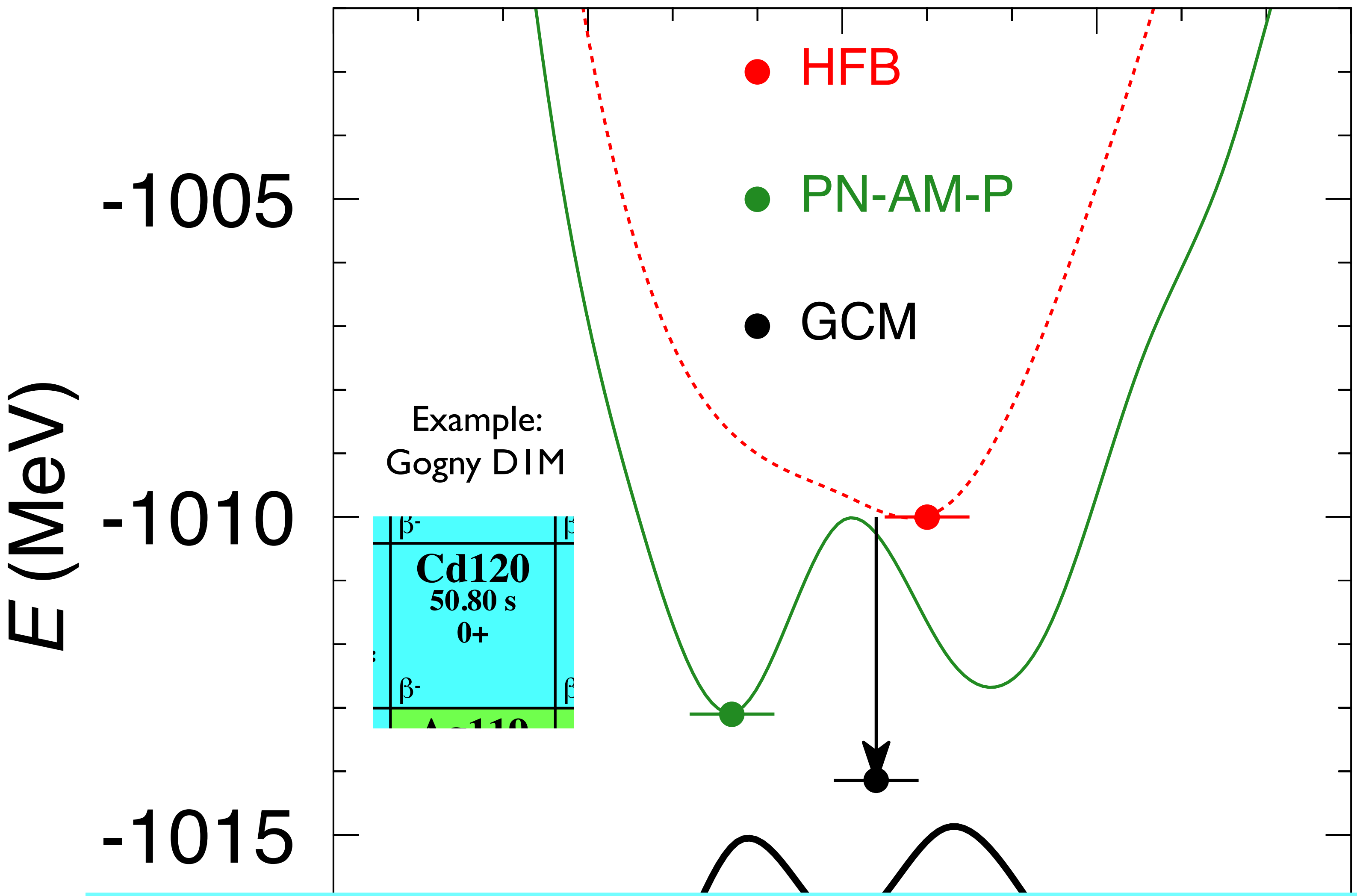

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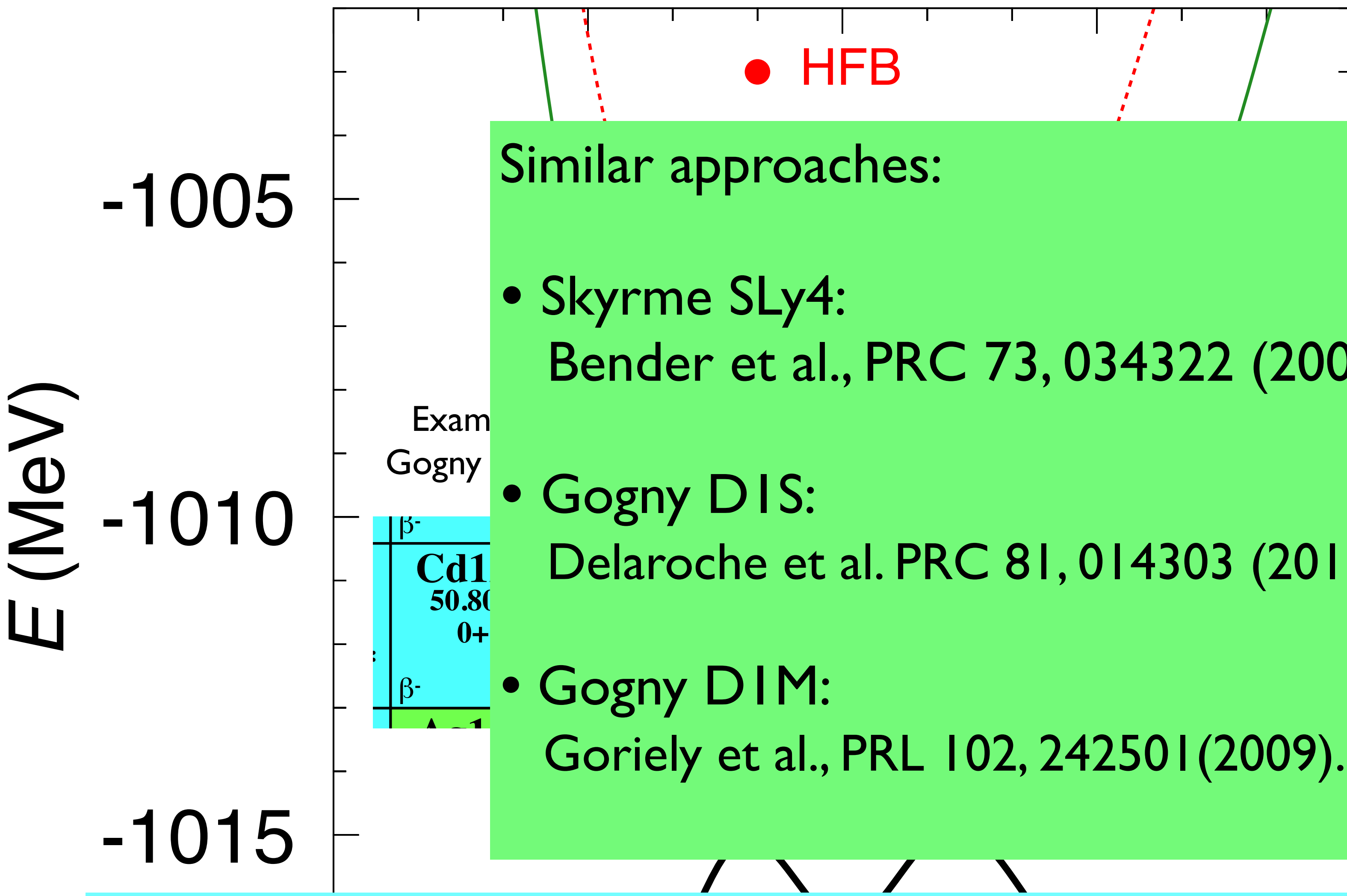
- Beyond mean field (II):

- **Correlations:** Energy difference between the binding energies calculated with the mean-field approximation (HFB) and any other method, using the same underlaying interaction.
If the beyond mean field method is **variational, correlations must give extra binding energy.**

Self-consistent beyond mean field description



• Mean field: Hartree-Fock-
…). No
…rvation and no
…xing.

…field (I):
… on particle
…ular

…lation energy)

• Beyond mean field (II):

Similar approaches:

• Skyrme SLy4:
Bender et al., PRC 73, 034322 (2006). GCM

• Gogny D1S:
Delaroche et al. PRC 81, 014303 (2010). 5DCH

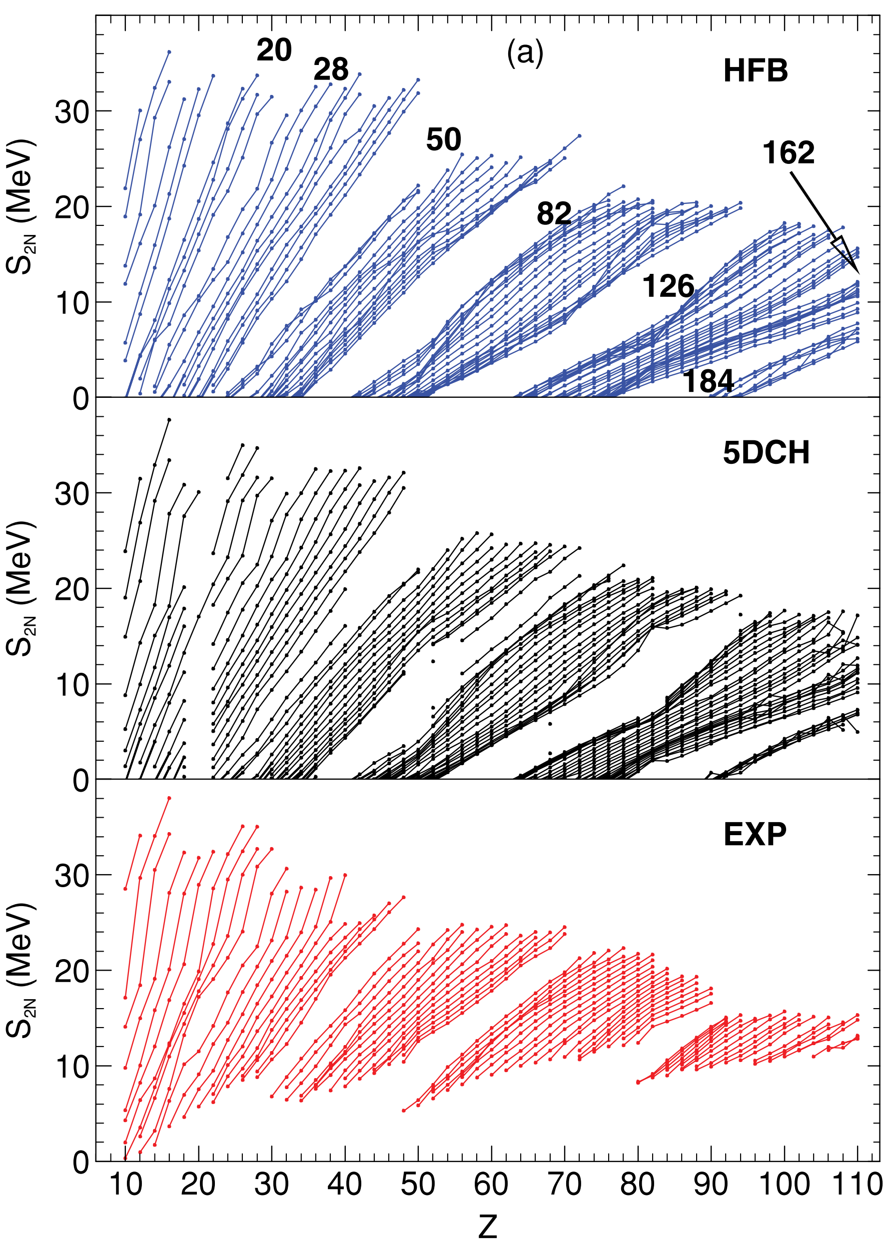
• Gogny D1M:
Goriely et al., PRL 102, 242501(2009). 5DCH

• **Correlations:** Energy difference between the binding energies calculated with the mean-field approximation (HFB) and any other method, using the same underlaying interaction.

If the beyond mean field method is **variational, correlations must give extra binding energy.**

Mean field vs. Beyond mean field. Global systematics

Gogny D1S



Delaroche et al. PRC 81, 014303 (2010)

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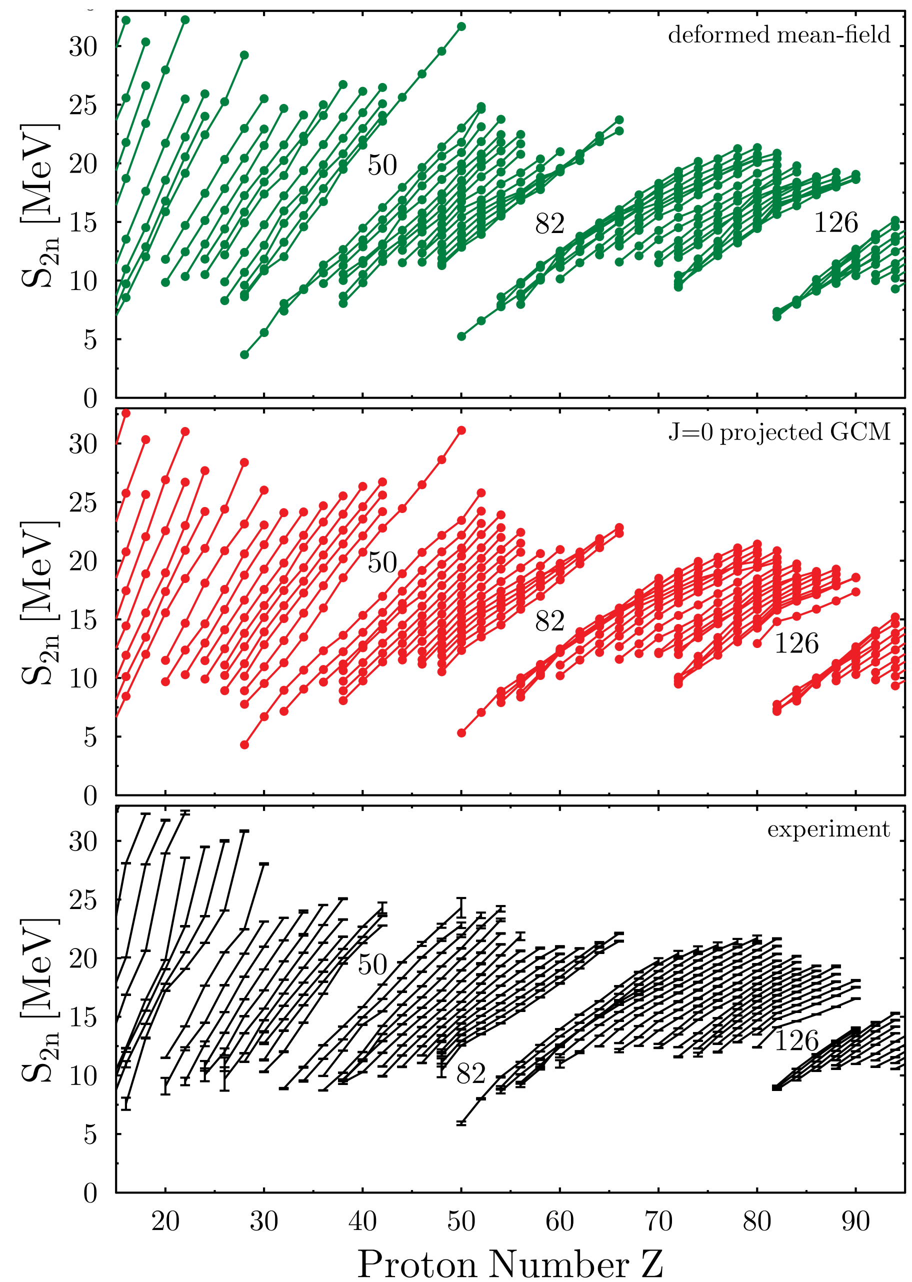

Bender et al., PRC 73, 034322 (2006)

- Beyond mean field effects tend to reduce the shell gaps
- Separation energies are smoother when beyond mean field are included.

Mean field vs. Beyond mean field. Global systematics

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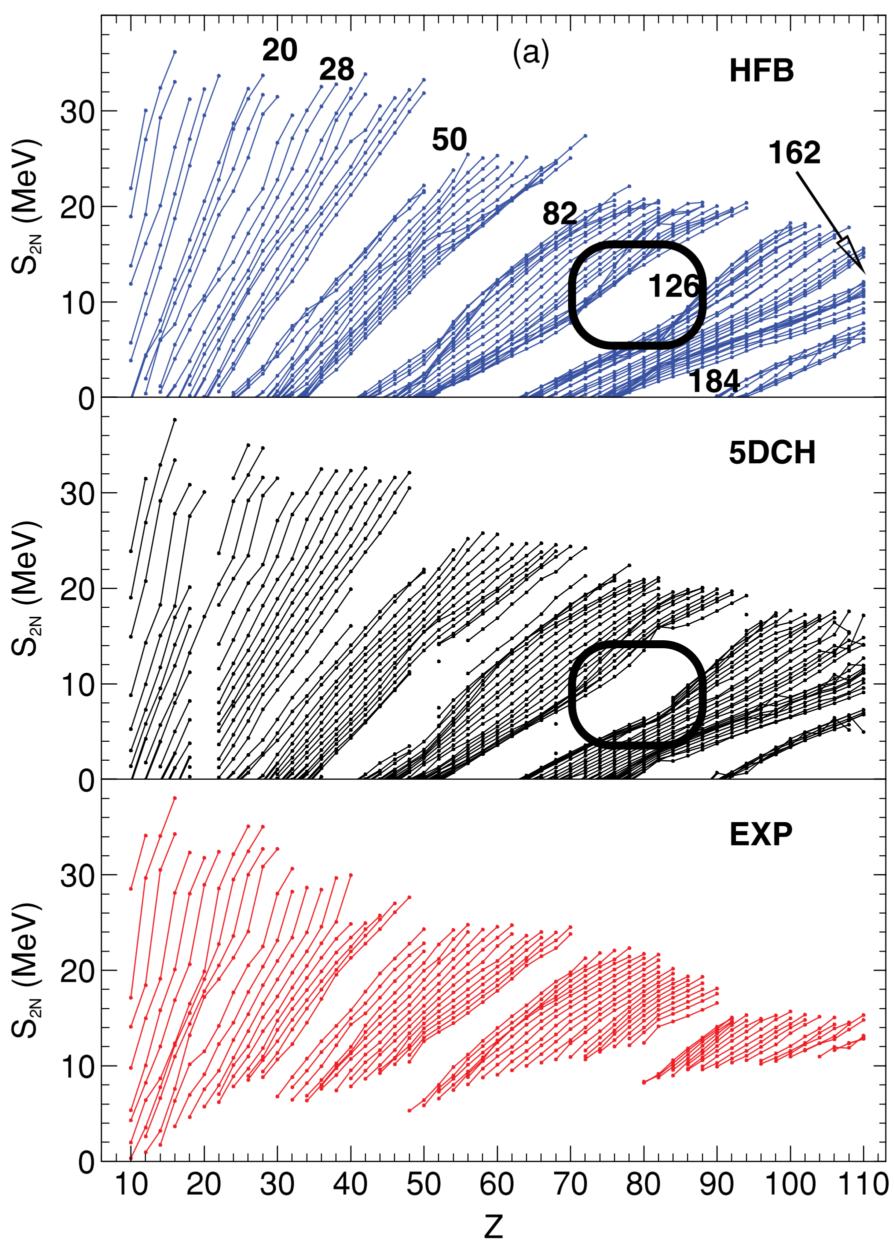

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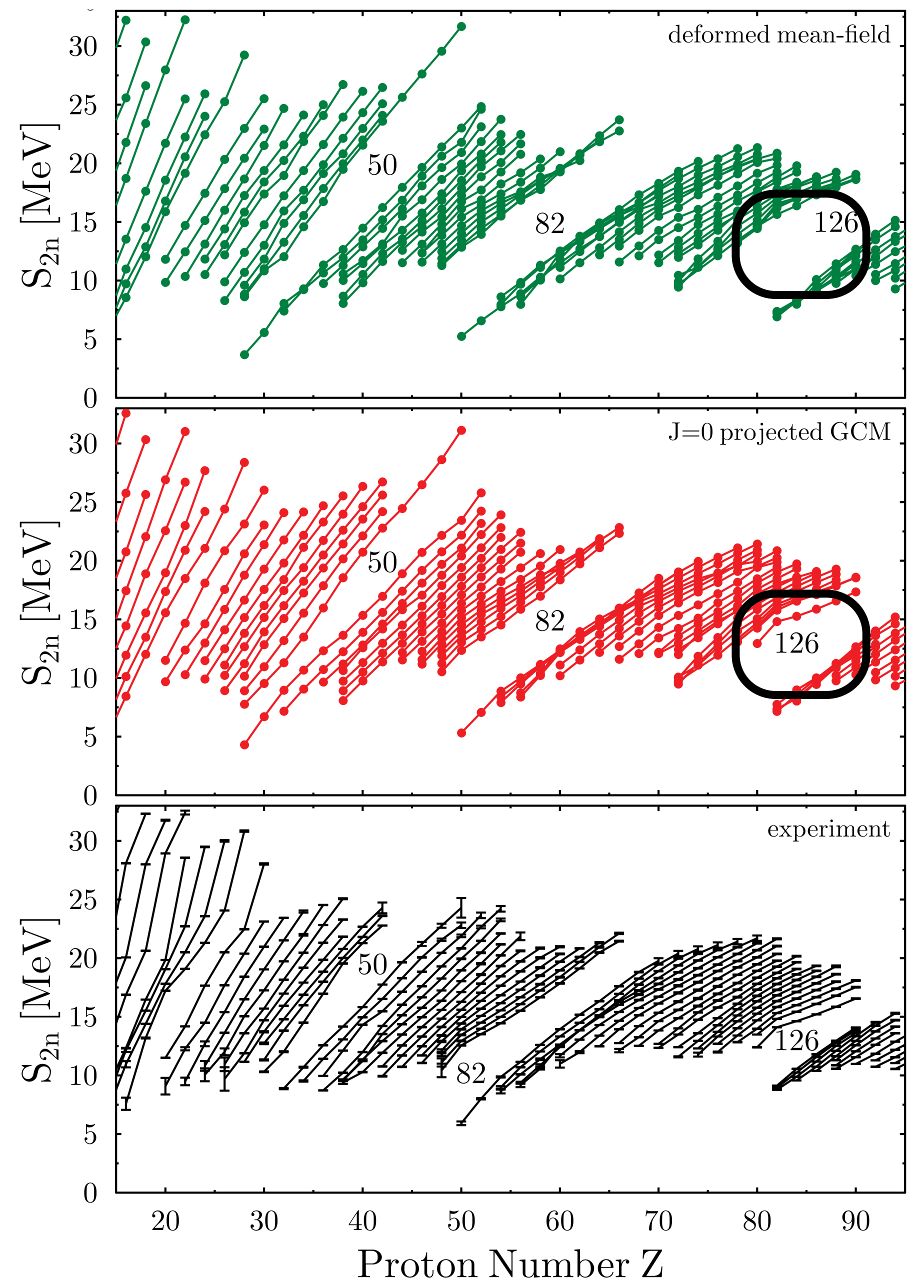

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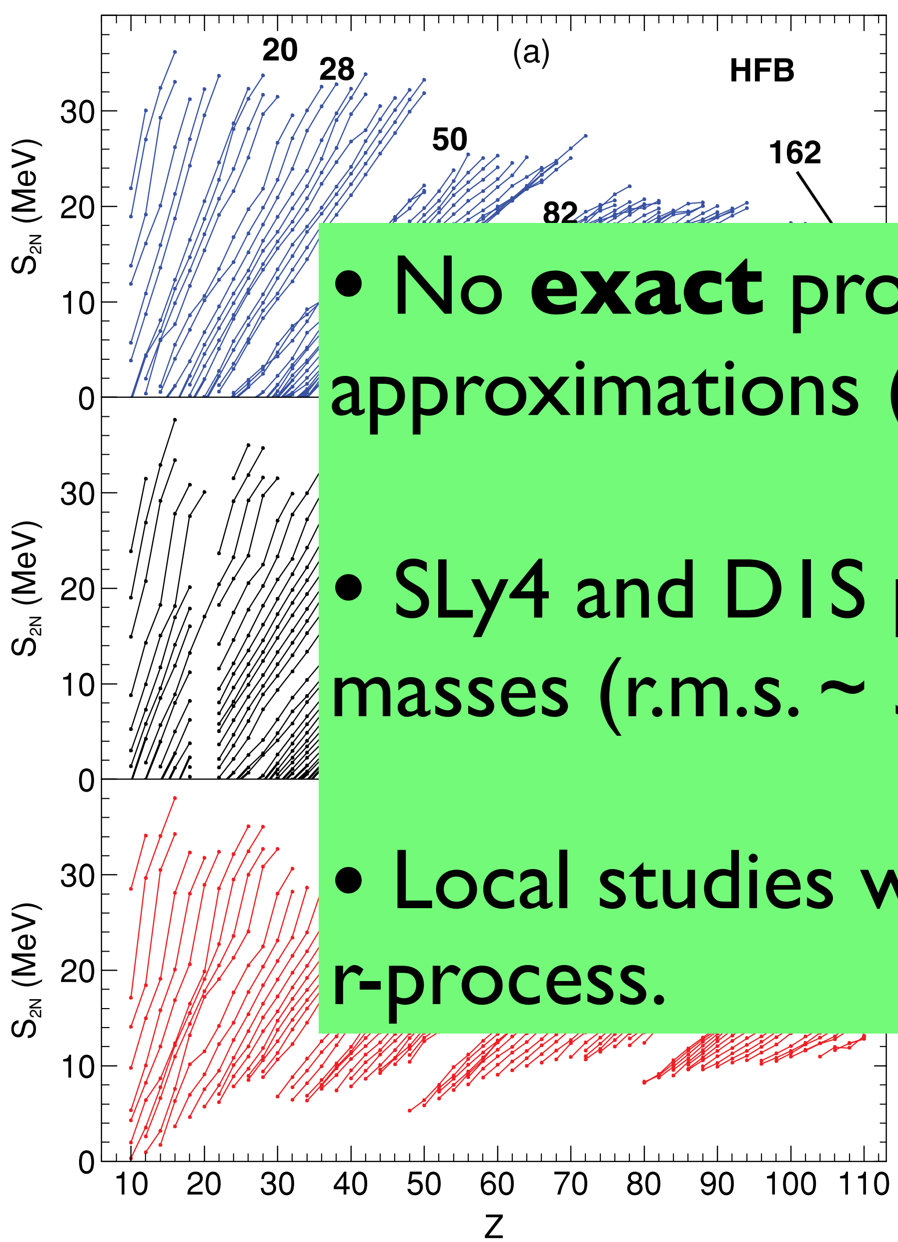

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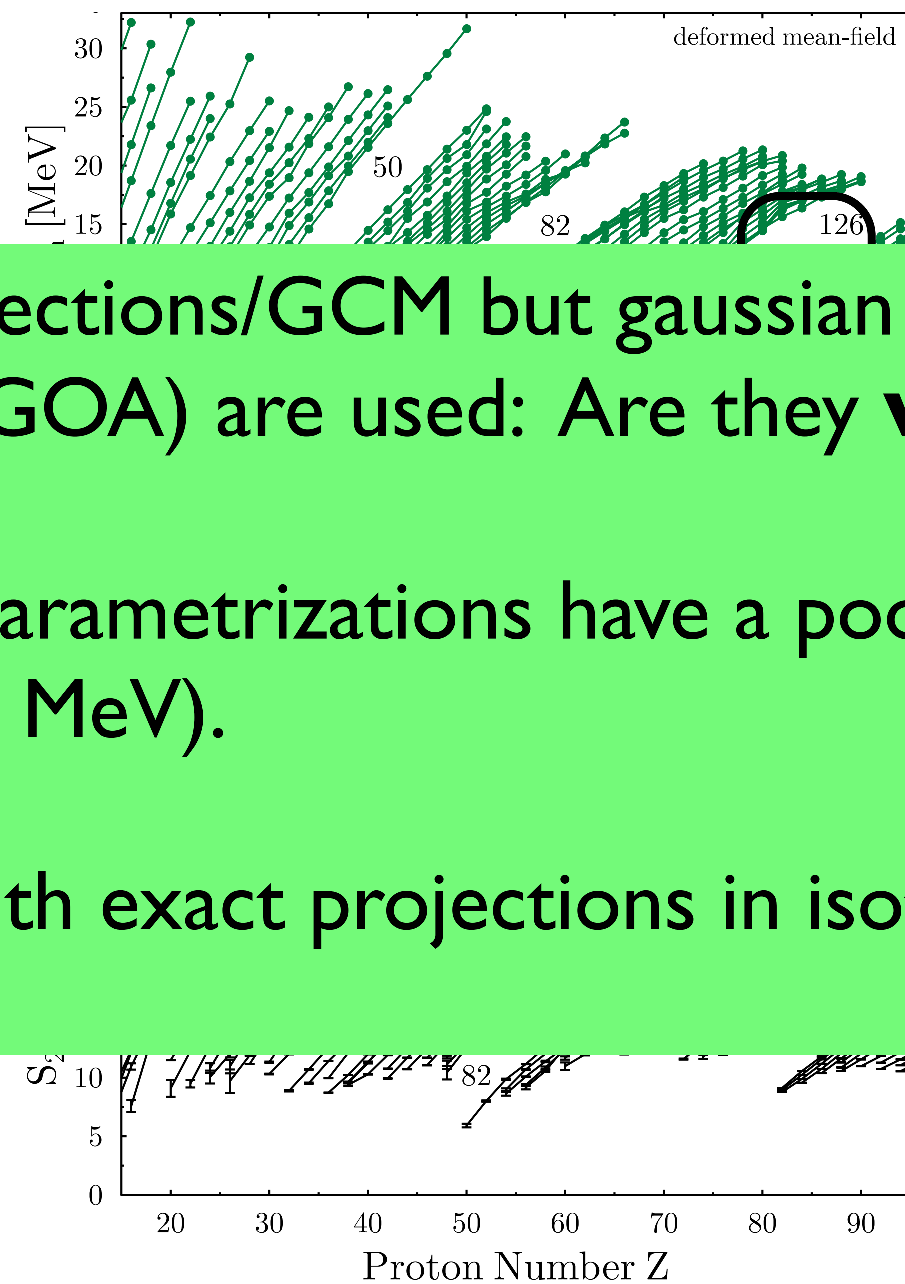


Bender et al., PRC 73, 034322 (2006)

- No **exact** projections/GCM but gaussian overlap approximations (GOA) are used: Are they **variational?**

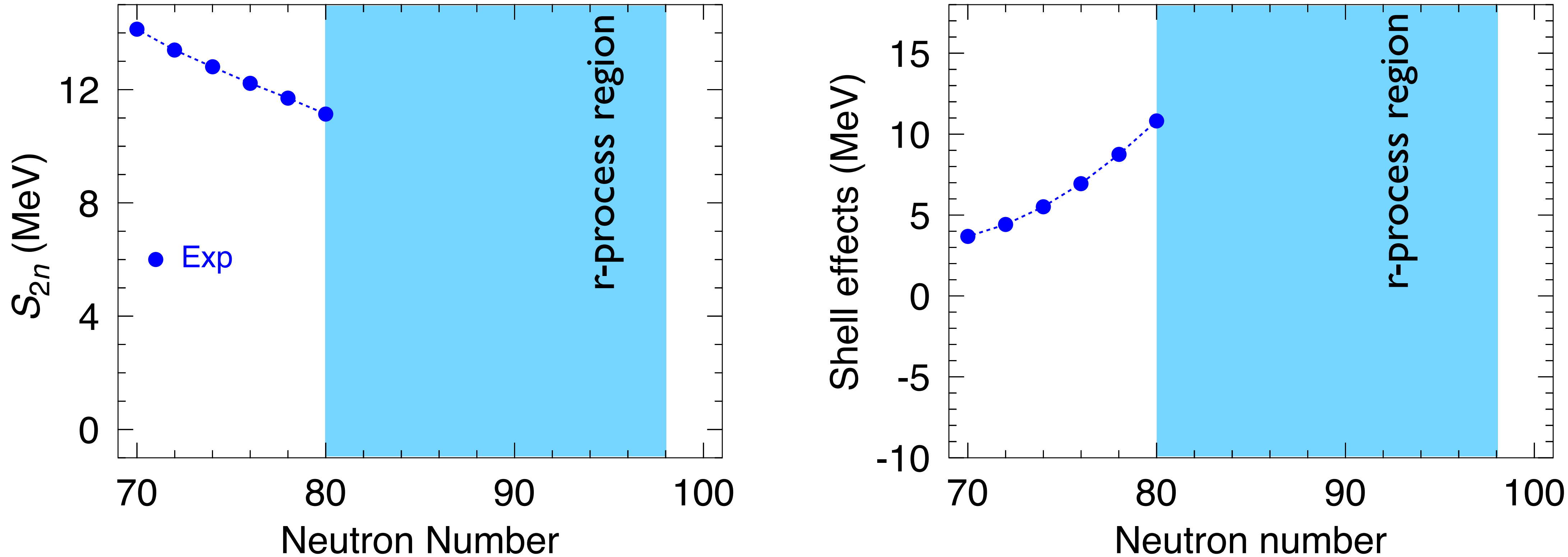
- SLy4 and D1S parametrizations have a poor performance for masses (r.m.s. ~ 5 MeV).

- Local studies with exact projections in isotopes relevant for r-process.

Mean field vs. Beyond mean field. Local systematics

TECHNISCHE UNIVERSITÄT DARMSTADT

Cadmium isotopes. Gogny D1S parametrization



- Similar behavior of the two-neutron separation energies in all approaches and close to the experiment in the experimental region.
- GCM approach always includes correlation energies (variational) while 5DCH fails close to the shell closure.
- 5DCH approach removes the shell gap at N=82 while the others still give a sizable gap. This quenching is an artifact of the 5DCH and not an effect of including correlations beyond mean field (NOT VARIATIONAL).

Mean field vs. Beyond mean field. Local systematics

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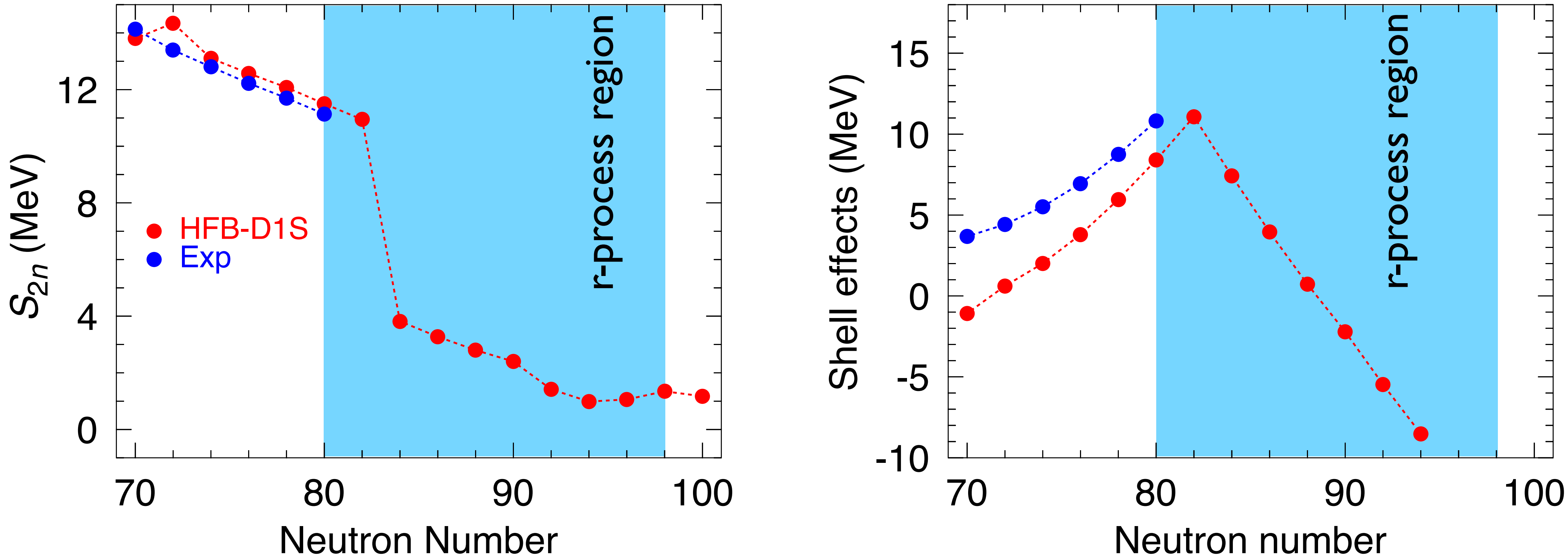

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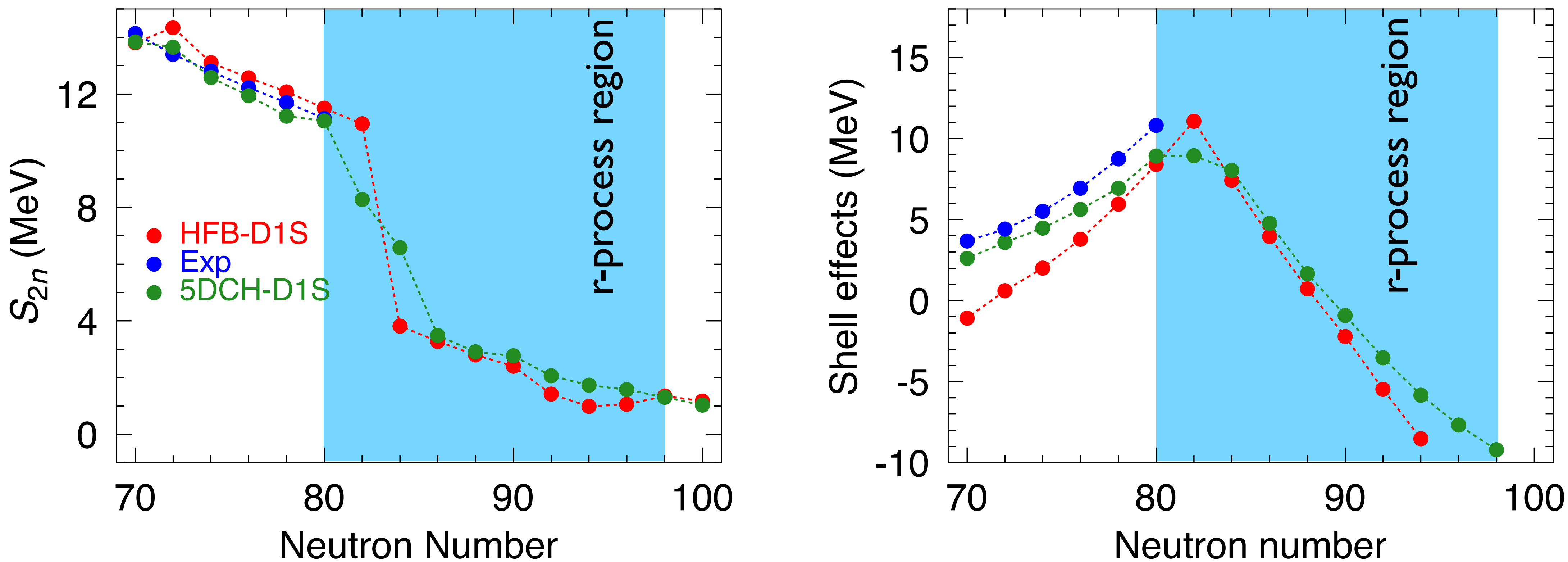

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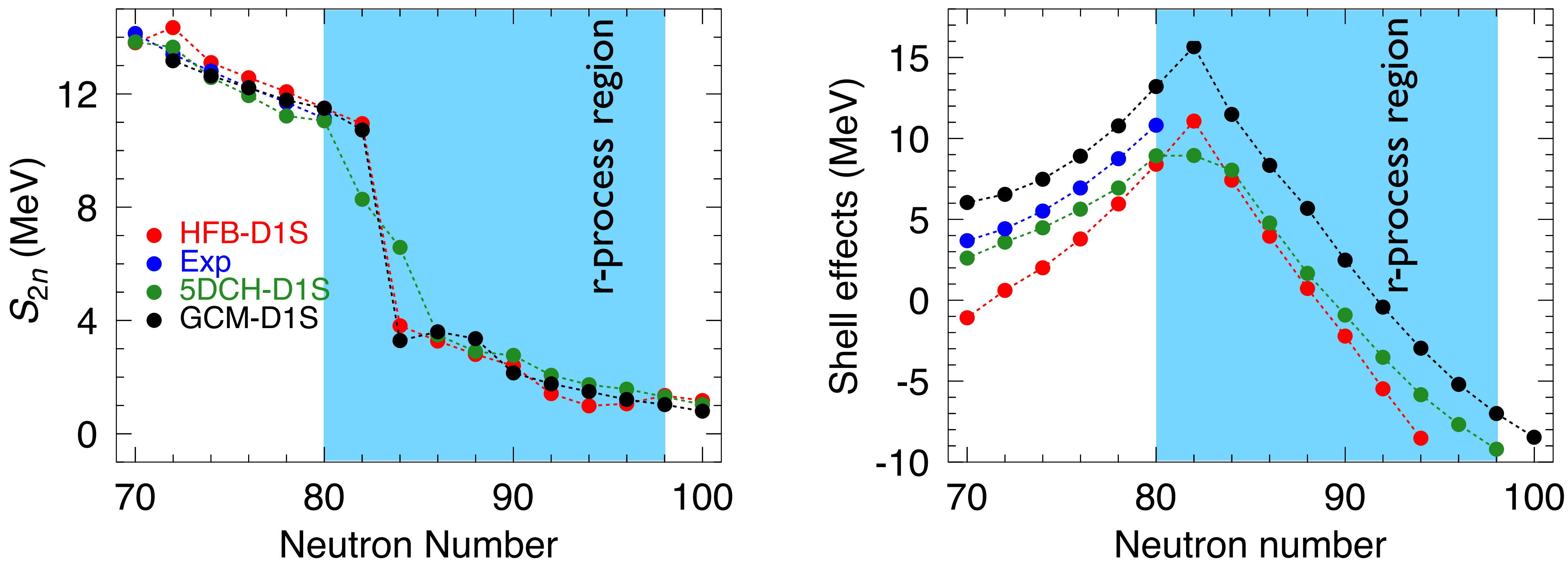

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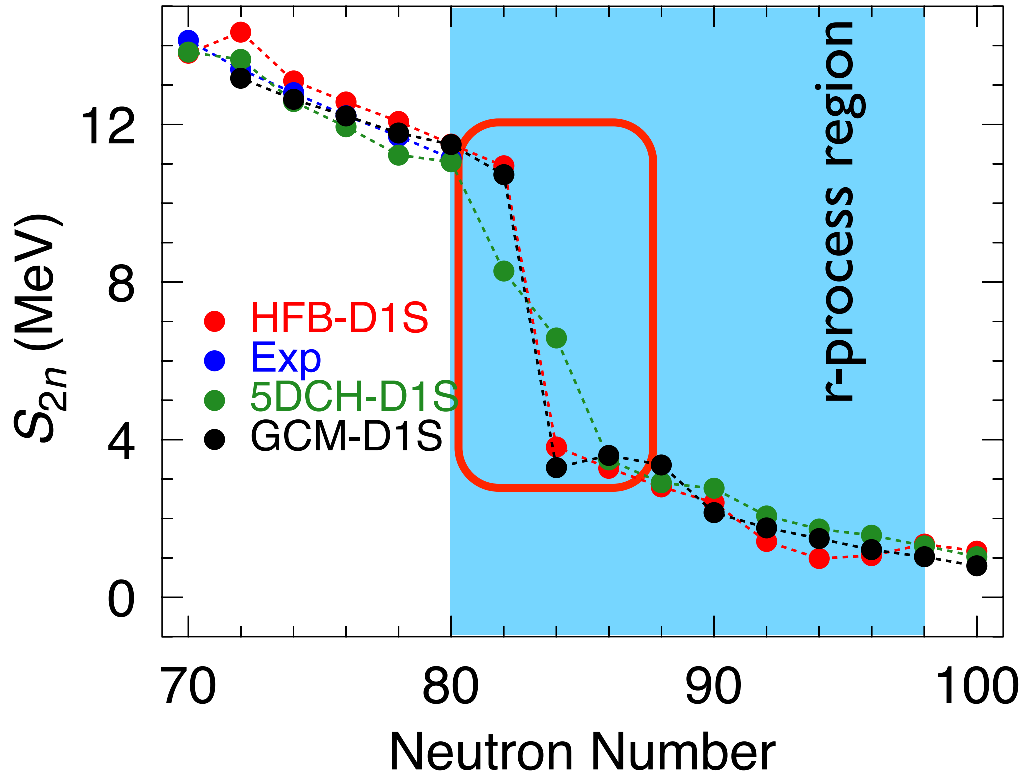

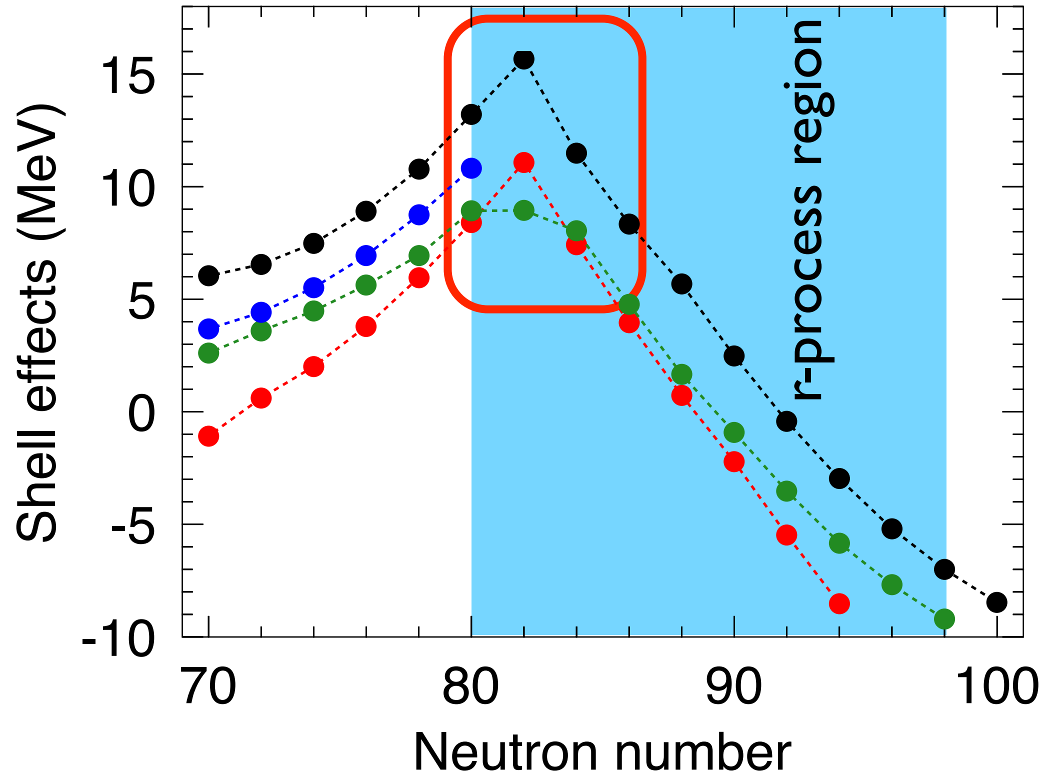

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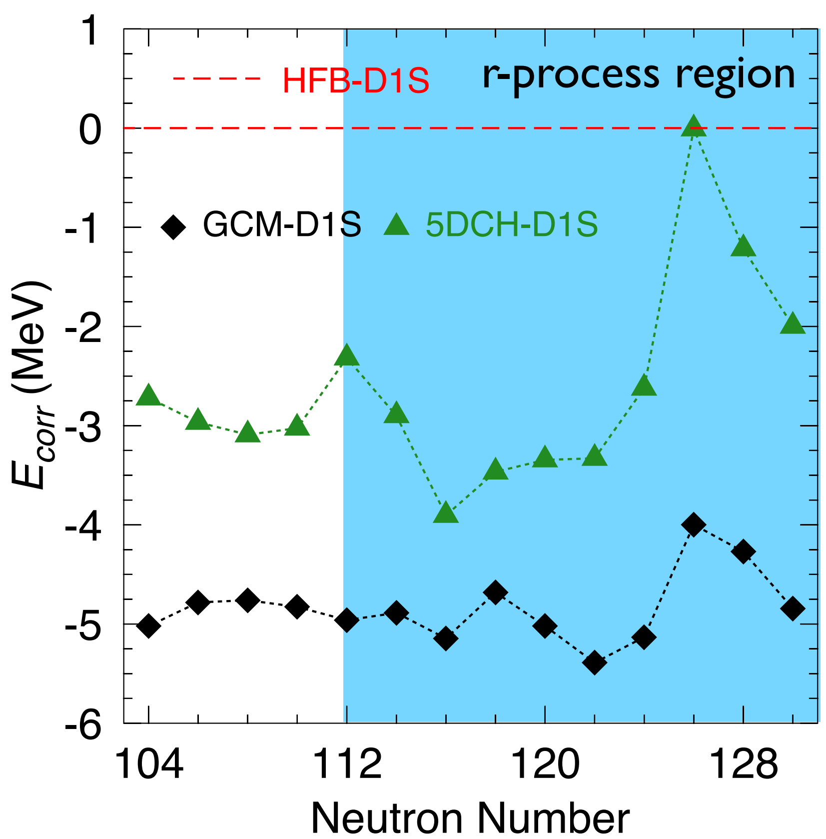
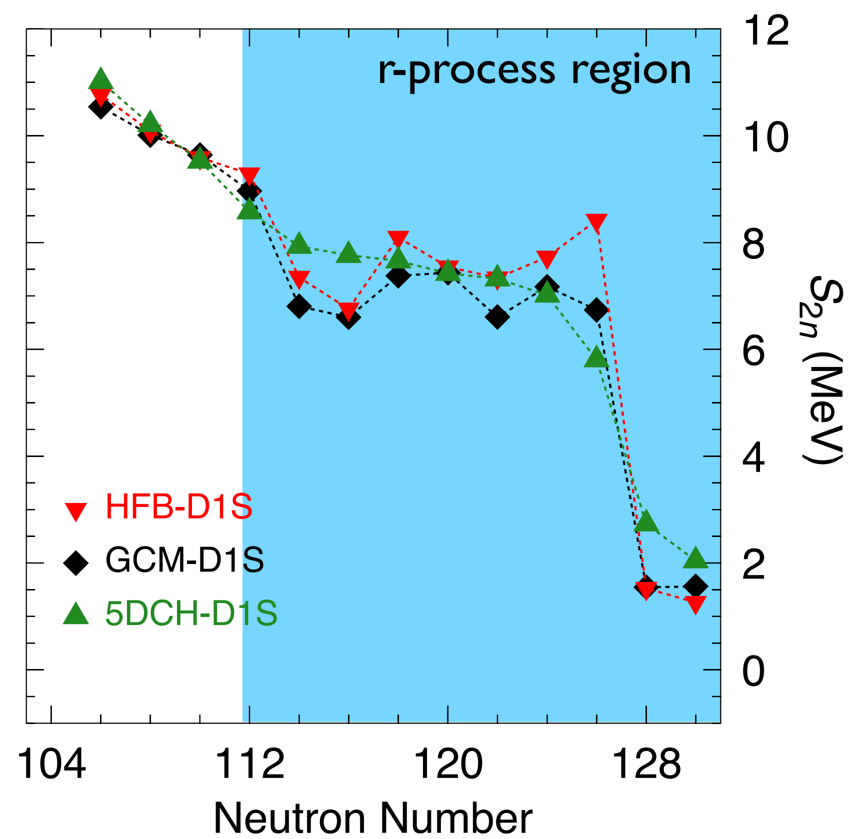
Mean field vs. Beyond mean field. Local systematics

Erbium isotopes. Gogny D1S parametrization

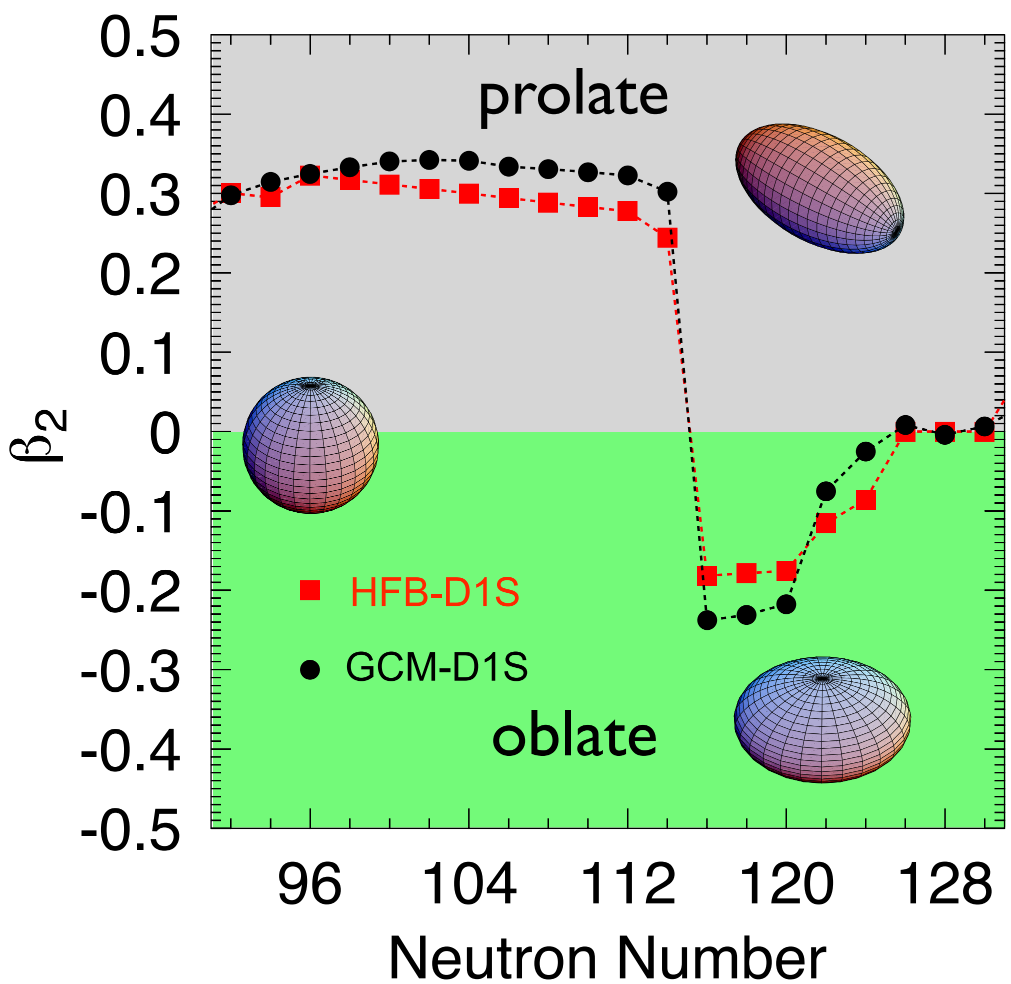


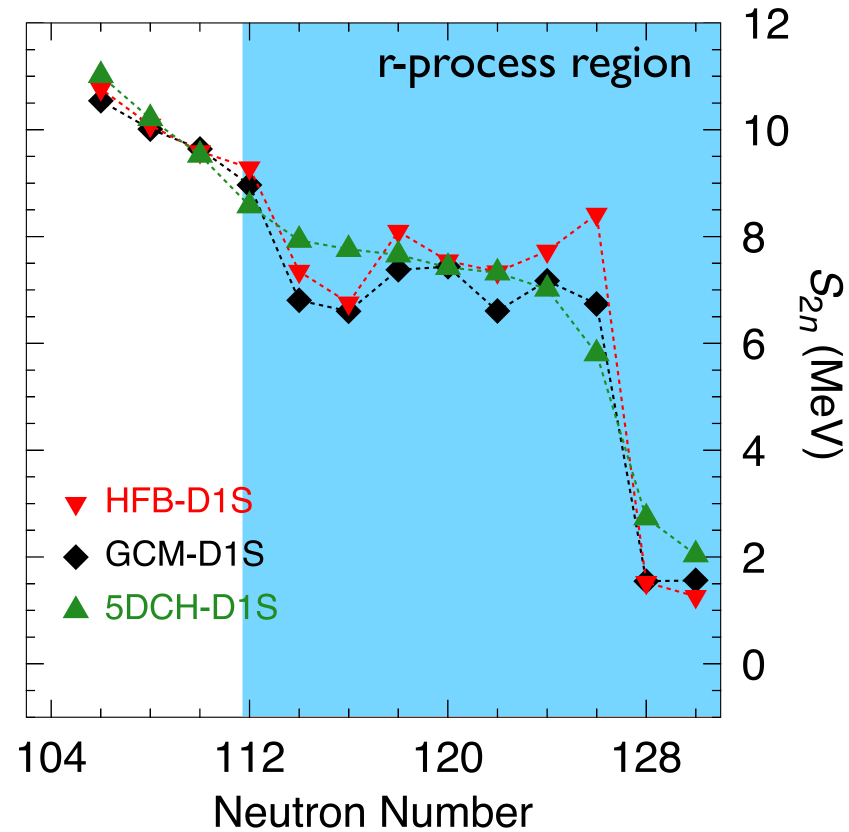


- 5DCH fails in accounting for correlations at N=126 shell closure.
- 5DCH artificially smooths out the trough and the shell gap in the S_{2n}.
- Minima in the S_{2n} are produced by changes in deformation.

Mean field vs. Beyond mean field. Local systematics

Erbium isotopes. Gogny D1S parametrization





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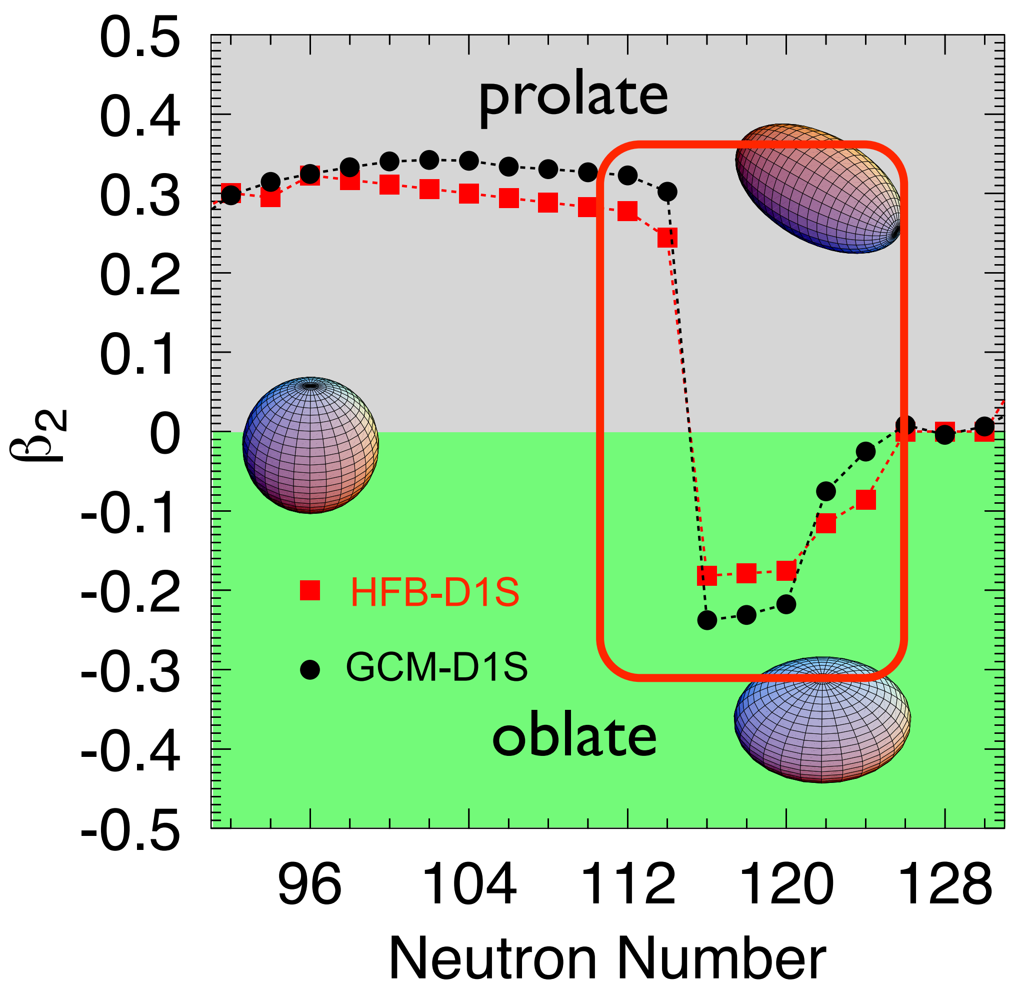

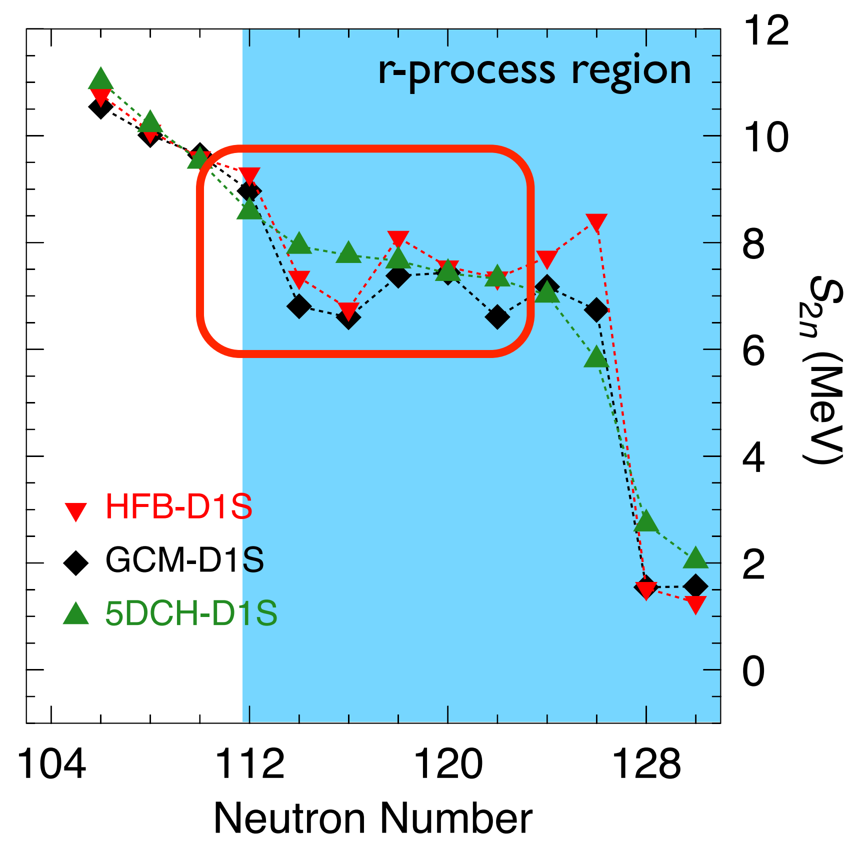

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- Trough appearing both in S_{2n} and shell effects for Er isotopes is produced by an oblate-prolate shape transition and it is not smoothing out with the BMF model used here.

Outlook

- Systematic analysis of the convergence/numerical noise.
- Perform global studies ensuring convergence of the results with the present variational BMF method.
- Study the impact on nucleosynthesis simulations.
- In the long-range plan:
  - Description of the odd systems at the same level of BMF approach.
  - Development of parametrizations of the interaction fitted with BMF functionals.

Acknowledgments

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Alexander Arzhanov (TU-Darmstadt, Germany)

Joel Mendoza-Temis (TU-Darmstadt, Germany)

Gabriel Martínez-Pinedo (TU-Darmstadt, Germany)