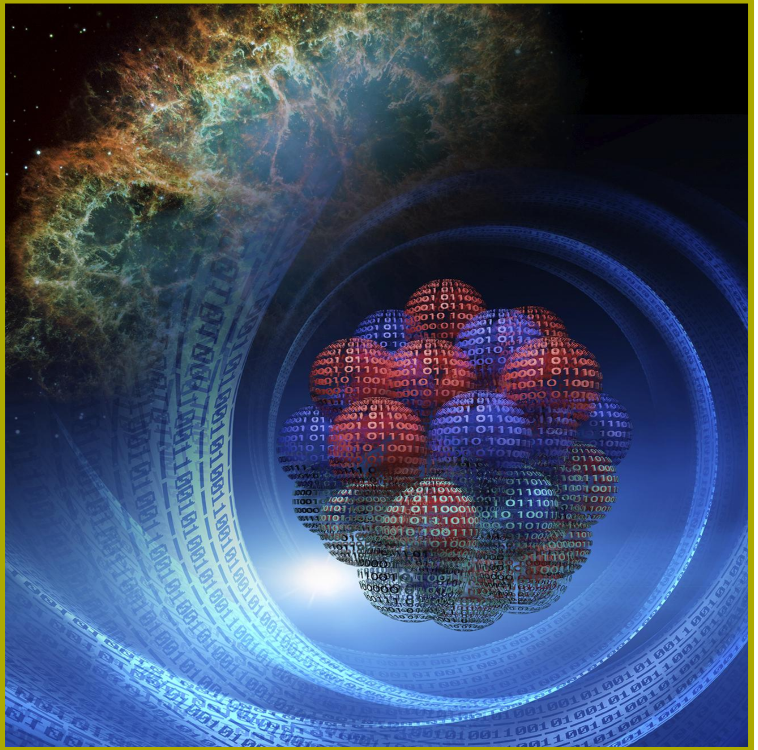
WOUTER RYSSENS



Andy Sproles, ORNL

The fission properties of ~~BSkG2~~ ....the BSkG models

W. Ryssens
G. Grams, M. Bender, G. Scamps and S. Goriely

17th of December 2024

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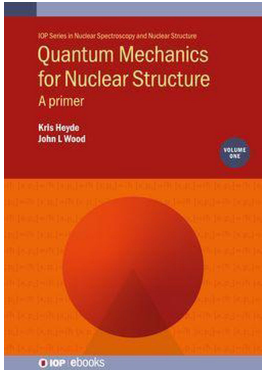
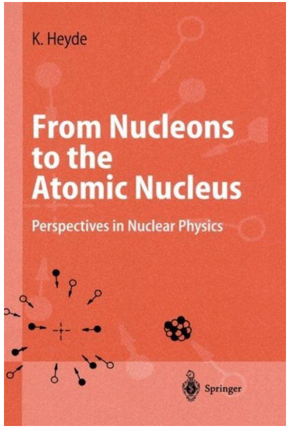
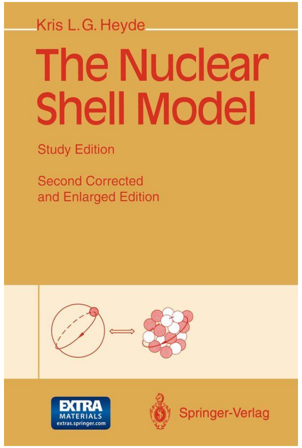
BRUSSELS LABORATORY OF THE UNIVERSE

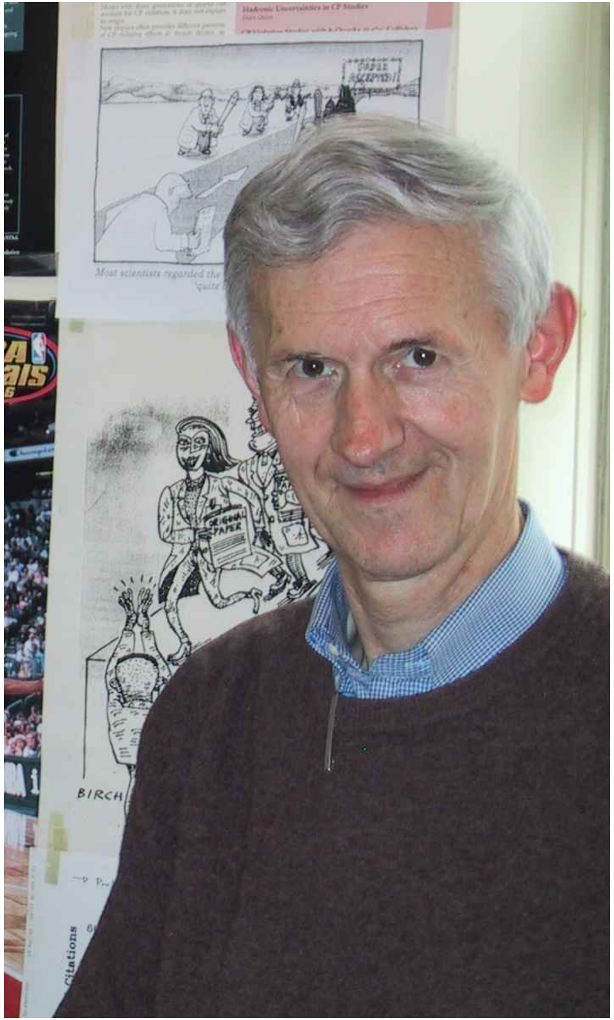
LA LIBERTÉ DE CHERCHER

In memory of Kris Heyde (1942 - 2024)



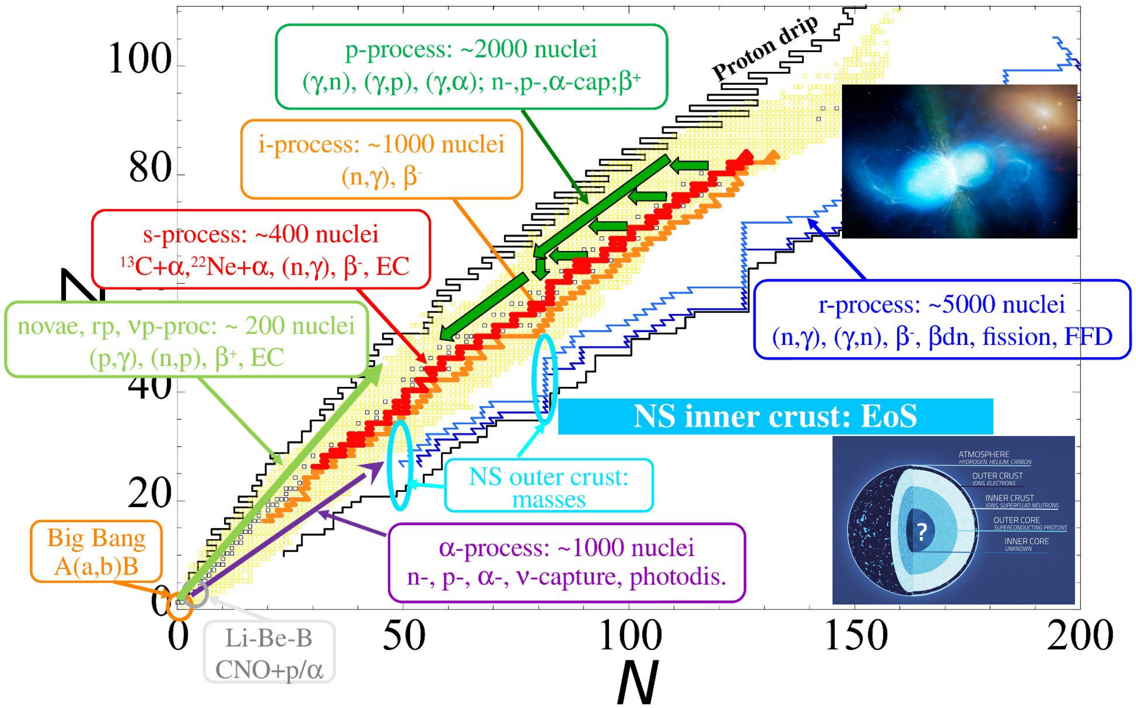






The nuclear chart and the processes traversing it

Predictions needed for
- **~7000** nuclei
- **many** reactions



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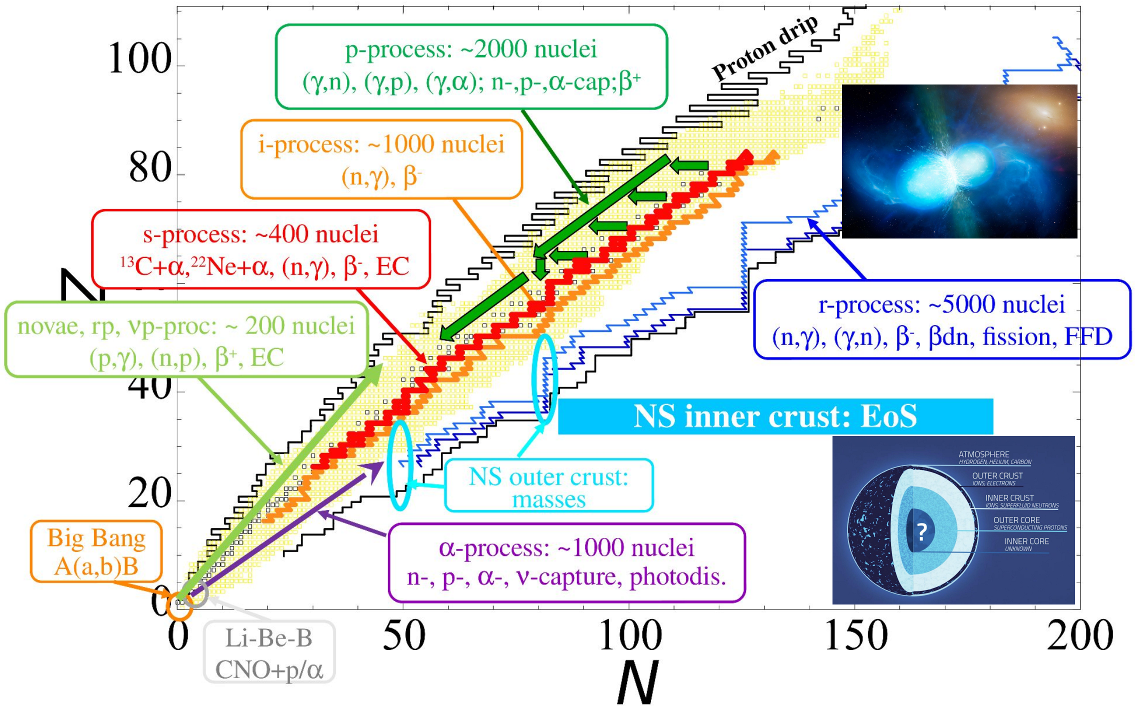

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- **~7000** nuclei
- **many** reactions

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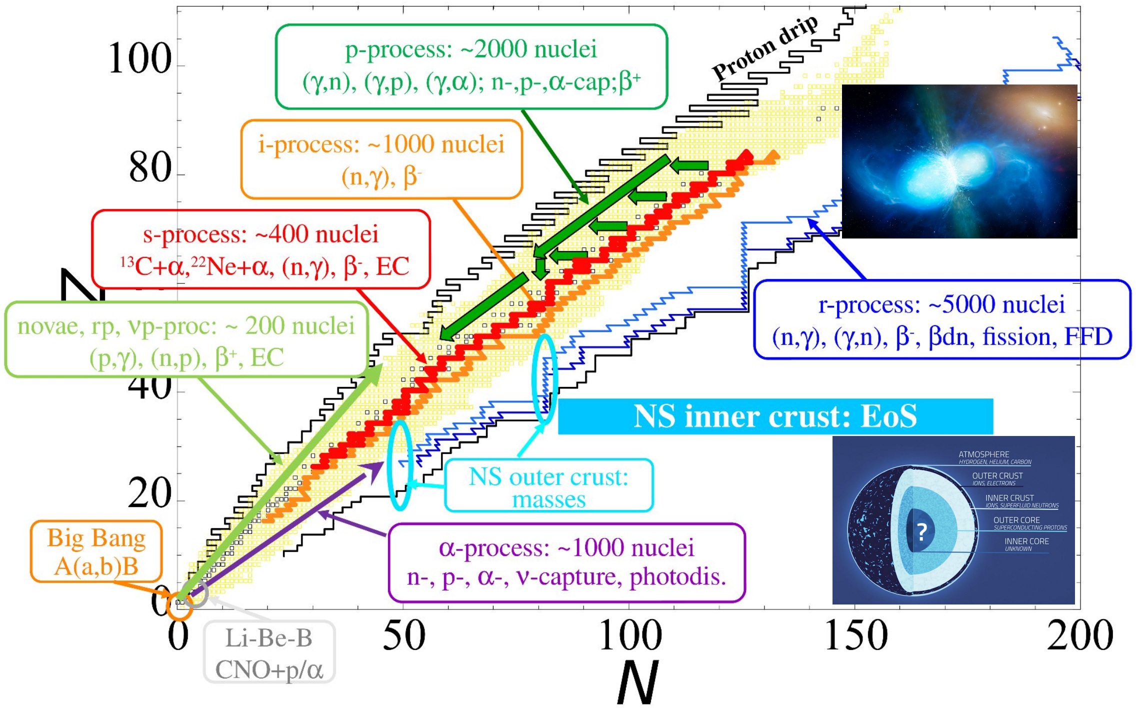
We need structure models that are

1. **predictive….**
2. but **complete!**



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Model	Fit	Triaxial		N_b	N_{iso}	E_{I}		E_{II}		E_{iso}		$(E_{\mathrm{I}} - E_{\mathrm{II}})$		References
		I	O			σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	
BSkG1	N	Y	Y	45	28	0.88	+0.80	0.87	+0.71	1.00	+0.67	0.56	+0.09	
BSkG2	Y	Y	Y	45	28	0.44	+0.24	0.47	+0.10	0.49	−0.36	0.53	+0.14	
BSk14	Y	N	N	45	28	0.60	−0.27	0.69	+0.20	1.05	+0.34	0.76	−0.47	[35]
BCPM	N	N	N	45	28	1.42	−1.07	0.72	−0.30	0.52	+0.09	1.22	−0.77	[106]
SkSC4	N	N	N	45	0	0.57	+0.04	2.03	+1.78	–	–	2.15	−1.74	[31]
FRLDM	Y	Y	N	45	28	0.81	+0.22	1.41	+0.66	1.02	−0.91	0.88	−0.44	[103]
YPE+WS	Y	Y	N	45	28	0.82	−0.66	0.84	−0.40	0.38	+0.07	0.72	−0.26	[110]
D1M	Y	Y	N	14	8	0.53	+0.23	0.43	+0.06	0.99	+0.50	0.47	+0.17	[57]
UNEDF1	Y	Y	N	10	4	0.72	−0.67	0.79	−0.41	0.16	−0.06	0.83	−0.26	[73]
	Y	Y	Y	12	8	0.71	−0.52	0.65	−0.28	0.69	−0.36	0.71	−0.24	[45]
SkM*	Y	Y	N	10	0	1.92	−1.86	1.93	−1.84	–	–	0.57	−0.01	[73]
SkI3	N	N	N	7	8	3.99	−3.59	1.59	−1.44	1.04	+0.35	2.51	−2.15	[81]
	N	N	N	14	0	3.26	−2.50	–	–	–	–	–	–	[111]
SkI4	N	N	N	7	8	4.35	−4.27	3.65	−3.49	0.95	−0.22	1.02	−0.78	[81]
SLy6	N	N	N	7	8	4.23	−3.90	2.19	−2.08	1.24	−1.28	2.24	−1.82	[81]
	N	N	N	14	0	3.89	−3.31	–	–	–	–	–	–	[111]
SV-bas	N	N	N	14	0	1.88	−1.10	–	–	–	–	–	–	[111]
SV-min	N	N	N	14	0	1.61	−0.50	–	–	–	–	–	–	[111]
NL-Z2	N	N	N	7	8	1.73	−0.93	1.28	+1.19	1.81	+1.91	2.68	−2.12	[81]
NL3	N	N	N	7	8	2.18	−1.26	1.03	+0.62	0.49	+0.39	2.73	−1.88	[81]
NL3*	N	N	N	14	0	2.16	−2.03	–	–	–	–	–	–	[112]
PC-PK1	N	N	N	14	0	1.84	−1.53	1.01	−0.60	–	–	1.43	−0.93	[43]
	N	Y	Y	14	0	0.37	+0.18	0.82	+0.13	–	–	0.73	+0.05	[43]
DD-ME2	N	N	N	14	0	3.35	−3.17	–	–	–	–	–	–	[112]
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SLy6	N	N	N	7	8	4.23	−3.90	2.19	−2.08	1.24	−1.28	2.24	−1.82	[81]
	N	N	N	14	0	3.89	−3.31	–	–	–	–	–	–	[111]
SV-bas	N	N	N	14	0	1.88	−1.10	–	–	–	–	–	–	[111]
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NL-Z2	N	N	N	7	8	1.73	−0.93	1.28	+1.19	1.81	+1.91	2.68	−2.12	[81]
NL3	N	N	N	7	8	2.18	−1.26	1.03	+0.62	0.49	+0.39	2.73	−1.88	[81]
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PC-PK1	N	N	N	14	0	1.84	−1.53	1.01	−0.60	–	–	1.43	−0.93	[43]
	N	Y	Y	14	0	0.37	+0.18	0.82	+0.13	–	–	0.73	+0.05	[43]
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Brussels-**Sk**yrme-on-a-**G**rid: BSkG

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BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741			
S_n [MeV]	0.466			
Radii [fm]	0.024			
Prim. barriers [MeV]				
Sec. barriers [MeV]				
Fission isomers [MeV]				
Max. NS mass [$M_\odot$]				

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Masses [MeV]	0.741	0.678		
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Radii [fm]	0.024	0.027		
Prim. barriers [MeV]	0.88	0.44		
Sec. barriers [MeV]	0.87	0.47		
Fission isomers [MeV]	1.0	0.49		
Max. NS mass [$M_\odot$]				

BSkG2

- **complete** time-reversal breaking
- fit to 45 reference fission barriers
+ 28 fission isomers

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Masses [MeV]	0.741	0.678	0.631	
S_n [MeV]	0.466	0.500	0.442	
Radii [fm]	0.024	0.027	0.024	
Prim. barriers [MeV]	0.88	0.44	0.33	
Sec. barriers [MeV]	0.87	0.47	0.51	
Fission isomers [MeV]	1.0	0.49	0.34	
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	

BSkG2

- <u>**complete**</u> time-reversal breaking
- fit to 45 reference fission barriers
+ 28 fission isomers

BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

Brussels-**Sk**yrme-on-a-**G**rid: BSkG

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
Prim. barriers [MeV]	0.88	0.44	0.33	0.36
Sec. barriers [MeV]	0.87	0.47	0.51	0.53
Fission isomers [MeV]	1.0	0.49	0.34	0.33
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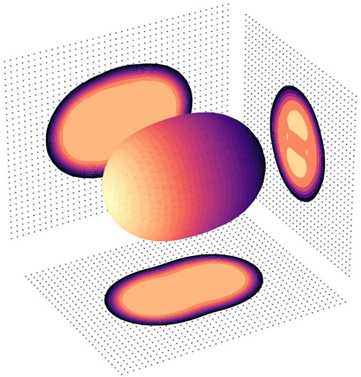
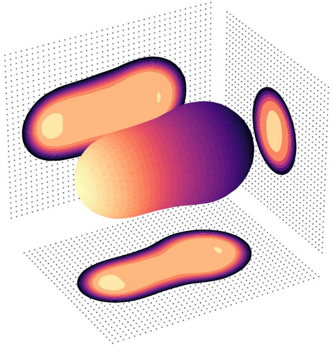
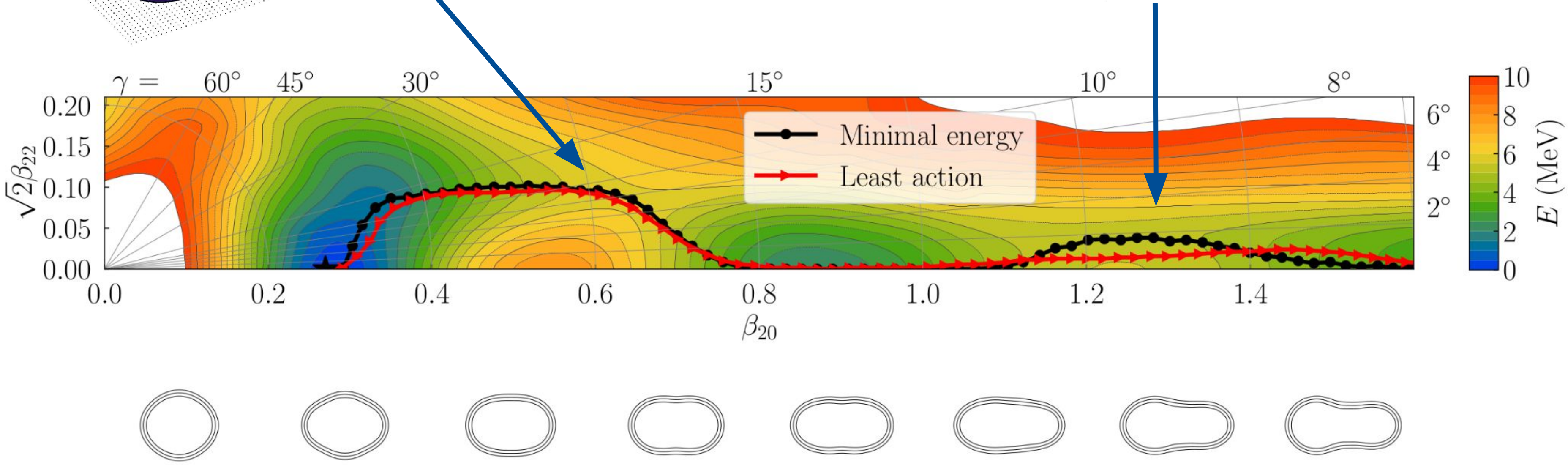
- supports massive neutron stars

Fission barriers

W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.

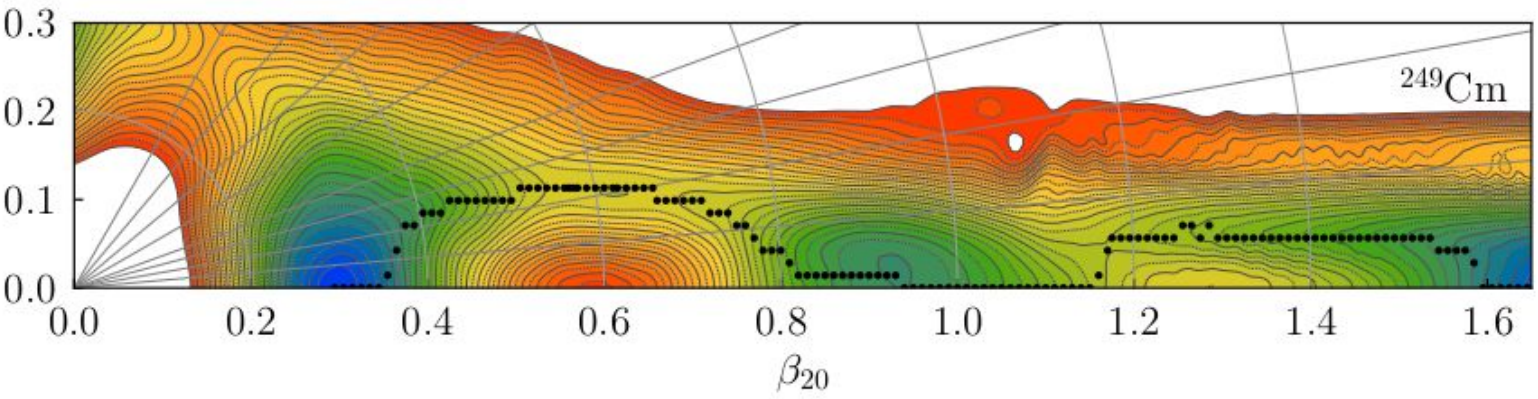






.... odd-mass and odd-odds!

W. R. et al., EPJA **59**, 96 (2023).



Blocked PES

- lowest E solution at every point
- perturbative inertia's ill-defined for odd-mass and odd-odds
- .... but can be "massaged"

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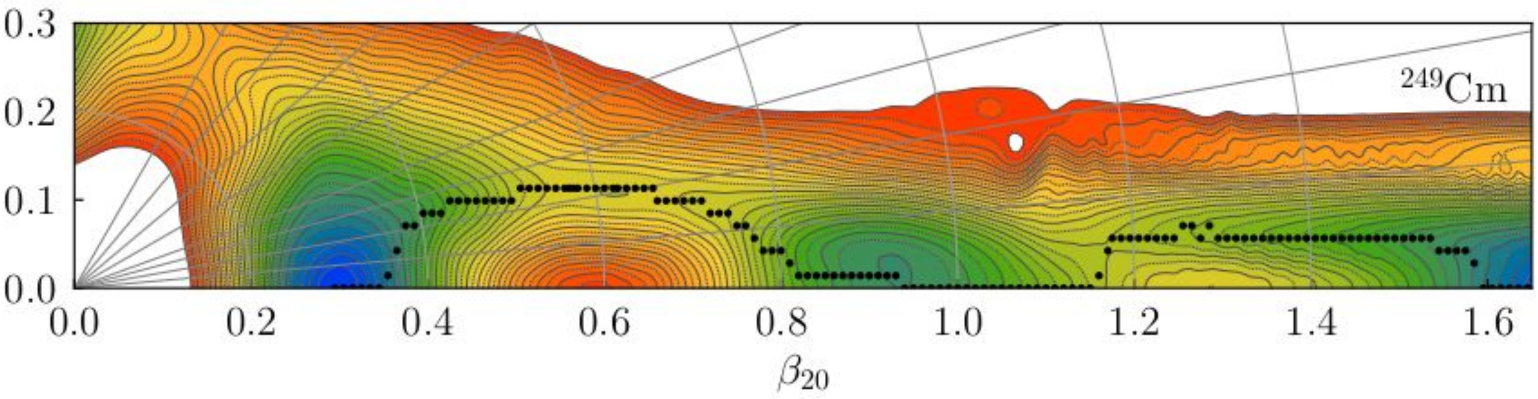
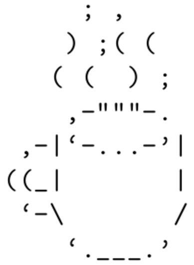




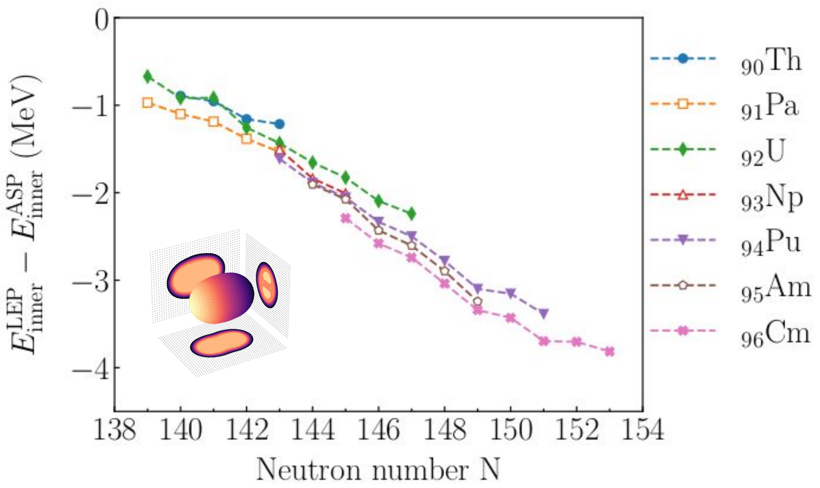
Blocked PES

- lowest E solution at every point
- perturbative inertia's ill-defined for odd-mass and odd-odds
- …. but can be "massaged"

MOCCa

- gradient solver => stable blocking
- predictor-corrector technique => simultaneous constraints
- heavy-ball method => raw speed

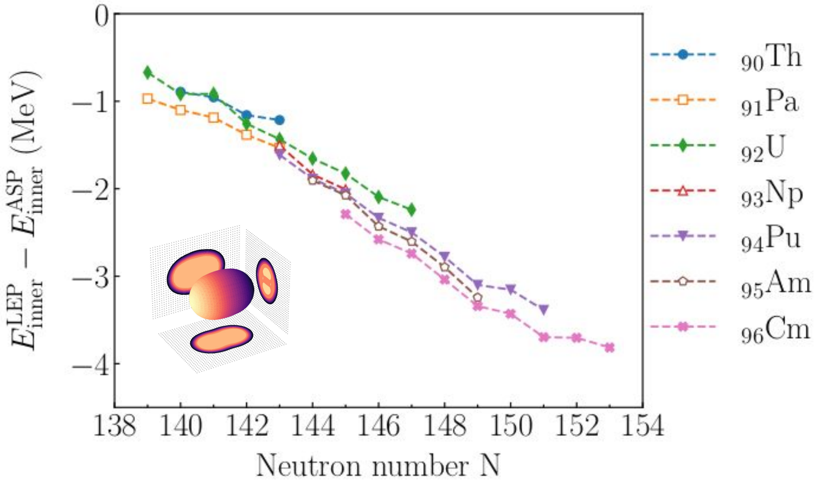
Impact of triaxial deformation

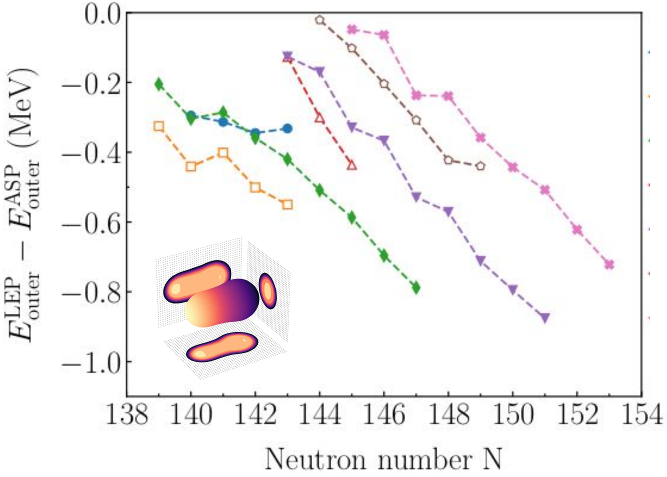


Inner barriers

- <u>**all**</u> triaxial
- effect increases with N
- remarkably insensitive to Z

Impact of triaxial deformation





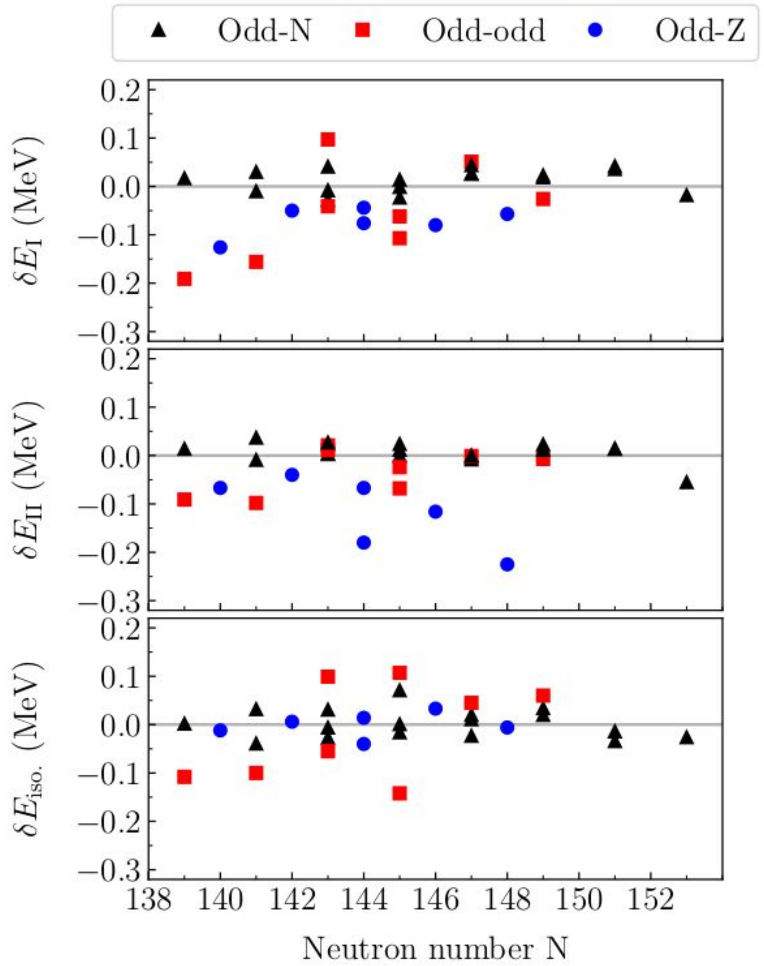
Inner barriers

- <u>**all**</u> triaxial
- effect increases with N
- remarkably insensitive to Z

Outer barriers

- <u>**all**</u> octupole + triaxial
- effect increases with N
- somewhat sensitive to Z

Impact of time-odd terms



How did we manage this agreement?

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
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Ingredients

1. coordinate space representation

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1. coordinate space representation
2. COM-correction

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Ingredients

1. coordinate space representation
2. COM-correction
3. collective corrections refit
4. triaxiality

Model ingredients

$$E_{\mathrm{tot}}(|\Phi\rangle) = E_{\mathrm{HFB}} + E_{\mathrm{corr}} ,$$

$$E_{\mathrm{HFB}} = E_{\mathrm{kin}} + E_{\mathrm{Sk}} + E_{\mathrm{pair}} + E_{\mathrm{Coul}} + E_{\mathrm{cm}}^{(1)} ,$$

$$E_{\mathrm{corr}} = E_{\mathrm{rot}} + E_{\mathrm{vib}} + E_{\mathrm{cm}}^{(2)} + E_{\mathrm{W}} ,$$

Mean-field energy

- Usual terms
- 1-body COM correction
- ~ 16 parameters
- treated **self-consistently**

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Mean-field energy

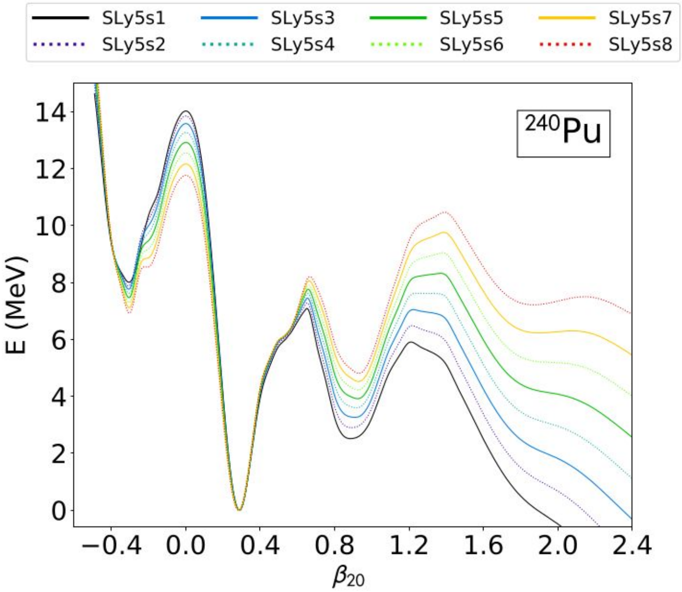
- Usual terms
- 1-body COM correction
- ~ 16 parameters
- treated **self-consistently**

Collective corrections

- rotational correction
- vibrational correction
- 2-body COM correction
- treated **semi-variationally**

Center-of-mass-correction

M. Bender et al., Eur. Phys. J. A **7**, 467–478 (2000)
P. Da Costa et al., PRC **109**, 034316 (2024).



surface tension a_{surf} determines barriers but...

Center-of-mass-correction

M. Bender et al., Eur. Phys. J. A **7**, 467–478 (2000).
W. R. et al. PRC **99**, 044315 (2019).
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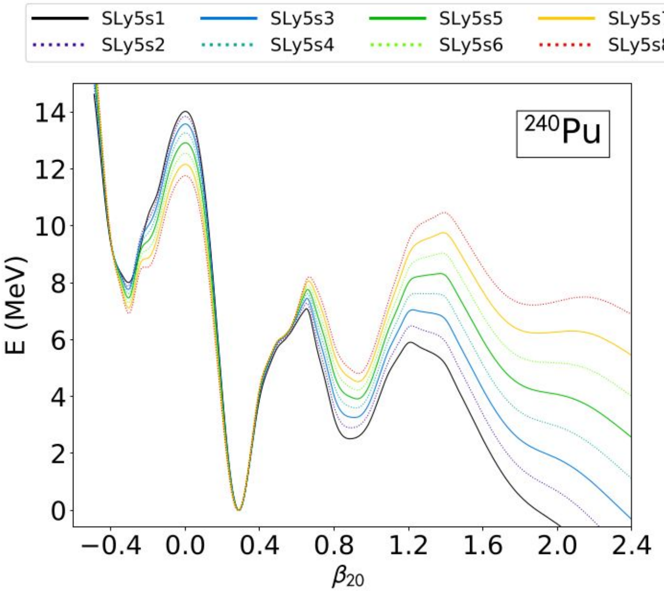

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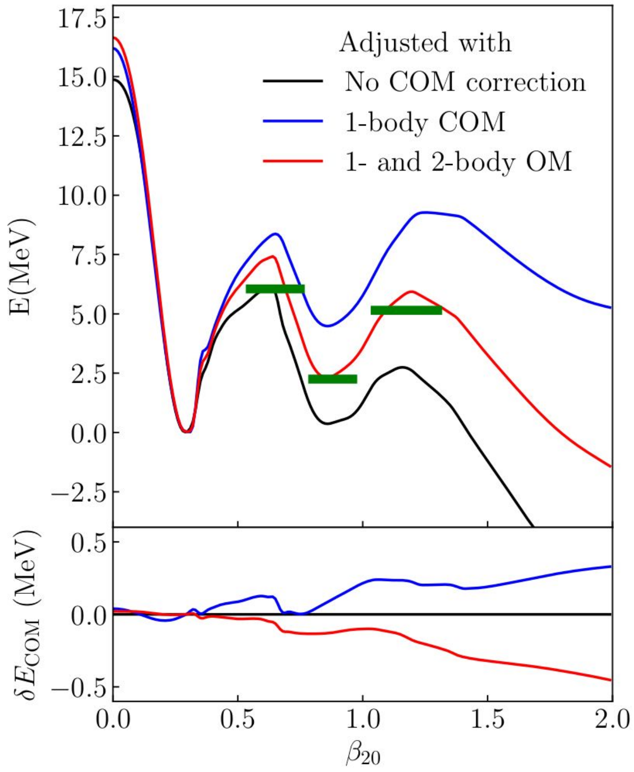

…. masses + COM correction determine a_{surf}!

Collective corrections

Fission fitting

1. Fit to non-fission observables

Collective corrections

Rms σ	BSkG1	BSkG2
Masses [MeV]	0.741	0.678
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1. Fit to non-fission observables
2. Refit 5 collective parameters to fission (requires no MOCCa calculations)

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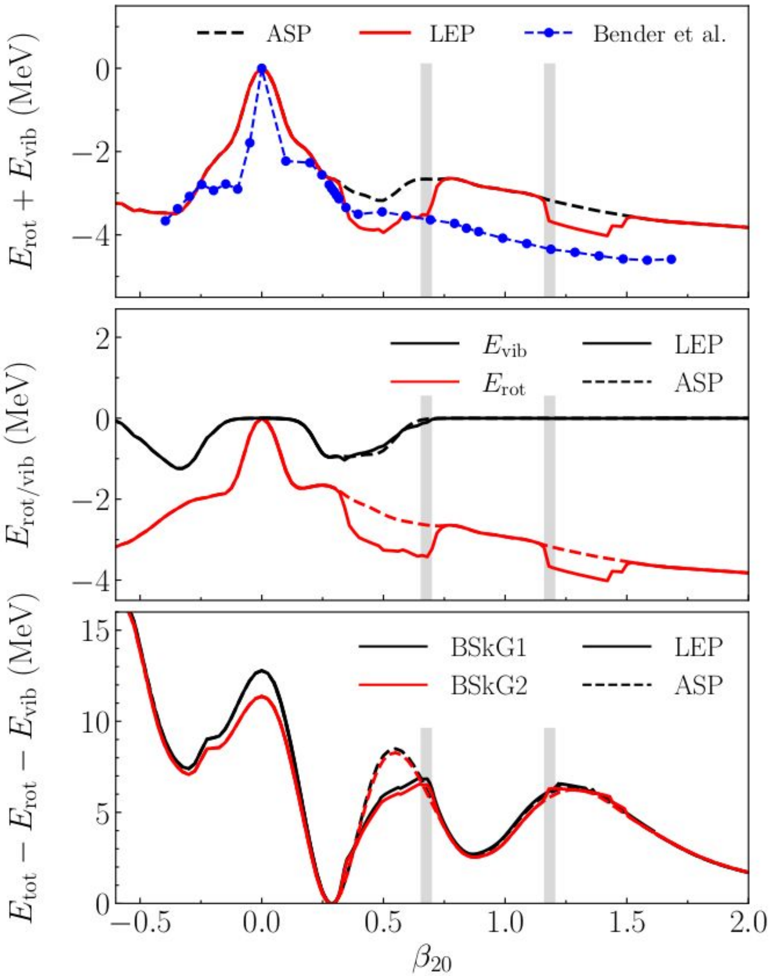

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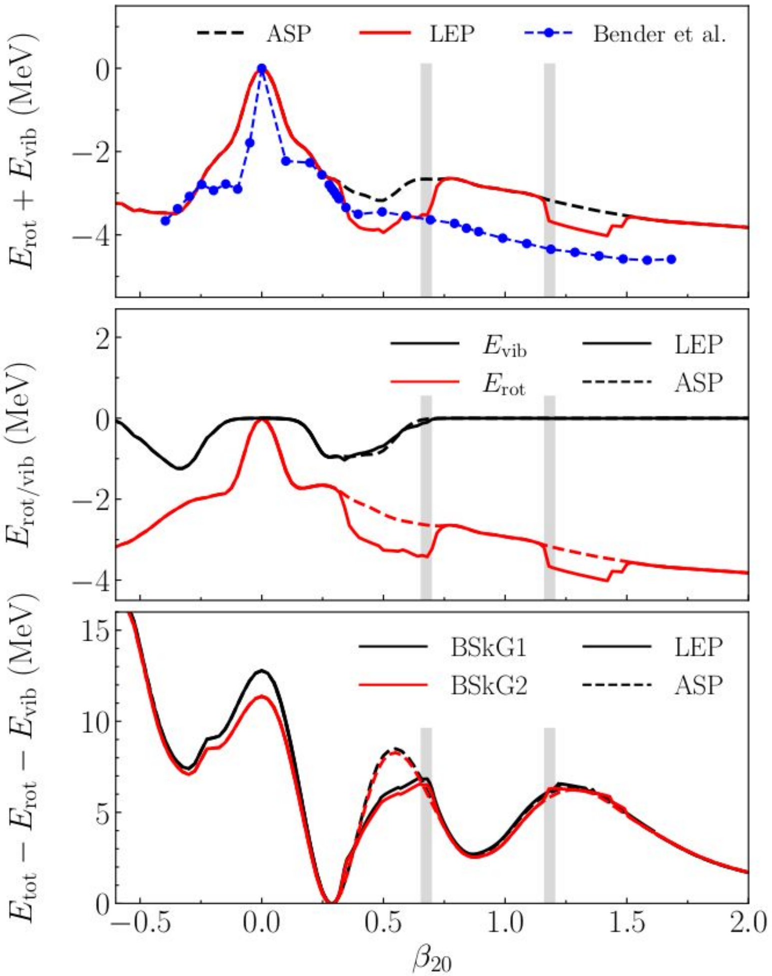
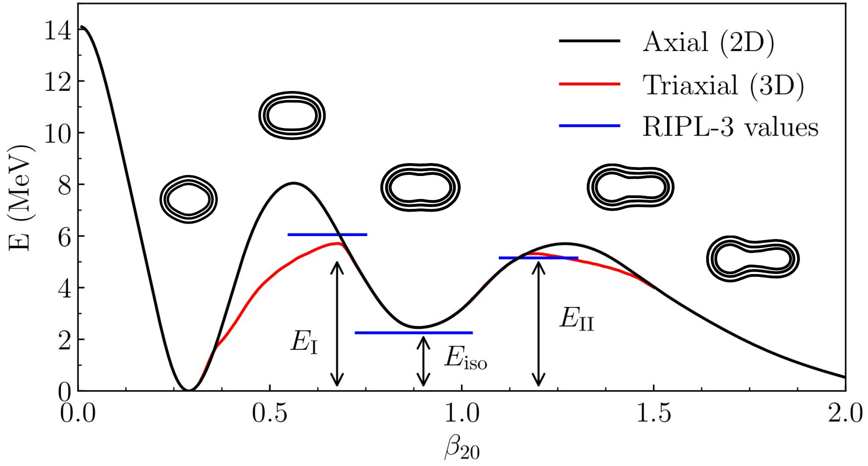


Fission fitting

1. Fit to non-fission observables
2. Refit 5 collective parameters to fission (requires no MOCCa calculations)
3. Check non-fission observables; go to 1 if necessary

➢ fit is fine-tuning, no dramatic changes

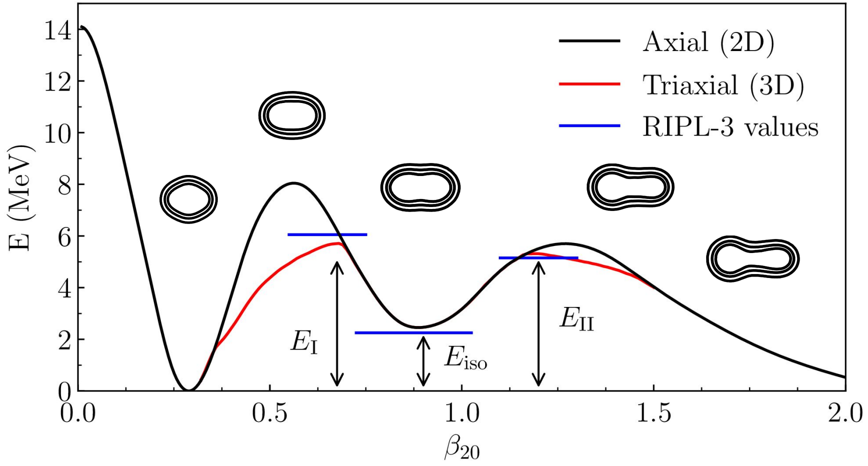
Triaxiality = ...

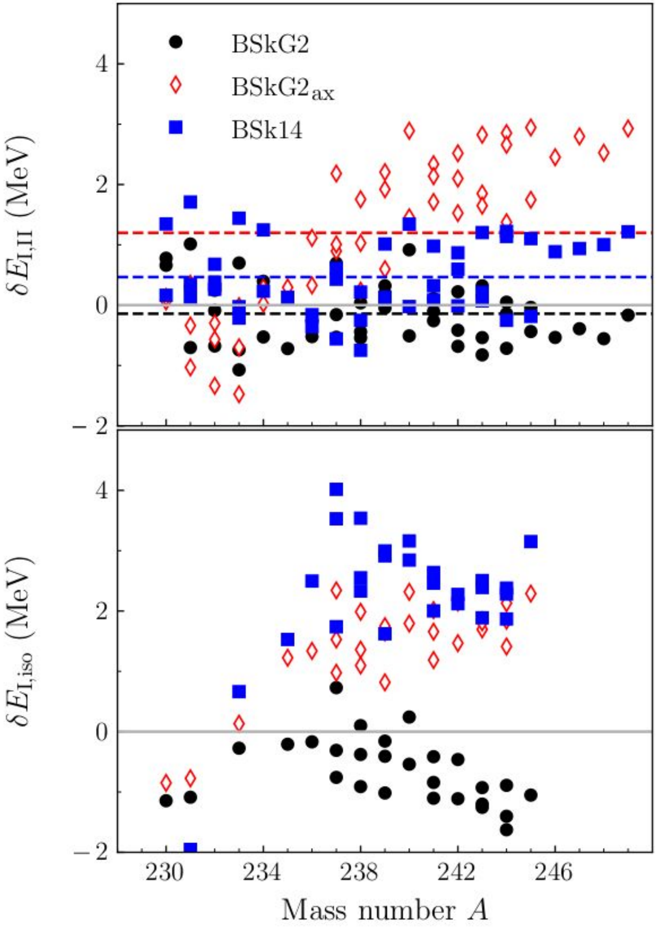


..... getting everything simultaneously

- different impact on different quantities

Triaxiality = ...





..... getting everything simultaneously

- different impact on different quantities
- differential quantities especially sensitive

Triaxiality (somehow) included

No triaxiality

Table 3 Rms deviations (σ) and mean ($\bar{\epsilon}$) errors ($\delta E_X = E_X^{\mathrm{emp}} - E_X^{\mathrm{calc}}$) for the height of the primary (E_{I}) and secondary (E_{II}) barriers, the excitation energy of the isomer (E_{iso}) and the barrier difference ($E_{\mathrm{I}} - E_{\mathrm{II}}$) for various models

Model	Fit	Triaxial		N_{b}	N_{iso}	E_{I}		E_{II}		E_{iso}		$(E_{\mathrm{I}} - E_{\mathrm{II}})$		References
		I	O			σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$	
BSkG1	N	Y	Y	45	28	0.88	+0.80	0.87	+0.71	1.00	+0.67	0.56	+0.09	
BSkG2	Y	Y	Y	45	28	0.44	+0.24	0.47	+0.10	0.49	−0.36	0.53	+0.14	
BSk14	Y	N	N	45	28	0.60	−0.27	0.69	+0.20	1.05	+0.34	0.76	−0.47	[35]
BCPM	N	N	N	45	28	1.42	−1.07	0.72	−0.30	0.52	+0.09	1.22	−0.77	[106]
SkSC4	N	N	N	45	0	0.57	+0.04	2.03	+1.78	–	–	2.15	−1.74	[31]
FRLDM	Y	Y	N	45	28	0.81	+0.22	1.41	+0.66	1.02	−0.91	0.88	−0.44	[103]
YPE+WS	Y	Y	N	45	28	0.82	−0.66	0.84	−0.40	0.38	+0.07	0.72	−0.26	[110]
D1M	Y	Y	N	14	8	0.53	+0.23	0.43	+0.06	0.99	+0.50	0.47	+0.17	[57]
UNEDF1	Y	Y	N	10	4	0.72	−0.67	0.79	−0.41	0.16	−0.06	0.83	−0.26	[73]
	Y	Y	Y	12	8	0.71	−0.52	0.65	−0.28	0.69	−0.36	0.71	−0.24	[45]
SkM*	Y	Y	N	10	0	1.92	−1.86	1.93	−1.84	–	–	0.57	−0.01	[73]
SkI3	N	N	N	7	8	3.99	−3.59	1.59	−1.44	1.04	+0.35	2.51	−2.15	[81]
	N	N	N	14	0	3.26	−2.50	–	–	–	–	–	–	[111]
SkI4	N	N	N	7	8	4.35	−4.27	3.65	−3.49	0.95	−0.22	1.02	−0.78	[81]
SLy6	N	N	N	7	8	4.23	−3.90	2.19	−2.08	1.24	−1.28	2.24	−1.82	[81]
	N	N	N	14	0	3.89	−3.31	–	–	–	–	–	–	[111]
SV-bas	N	N	N	14	0	1.88	−1.10	–	–	–	–	–	–	[111]
SV-min	N	N	N	14	0	1.61	−0.50	–	–	–	–	–	–	[111]
NL-Z2	N	N	N	7	8	1.73	−0.93	1.28	+1.19	1.81	+1.91	2.68	−2.12	[81]
NL3	N	N	N	7	8	2.18	−1.26	1.03	+0.62	0.49	+0.39	2.73	−1.88	[81]
NL3*	N	N	N	14	0	2.16	−2.03	–	–	–	–	–	–	[112]
PC-PK1	N	N	N	14	0	1.84	−1.53	1.01	−0.60	–	–	1.43	−0.93	[43]
	N	Y	Y	14	0	0.37	+0.18	0.82	+0.13	–	–	0.73	+0.05	[43]
DD-ME2	N	N	N	14	0	3.35	−3.17	–	–	–	–	–	–	[112]
DD-PC1	N	N	N	14	0	2.45	−1.76	–	–	–	–	–	–	[112]

The second column indicate whether the models parameter adjustment included information on the physics of large deformation, in one form or another. The third and fourth column indicate whether or not the calculations considered triaxial deformation near the inner and outer barrier respectively. N_{b} and N_{iso} respectively refer to the number of barriers and isomers included in the calculated deviations

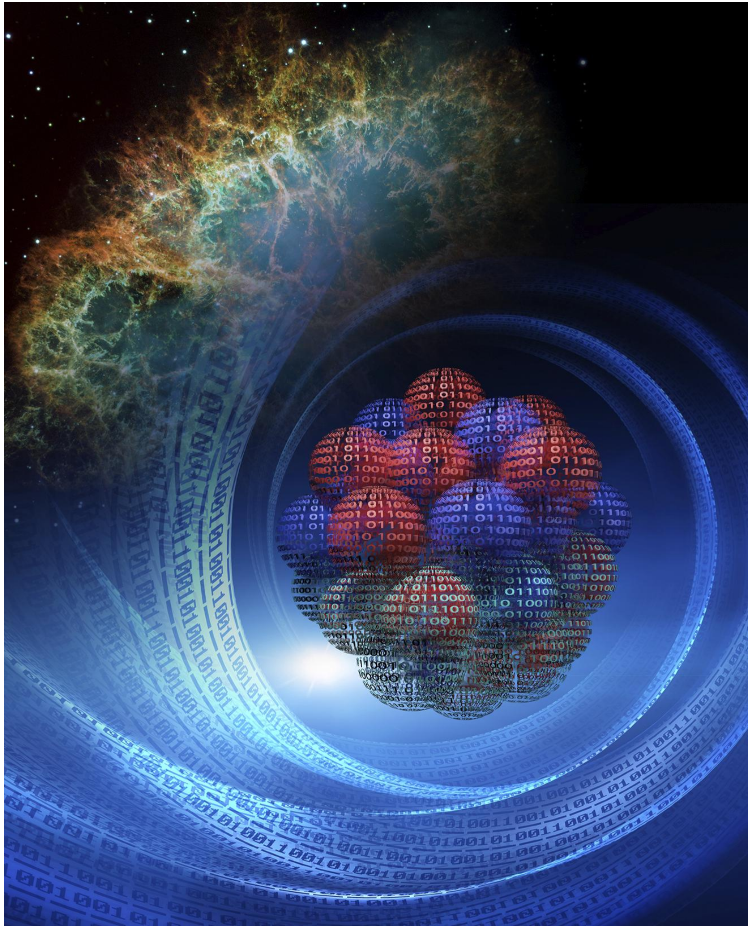
Conclusion & perspectives

The BSkG models

Now:

- **excellent** ground state properties

- **simultaneous** reproduction of static fission properties within 500 keV
  - coordinate space representation
  - realistic surface properties through COM correction
  - fine-tuning of collective corrections
  - triaxial deformation of inner and outer barriers



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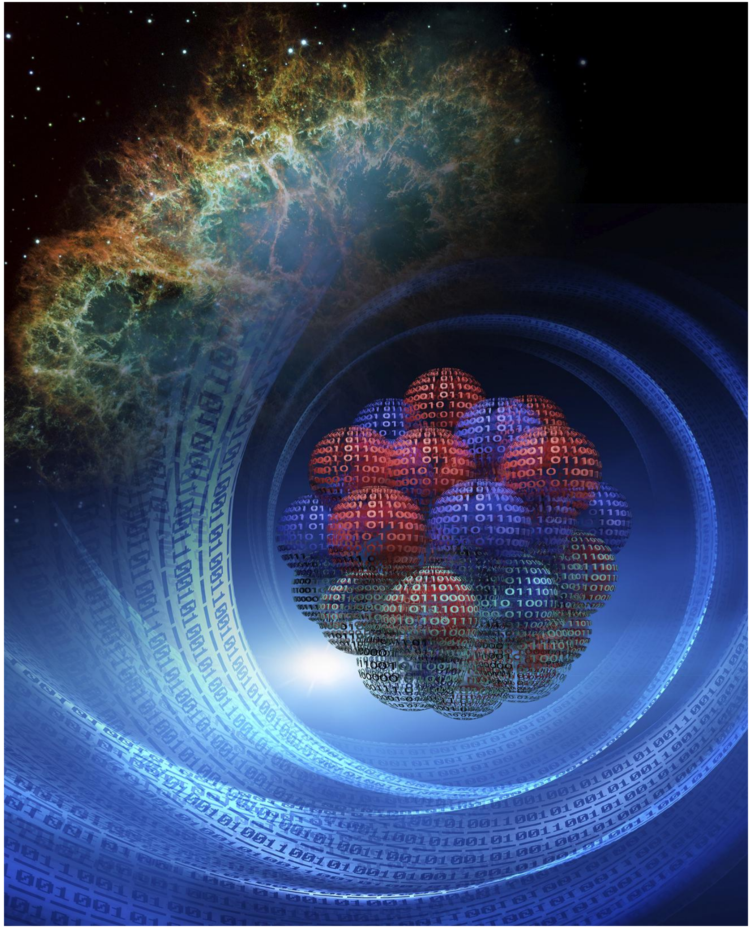
Soon:

- database with ~3000 fission paths in ‘poor-mans 3D’



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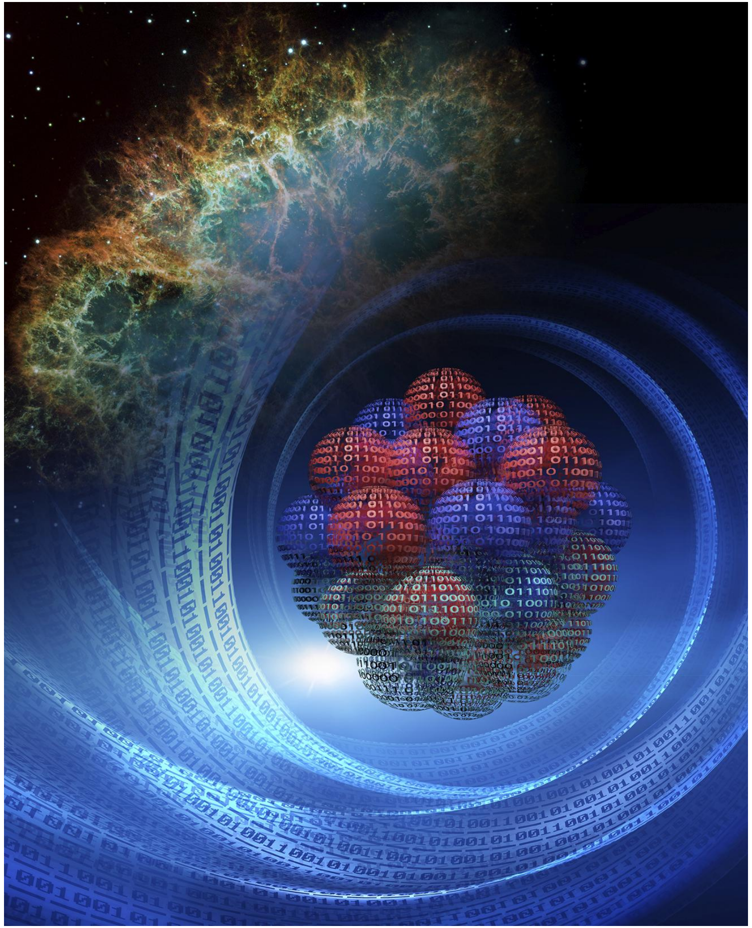

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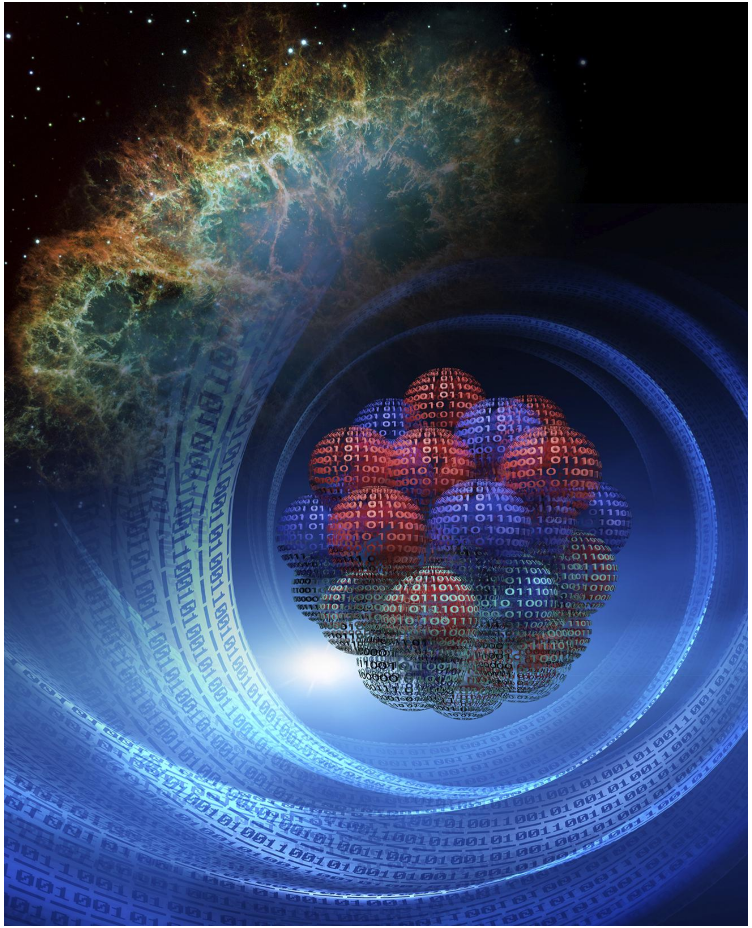
Model construction

- COM correction => undefined in time-dependent approaches

- No COM correction => bad surface properties

- This is an issue since time-dependent <-> static approaches
    - fission of odd-mass and odd-odd nuclei
    - dynamics in neutron star crust
    - .....



Thank you for…

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EuroHPC Joint Undertaking

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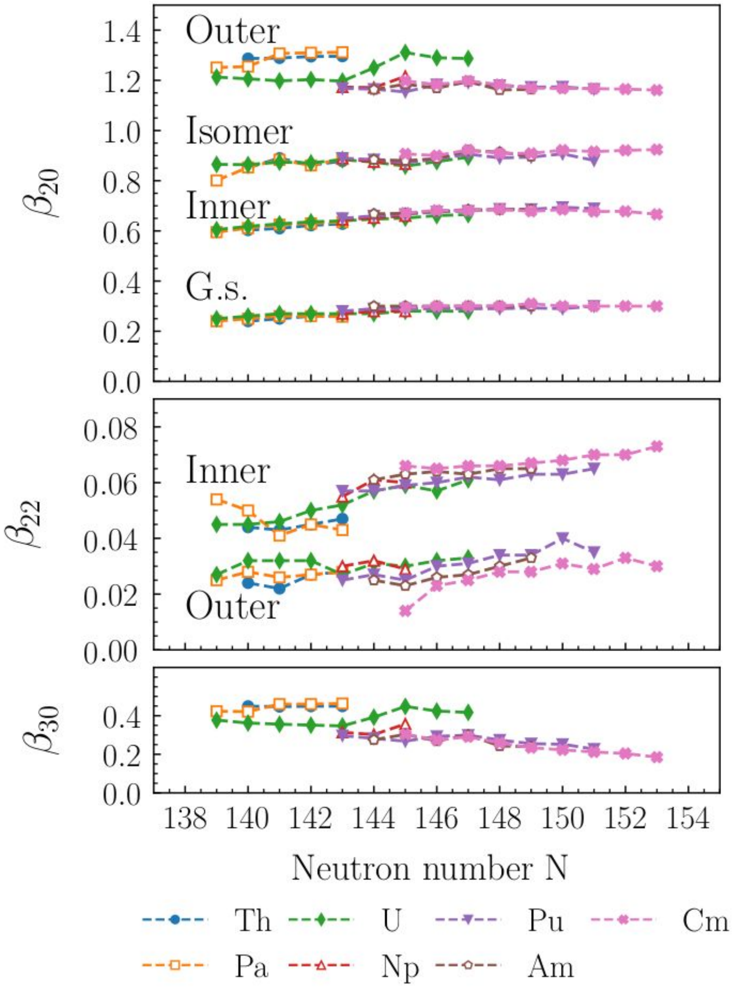

Outer
Isomer
Inner
G.s.
β_{20}
Inner
Outer
β_{22}
β_{30}
Neutron number N
Th
U
Pu
Cm
Pa
Np
Am

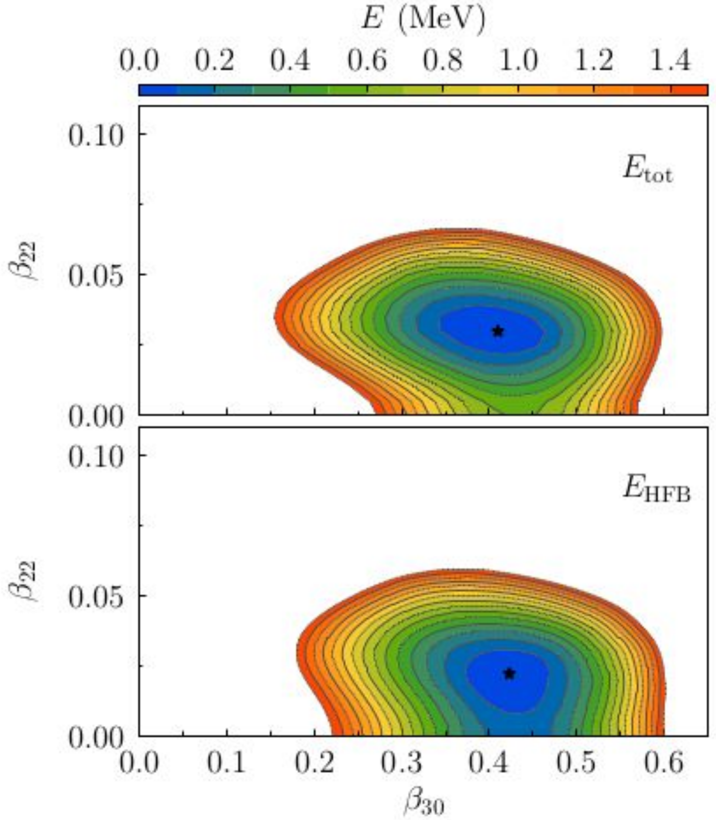

Fig. 4 The total energy E_{tot} (top panel) and the mean-field energy E_{HFB} (bottom panel) of ^{240}Pu at (fixed) elongation $\beta_{20} = 1.30$, normalized to their respective minima, as a function of β_{22} and β_{30}. Respective minima are indicated by black stars and contour lines are 100 keV apart

Table 2 Rms $\sigma(O)$ and mean deviations $\bar{\epsilon}(O)$ of the BSkG1 and BSkG2 models, with respect to RIPL-3 reference values for the primary and secondary barriers [38] and isomer excitation energies from Ref. [67] for different subsets of nuclei: even-even nuclei, odd-mass nuclei with odd Z, odd-mass nuclei with odd N and odd-odd nuclei. M indicates the number of empirical values available for each subset. All energies are expressed in MeV

			BSkG1		BSkG2	
		M	σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$
Even-even	E_{I}	14	0.94	+0.90	0.45	+0.31
	E_{II}	14	0.83	+0.67	0.46	+0.01
	E_{iso}	8	0.63	+0.52	0.53	−0.38
Odd-Z	E_{I}	6	0.66	+0.52	0.41	−0.03
	E_{II}	6	0.69	+0.62	0.28	+0.10
	E_{iso}	4	0.66	+0.62	0.40	−0.29
Odd-N	E_{I}	17	0.96	+0.87	0.5	+0.34
	E_{II}	17	0.93	+0.72	0.55	+0.12
	E_{iso}	12	1.35	+0.85	0.46	−0.35
Odd-odd	E_{I}	8	0.73	+0.67	0.28	+0.13
	E_{II}	8	0.95	+0.84	0.43	+0.24
	E_{iso}	4	0.62	+0.50	0.57	−0.43
Total	E_{I}	45	0.88	+0.80	0.44	+0.24
	E_{II}	45	0.87	+0.71	0.47	+0.10
	E_{iso}	28	1.00	+0.67	0.49	−0.36

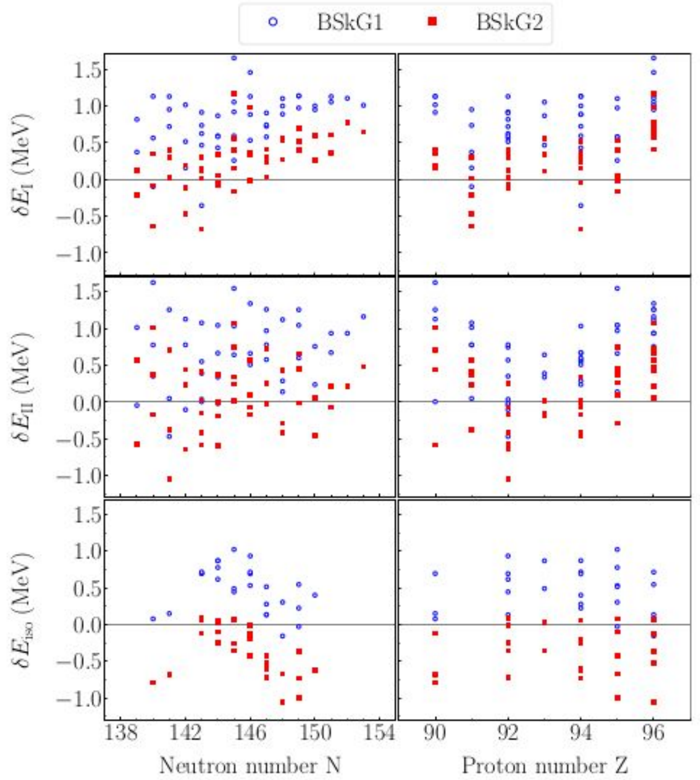

Fig. 6 Difference between calculated and reference values for the primary barrier heights (top panel), secondary barrier heights (middle) and isomer excitation *energies* (bottom panel), using BSkG1 (blue open circles) and BSkG2 (red filled squares). Positive (negative) values for all three differences mean that calculated results are smaller (larger) than the reference values