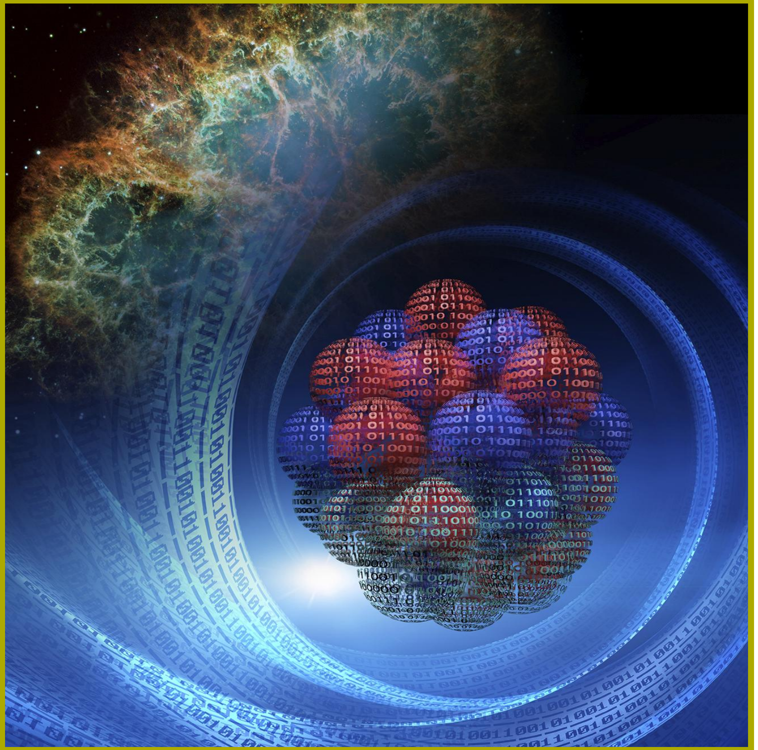
WOUTER RYSSENS



Andy Sproles, ORNL

Symmetry breaking on the scale of the nuclear chart

W. Ryssens, G. Scamps and S. Goriely

April 21th 2022

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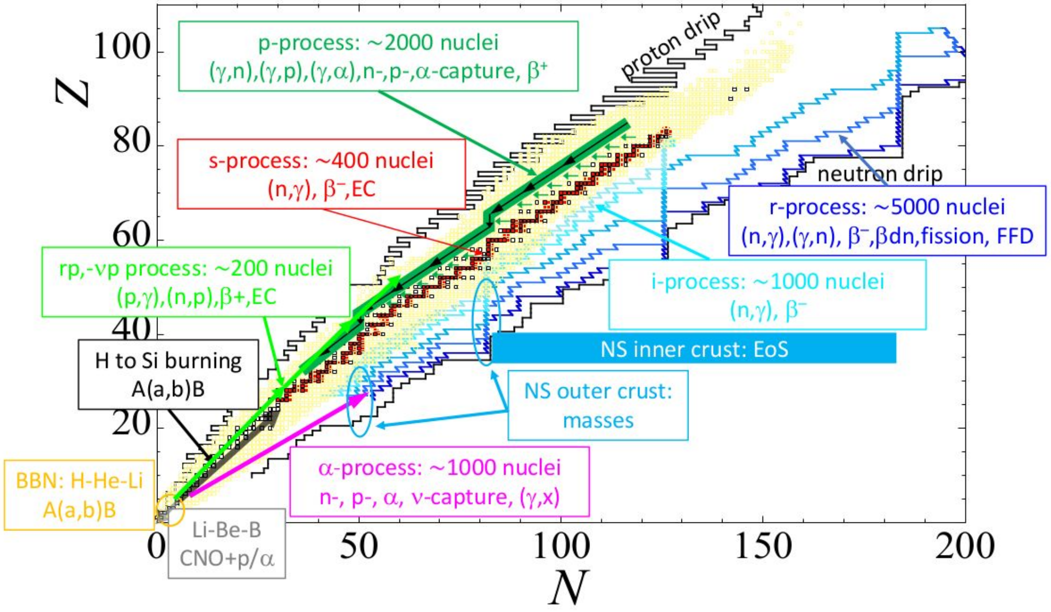
The challenge for nuclear theory



M. Arnould & S. Goriely, Prog. Part. Nuc. Phys. 112, 103766 (2020).

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

Coupling constants

$$\boxed{E} \sim \int d^3r \left[\boxed{C^{\rho}}\,\boxed{\rho(\mathbf{r})\rho(\mathbf{r})} + \boxed{C^{\tau}}\,\boxed{\tau(\mathbf{r})\rho(\mathbf{r})} + \dots \right]$$

Energy (to be varied)

Local densities of a mean-field state

Strong points

- **Microscopic** approach
- # of **observables** accessible
- Feasible for **1000s** of nuclei

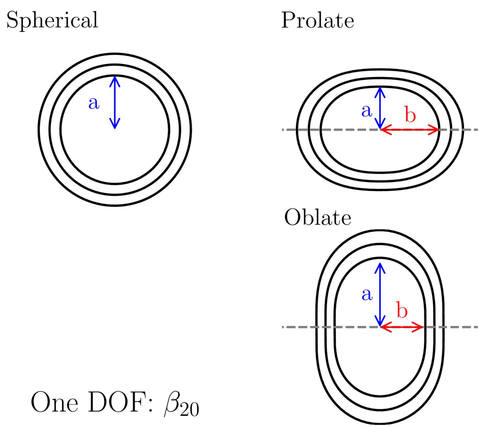
Weak points

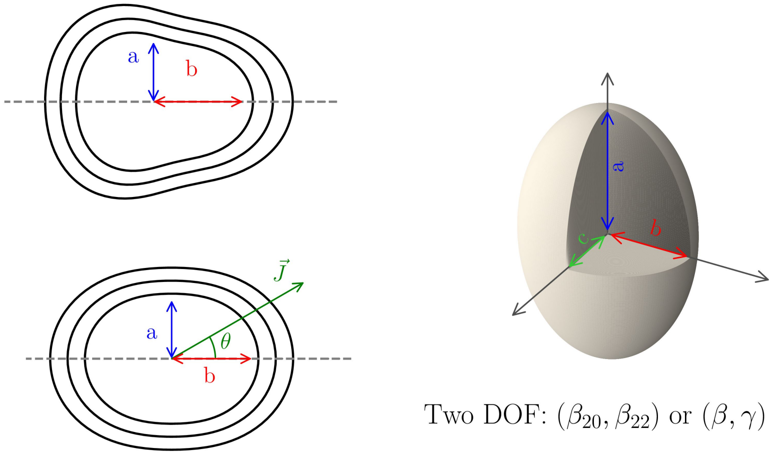
- Simple ansatz
- **Phenomenological** form
- Fitting of **coupling constants**

Brussels models

- **20-25** parameters
- grasp physics of the entire chart
- Fit protocol includes:
  - 1000s of masses
  - 100s of charge radii
  - INM properties

Symmetry breaking





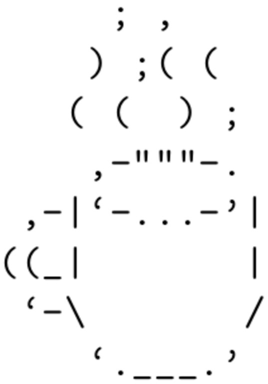
Nuclear deformation

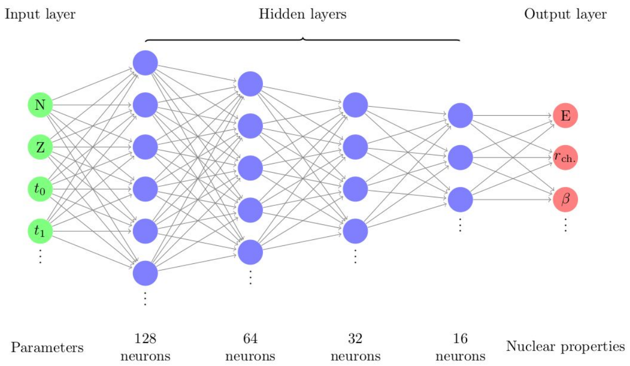
- Cheap way to grasp more **correlations**
- **intuitive interpretation** of results
- State-of-the-art for global models:
  - time-reversal invariance
  - reflection symmetry
  - axial symmetry

Including complicated geometries

- **reflection-asymmetric** shapes
- **time-reversal** breaking
- **cluster** structures
- **triaxial** shapes
- ....

Tools: MOCCa and machine learning





W. R. PhD Thesis, ULB (2016).
W. R. et. al., PRC 92, 064318 (2015).
W. R. et. al., EPJA 55, 93 (2019).

G. Scamps et al., EPJA 57, 333 (2021).

MOCCa

- Skyrme-HFB solver in **3D coordinate space**
- Very flexible for **symmetries/shapes**
- High numerical **accuracy**
- New algorithms for **speed** and **robustness**

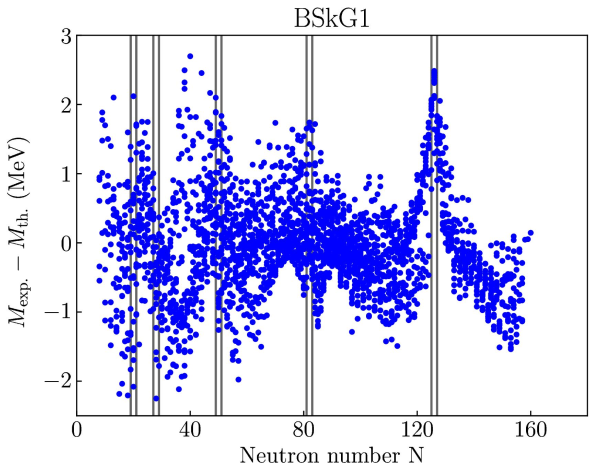
Machine learning

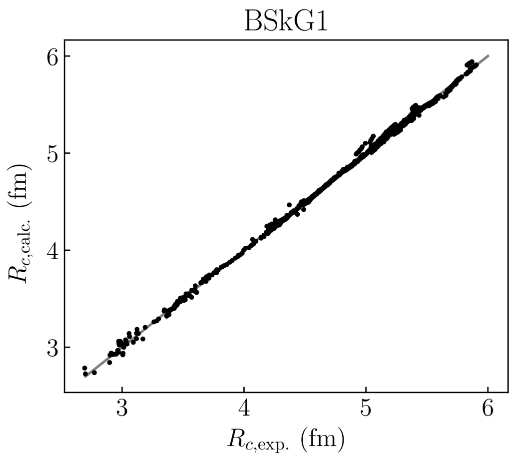
- **100's** of neural networks
- each trained to emulate MOCCa
- exploration of parameter space

There are no ML extrapolations!

Brussels **Sk**yrme on a **G**rid: BSkG1 and BSkG2

Wouter Ryssens (ULB)





BSkG1: G. Scamps et al., EPJA 57, 333 (2021).
BSkG2: W. Ryssens et al., in preparation
HFB-21: S. Goriely et al., PRC 82, 035804 (2010).
FRDM: P. Möller et al., At. Data Nucl. Data Tables, 109-110 (2016).

Both models fitted with

- >2400 masses
- >800 charge radii
- triaxial deformation
- high numerical accuracy

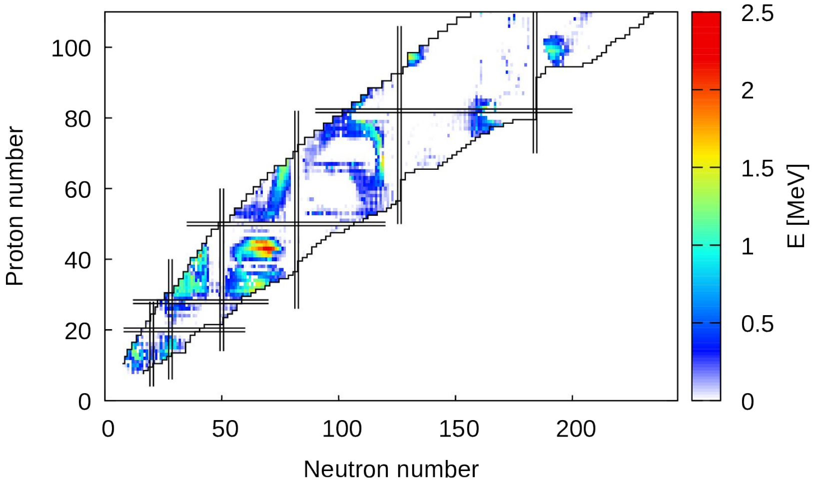
Extra for BSkG2:

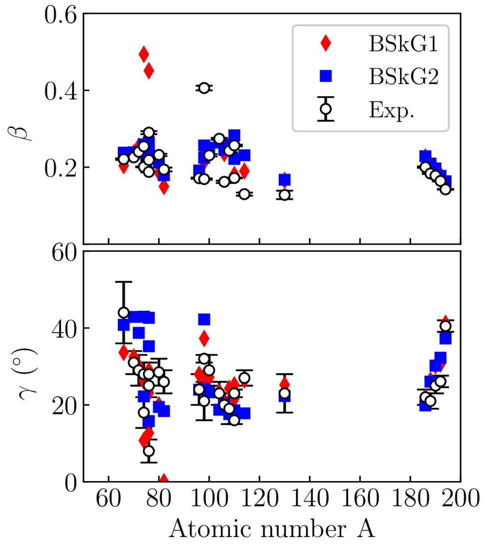
- **time-reversal** breaking
- **vibrational** correction
- **12 fission barriers**

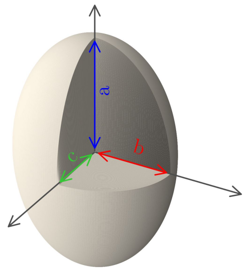
Global performance

σ^2	**BSkG1**	**BSkG2**	HFB-21	FRDM
Masses (MeV)	**0.741**	**0.678**	0.577	0.560
Charge radii (fm)	**0.027**	**0.027**	0.027	0.038

Triaxial deformation







Two DOF: (β_{20}, β_{22}) or (β, γ)

All refs in G. Scamps et al., EPJA 57, 333 (2021).

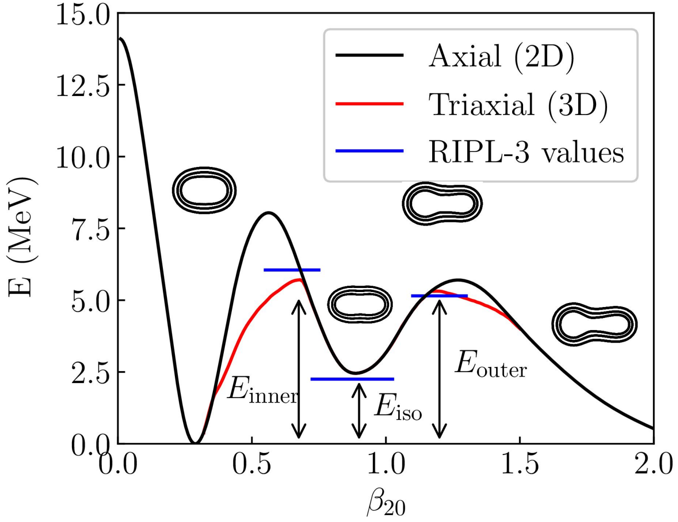
Energy gain by triaxial deformation

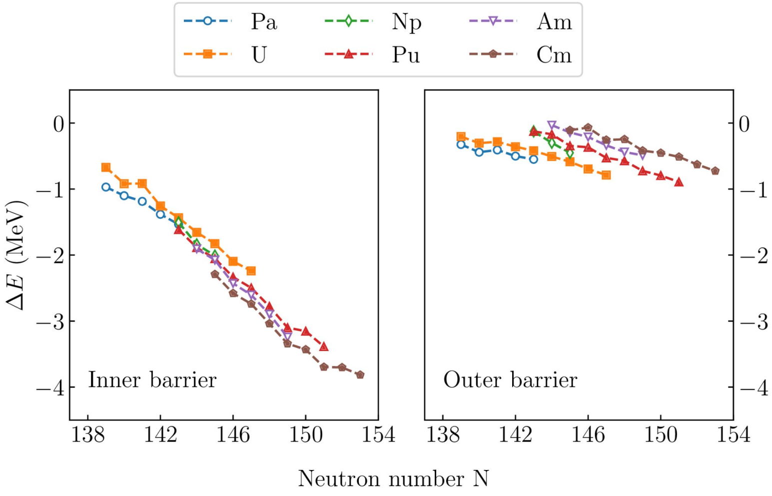
- Many nuclei gain **0.5-2.5** MeV
- Highest gains for Z~43 (Rh)

Rotational invariants

- obtained from COULEX
- data compiled by M. Zielińska

Fission barriers of actinides





HFB-14: S. Goriely et al., PRC 75, 064312 (2007).
FRLDM: P. Möller et al., PRC 79, 064304 (2009).

Fission barriers with BSkG2

- collective correction parameters (5)
- refit to 12 actinide barriers after mass fit

Performance on 41 barriers (Z>90) + 25 isomers

σ^2(MeV)	BSkG1	**BSkG2**	HFB-14	FRLDM
Primary barriers	0.87	**0.45**	0.61	0.79
Secondary barriers	0.86	**0.45**	0.70	1.35
Isomers	0.45	**0.48**	0.93	1.04

The BSkGX models

Today's models:

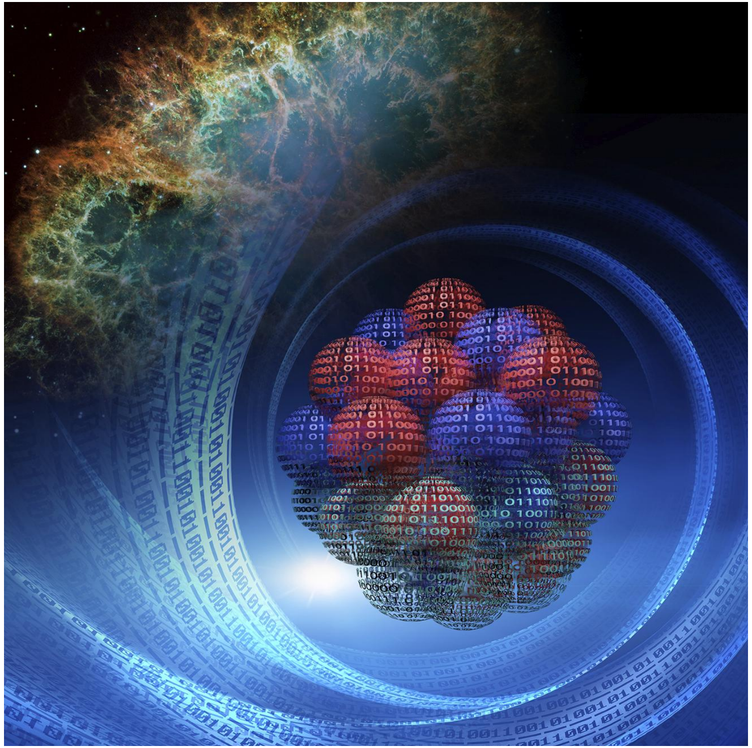
- fitted to > 2400 masses and > 800 radii
- among the best for **masses** and **charge radii**
- include **triaxiality** (BSkG1/2)
- include **time-odd** channel (BSkG2)
- the best for actinide fission barriers (BSkG2)

We are working on constructing:

- nuclear level densities
- complete fission model

Tomorrow's models:

- improved neutron matter equation-of-state
- improved spectroscopy
- octupole deformation



Thank you for...

...... the help!

ULB

S. Goriely
G. Grams

iP2i LES 2 INFINIS LYON

M. Bender

UNIVERSITY of WASHINGTON

G. Scamps

...... the computing time!

CÉCI

Cenaero

...... the funding!

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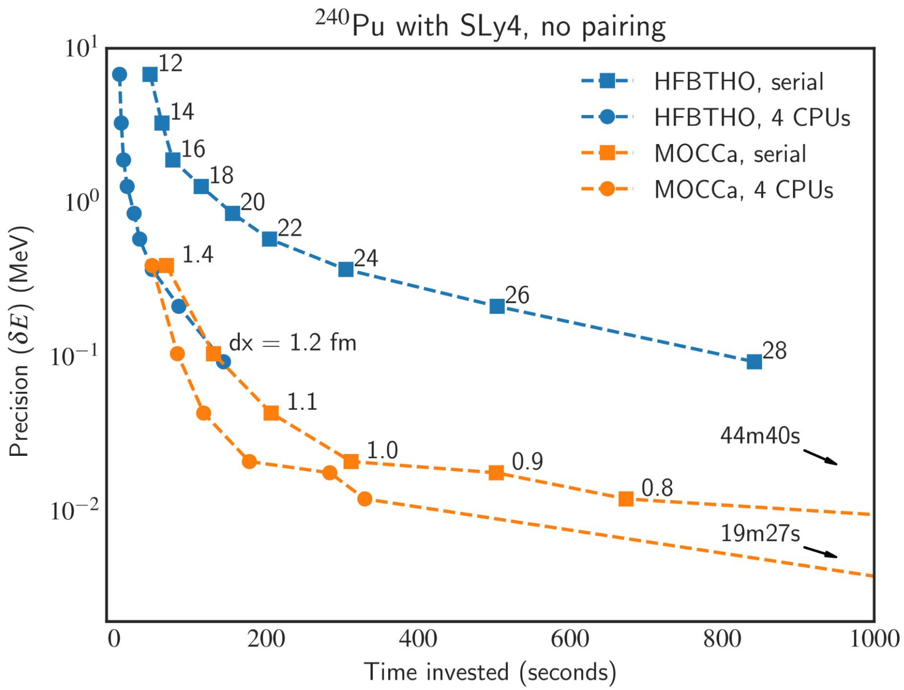
...... your attention!

Bonus!

MOCCa is **fast** and **accurate**



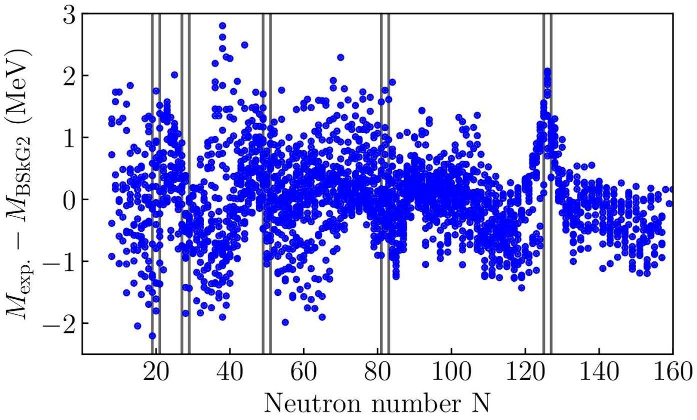
W. R., unpublished.

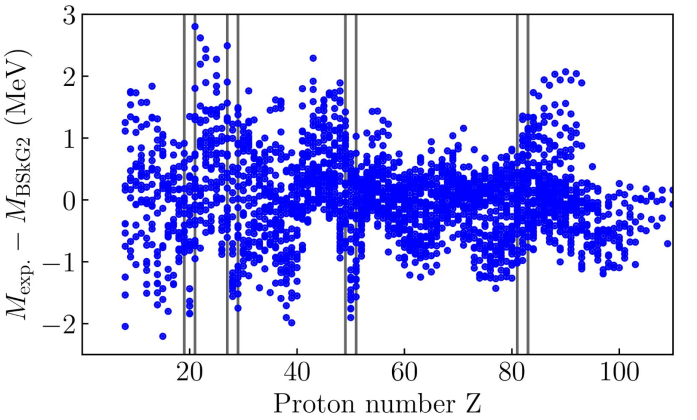
BSkG models: details

W. R. et al., in preparation.

Table IV. Rms σ and mean $\bar{\epsilon}$ (exp.-theory) deviations with respect to the 2457 known masses ($Z, N \geq 8$) M [57], the 2309 neutron separation energies S_n, the 2173 β-decay energies Q_β, and the 884 measured charge radii R_c [58] for the BSkG1 and BSkG2 mass models. The first line gives the model error [59] on all the 2457 measured masses. [a]

Results	BSkG1	BSkG2
$\sigma_{\mathrm{mod}}(M)$ [MeV]	0.734	0.668
$\sigma(M)$ [MeV]	0.741	0.678
$\bar{\epsilon}(M)$ [MeV]	−0.026	0.026
$\sigma(S_n)$ [MeV]	0.466	0.500
$\bar{\epsilon}(S_n)$ [MeV]	0.000	−0.006
$\sigma(Q_\beta)$ [MeV]	0.645	0.619
$\bar{\epsilon}(Q_\beta)$ [MeV]	0.000	−0.019
$\sigma(R_c)$ [fm]	0.0267	0.0274
$\bar{\epsilon}(R_c)$ [fm]	−0.0008	−0.007
$\sigma(\Delta R_c)$ [fm]	0.0150	0.0169



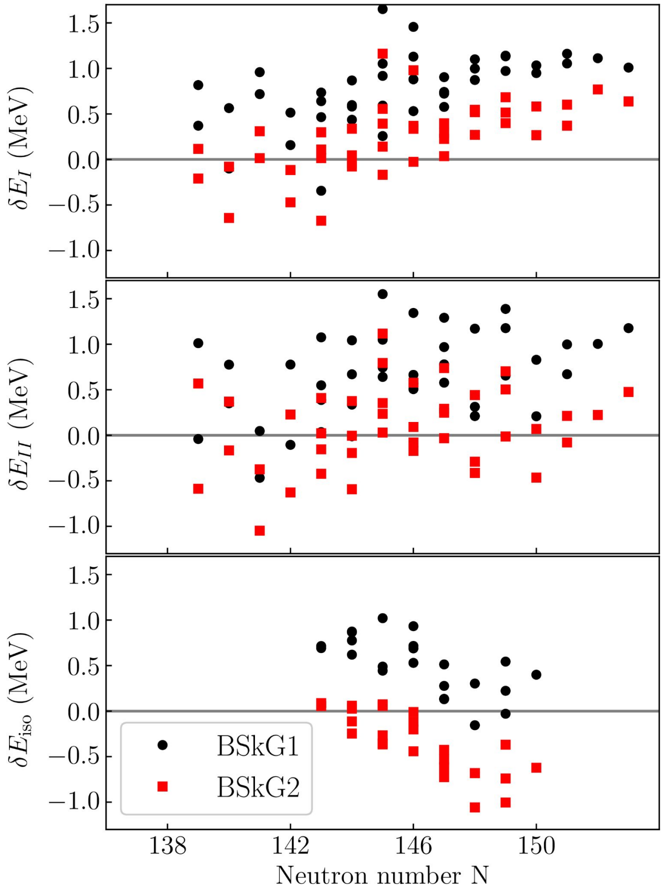


BSkG models: fission

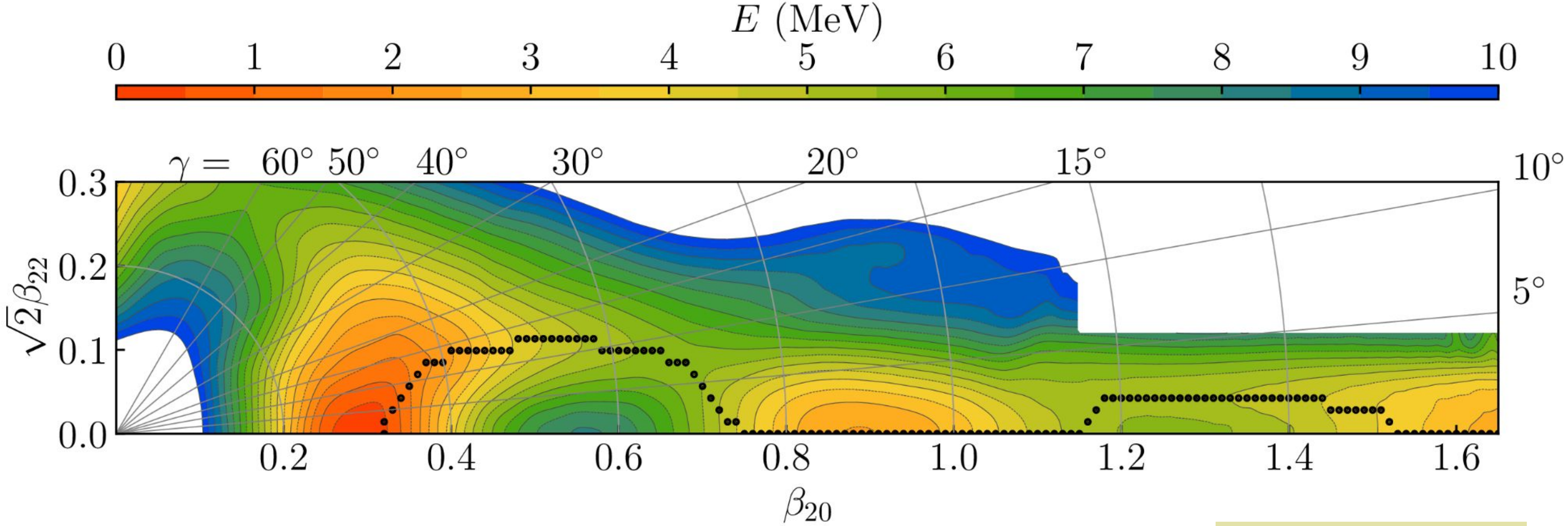
W. R. et al., in preparation.

			BSkG1		BSkG2	
			σ	$\bar{\epsilon}$	σ	$\bar{\epsilon}$
Fit-data	Primary	12	+0.92	+0.88	+0.47	+0.32
	Secondary	12	+0.71	+0.57	+0.38	−0.10
	Isomers	7	+0.67	+0.58	+0.48	−0.32
Even-even	Primary	12	+0.92	+0.88	+0.47	+0.32
	Secondary	12	+0.71	+0.57	+0.38	−0.10
	Isomers	7	+0.67	+0.58	+0.48	−0.32
Other	Primary	29	+0.84	+0.74	+0.45	+0.21
	Secondary	29	+0.91	+0.76	+0.48	+0.16
	Isomers	18	+0.47	+0.77	+0.47	−0.35
Total	Primary	41	+0.87	+0.78	+0.45	+0.24
	Secondary	41	+0.86	+0.70	+0.45	+0.08
	Isomers	25	+0.45	+0.77	+0.48	−0.34

Table VI. Rms deviations σ_X and mean deviations $\bar{\epsilon}_X$ between RIPL-3 [29] and BSkG1 and BSkG2 calculated values for the primary and secondary barrier heights (data for 41 nuclei with for $90 < Z \leq 96$), as well as isomer excitation energies from Ref. [30] (data for 25 nuclei with for $90 < Z \leq 96$). All quantities in MeV.

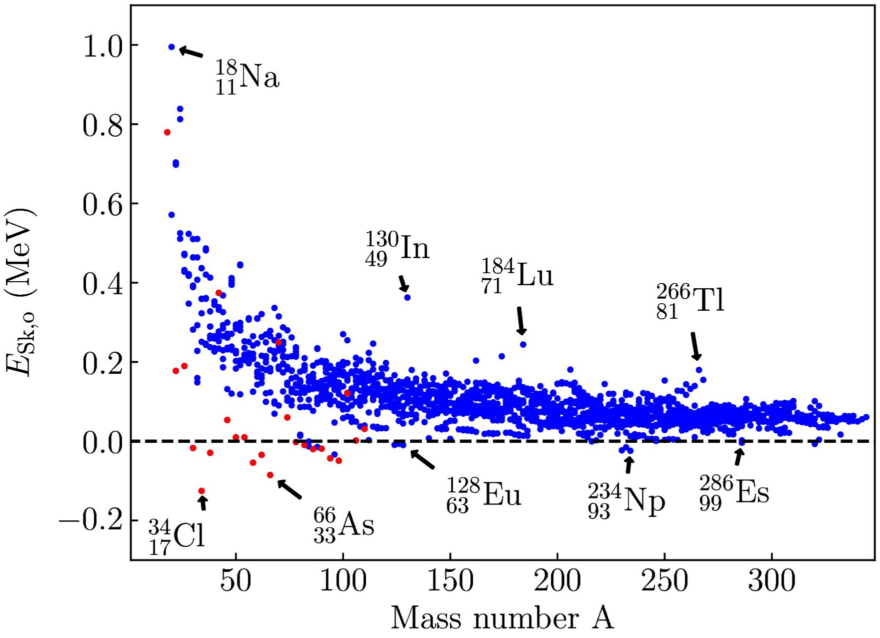


BSkG models: fission

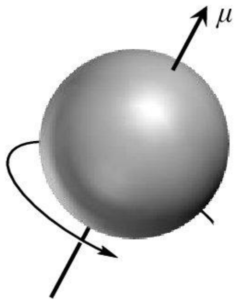


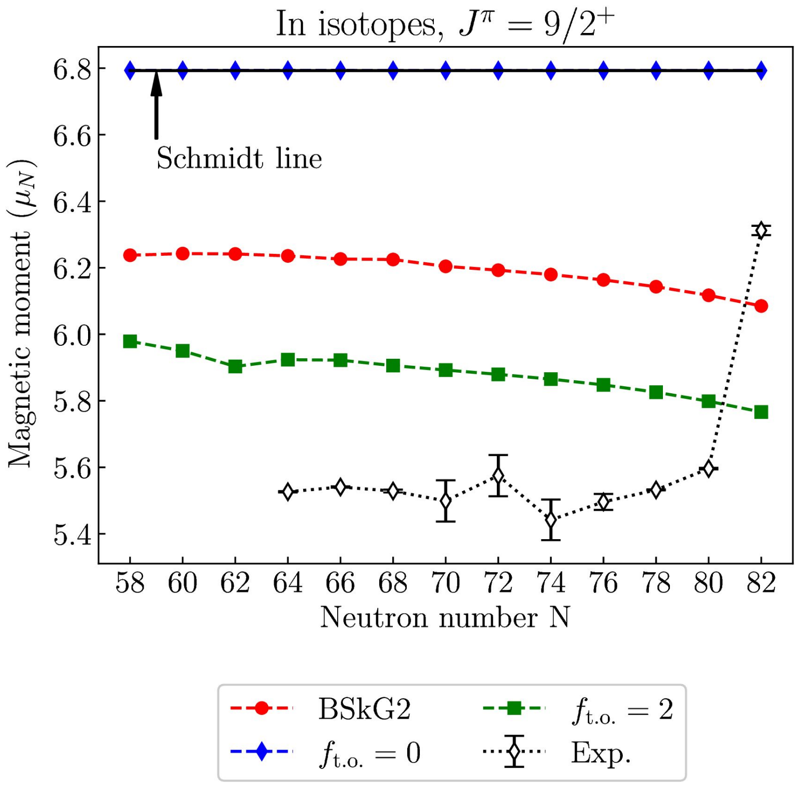
W. R. et al., in preparation.

BSkG models: time-odd energy contribution



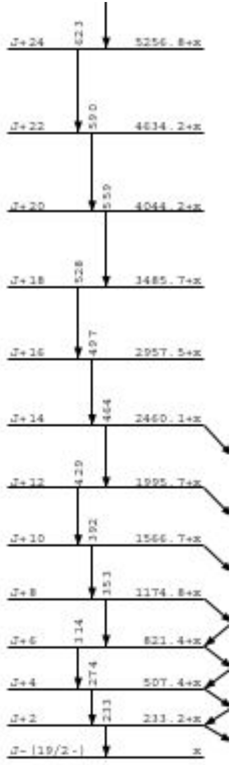
BSkG models: magnetic moments



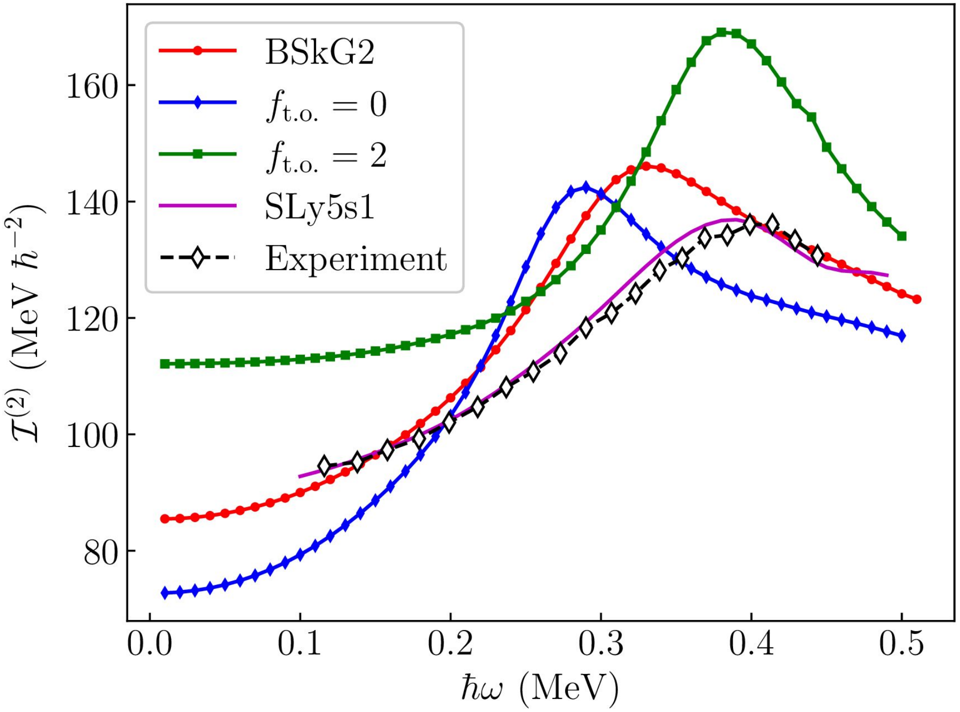


Exp. data from A. Vernon et al., under review at Nature.
DOI:10.21203/rs.3.rs-611360/v1

BSkG models: rotational bands



SD-1 band
(1998Bu03,1994Jo10)



Exp. data from B. Singh, Nuclear Data Sheets 97, 241 (2002).