Theory, a Summary

Witold Nazarewicz/Dario Vretenar

FUSHE 2012, May 17, 2012

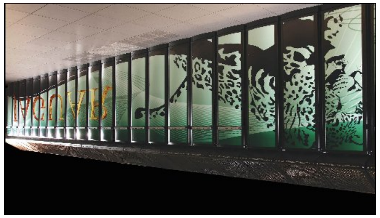
Periodic Table of Elements 2012

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 1																	He 2
Li 3	Be 4											B 5	C 6	N 7	O 8	F 9	Ne 10
Na 11	Mg 12											Al 13	Si 14	P 15	S 16	Cl 17	Ar 18
K 19	Ca 20	Sc 21	Ti 22	V 23	Cr 24	Mn 25	Fe 26	Co 27	Ni 28	Cu 29	Zn 30	Ga 31	Ge 32	As 33	Se 34	Br 35	Kr 36
Rb 37	Sr 38	Y 39	Zr 40	Nb 41	Mo 42	Tc 43	Ru 44	Rh 45	Pd 46	Ag 47	Cd 48	In 49	Sn 50	Sb 51	Te 52	I 53	Xe 54
Cs 55	Ba 56	La* 57	Hf 72	Ta 73	W 74	Re 75	Os 76	Ir 77	Pt 78	Au 79	Hg 80	Tl 81	Pb 82	Bi 83	Po 84	At 85	Rn 86
Fr 87	Ra 88	Ac+ 89	Rf 104	Db 105	Sg 106	Bh 107	Hs 108	Mt 109	Ds 110	Rg 111	Cn 112	113	Fl 114	115	Lv 116	117	118

* Lanthanides														
Ce 58	Pr 59	Nd 60	Pm 61	Sm 62	Eu 63	Gd 64	Tb 65	Dy 66	Ho 67	Er 68	Tm 69	Yb 70	Lu 71	

+ Actinides														
Th 90	Pa 91	U 92	Np 93	Pu 94	Am 95	Cm 96	Bk 97	Cf 98	Es 99	Fm 100	Md 101	No 102	Lr 103	

- Metals
- Non-metals
- Not confirmed



Happy the man who has been able to discern the cause of things

Virgil, Georgica

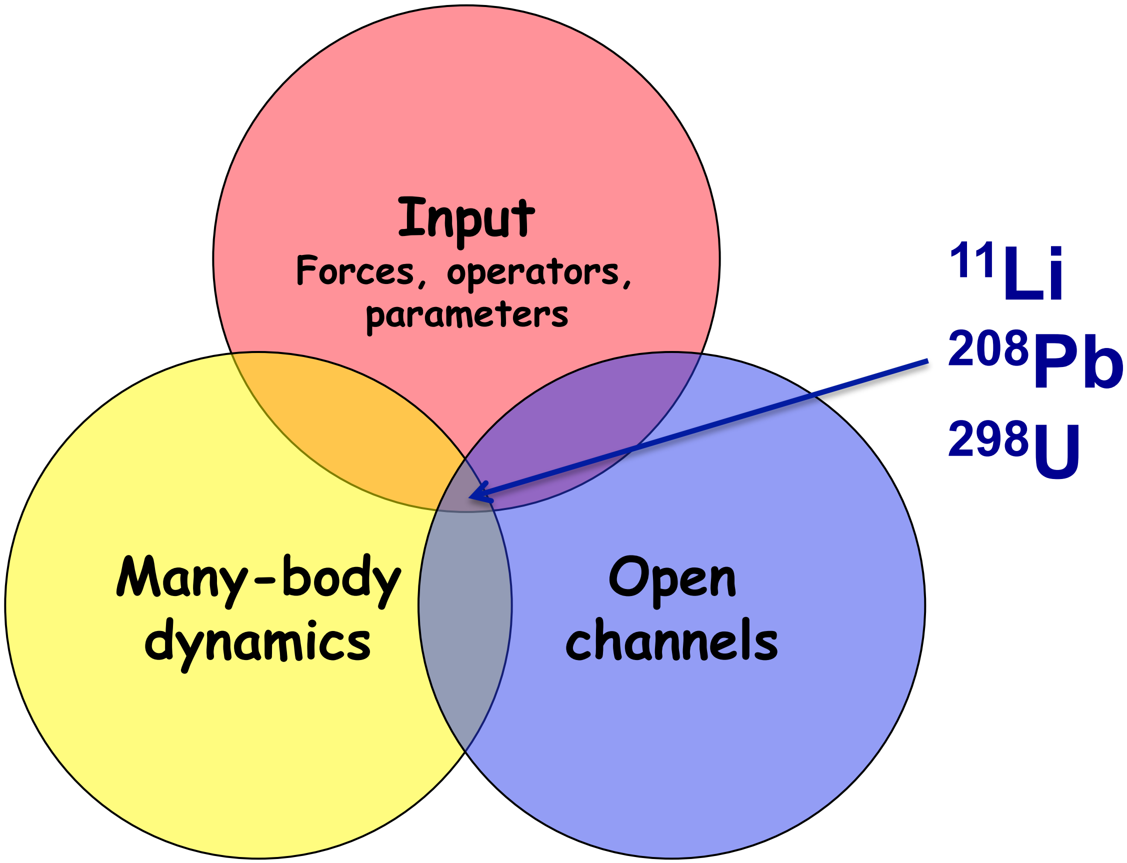
Theories
Models

- A third rate theory forbids
- A second rate theory explains after the fact
- A first rate theory predicts

A. Lomonosov

$$|T\rangle = \alpha_1|T_1\rangle + \alpha_2|T_2\rangle + \alpha_3|T_3\rangle + \cdots$$

Physics of nuclei is demanding



Are superheavy nuclei different?

Yes!

Competition between short-range nuclear force and long-range electrostatic repulsion results in the Coulomb frustration effects

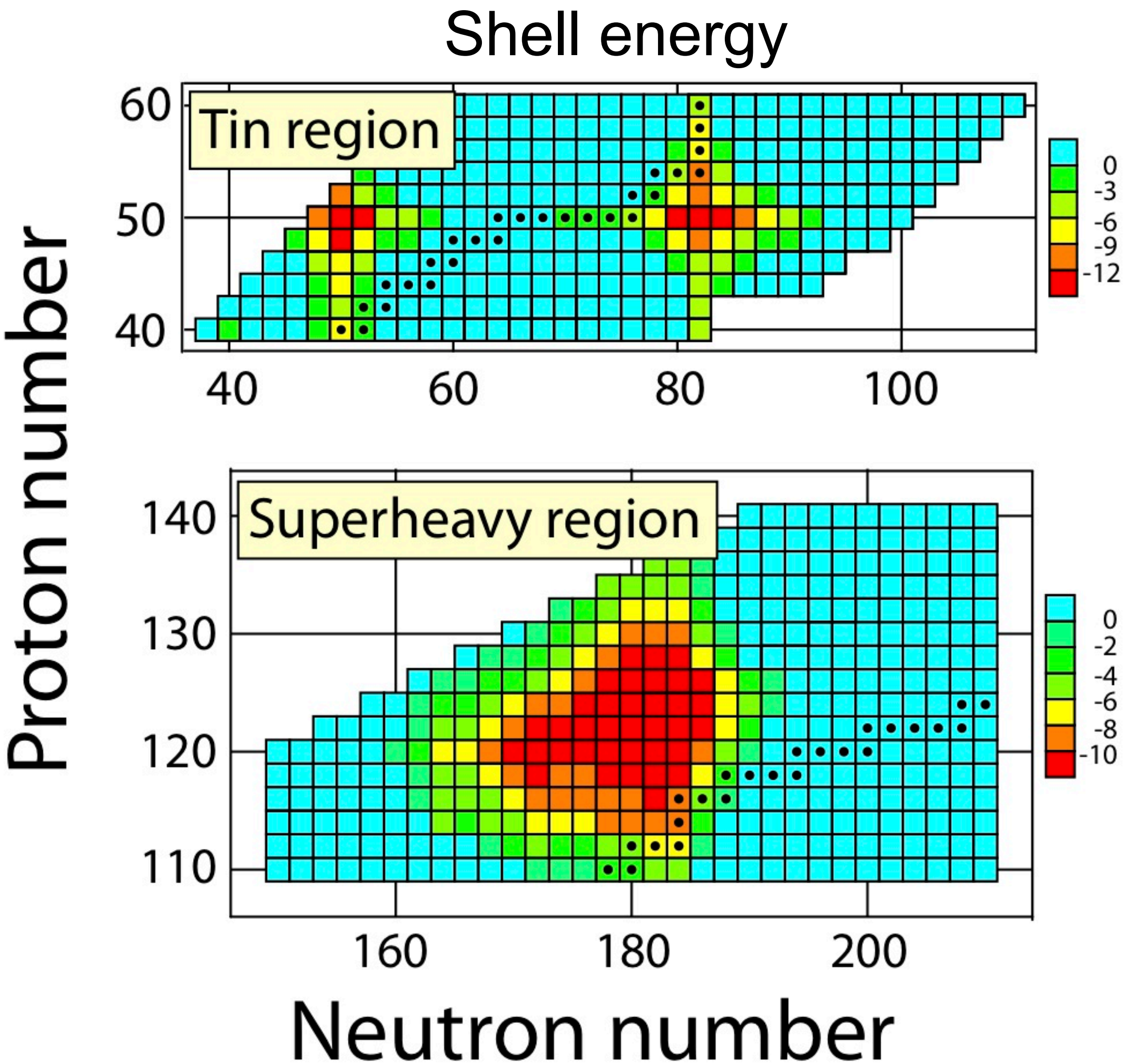
Electromagnetic interaction highly nonperturbative – gives rise to huge self-consistent polarization effects/ rearrangements

Is the concept of magicity useful in superheavy nuclei?

Probably not

Because of very high level density and the Coulomb frustration effects

Shell structure and Coulomb frustration

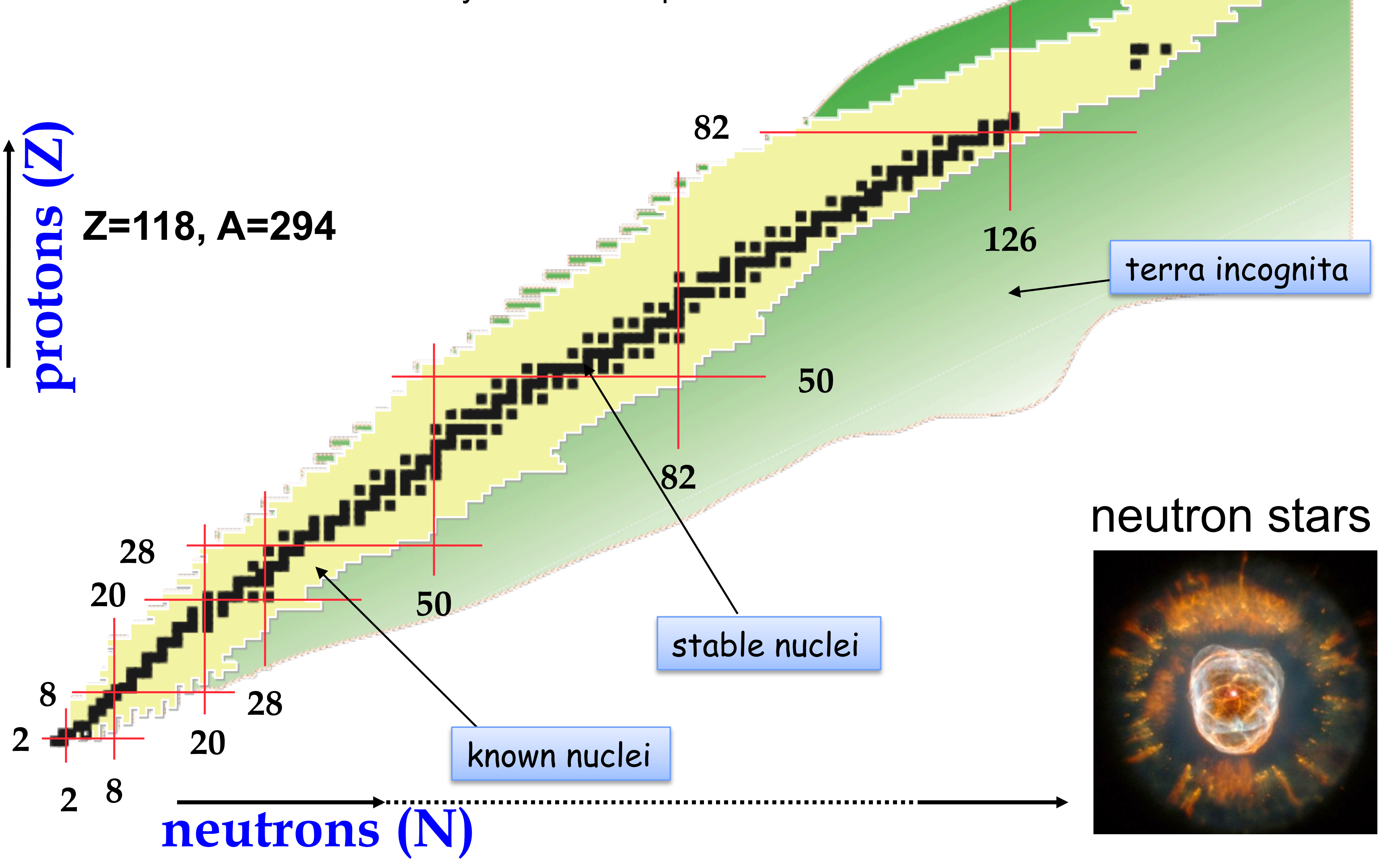


M. Bender et al. Phys. Lett. B 515, 42–48 (2001)

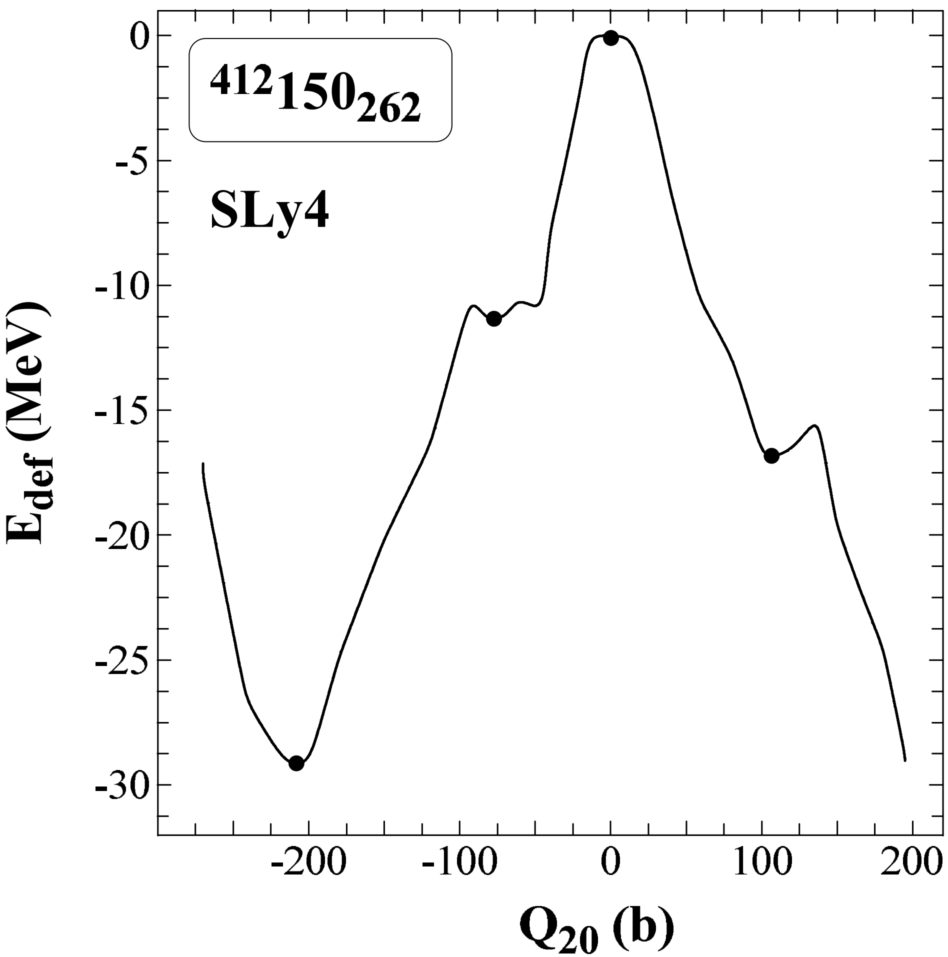
Where is the end
of the nuclear landscape
at extreme A and Z?

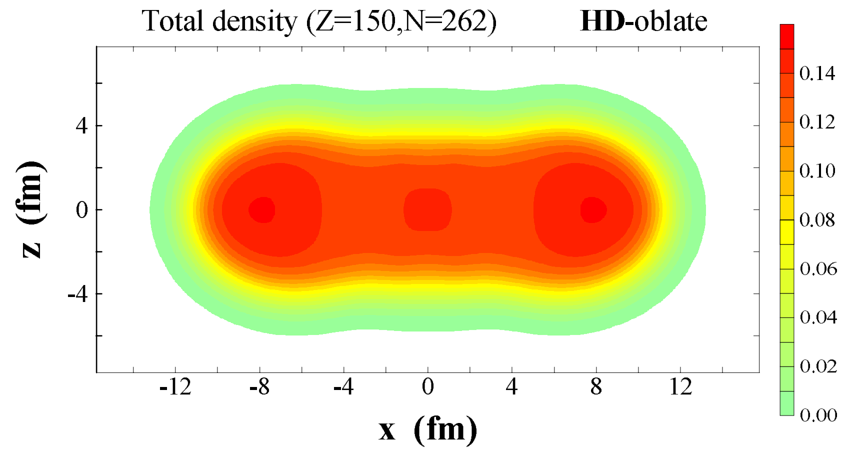
The Nuclear Landscape

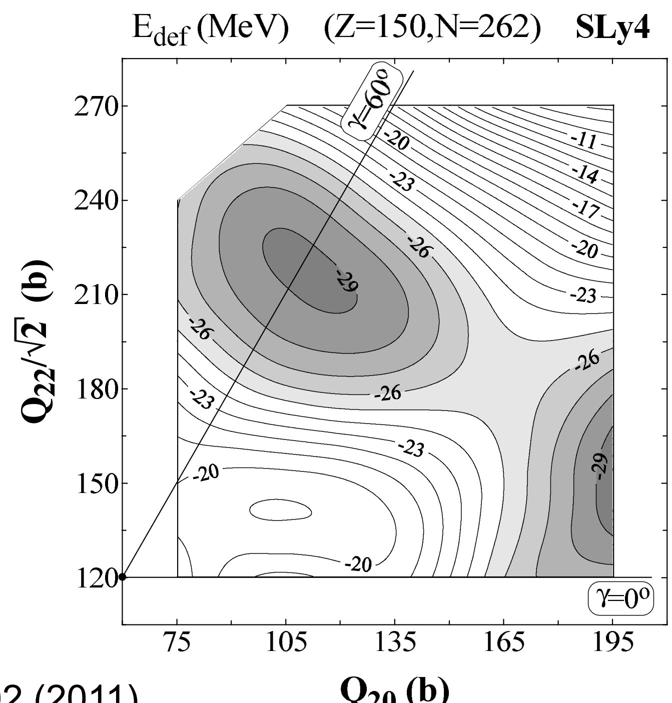
- Protons and neutrons formed 10^{-6}s-1s after Big Bang
- H, D, He, Li, Be, B formed 3-20 min after Big Bang
- Other nuclei born later in heavy stars and supernovae



Exotic topologies of superheavy nuclei: Coulomb frustration



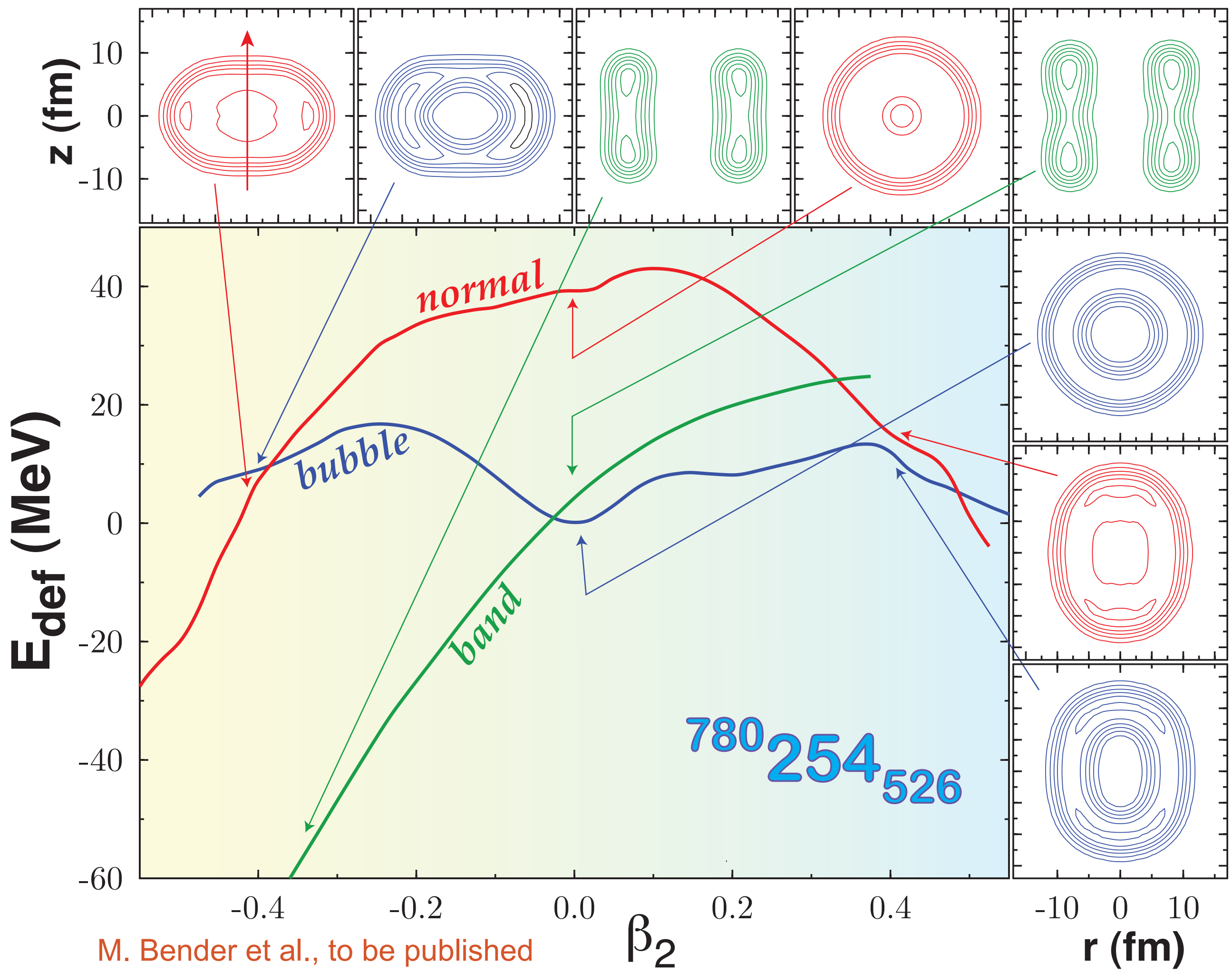




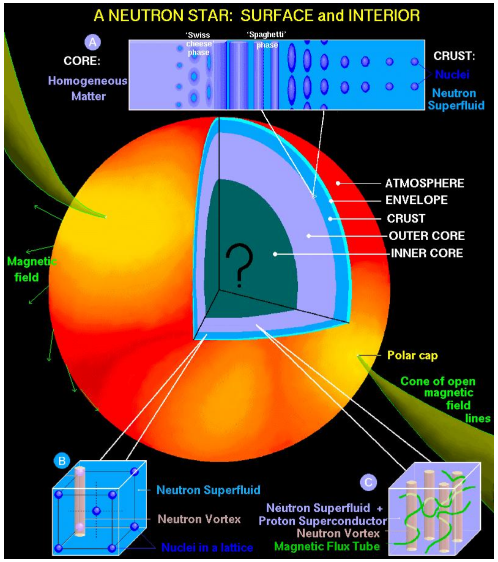
S. Ćwiok et al

see also Jachimowicz, Kowal, Skalski, Phys. Rev. C **83**, 054302 (2011)

Exotic topologies of superheavy nuclei: Coulomb frustration



M. Bender et al., to be published



Self-consistent calculations confirm the fact that the "pasta phase" might have a rather complex structure, various shapes can coexist, at the same time significant lattice distortions are likely and the neutron star crust could be on the verge of a disordered phase.

A challenge is to assess stability of such forms

WORK IN PROGRESS

Since we are dealing with extrapolations, error estimation crucial

Systematic errors (due to incorrect assumptions/poor modeling)

Statistical errors (optimization and numerical errors)

Statistical uncertainty in variable A:

$$\overline{\Delta A^2} = \sum_{ij} \partial_{p_i} A (\hat{M}^{-1})_{ij} \partial_{p_j} A, \quad \partial_{p_i} A = \partial_{p_i} A\Big|_{\mathbf{p}_0}$$

Correlation between variables A and B:

$$\overline{\Delta A \, \Delta B} = \sum_{ij} \partial_{p_i} A (\hat{M}^{-1})_{ij} \partial_{p_j} B$$

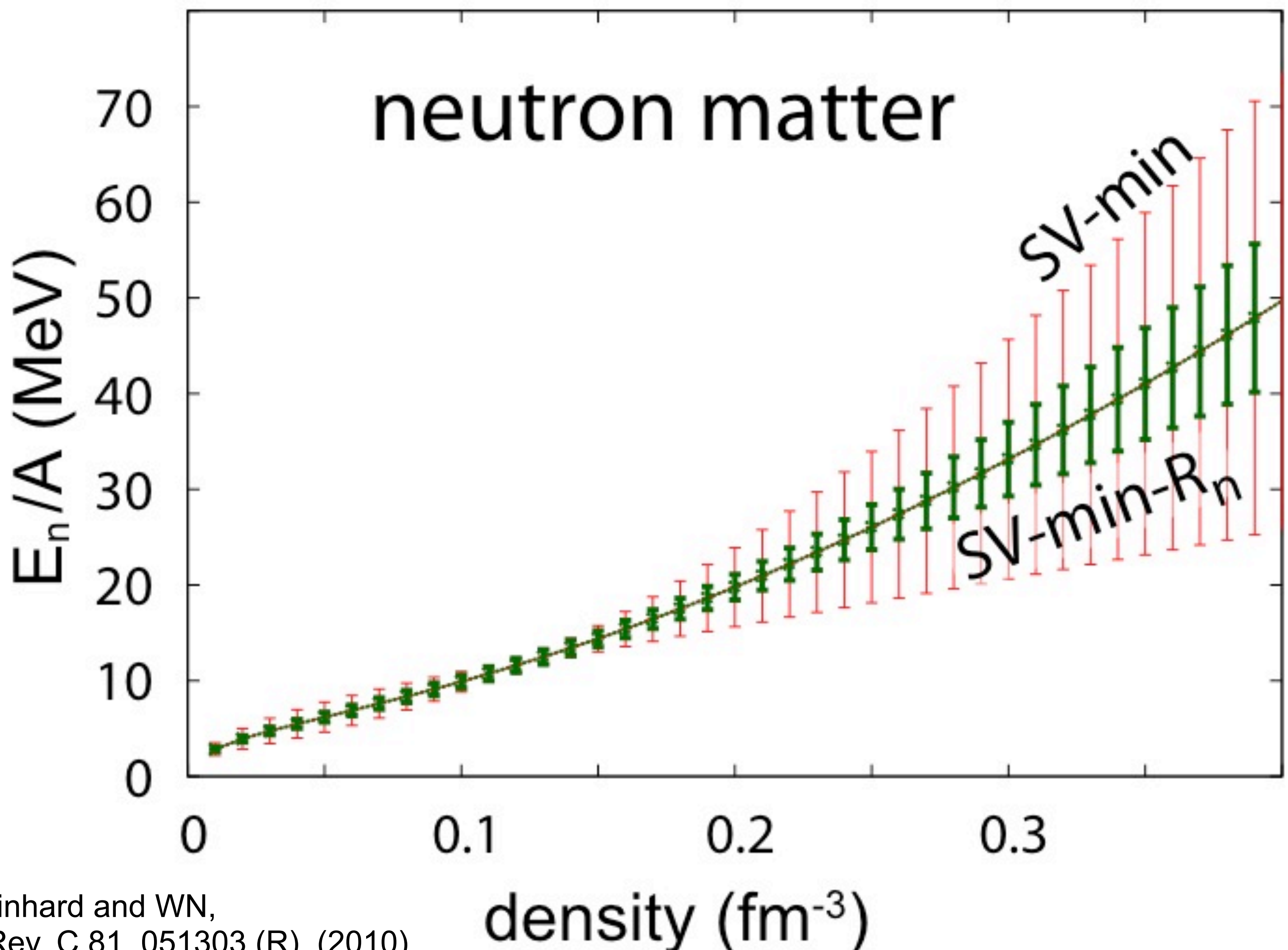
Product-moment correlation coefficient between two observables/variables A and B:

$$c_{AB} = \frac{\overline{\Delta A \, \Delta B}}{\sqrt{\overline{\Delta A^2} \; \overline{\Delta B^2}}}$$

=1: full alignment/correlation

=0: not aligned/statistically independent

To estimate the impact of precise experimental determination of neutron skin, we generated a new functional SV-min-R_n by adding the value of neutron radius in 208Pb, r_n=5.61 fm, with an adopted error 0.02 fm, to the set of fit observables. With this new functional, calculated uncertainties on isovector indicators shrink by about a factor of two.



P.G. Reinhard and WN, Phys. Rev. C 81, 051303 (R) (2010)

How to estimate systematic (model) error?

Take a set of reasonable models M_i

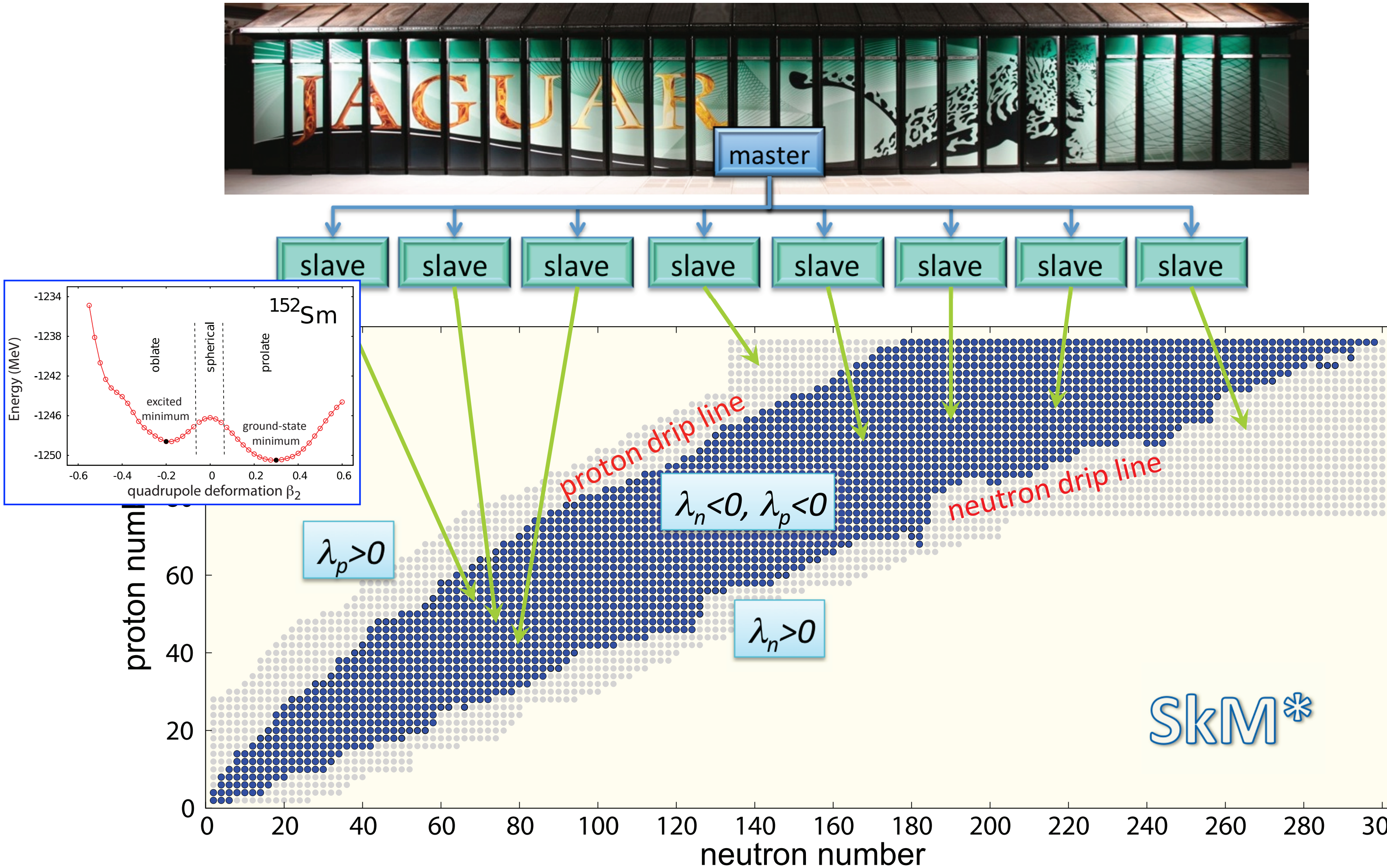
Make a prediction $O(M_i)$

Compute average and variation within this set

$$C_{AB}^{\mathrm{models}} = \frac{|\overline{\Delta A\, \Delta B}|_M}{\sqrt{(\overline{\Delta A^2}))_M\ (\overline{\Delta B^2})_M}}$$

Example: Large Scale Mass Table Calculations

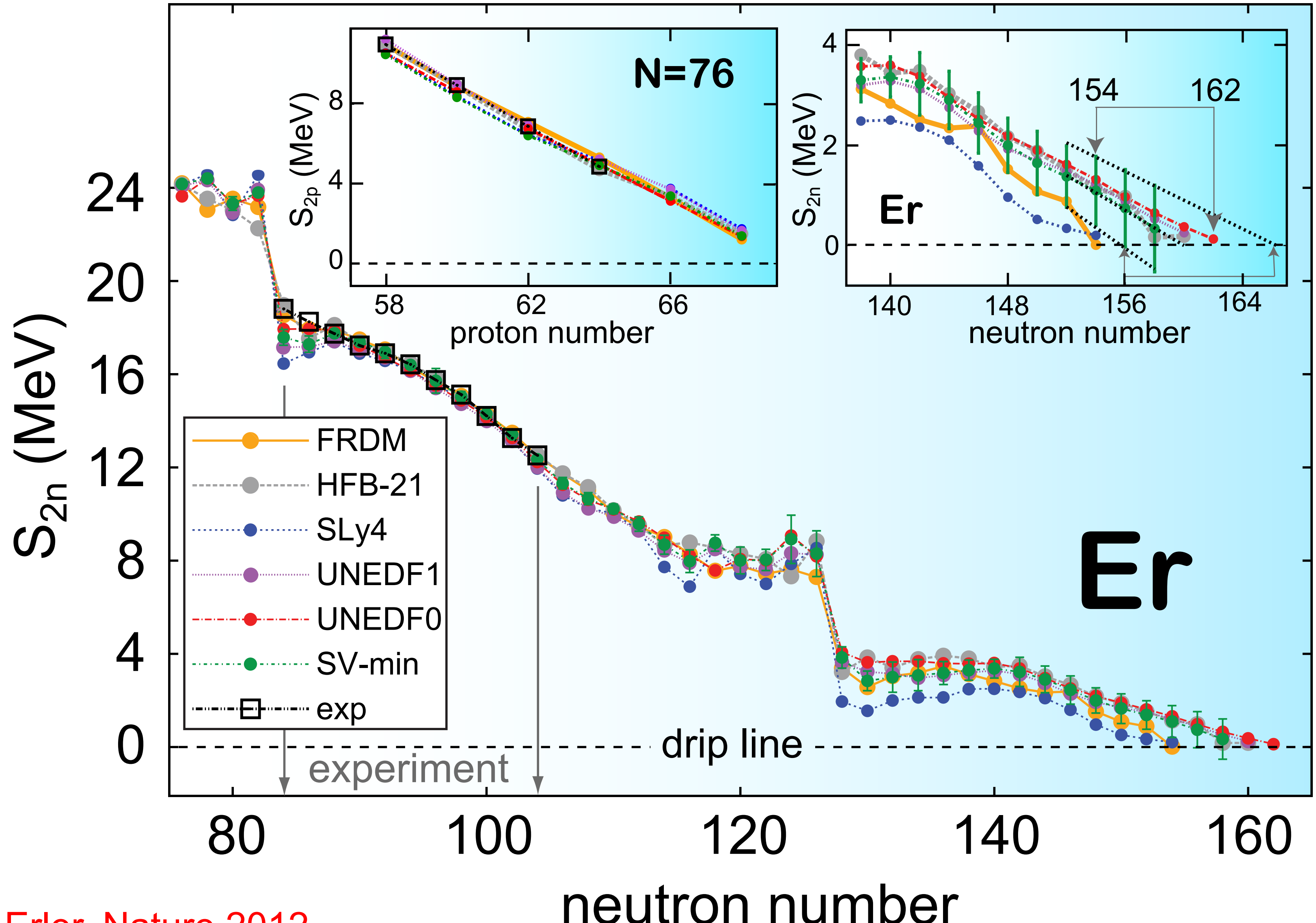
Skyrme-DFT mass table



- 5,000 even-even nuclei, 250,000 HFB runs, 9,060 processors – about 2 CPU hours
- Full mass table: 20,000 nuclei, 12M configurations — full JAGUAR Cray XT5

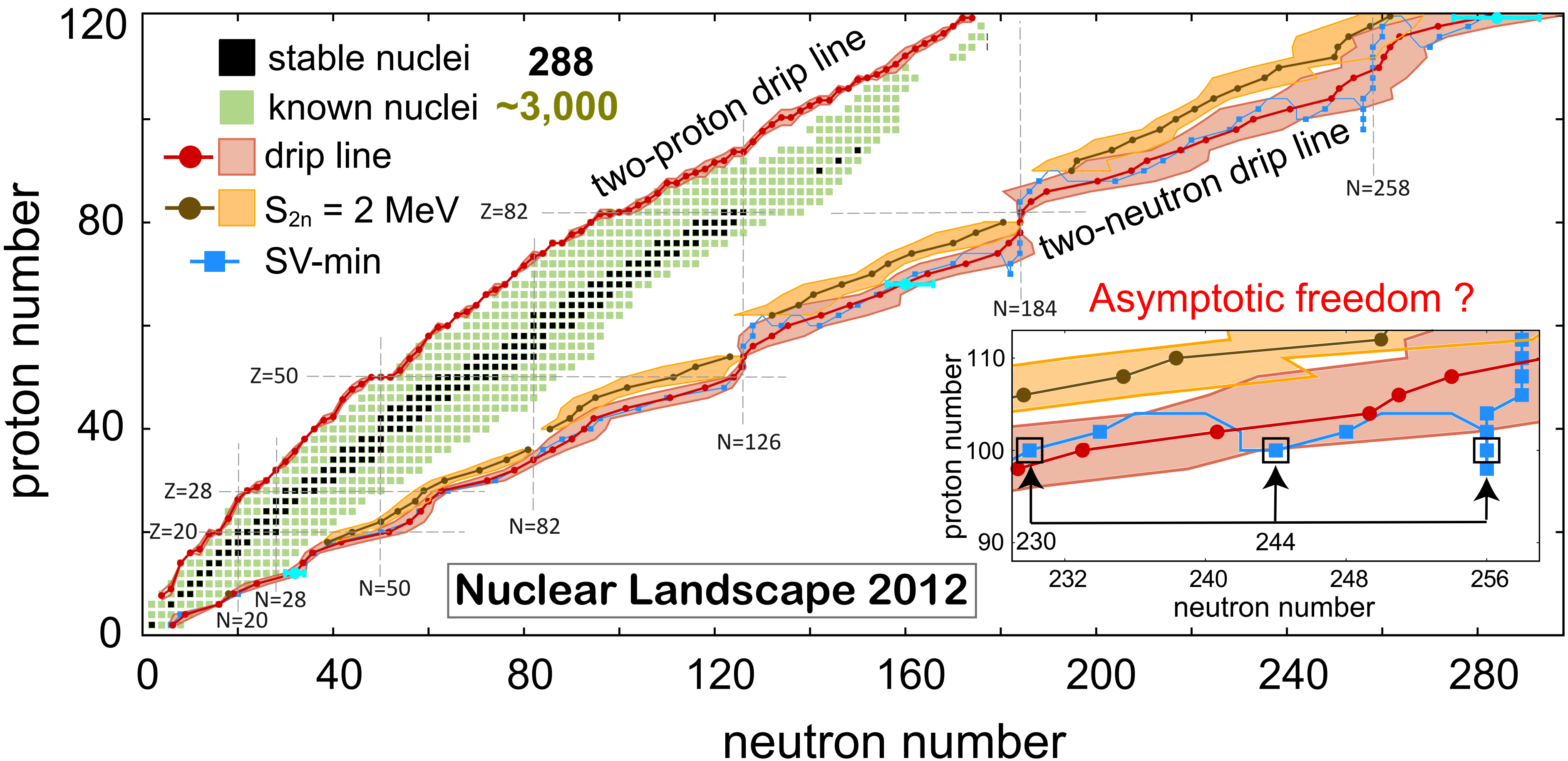
Description of observables and model-based extrapolation

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)



J. Erler, Nature 2012

The limits: Skyrme-DFT Benchmark 2012



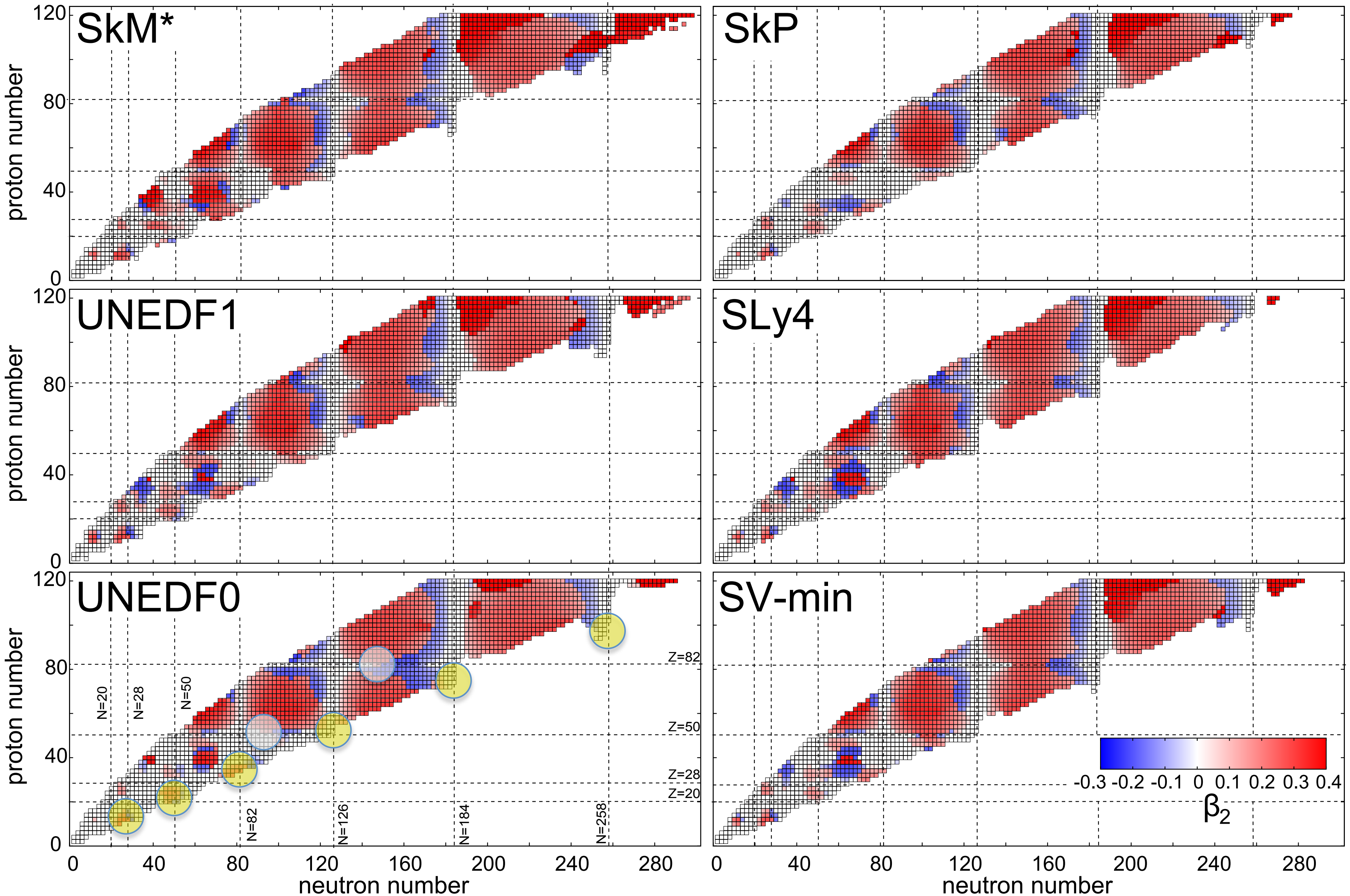
How many protons and neutrons can be bound in a nucleus?

Literature: 5,000-12,000

Skyrme-DFT: 6,900±500$_{syst}$

J. Erler, Nature 2012

Quadrupole ground-state shape deformations



J. Erler, Nature 2012

PHYSICAL REVIEW A 83, 040001 (2011): Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in Physical Review A without a detailed discussion of the uncertainties involved in the measurements. For example, a graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement. Even papers reporting the observation of entirely new phenomena need to contain enough information to convince the reader that the effect being reported is real. The standards become much more rigorous for papers claiming high accuracy.

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done.

(…) there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.

2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.

3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

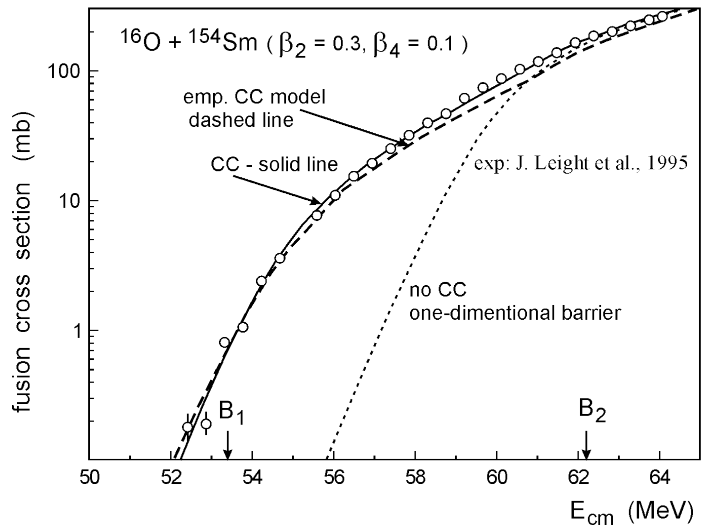
These guidelines have been used on a case-by-case basis for the past two years. Authors have adapted well to this, resulting in papers of greater interest and significance for our readers.

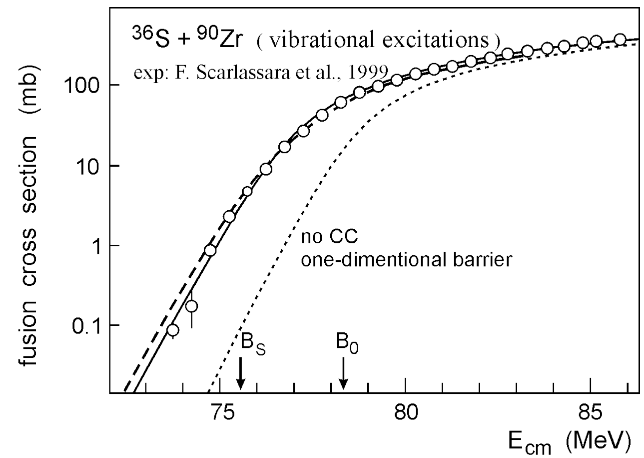
The major challenge: towards N=184

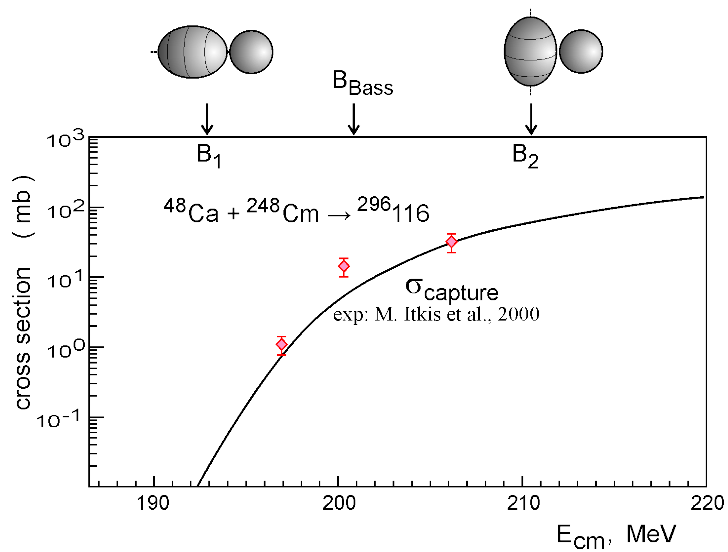
The Holy Grail

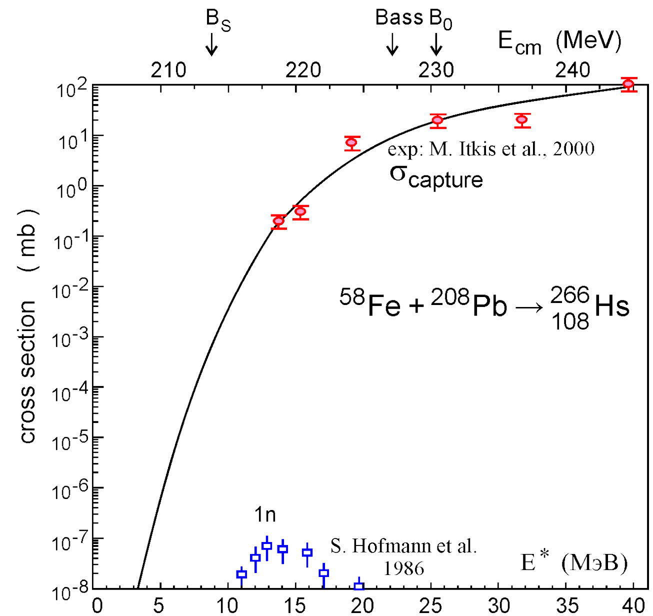
How to get there experimentally?
How to inform experiment about optimal conditions?
How can spectroscopic data on the heaviest nuclei help?

Zagrebaev



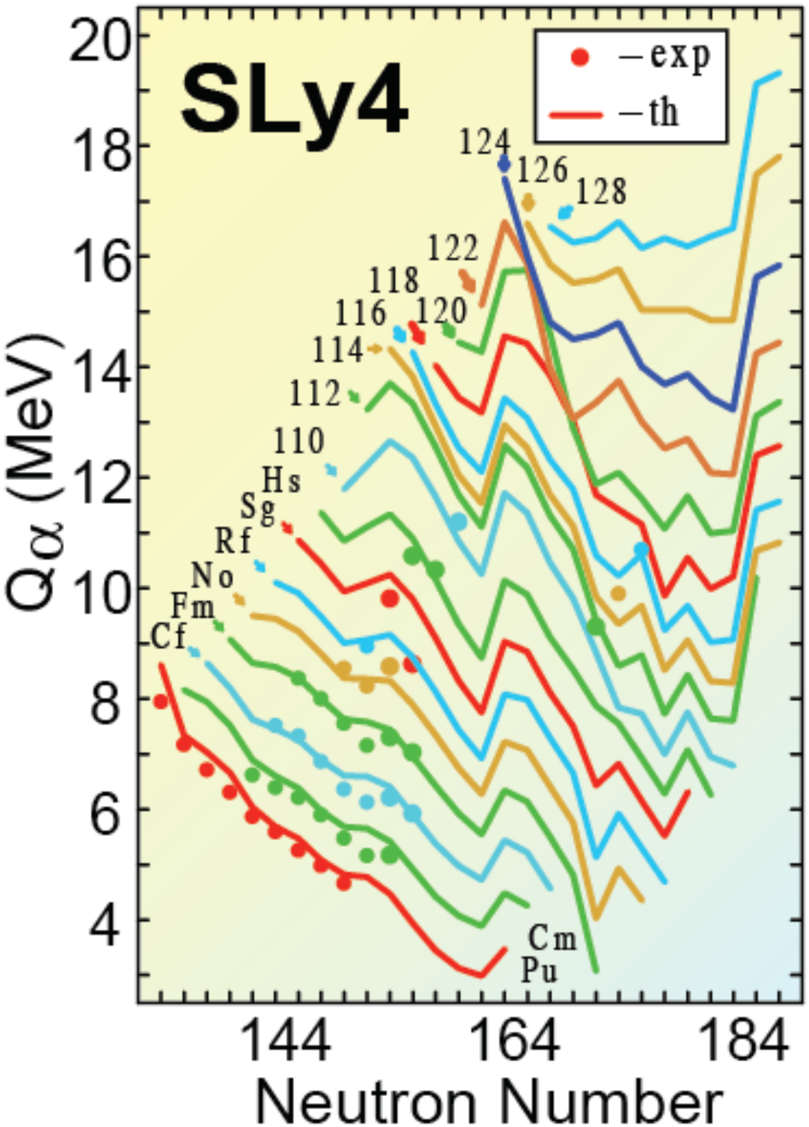




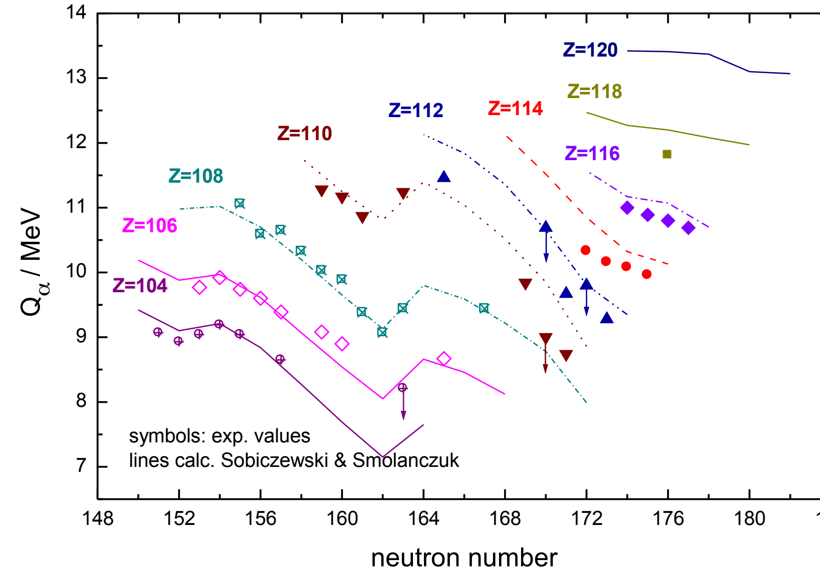


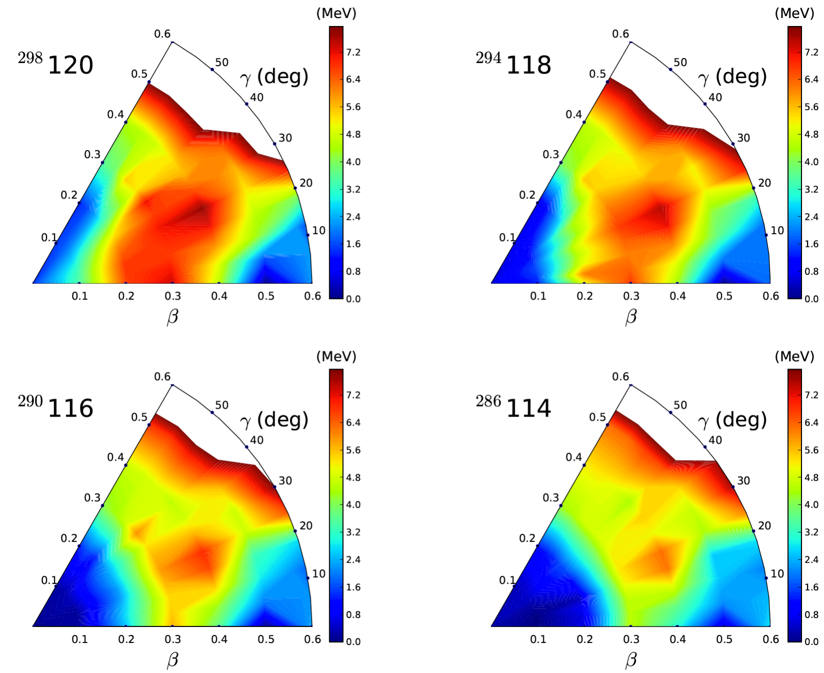
- Spectacular agreement in some cases, but… no predictive power yet
- More investments in this area badly needed!

Q_α values and deformations fairly robust; easier to predict



S. Cwiok et al , Nature 285 (2005) 705



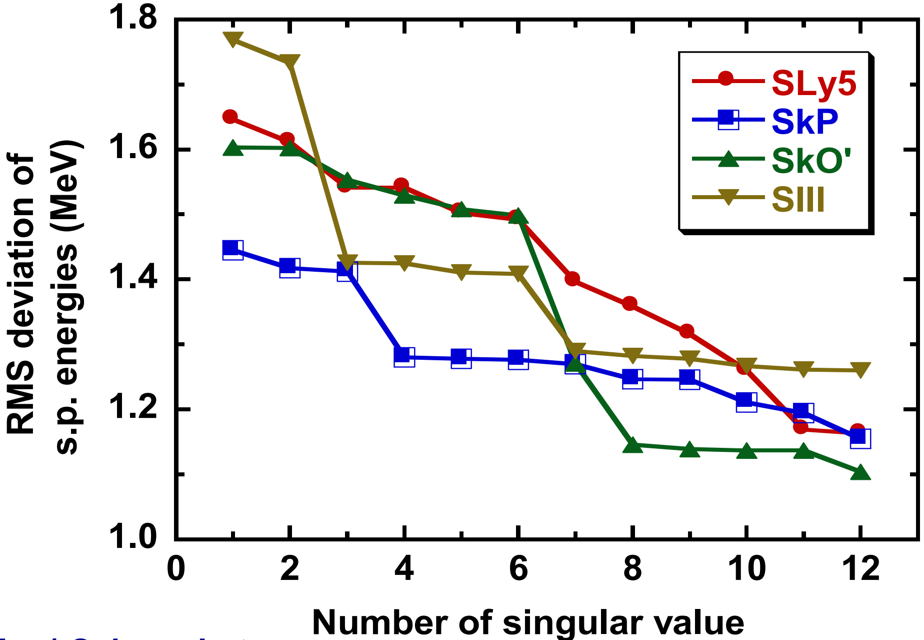


V. Prassa et al., arXiv:1205.2568 (Zagreb, Thessaloniki)

Spectroscopic quality: challenge for the self-consistent theory

"We show that the obtained rms deviations from experimental data are still quite large, of the order of 1.1 MeV. This suggests that the current standard form of the Skyrme functional cannot ensure spectroscopic-quality description of single-particle energies, and that extensions of this form are very much required."

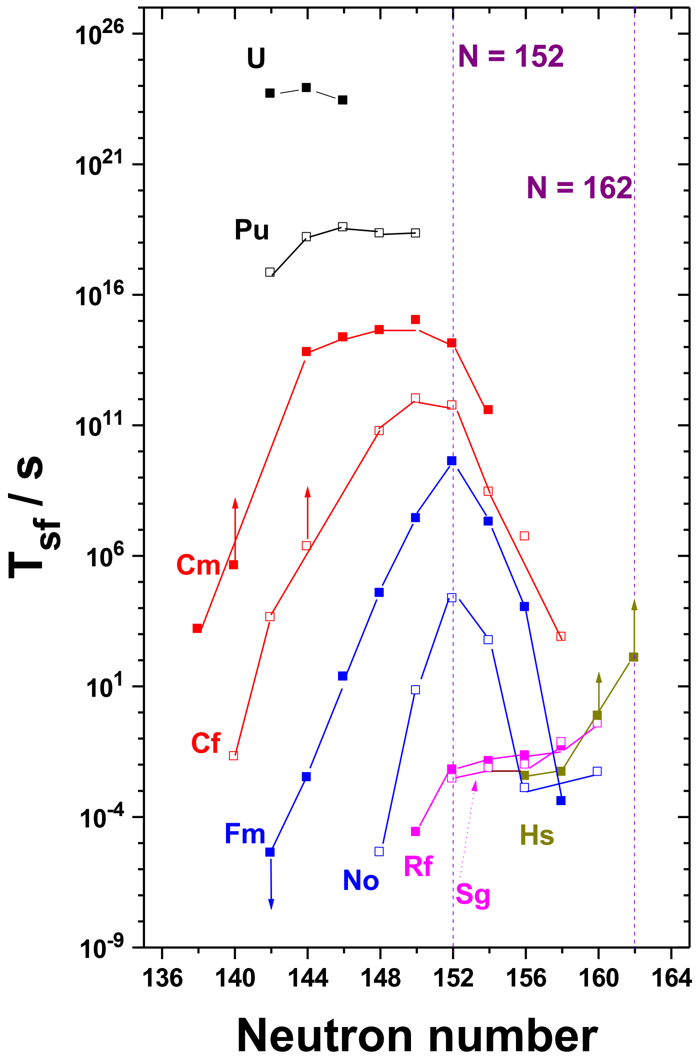
M . Kortelainen et al., Phys. Rev. C 77, 064307 (2008)



- Unique spectroscopic data on 100≤Z≤104 exist
- Systematic deviations from the data need to be identified
- Uncertainties need to be assigned; what is the meaning of "agreement"
- Crucial test ground: actinides around ^{235}U
- The s.p. bandheads in the heaviest elements should be used in the optimization process
- Results for Z>100 strongly impacted by Coulombic effects
- The ball is in the theory court

Fission: the major uncertainty

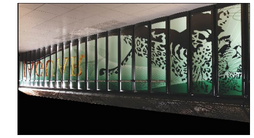
- need to concentrate on observables
- fission barriers are theoretical constructs, not observables



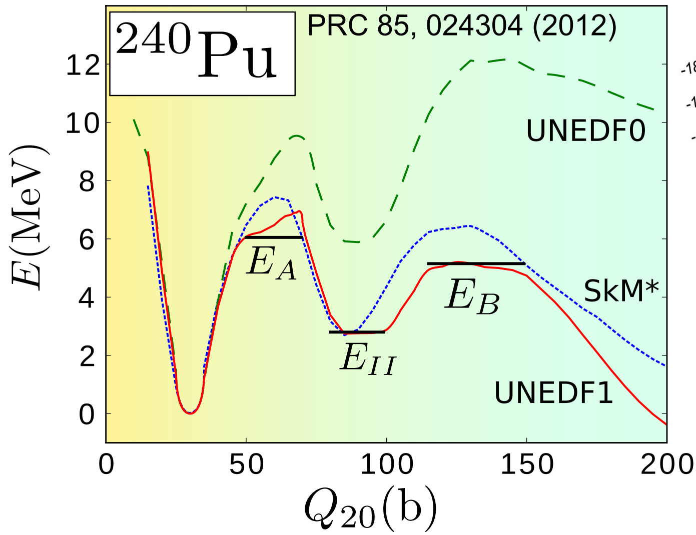
Status: 6.3.2012

LACM, Fission: the ultimate challenge

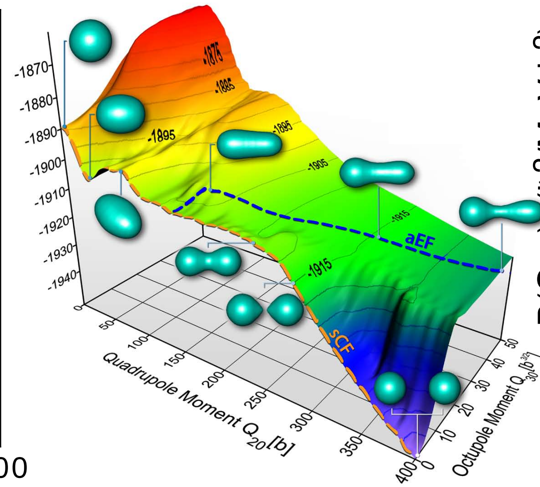
Stability of the heaviest nuclei, r-process, advanced fuel cycle, stockpile stewardship…



Optimized Functionals

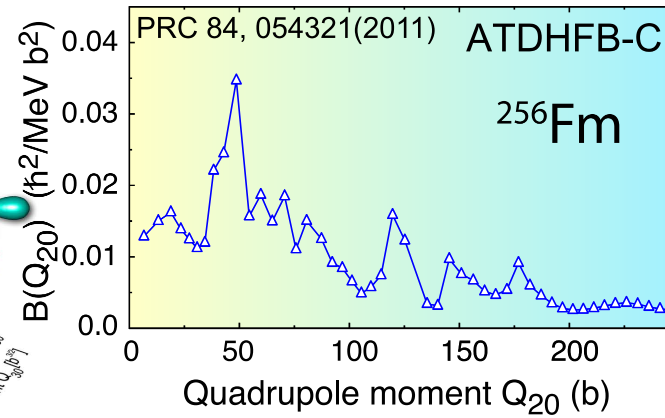


Large-scale DFT

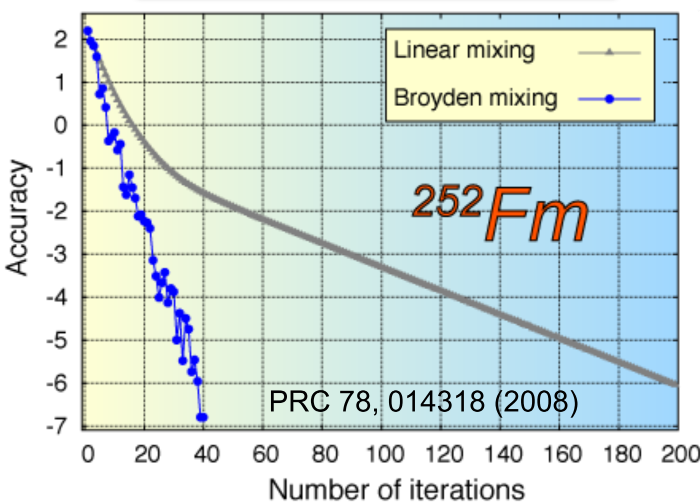


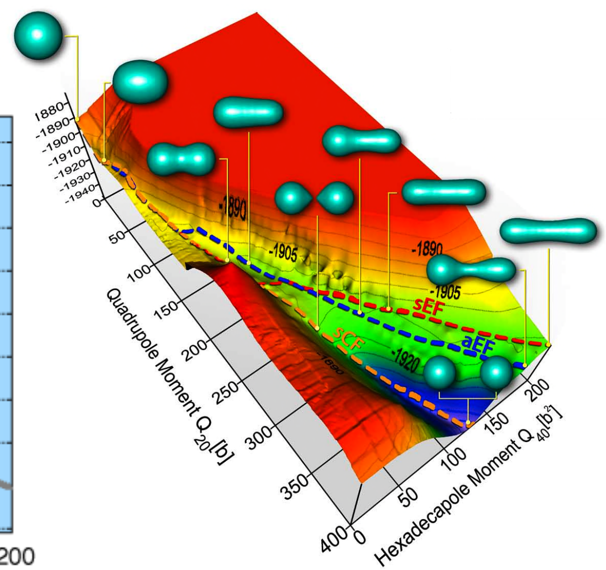
PRC 80, 014309 (2009)

Collective dynamics



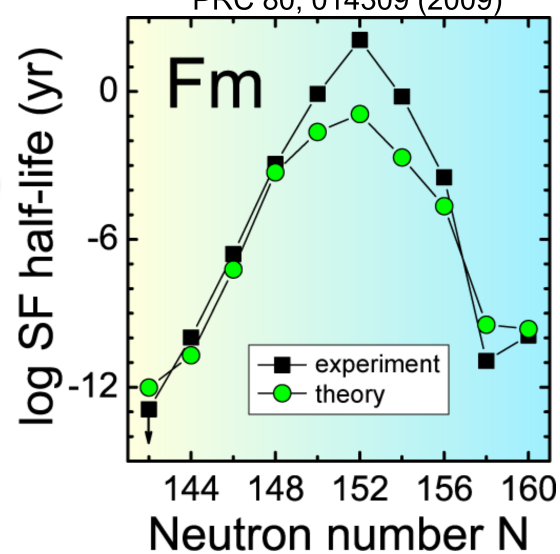
Numerical Techniques





Confrontation with experiment; predictions

PRC 80, 014309 (2009)



Surface symmetry energy and fission of neutron-rich nuclei

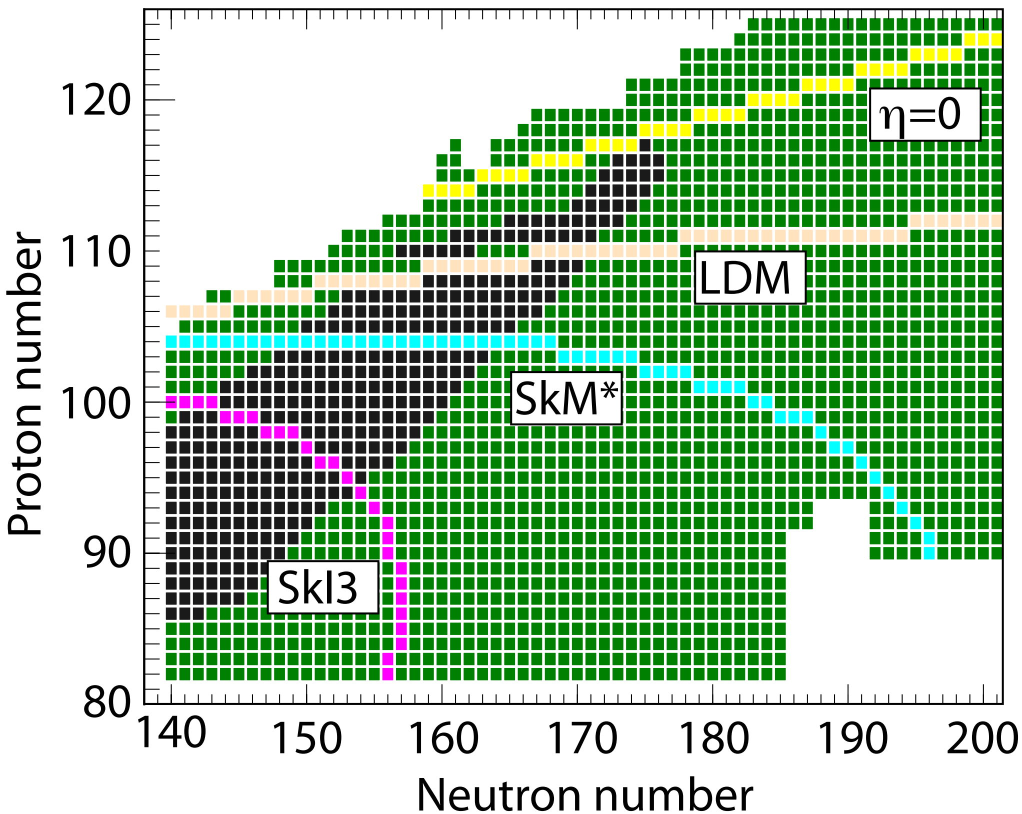
$$\mathcal{E}^{(\mathrm{LDM})} = \mathcal{E}^{(\mathrm{smooth})}(A,I)$$

$$= a_{\mathrm{vol}} \;\Big|\; + a_{\mathrm{surf}}A^{-1/3} + a_{\mathrm{sym}}I^2 \;\Big|\; + a_{\mathrm{curv}}A^{-2/3} + a_{\mathrm{ssym}}I^2A^{-1/3} + a^{(2)}_{\mathrm{sym}}I^4 \; .$$

O(0) | O(1) | O(2)

$$I = \frac{N-Z}{N+Z}$$

N. Nikolov et al., PRC 83, 034305 (2011)



fissility parameter

$$x = \frac{E_{\mathrm{Coul}}(\mathrm{sph})}{2E_{\mathrm{surf}}(\mathrm{sph})} \approx \frac{Z^2}{47A\,(1-\eta I^2)}$$

$$\eta \equiv -\frac{a_{\mathrm{ssym}}}{a_{\mathrm{surf}}}$$

strong correlation between a_{surf} and a_{ssym}

UNEDF1 functional: focus on heavy nuclei and fission

PHYSICAL REVIEW C 85, 024304 (2012)

Nuclear energy density optimization: Large deformations

M. Kortelainen,[1,2] J. McDonnell,[1,2] W. Nazarewicz,[1,2,3] P.-G. Reinhard,[4] J. Sarich,[5] N. Schunck,[1,2,6]
M. V. Stoitsov,[1,2] and S. M. Wild[5]
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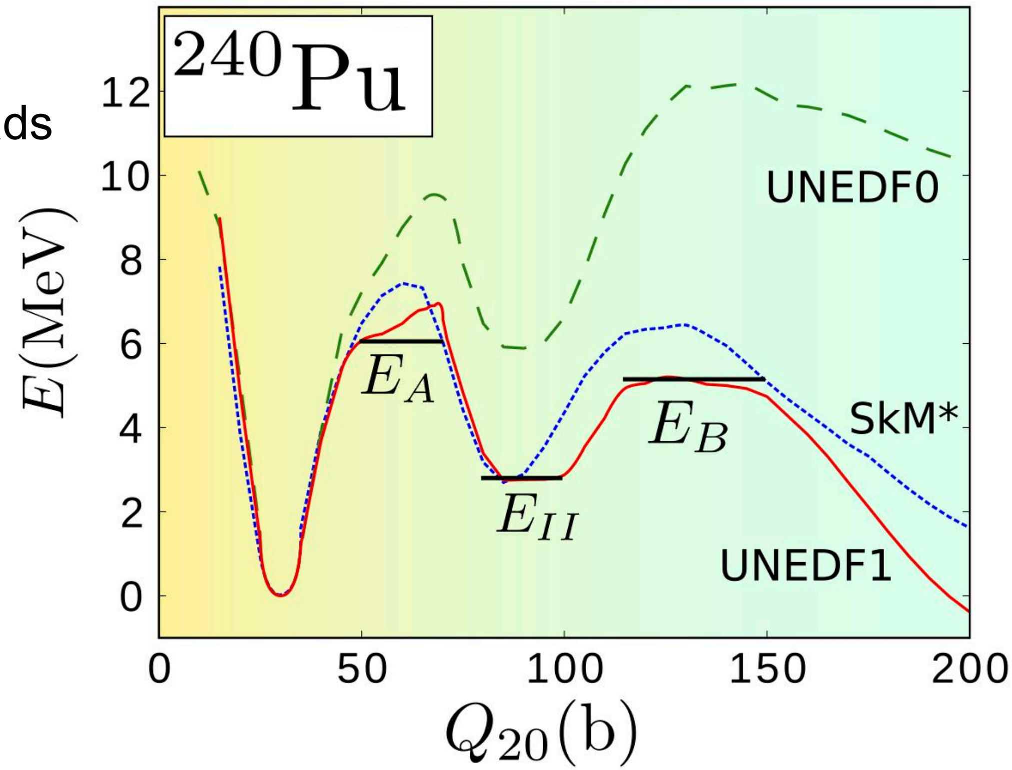
[3]*Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, PL-00681, Warsaw, Poland*
[4]*Institut für Theoretische Physik, Universität Erlangen, D-91054 Erlangen, Germany*
[5]*Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[6]*Physics Division, Lawrence Livermore National Laboratory, Livermore, California 94551, USA*
(Received 18 November 2011; published 8 February 2012)

- Center-of-mass correction neglected
- Data on fission isomers bandheads included
- Coulomb exchange tested

Fission isomer data:

Z	N	E (MeV)
92	144	2.750
92	146	2.557
94	146	2.800
96	146	1.900

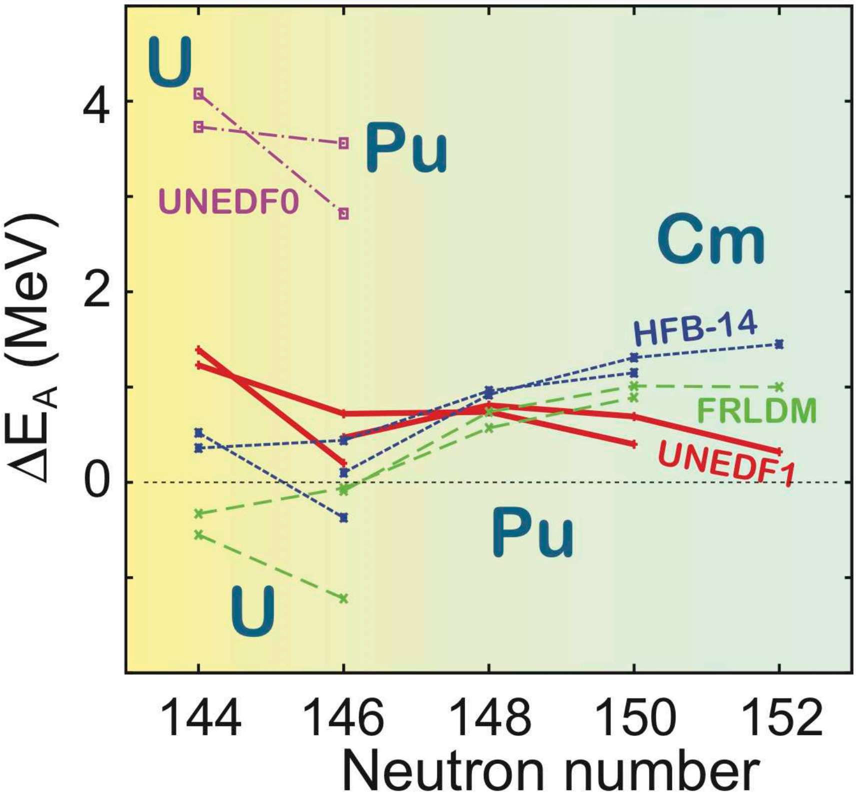


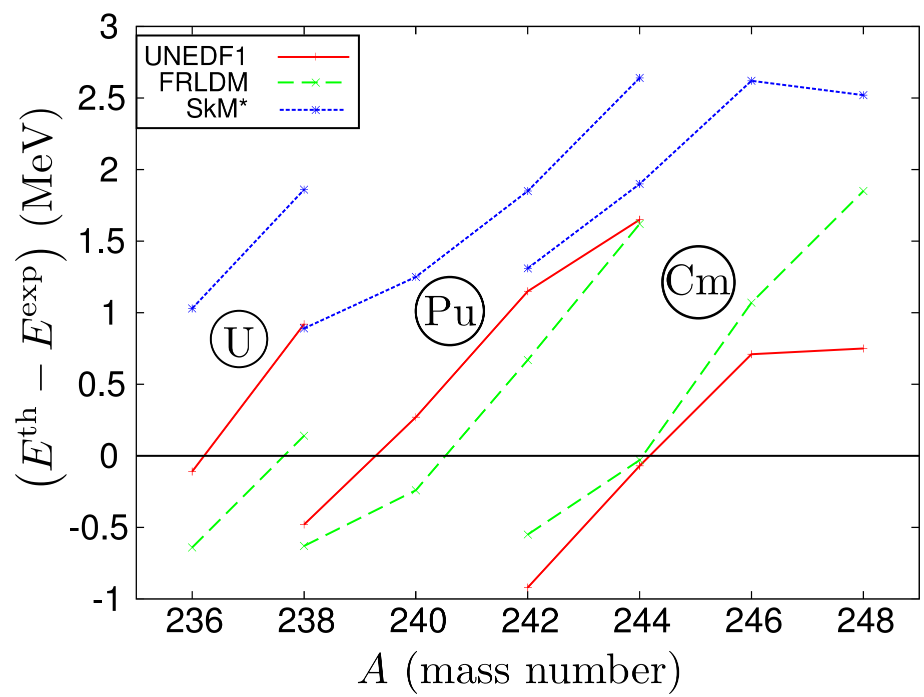
UNEDF1 functional: focus on heavy nuclei and fission

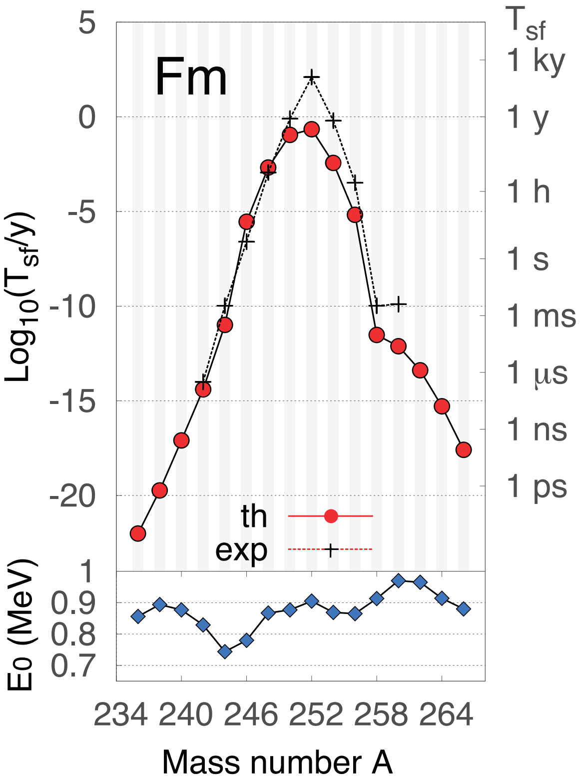
Nucleus	UNEDF0	UNEDF1	Exp.
^{236}U	5.276	2.423	2.75
^{238}U	5.727	2.709	2.557
^{240}Pu	5.738	2.510	2.8
^{242}Cm	5.273	1.851	1.9

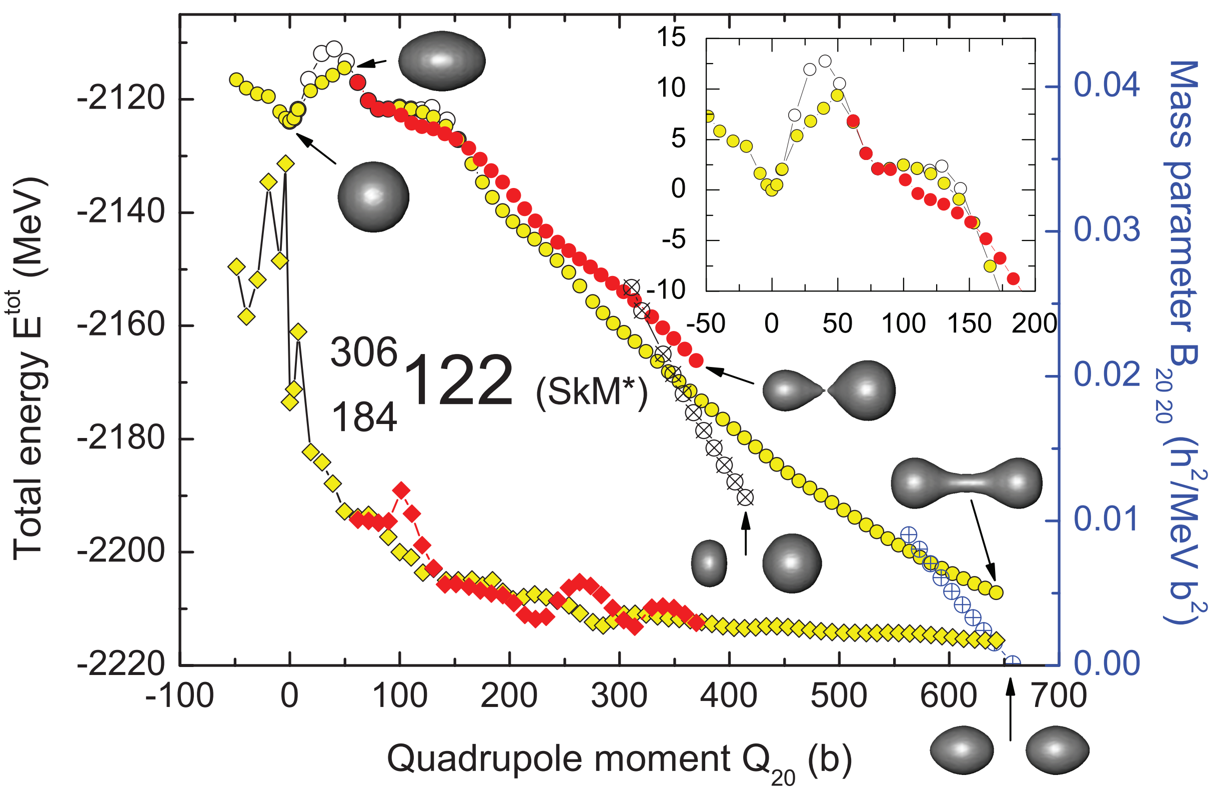
big improvement for fission

Comparison with RIPL-3 (IAEA) data:

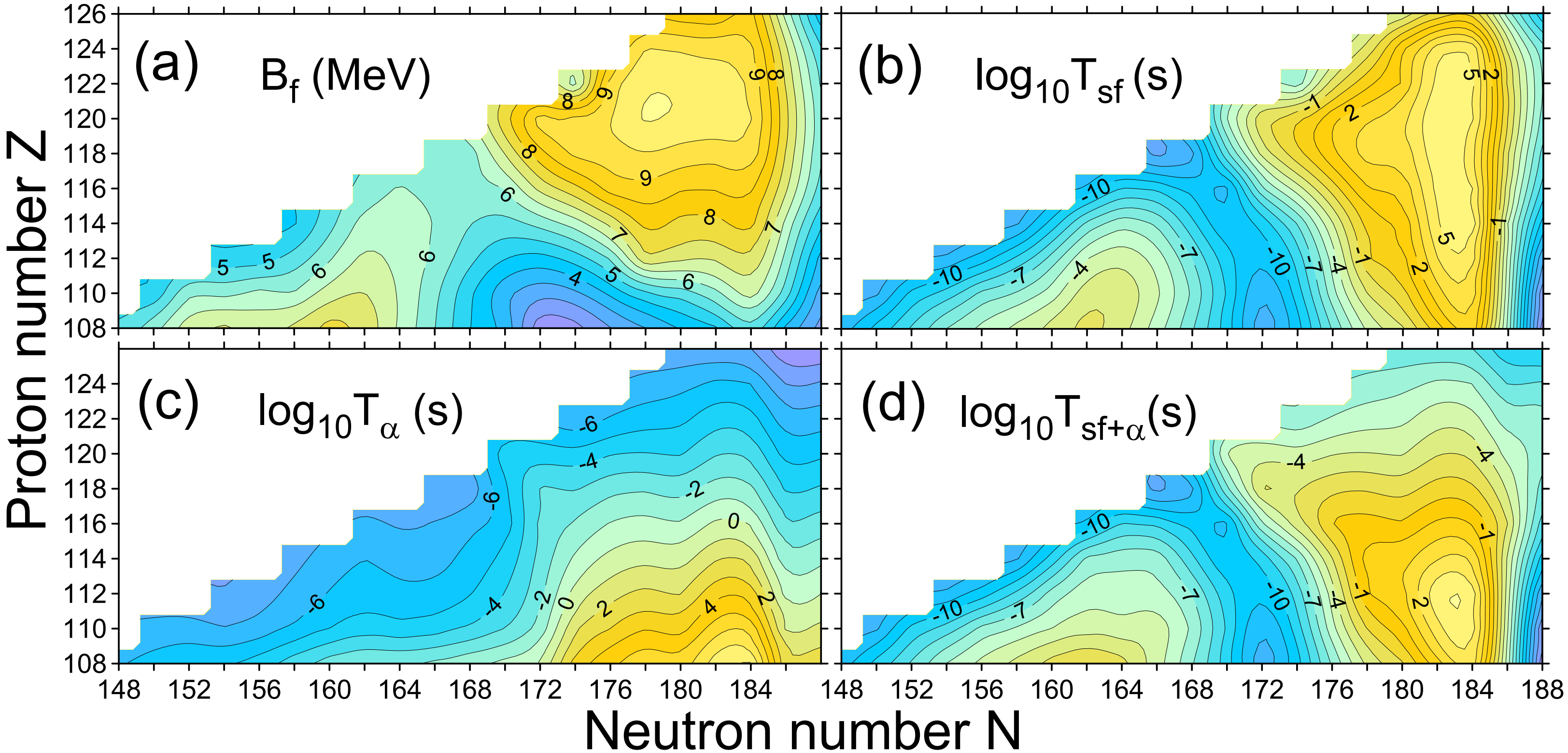






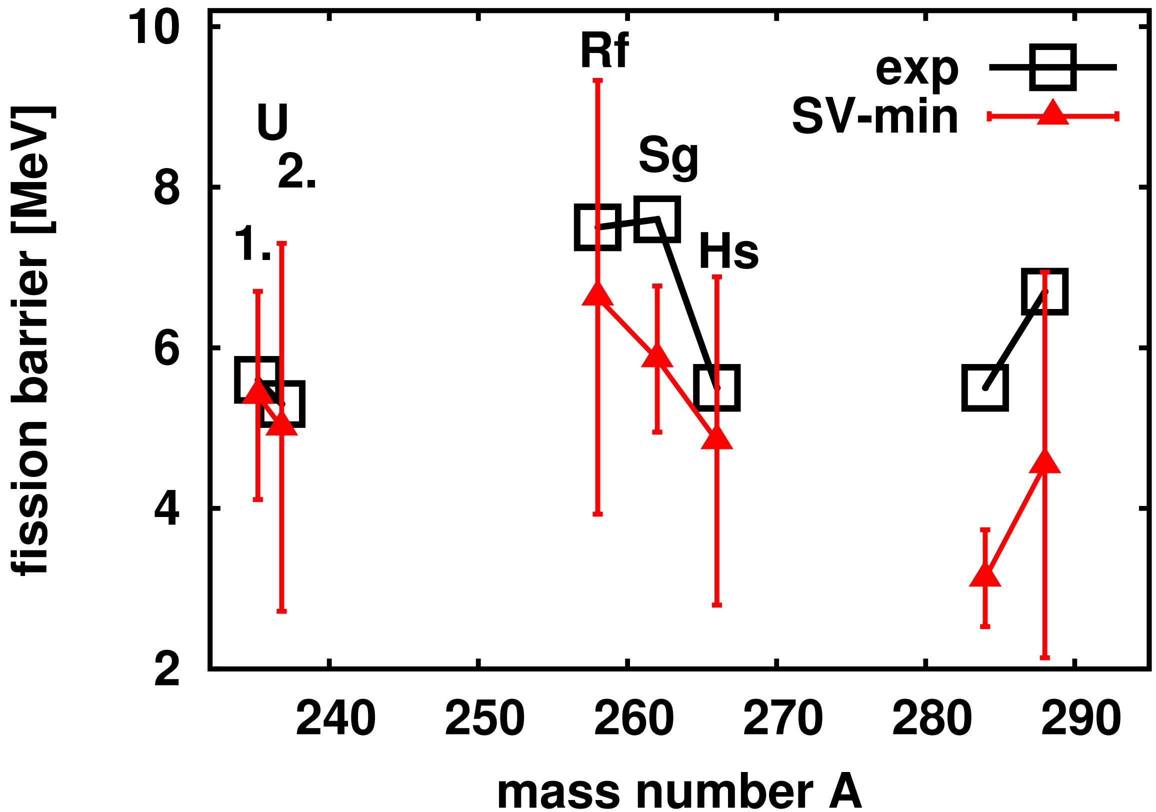


A. Staszczak, A, Baran, WN



A. Staszczak, A, Baran, WN

See also talks/papers by Kowal, Warda, Afanasjev, Erler et al., Prassa et al …



Fission properties for r-process nuclei

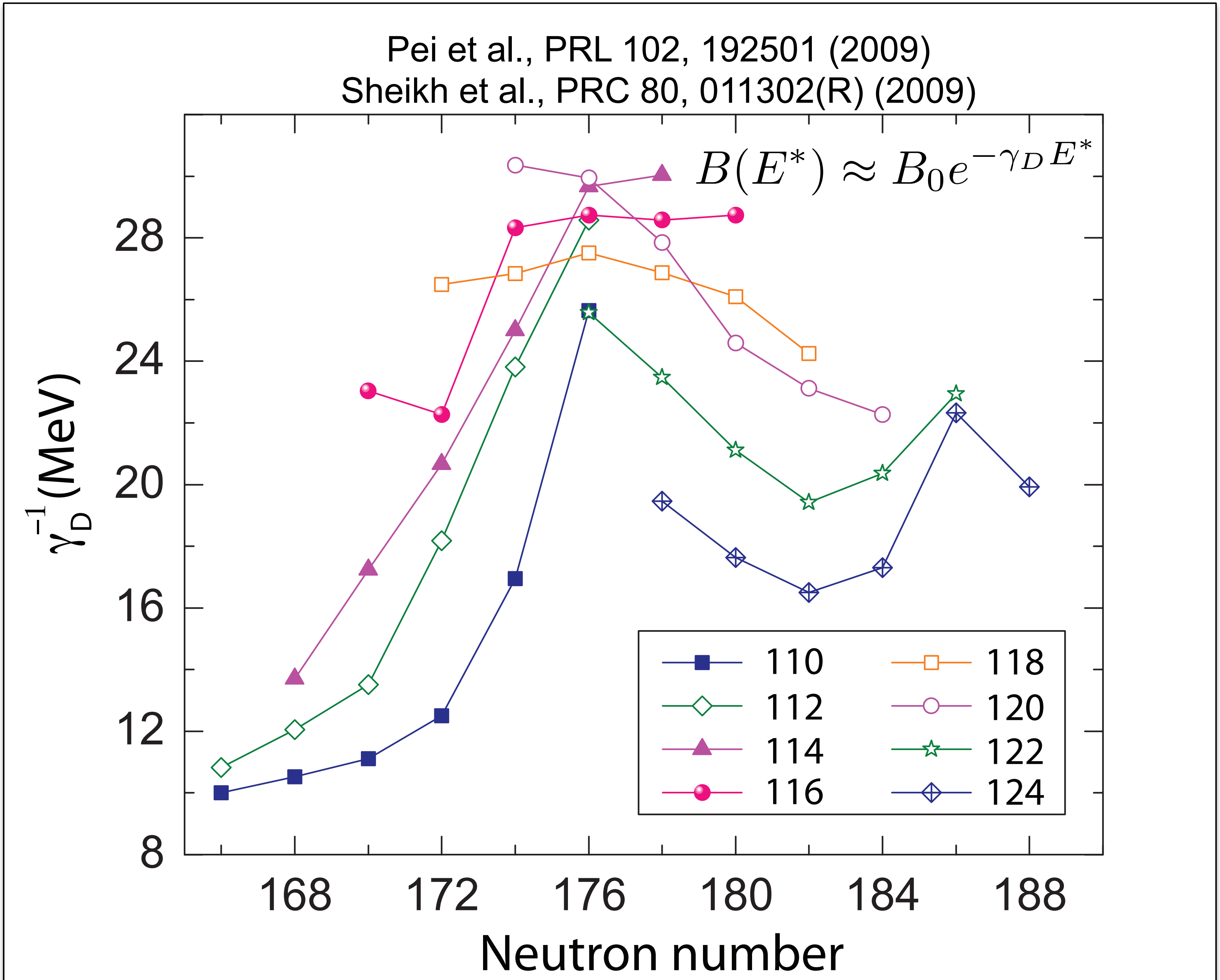
J. Erler et al, Phys. Rev. C 85, 025802 (2012)

The meaning of the fission barrier

- The barrier is a theoretical construct. It is not observable.
- Nucleus is not a molecule (the barrier is internal not external)
- Fission is slow, adiabatic
- The collective pathway must depends on configuration
- Penalty when level crossing occurs

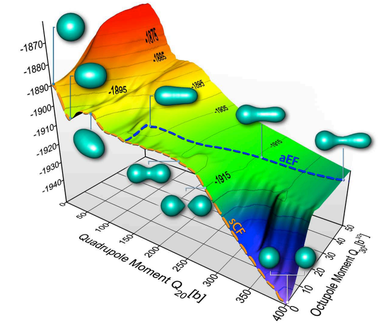
Adiabatic => Isentropic

Kerman, Levit, and Troudet, Ann. Phys. 148, 443 (1983)



Pei et al., PRL 102, 192501 (2009)
Sheikh et al., PRC 80, 011302(R) (2009)
$B(E^*) \approx B_0 e^{-\gamma_D E^*}$
γ_D^{-1} (MeV)
28
24
20
16
12
8
168
172
176
180
184
188
Neutron number
110
112
114
116
118
120
122
124

Program announcement:



Quantitative Large Amplitude Shape Dynamics: fission and heavy ion fusion
Institute for Nuclear Theory, Seattle
September 23 – November 15, 2013

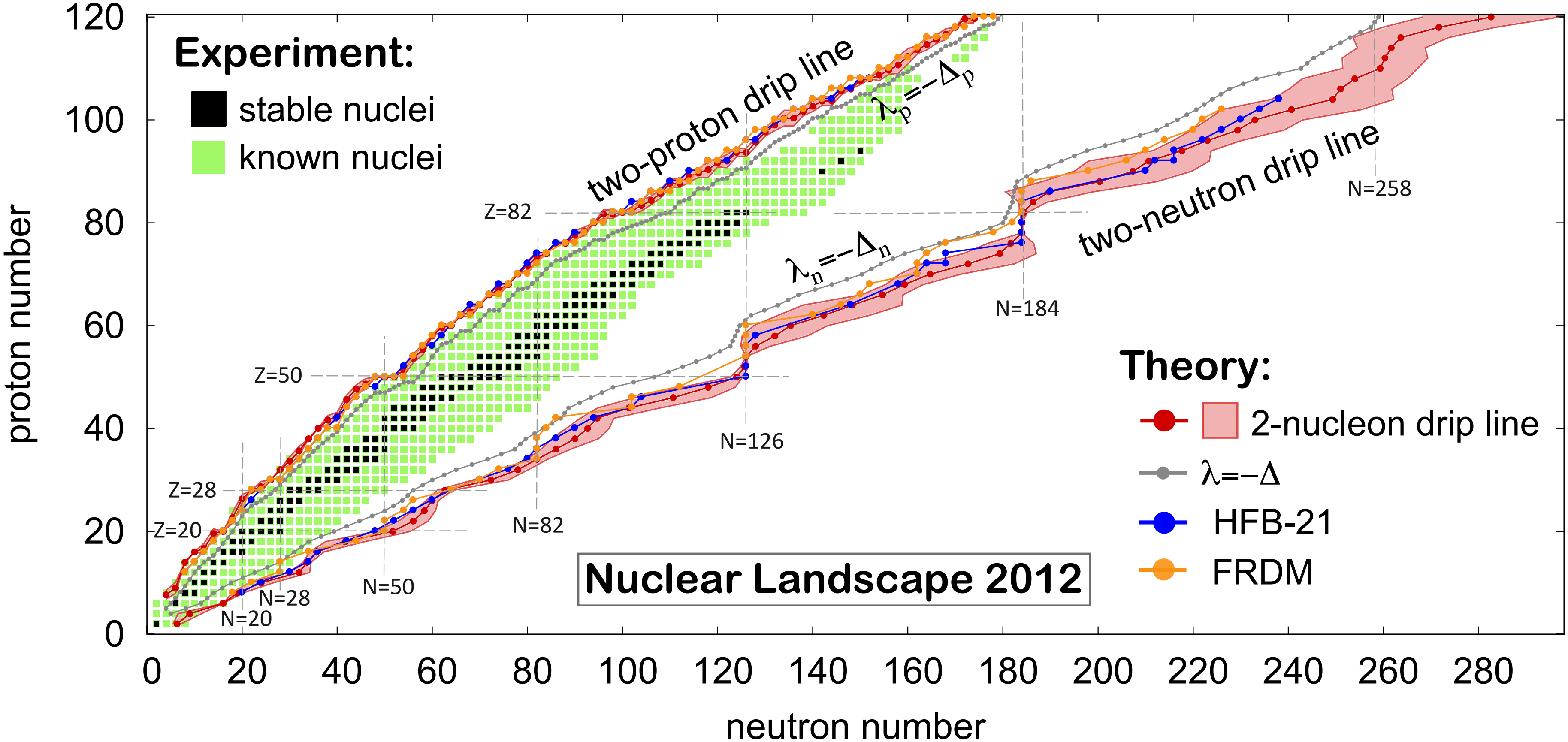
Organizers: W. Nazarewicz (witek@utk.edu), A. Andreyev, G. Bertsch, W. Loveland

Main topics:

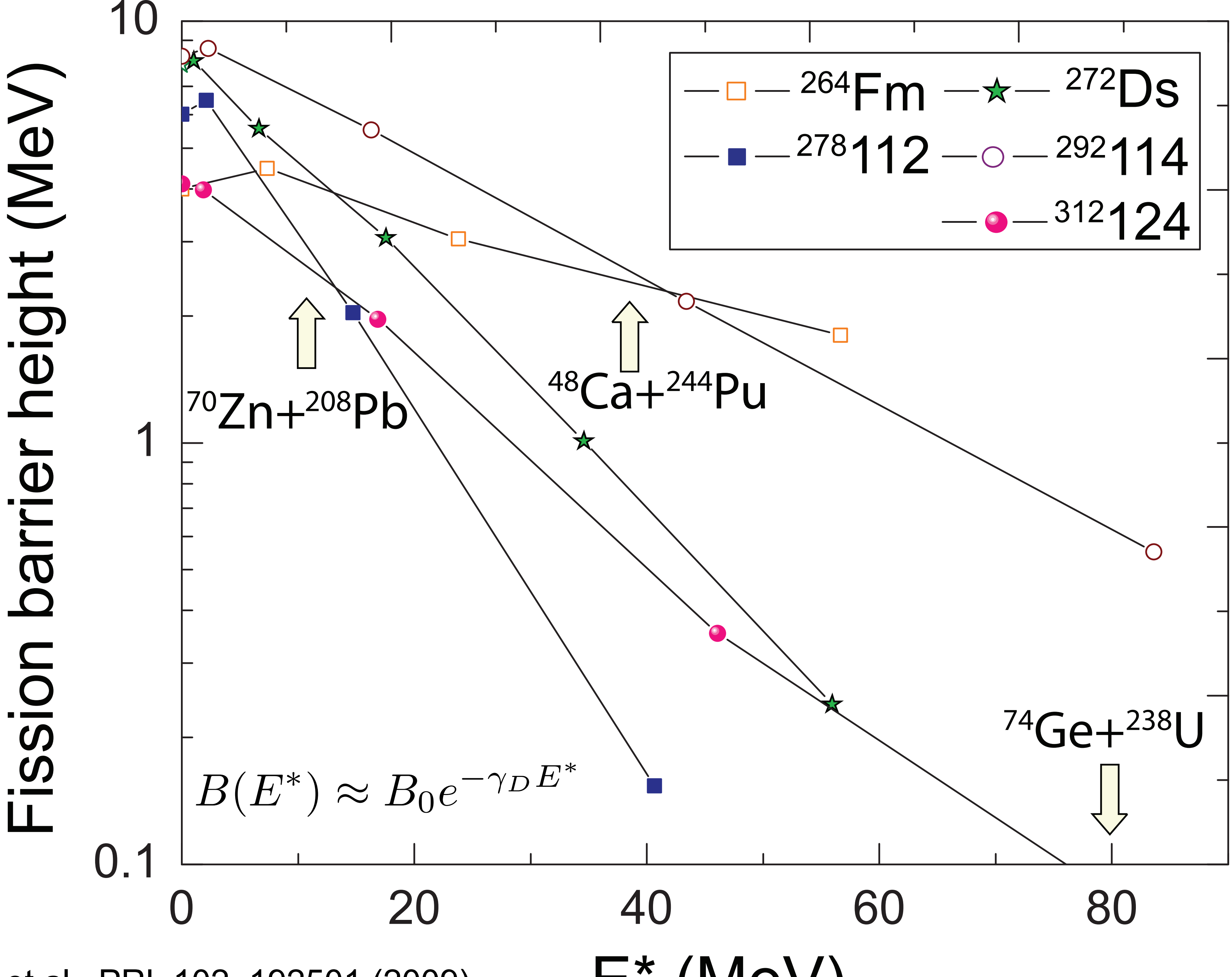
- Reevaluation of basic concepts
- Microscopic theory and phenomenological approaches
- Nuclear interactions and energy density functionals
- Time-dependent many-body dynamics
- Key experimental tests
- Experimental data needs
- Spectroscopic implications
- Computational methodologies for dynamics
- Quality data for nuclear applications.

Keywords: fission, fusion, shape coexistence, self-consistent mean field theory, nuclear density functional theory and its extensions, time dependent methods, adiabatic and diabatic dynamics, synthesis of superheavy elements, fission recycling in the r-process, stockpile stewardship, advanced fuel cycle

BACKUP



J. Erler, Nature 2012



Pei et al., PRL 102, 192501 (2009)

P. Pyykkö: A suggested Periodic Table up to Z ≤ **172**, based on Dirac-Fock calculations on atoms and ions, Phys. Chem. Chem. Phys. 13, 161-168 (2011)

Periodic Table 1-172

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	Orbitals
1	1 H																	2 He	1s
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	2s2p
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3s3p
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	4s3d4p
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	5s4d5p
6	55 Cs	56 Ba	57-71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	6s5d6p
7	87 Fr	88 Ra	89-103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113	114	115	116	117	118	7s6d7p
8	119	120	121-	156	157	158	159	160	161	162	163	164	139	140	169	170	171	172	8s7d8p
9	165	166											167	168					9s9p

6	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	4f
7	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	5f
8	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	6f

8	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	5g

"Half of chemistry is still undiscovered. We don't know what it looks like and that's the challenge"

The limit of mass and charge is still undiscovered. We don't know what it looks like and that's the challenge.

Based on:

P.G. Reinhard and WN, Phys. Rev. C 81, 051303 (R) (2010)

To what extent is a new observable independent of existing ones and what new information does it bring in? Without any preconceived knowledge, all different observables are independent of each other and can usefully inform theory. On the other extreme, new data would be redundant if our theoretical model were perfect. Reality lies in between.

Consider a model described by coupling constants $\mathbf{p} = (p_1, ..., p_F)$
Any predicted expectation value of an observable is a function of these parameters. Since the number of parameters is much smaller than the number of observables, there *must exist correlations* between computed quantities. Moreover, since the model space has been optimized to a limited set of observables, there may also exist correlations between model parameters.

How to confine the model space to a *physically reasonable* domain?

Statistical methods of linear-regression and error analysis

$$\chi^2(\mathbf{p}) = \sum_{\mathcal{O}} \left(\frac{\mathcal{O}^{(\mathrm{th})}(\mathbf{p}) - \mathcal{O}^{(\mathrm{exp})}}{\Delta \mathcal{O}} \right)^2$$

Objective function

Expected uncertainties

fit-observables
(may include pseudo-data)

Superheavy Elements in Nuclear DFT