Nuclear structure IV (nuclear theory, open quantum systems, superheavies)

Witek Nazarewicz (UTK/ORNL)

National Nuclear Physics Summer School 2014
William & Mary, VA

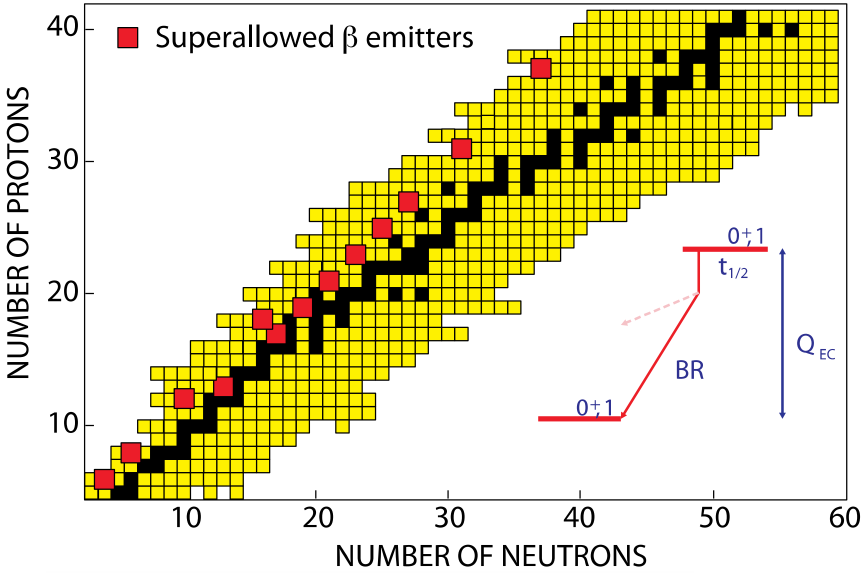
- Recent developments
- Perspectives

Microscopic calculations of isospin-breaking corrections to superallowed β-decay

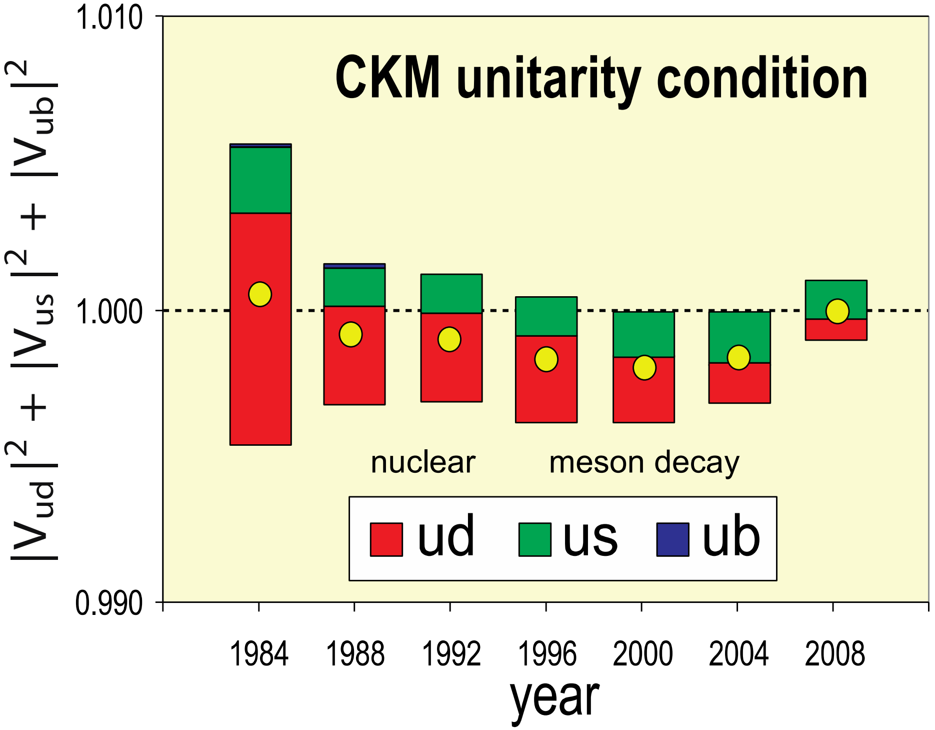
W. Satuła et al. Phys. Rev. Lett 106, 132502 (2011)

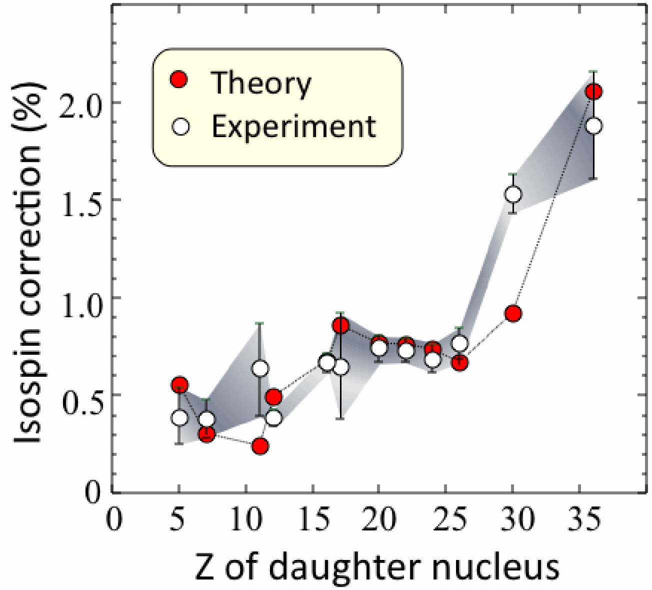
Superallowed Fermi 0+ → 0+ β-decay studies

Impressive experimental effort worldwide



Kobayashi and Maskawa: … for "the discovery of the origin of broken symmetry, which predicts the existence of at least three families of quarks in nature."

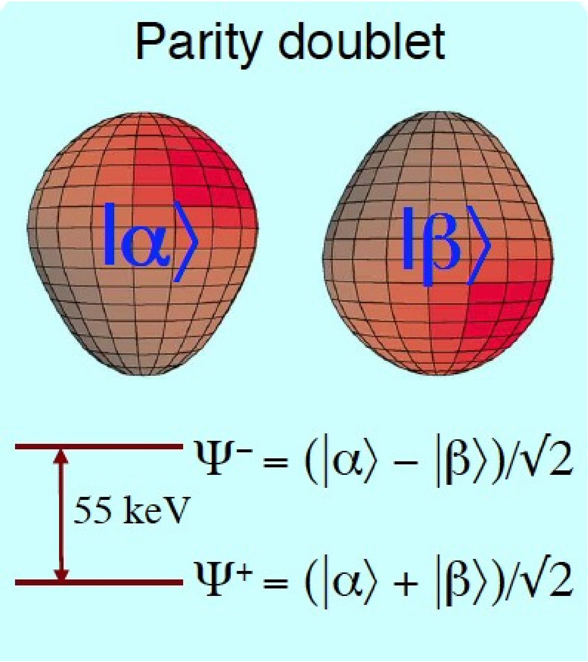


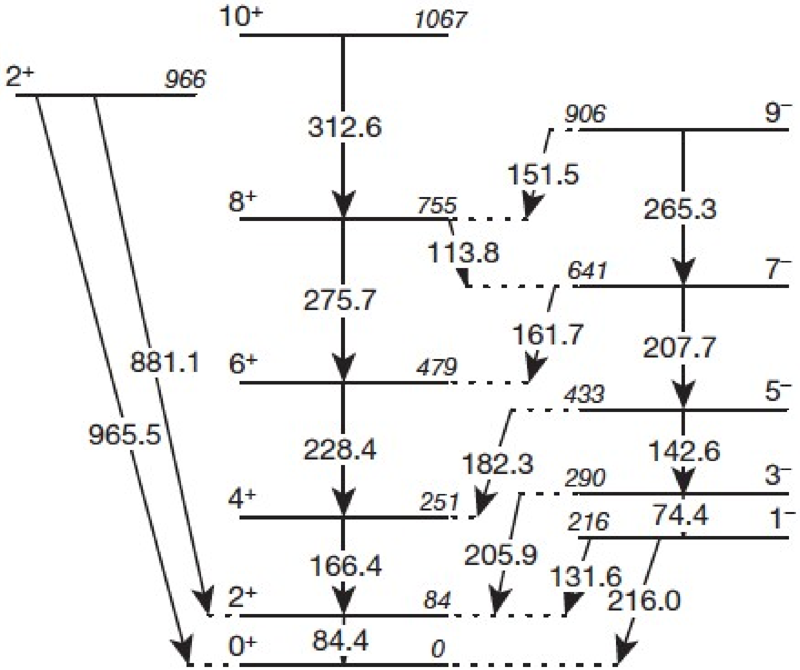


Towner and Hardy 2010

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9999(6)$$

The violation of CP-symmetry is responsible for the fact that the Universe is dominated by matter over anti-matter



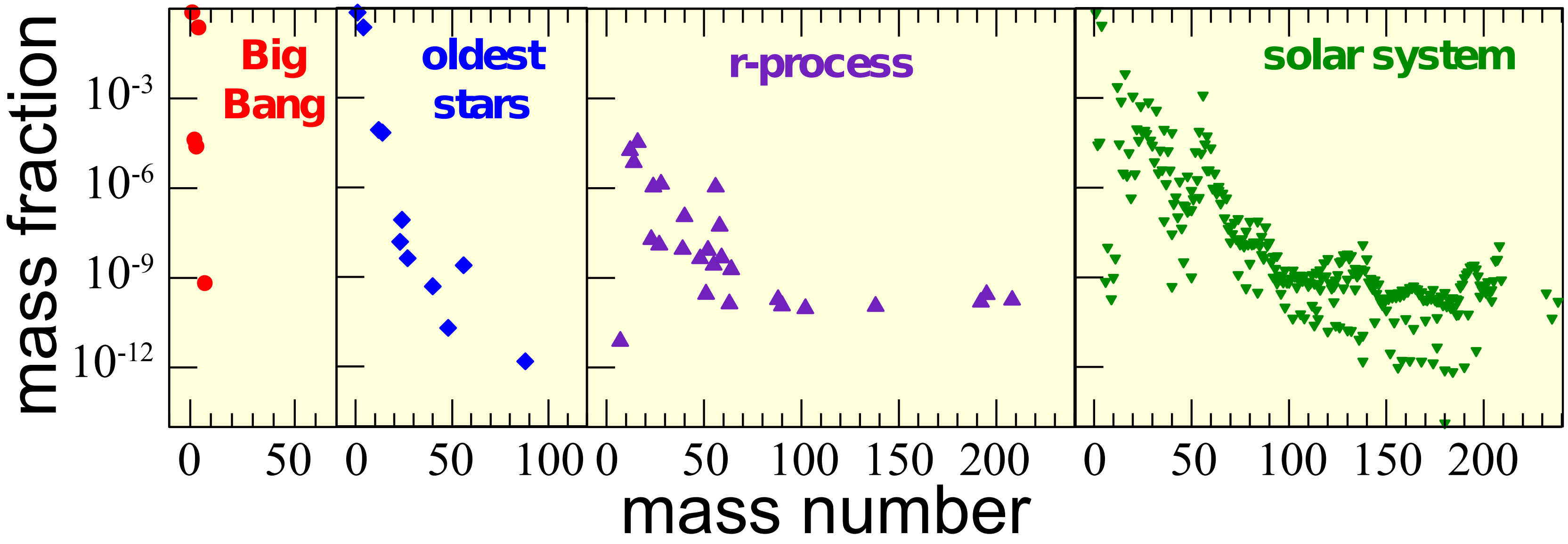


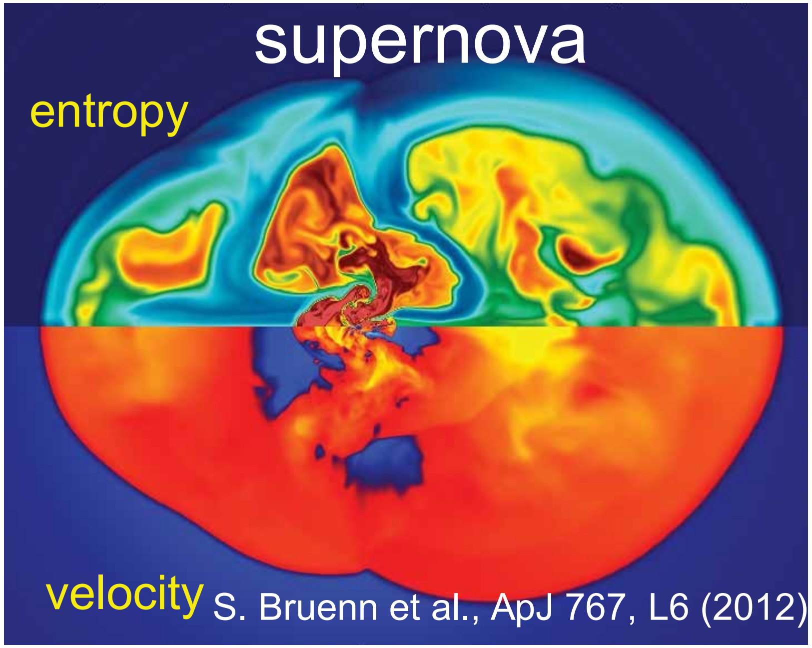
Gaffney et al., Nature 199, 497 (2013)

- Closely spaced parity doublet gives rise to enhanced electric dipole correlations
- Large intrinsic Schiff moment
- 199Hg (Seattle, 1980's – present)
- 225Ra (Starting at ANL and KVI)
- 223Rn at TRIUMF
- Potential at FRIB (1012/s w ISOL target (far future); 1010 initially

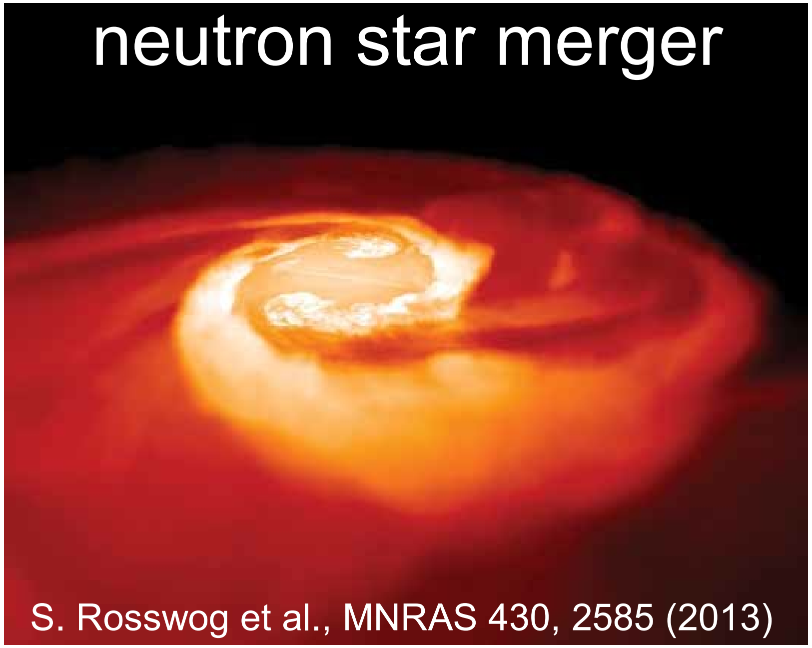
Theory!

The radioactive galaxy demonstrates the continuing formation of new radioactive isotopes




supernova

S. Bruenn et al., ApJ 767, L6 (2012)


neutron star merger

S. Rosswog et al., MNRAS 430, 2585 (2013)

Quality control
Uncertainty quantification

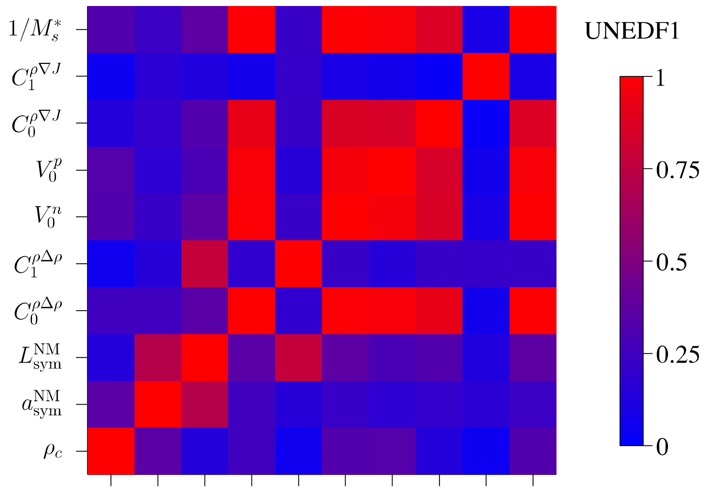
“Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful*”

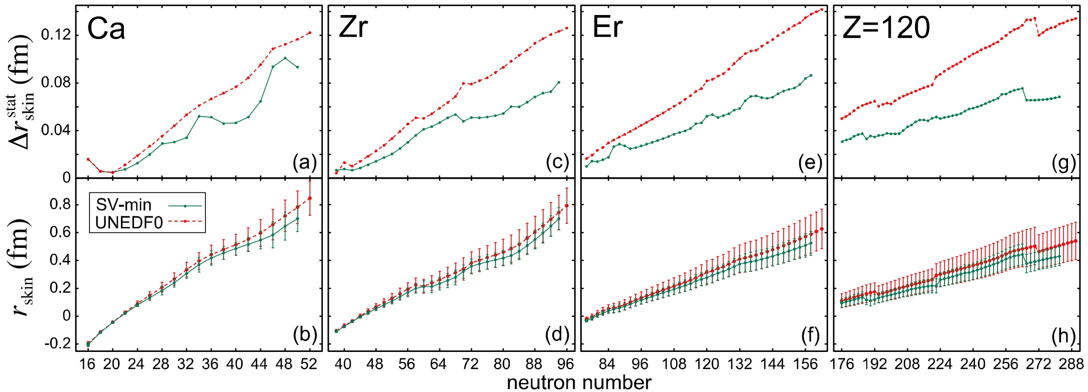
(E.P. Box)

Information content of future measurements

Nuclear theory is developing tools to deliver uncertainty quantification and error analysis for the assessment of new experimental data. Theoretical tools can also be used to assess the information content of an observable with respect to current theoretical models, and evaluate the degree of correlation between different observables.

see "Error Estimates of Theoretical Models: a Guide" (arXiv:1402.4657)





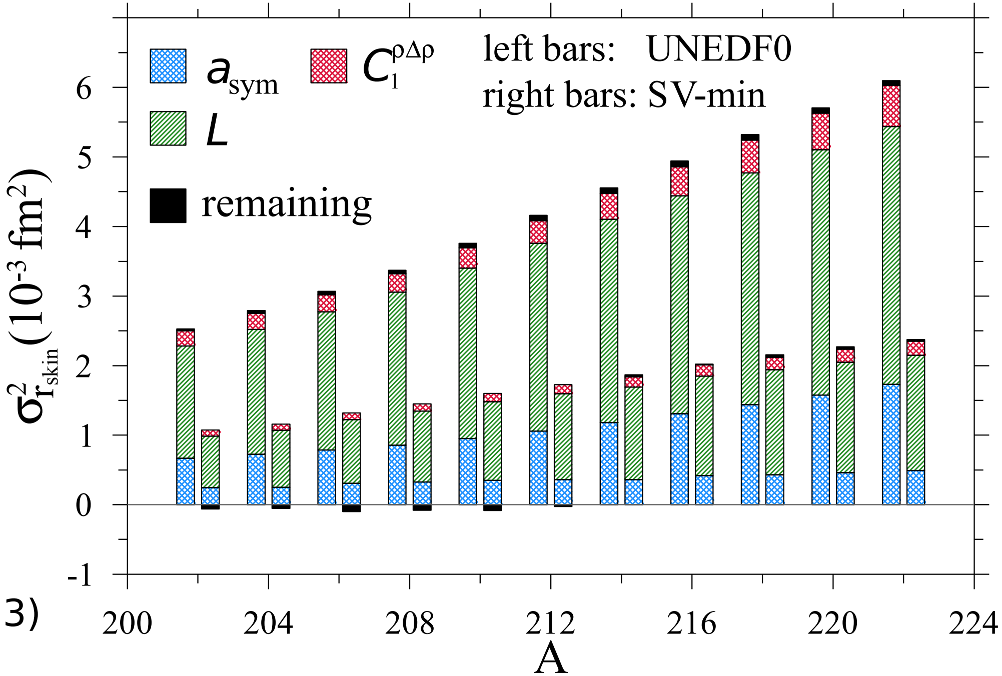


TABLE I. Theoretical uncertainties on $r_{\rm skin}$ in ^{208}Pb and ^{48}Ca (in fm). Shown are statistical errors of UNEDF0 and SV-min, systematic error $\Delta r_{\rm skin}^{\rm syst}$, the model-averaged deviation of Ref. [9], and errors of PREX [25] and planned PREX-II [29] and CREX [30] experiments.

nucleus	$\Delta r_{\rm skin}^{\rm stat}$ UNEDF0	$\Delta r_{\rm skin}^{\rm stat}$ SV-min	$\Delta r_{\rm skin}^{\rm syst}$	Ref. [9]	Experiment
^{208}Pb	0.058	0.037	0.013	0.022	0.18 [25], 0.06[29]
^{48}Ca	0.035	0.026	0.019	0.018	0.02 [30]

Kortelainen et al., Phys. Rev. C 88, 031305 (2013)

Theoretical Tools and Connections to Computational Science

1teraflop=10^{12} flops

1peta=1015 flops (today)

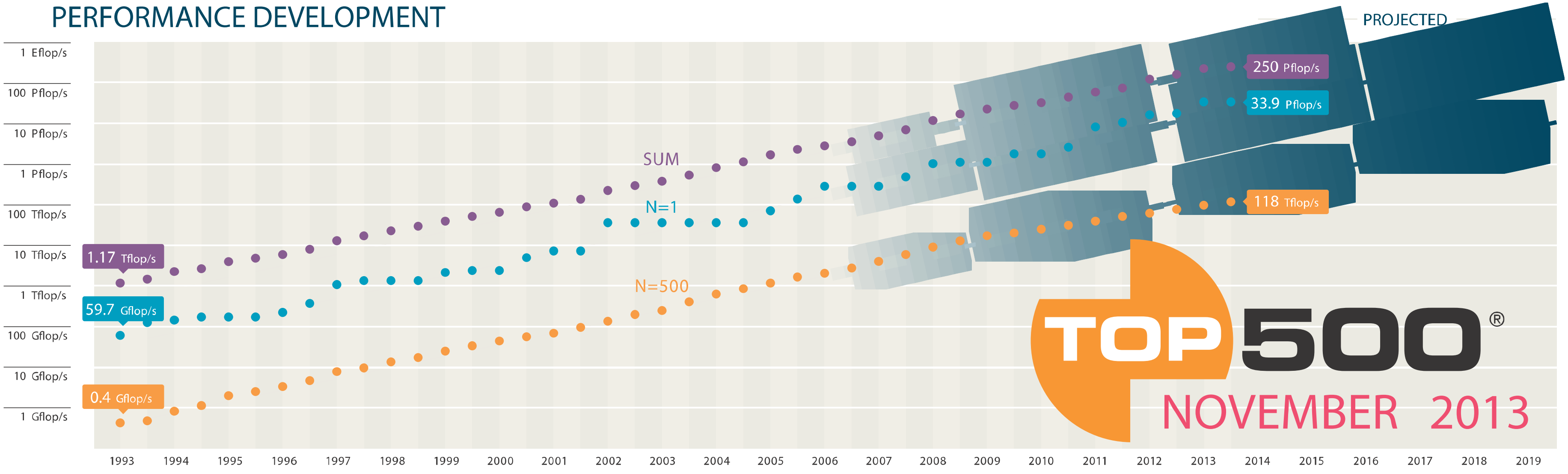
1exa=1018 flops (next 10 years)

Tremendous opportunities for nuclear theory!

33.9 pflops

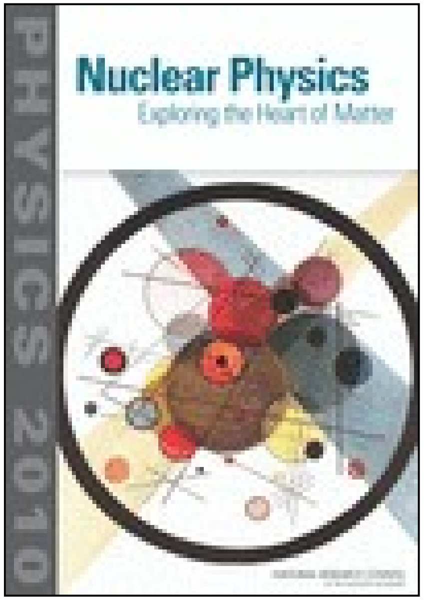
	NAME	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	NUDT, Intel Ivy Bridge (12C, 2.2 GHz) & Xeon Phi (57C, 1.1 GHz), Custom interconnect	NSCC Guangzhou	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Operon 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.2
3	Sequoia	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C, 2.0GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
5	Mira	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	8.59	3.95

PERFORMANCE DEVELOPMENT



“High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, *it becomes a third leg supporting the field of nuclear physics*.”

NAS Decadal Study



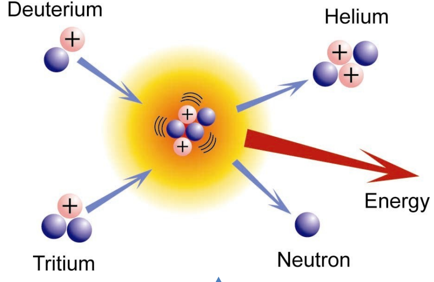
Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math

NUCLEI

Nuclear Computational Low-Energy Initiative

computingnuclei.org

fusion



Validated Nuclear Interactions

Chiral EFT
Ab-initio

Optimization
Model validation
Uncertainty Quantification

Structure and Reactions: Light and Medium Nuclei

Ab-initio
RGM
CI

Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification

Neutron drops

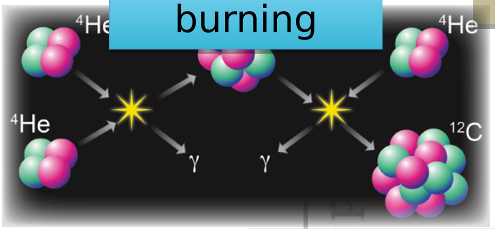
EOS
Correlations

Structure and Reactions: Heavy Nuclei

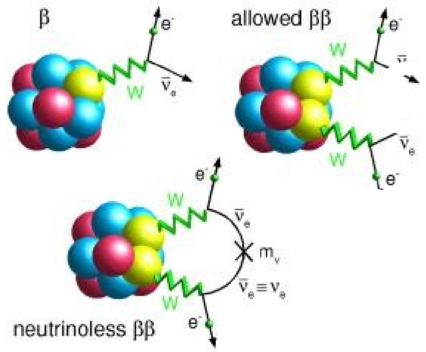
DFT
TDDFT

Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis

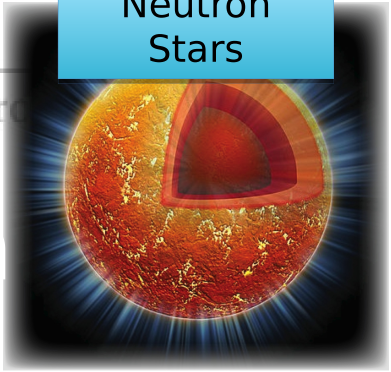
Stellar burning



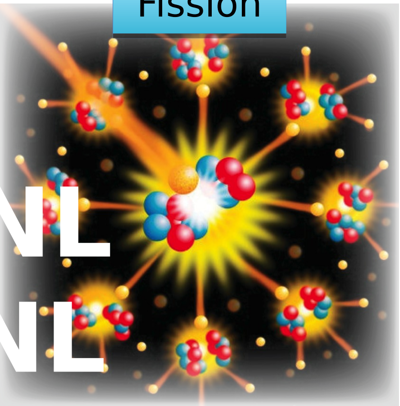
Neutrinos and Fundamental



Neutron Stars

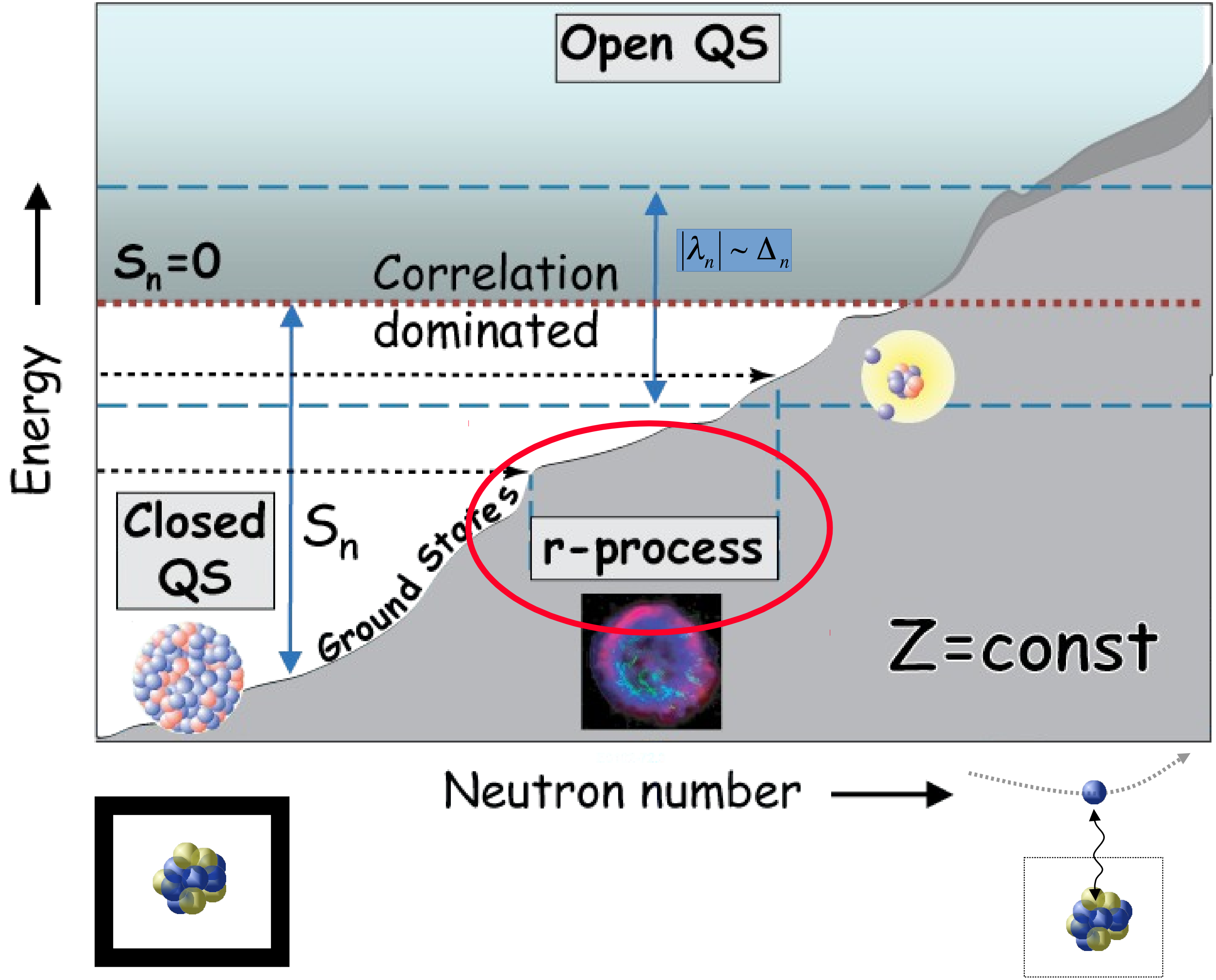


Fission

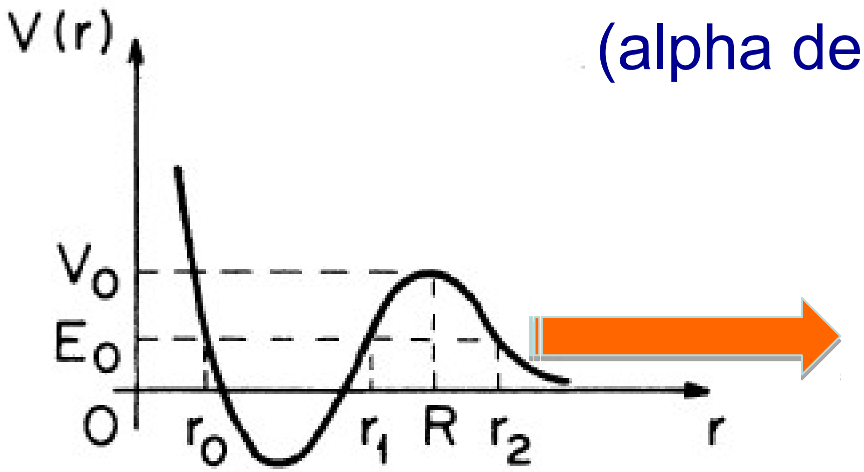


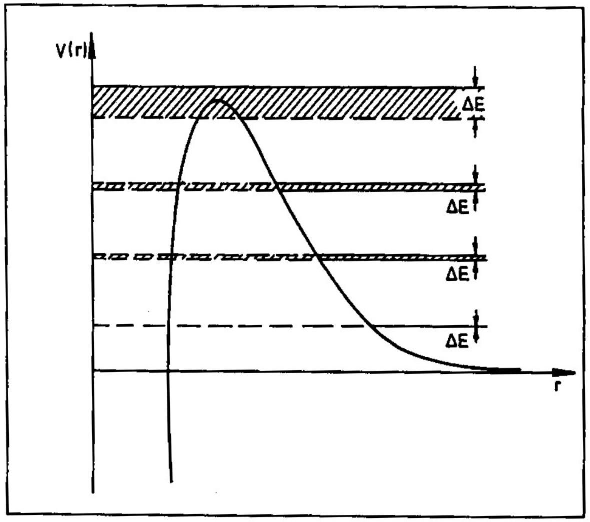
Open quantum systems

Prog. Part. Nucl. Phys. 59, 432 (2007)



Quasistationary States
(alpha decay)





$$\frac{dN}{dt} = -wN; \quad N = N_0 e^{-wt}$$

N is a number of radioactive nuclei, i.e., number of particles inside of sphere *r=R:*

$$N \sim \int |\psi^2| d^3r$$

$$\psi = \psi(r) e^{-iE_0 t/\hbar - wt/2} = \psi(r) e^{-iEt/\hbar}$$

$$E = E_0 - i\frac{\Gamma}{2}; \quad \Gamma = \hbar w$$

J.J. Thompson, 1884
G. Gamow, 1928

relation between decay width and decay probability

Basic Equations

Time Dependent (Many Body) Schödinger Equation

$$i \, \text{ㄹE} \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

+ boundary conditions

Often impractical/impossible to solve but an excellent starting point

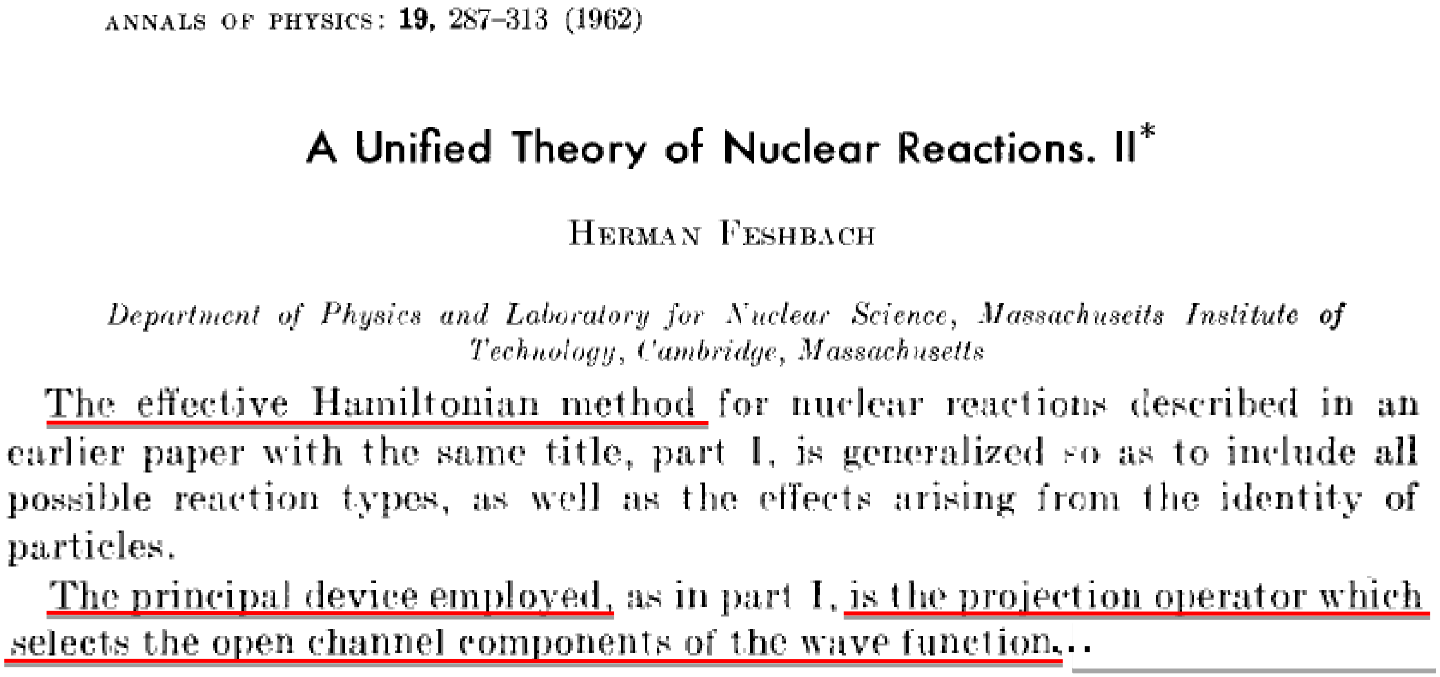
Time Independent (Many Body) Schödinger Equation

$$\hat{H} \psi = E \psi$$

Box boundary conditions (w.f. vanishes at large distances)
Decaying boundary conditions
Incoming or capturing boundary conditions
Scattering boundary conditions

Absorbing boundary conditions

choice depends on physics case



ANNALS OF PHYSICS: **19**, 287–313 (1962)

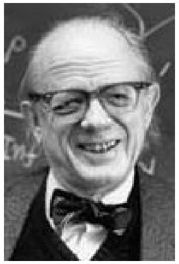
A Unified Theory of Nuclear Reactions. II*

HERMAN FESHBACH

Department of Physics and Laboratory for Nuclear Science, Massachusetts Institute of Technology, Cambridge, Massachusetts

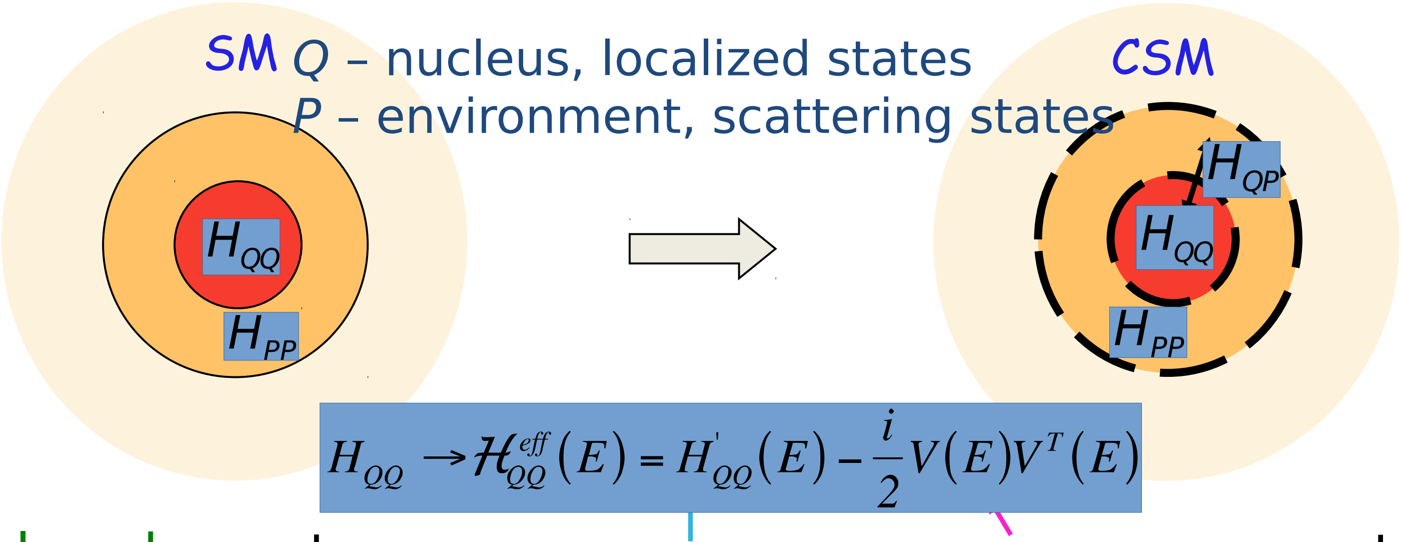
The effective Hamiltonian method for nuclear reactions described in an earlier paper with the same title, part I, is generalized so as to include all possible reaction types, as well as the effects arising from the identity of particles.

The principal device employed, as in part I, is the projection operator which selects the open channel components of the wave function...



H. Feshbach

Basic idea:



Q – nucleus, localized states

P – environment, scattering states

$$H_{QQ} \rightarrow \mathcal{H}^{eff}_{QQ}(E) = H'_{QQ}(E) - \frac{i}{2} V(E) V^{T}(E)$$

hermitian anti-hermitian

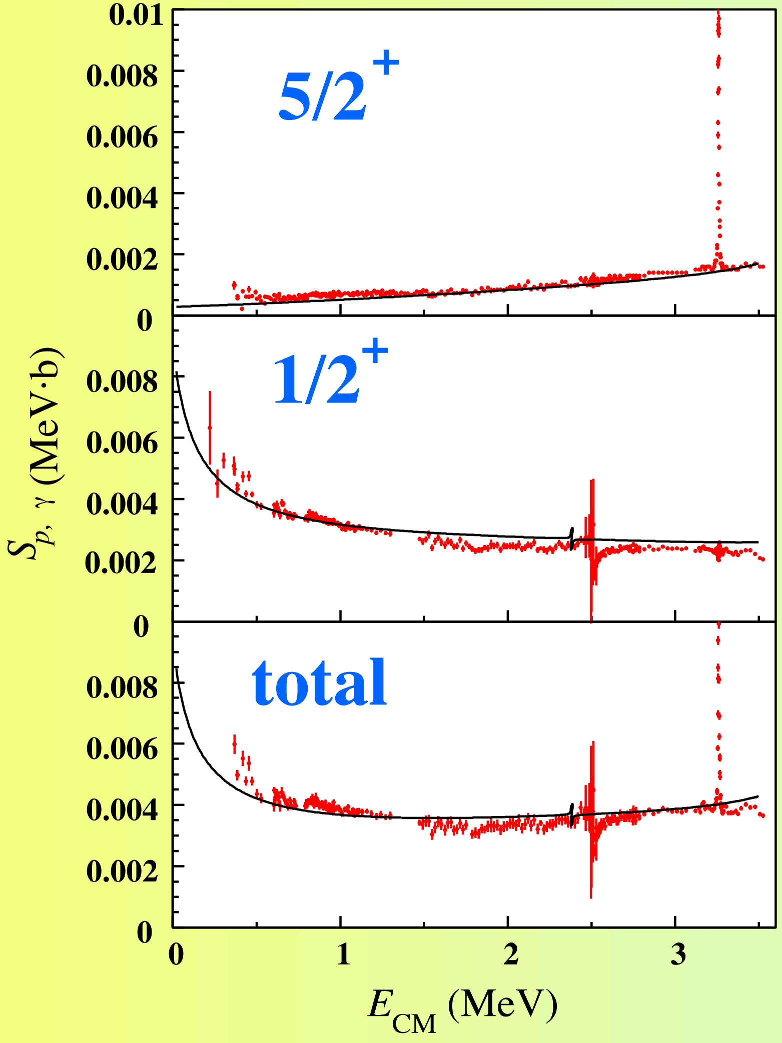
closed quantum system

open quantum system

Continuum Shell Model

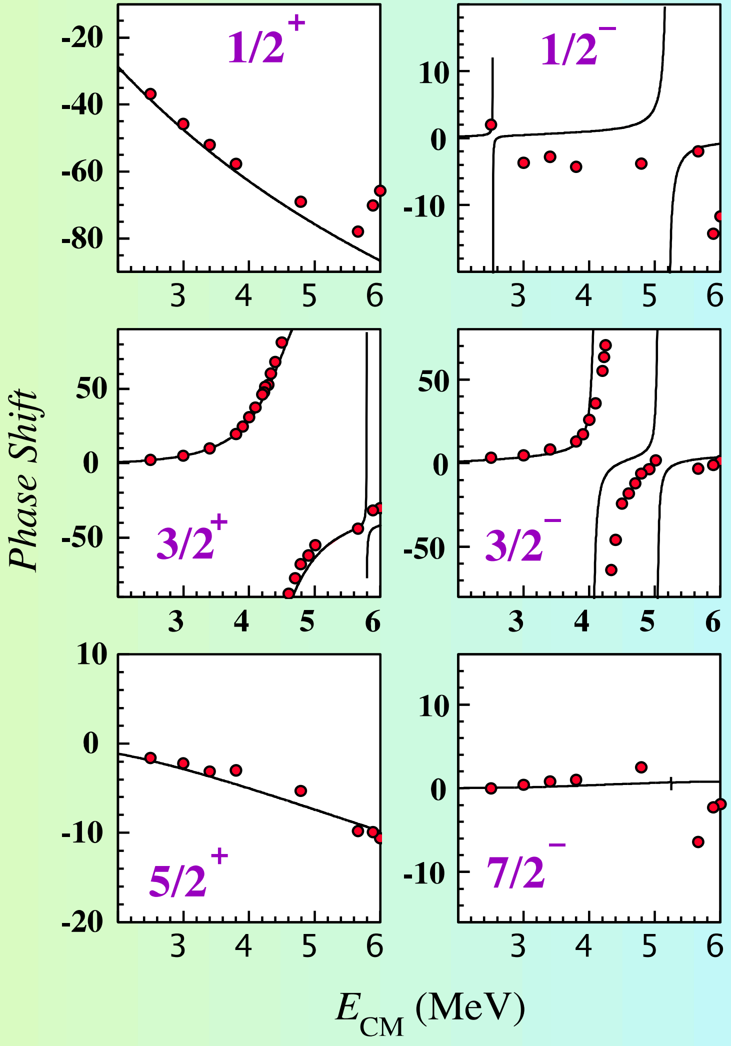
$^{16}O(p,\gamma)^{17}F$

Exp: Morlock et al., Phys. Rev. Lett. 79, 3837 (1997)



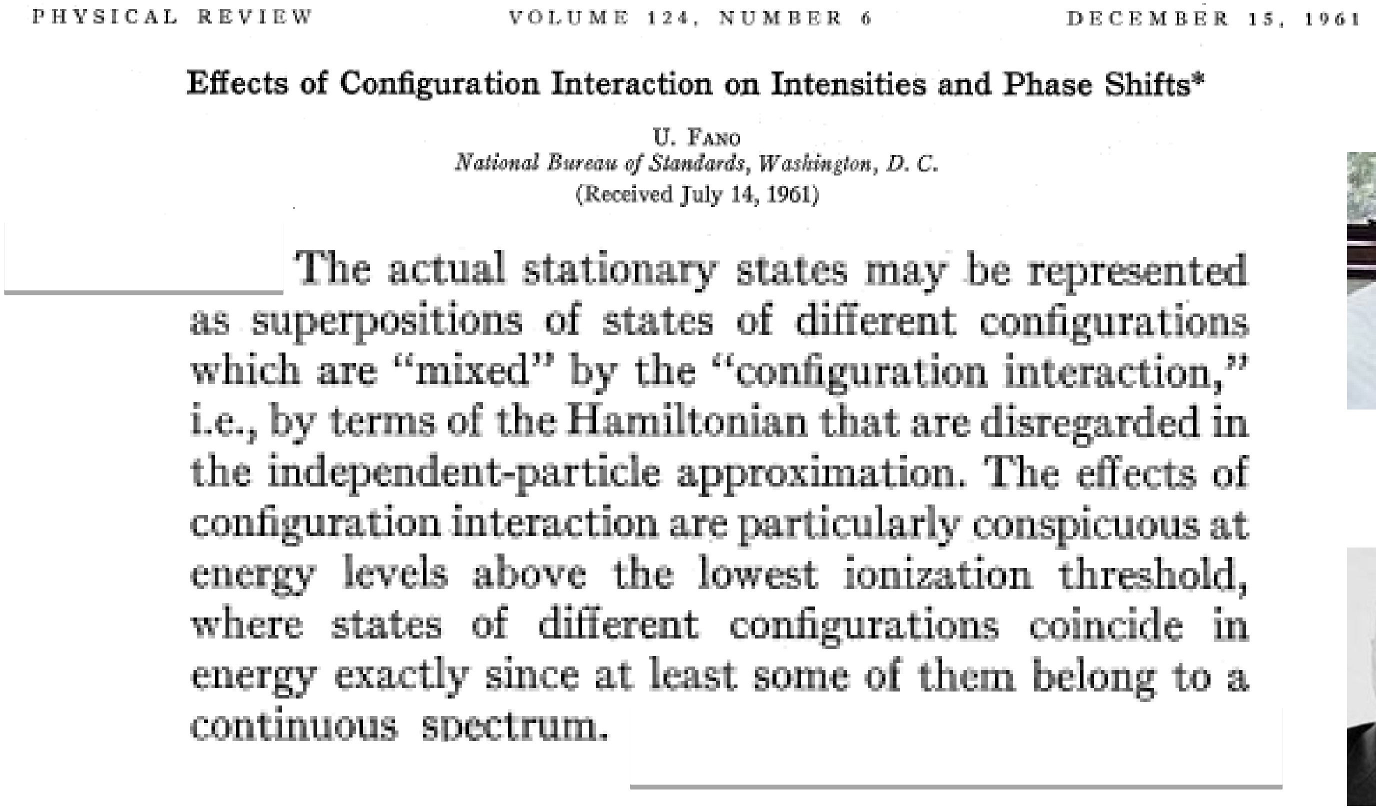
p+^{16}O elastic scattering

Exp: Blee and Haeberli , Phys. Rev. 137, B284 (1965)



Theory: K. Bennaceur et al., Nucl. Phys. A651, 289 (1999); Phys. Lett. B488, 75 (2000)

Shell Model for Open Quantum Systems
Gamow Shell Model



PHYSICAL REVIEW VOLUME 124, NUMBER 6 DECEMBER 15, 1961

Effects of Configuration Interaction on Intensities and Phase Shifts*

U. Fano
National Bureau of Standards, Washington, D. C.
(Received July 14, 1961)

The actual stationary states may be represented as superpositions of states of different configurations which are "mixed" by the "configuration interaction," i.e., by terms of the Hamiltonian that are disregarded in the independent-particle approximation. The effects of configuration interaction are particularly conspicuous at energy levels above the lowest ionization threshold, where states of different configurations coincide in energy exactly since at least some of them belong to a continuous spectrum.

U. Fano

I.M. Gelfand

T. Berggren

t took over 40 years and required the development of:

- New mathematical concepts: Rigged Hilbert Space (≥1964),…
- Generalized completeness relation including s.p. bound states, resonances, a scattering states (~1968)
- New many-body framework(s): Gamow Shell Model (2002), …

Rigged Hilbert Space: the natural framework to formulate quantum mechanics

In mathematics, a rigged Hilbert space (Gel’fand triple, nested Hilbert space, equipped Hilbert space) is a construction designed to link the distribution and square-integrable aspects of functional analysis. Such spaces were introduced to study spectral theory in the broad sense. They can bring together the 'bound state' (eigenvector) and 'continuous spectrum', in one place.

Mathematical foundations in the 1960s by Gel’fand et al. who combined Hilbert space with the theory of distributions. Hence, the RHS, rather than the Hilbert space alone, is the natural mathematical setting of Quantum Mechanics

I. M. Gel’fand and N. J. Vilenkin. Generalized Functions, vol. 4: Some Applications of Harmonic Analysis. Rigged Hilbert Spaces. Academic Press, New York, 1964.

The resonance amplitude associated with the Gamow states is proportional to the complex delta function and such amplitude can be approximated in the near resonance region by the Breit-Wigner amplitude (Nucl. Phys. A812, 13 (2008)):

$$\mathcal{A}(E_n \to E) \propto -\frac{1}{2\pi}\frac{1}{E - E_n}$$

For a pedagogical description, see R. de la Madrid, Eur. J. Phys. 26, 287 (2005)

Resonant (Gamow) states

$$\hat{H}\Psi = \left(e - i\frac{\Gamma}{2}\right)\Psi$$

$$\Psi(0,k) = 0, \quad \Psi(\hat{r},k) \xrightarrow[r\to\infty]{} O_l(kr)$$

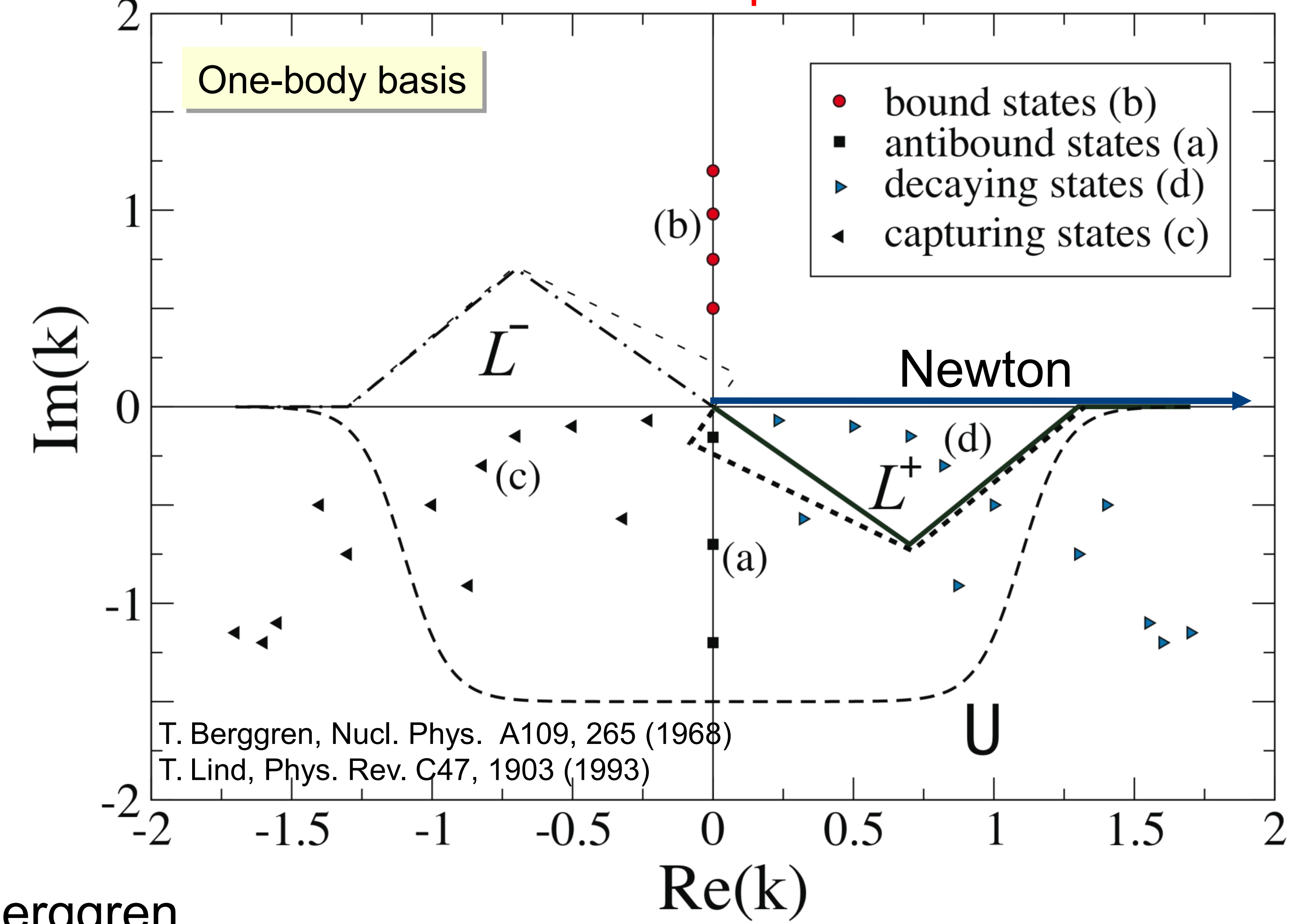
$$k_n = \sqrt{\frac{2m}{\hbar^{2}}\left(e_n - i\frac{\Gamma_n}{2}\right)}$$

complex pole
of the S-matrix

- Humblet and Rosenfeld, Nucl. Phys. **26**, 529 (1961)
- Siegert, Phys. Rev. **36**, 750 (1939)
- **Gamow, Z. Phys. 51, 204 (1928)**

Also true in many-channel case!

Gamow states and completeness relations

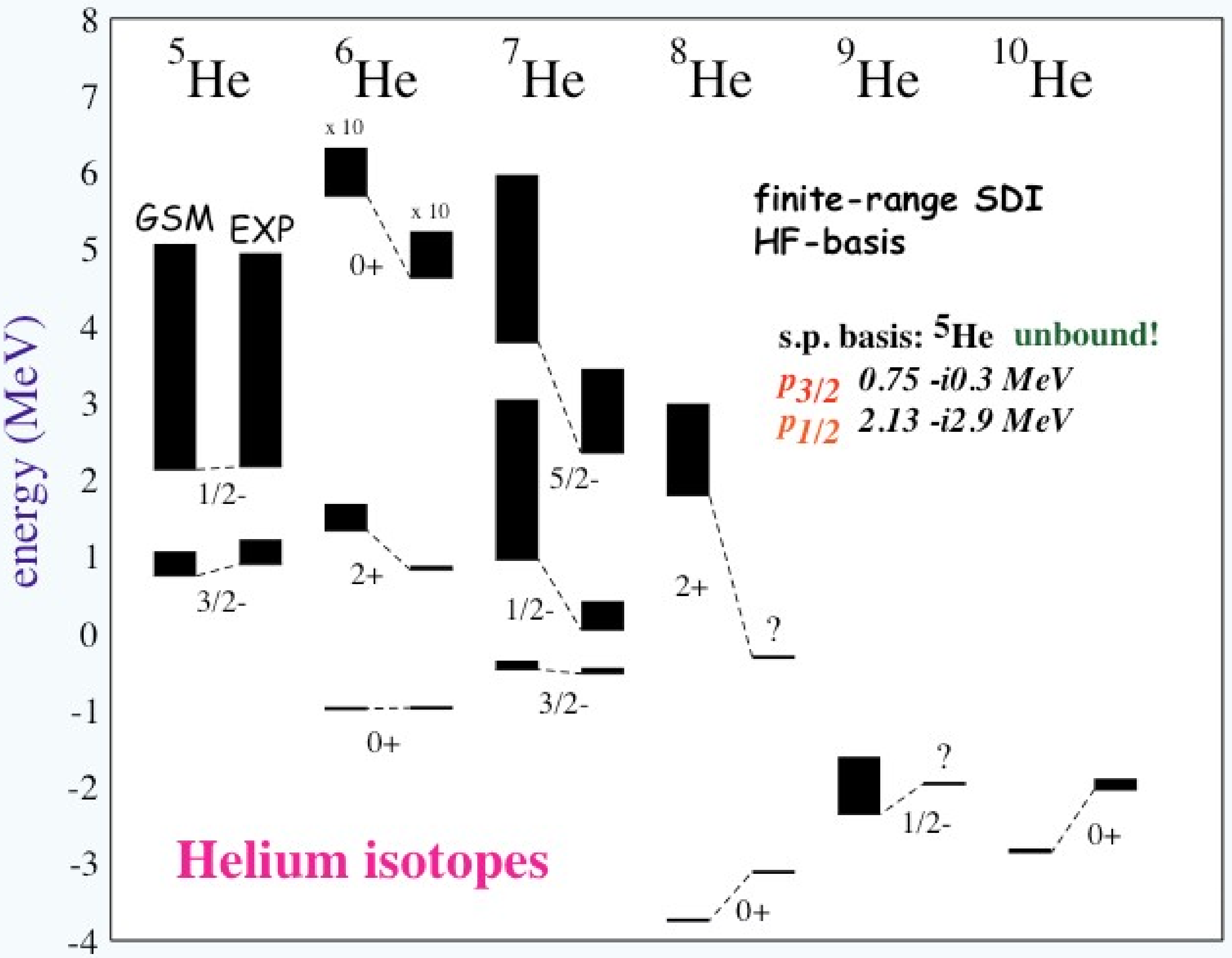


T. Berggren, Nucl. Phys. A109, 265 (1968)
T. Lind, Phys. Rev. C47, 1903 (1993)

Berggren ensemble for a given *jl* channel:

$$\sum_{n\in(b,d)} |u_n\rangle\langle u_n| + \int_{L^+} |u(k)\rangle\langle u(k)|dk = 1.$$

GSM: N. Michel et al., Phys.Rev.Lett. 89, 042502 (2002)



Helium isotopes

finite-range SDI
HF-basis

s.p. basis: ^{5}He unbound!
$p_{3/2}$ 0.75 -i0.3 MeV
$p_{1/2}$ 2.13 -i2.9 MeV

S_{2n} in 8He greater than S_{2n} in 6He

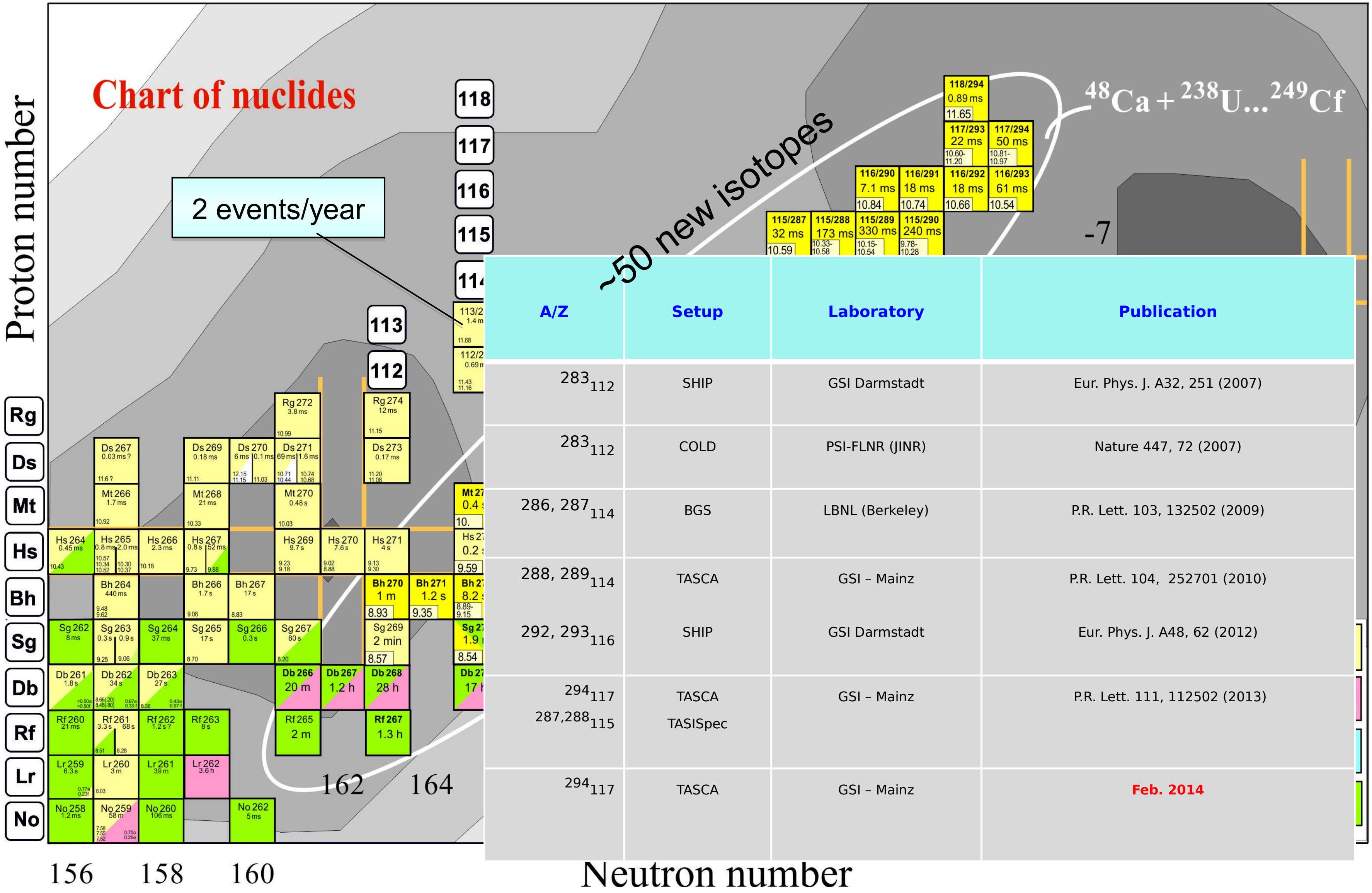
Open problems in the theory of nuclear open quantum systems

N. Michel et al., J. Phys. G **37**, 064042 (2010)

- What is the interplay between mean field and correlations in open quantum systems?
- What are properties of many-body systems around the reaction threshold?
- What is the origin of cluster states?
- What should be the most important steps in developing the theory that will treat nuclear structure and reactions consistently?
  - How to understand (Rigged) Quantum Mechanics of open quantum systems?
  - How are effective interactions modified in open quantum systems?

Superheavy nuclei

Limits of Mass and Charge: Superheavies



A/Z	Setup	Laboratory	Publication
$^{283}{}_{112}$	SHIP	GSI Darmstadt	Eur. Phys. J. A32, 251 (2007)
$^{283}{}_{112}$	COLD	PSI-FLNR (JINR)	Nature 447, 72 (2007)
$286, 287_{114}$	BGS	LBNL (Berkeley)	P.R. Lett. 103, 132502 (2009)
$288, 289_{114}$	TASCA	GSI – Mainz	P.R. Lett. 104, 252701 (2010)
$292, 293_{116}$	SHIP	GSI Darmstadt	Eur. Phys. J. A48, 62 (2012)
$^{294}{}_{117}$ $287{,}288_{115}$	TASCA TASISpec	GSI – Mainz	P.R. Lett. 111, 112502 (2013)
$^{294}{}_{117}$	TASCA	GSI – Mainz	Feb. 2014

Are superheavy atoms and nuclei different from lighter species?

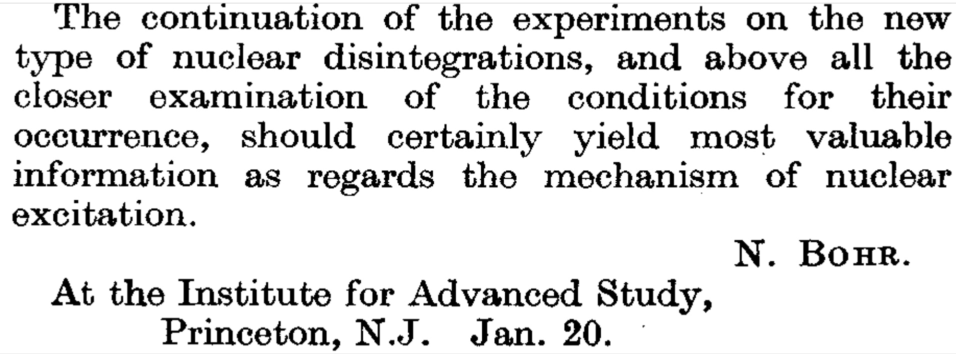
Yes!

Very large density of electronic and nucleonic levels

Electromagnetic interaction is huge

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

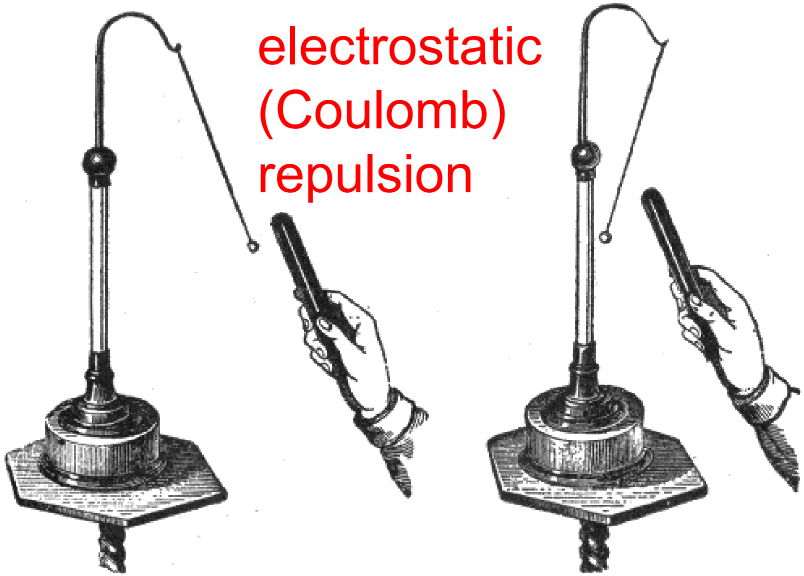
1939: Bohr’s paper on fission



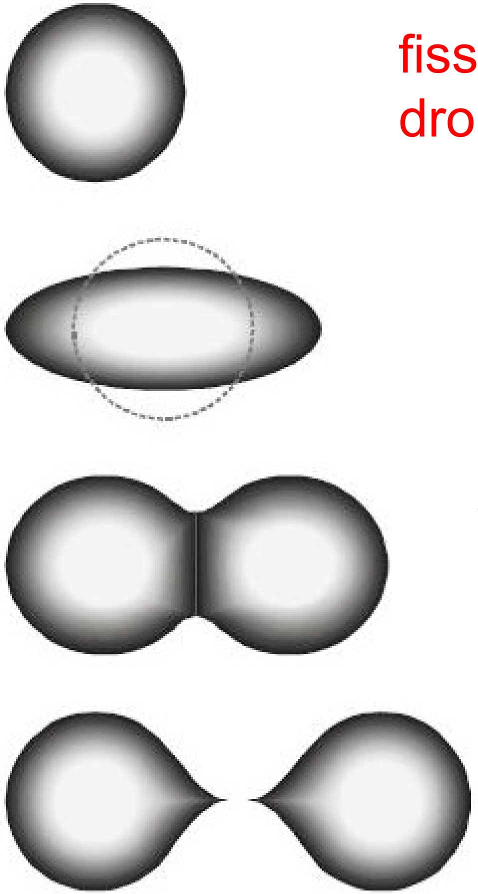
The continuation of the experiments on the new type of nuclear disintegrations, and above all the closer examination of the conditions for their occurrence, should certainly yield most valuable information as regards the mechanism of nuclear excitation.

N. Bohr.

At the Institute for Advanced Study,
Princeton, N.J. Jan. 20.



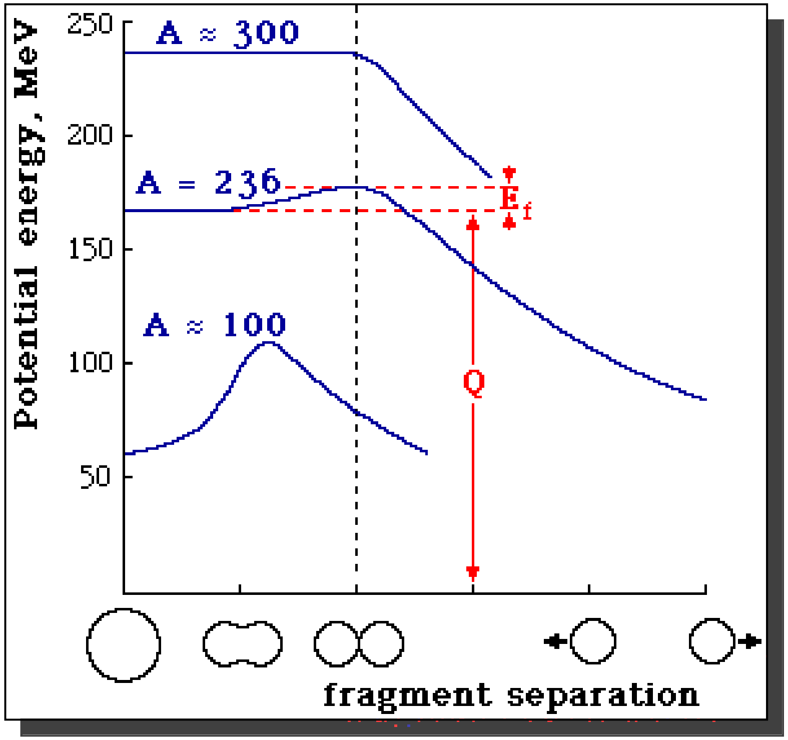
electrostatic (Coulomb) repulsion



fission of nuclear droplet

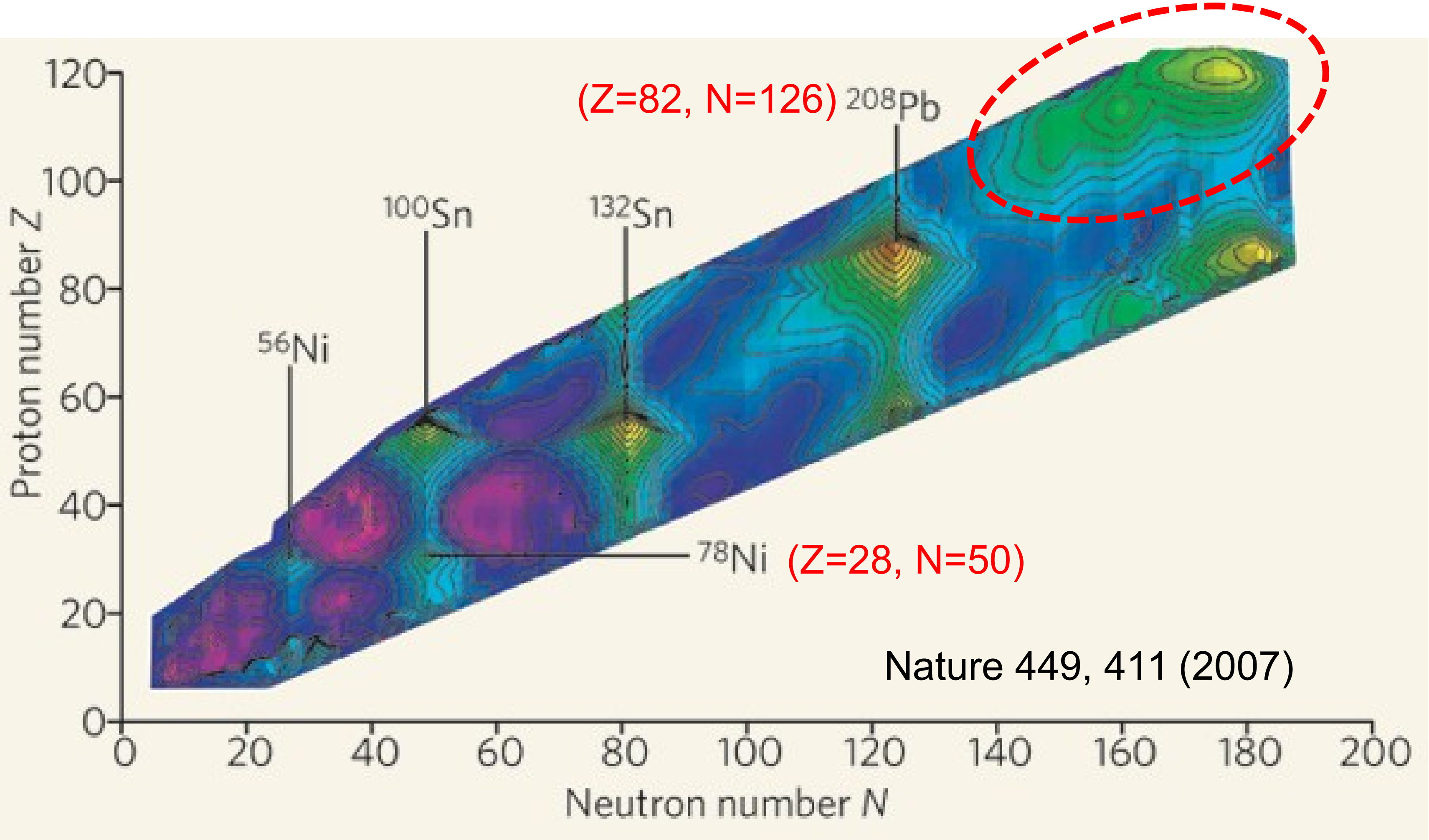
fissility parameter:

$$x = \frac{E_{\text{Coul}}}{2E_{\text{surf}}} \approx \frac{Z^2}{50A}$$



The nuclear droplet stays stable and spherical for x<1.
For x>1, it fissions immediately.
For ^{238}U, x=0.8

$$E_{\text{shell}} = E_{\text{total}} - E_{\text{LD}}$$



(Z=82, N=126)

(Z=28, N=50)

Nature 449, 411 (2007)

Magic numbers at Z or N= 2, 8, 20, 28, 50, 82,126

Is the concept of magicity useful in superheavy nuclei?

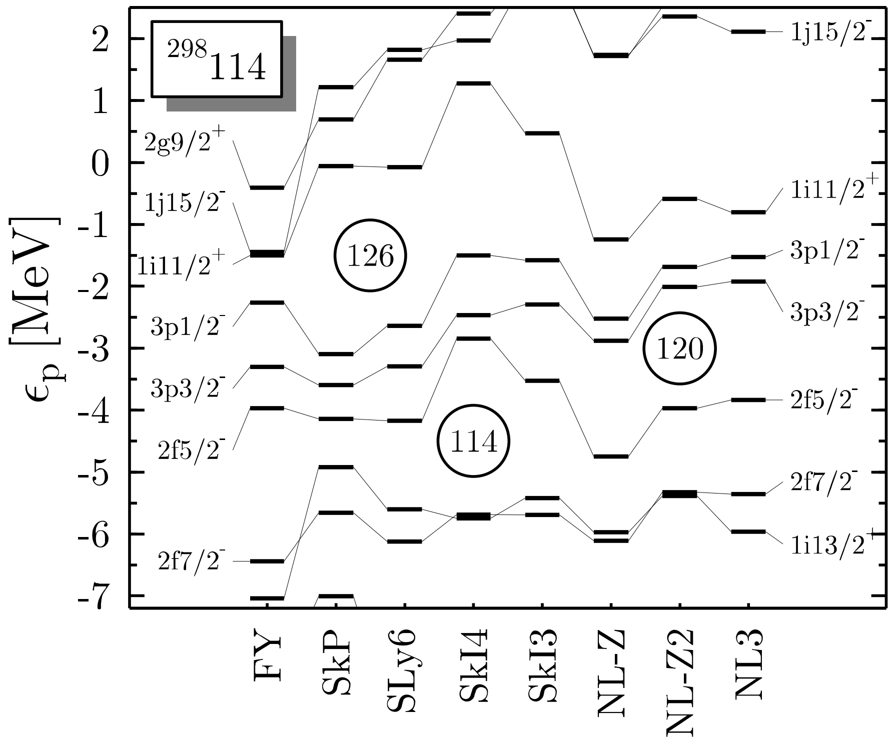
Probably not!

208Pb (Z=82, N=126) probably the last honest-to-goodness doubly-magic nucleus!

Shell structure and Coulomb frustration

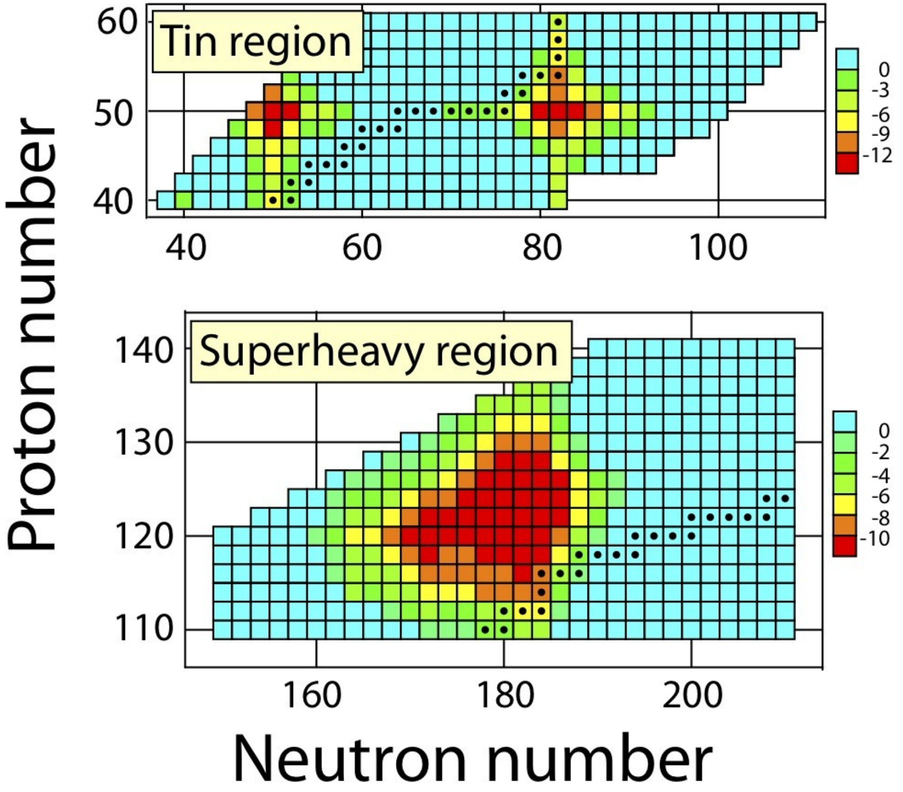
Small shifts of single-particle levels can impact shell structure significantly

Level density



M. Bender et al.
Phys. Rev. C 60, 034304 (1999)

Shell energy



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

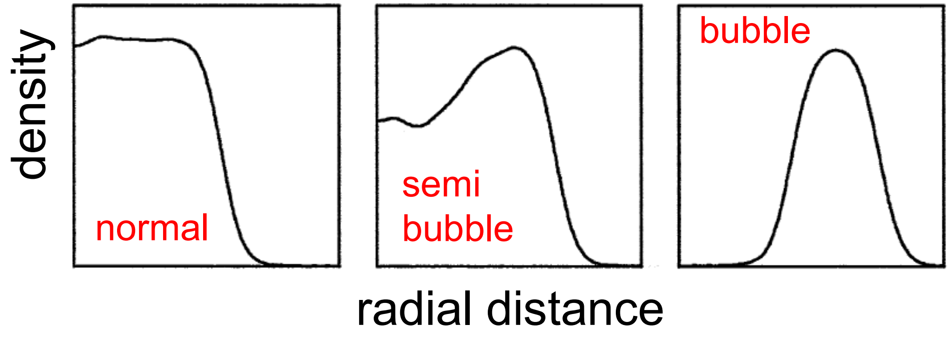
Because of the presence of highly-degenerate high-j levels and the smallness of the gaps in the single-particle spectrum, significant binding originates from the bunching of low-j orbits near the Fermi energy, not from the gaps

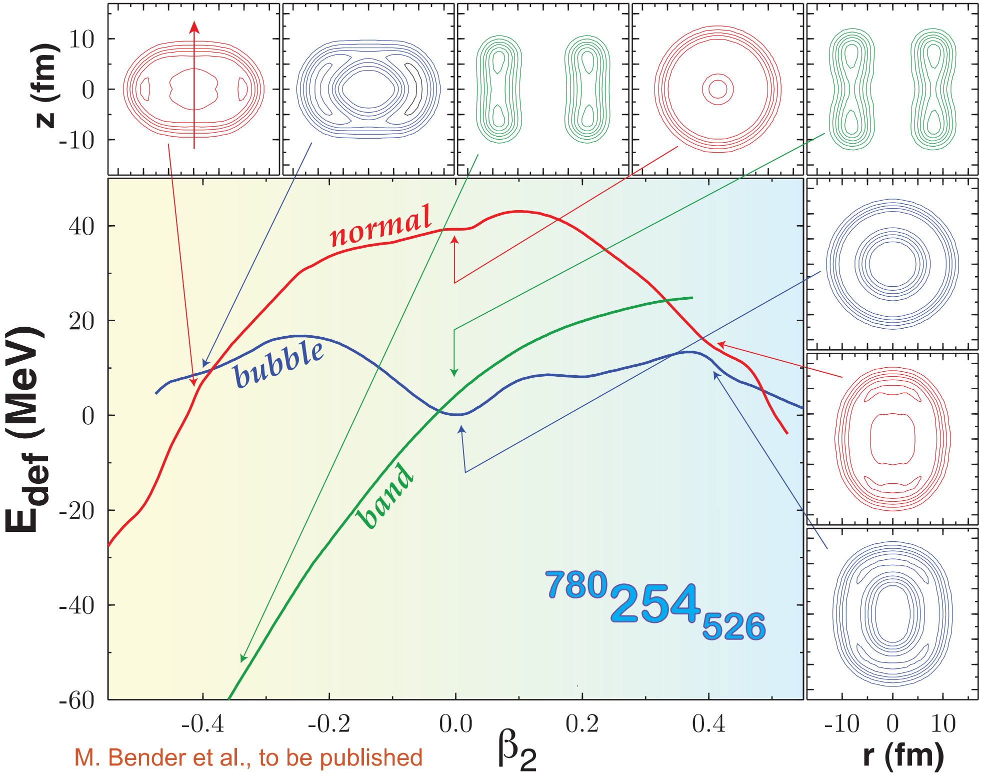
Where is the end of the nuclear landscape at the extremes of mass and charge?

We do not know…

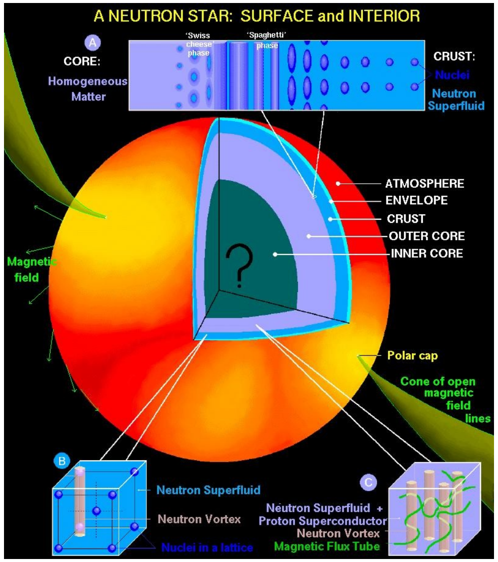
We really do not know!

Exotic topologies of superheavy nuclei: Coulomb frustration





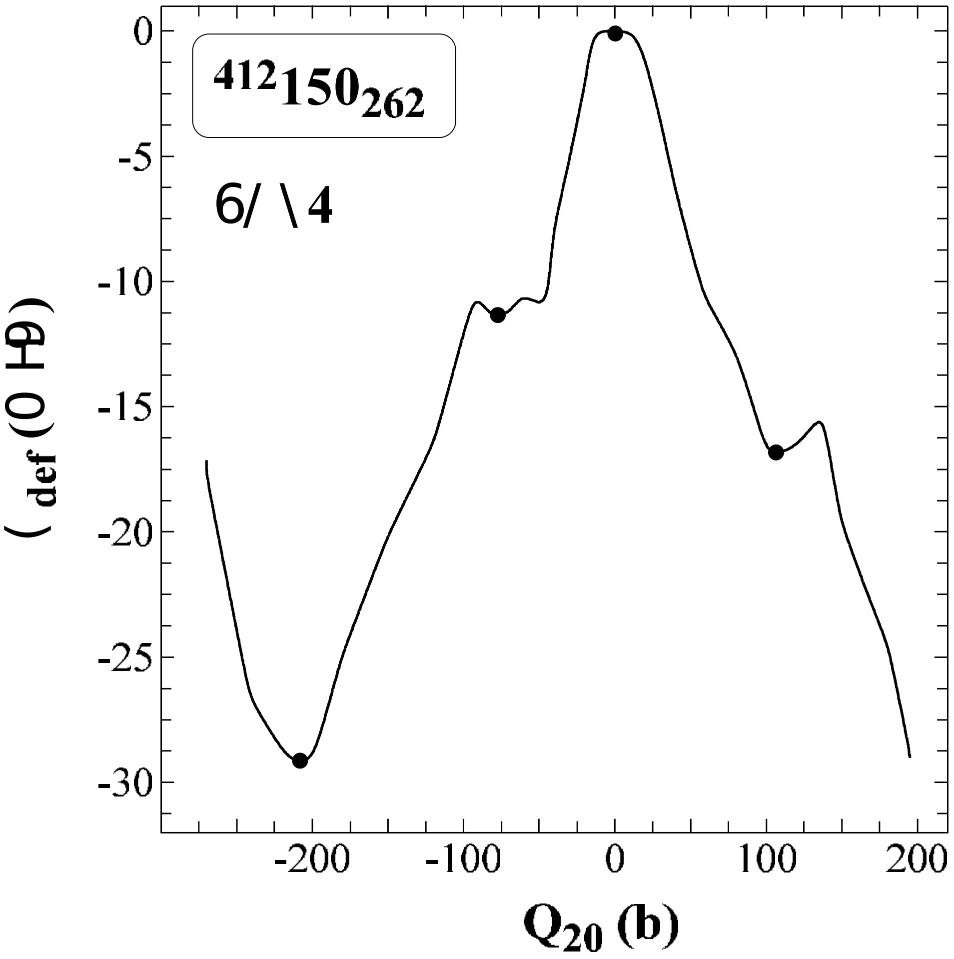
M. Bender et al., to be published



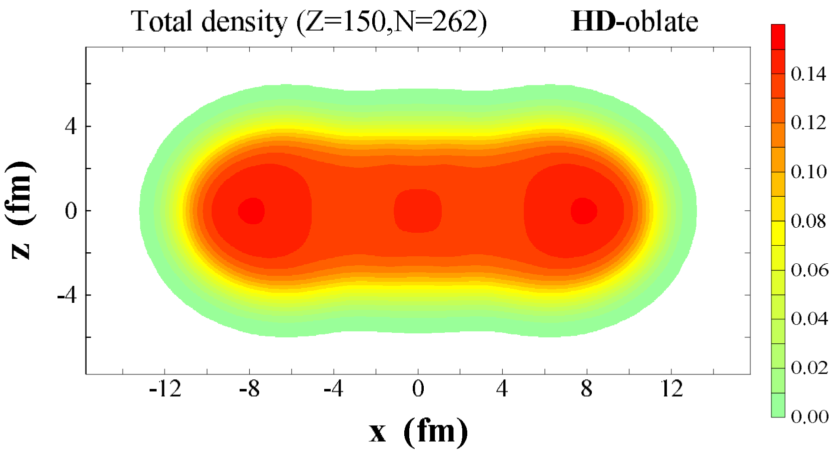
Self-consistent calculations confirm the fact that the “pasta phase” might have a rather complex structure, various shapes can coexist, at the same time significant lattice distortions are likely and the neutron star crust could be on the verge of a disordered phase.

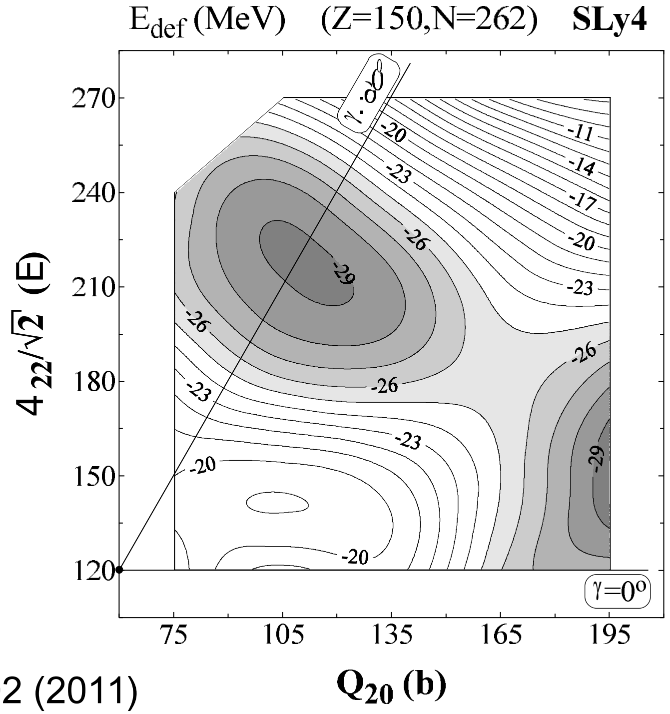
A challenge is to assess stability of such forms

Exotic topologies of superheavy nuclei: Coulomb frustration



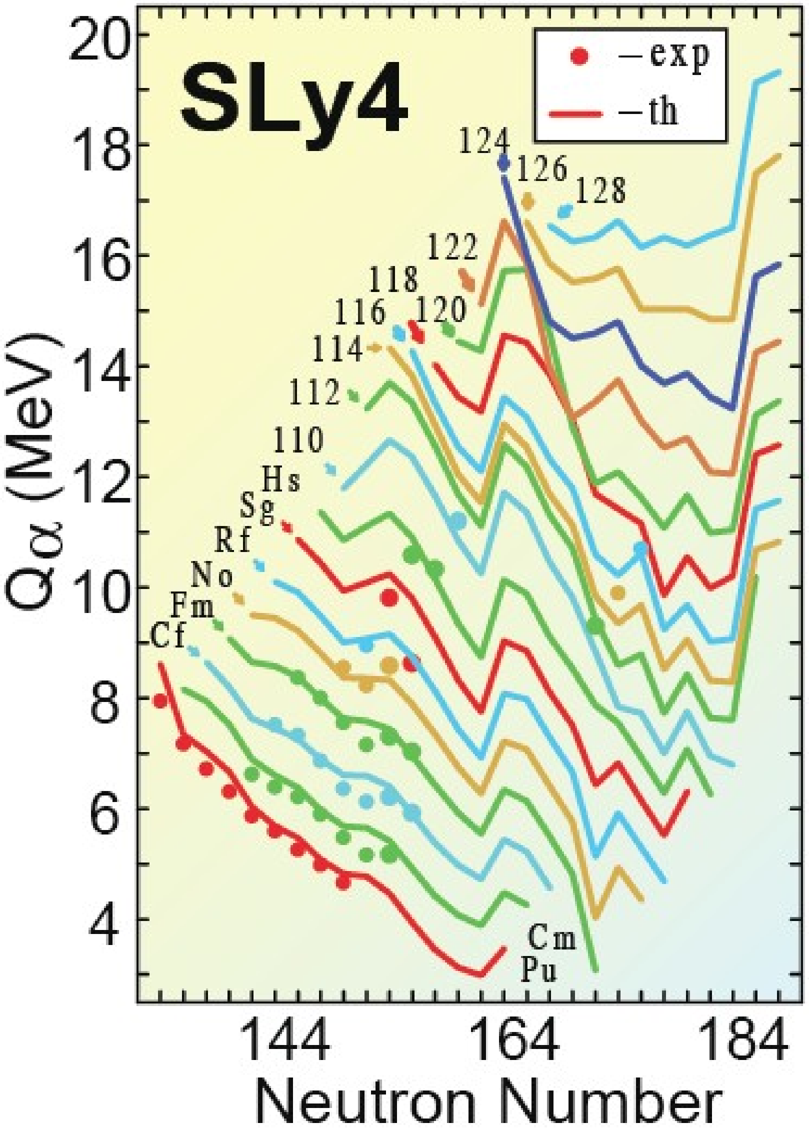
S. Ćwiok et al



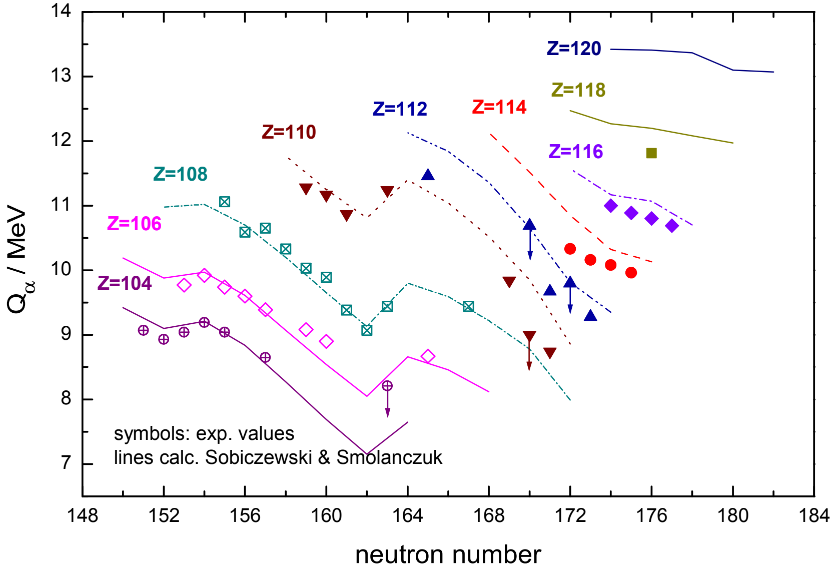


see also Jachimowicz, Kowal, Skalski, Phys. Rev. C **83**, 054302 (2011)

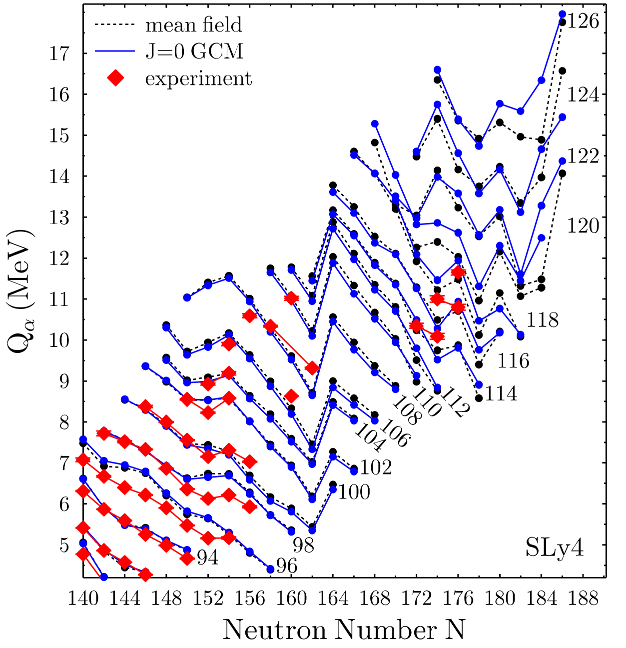
Q_{α} values and deformations fairly robust; easier to predict



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



V. Prassa et al., Phys. Rev. C86 (2012) 024317

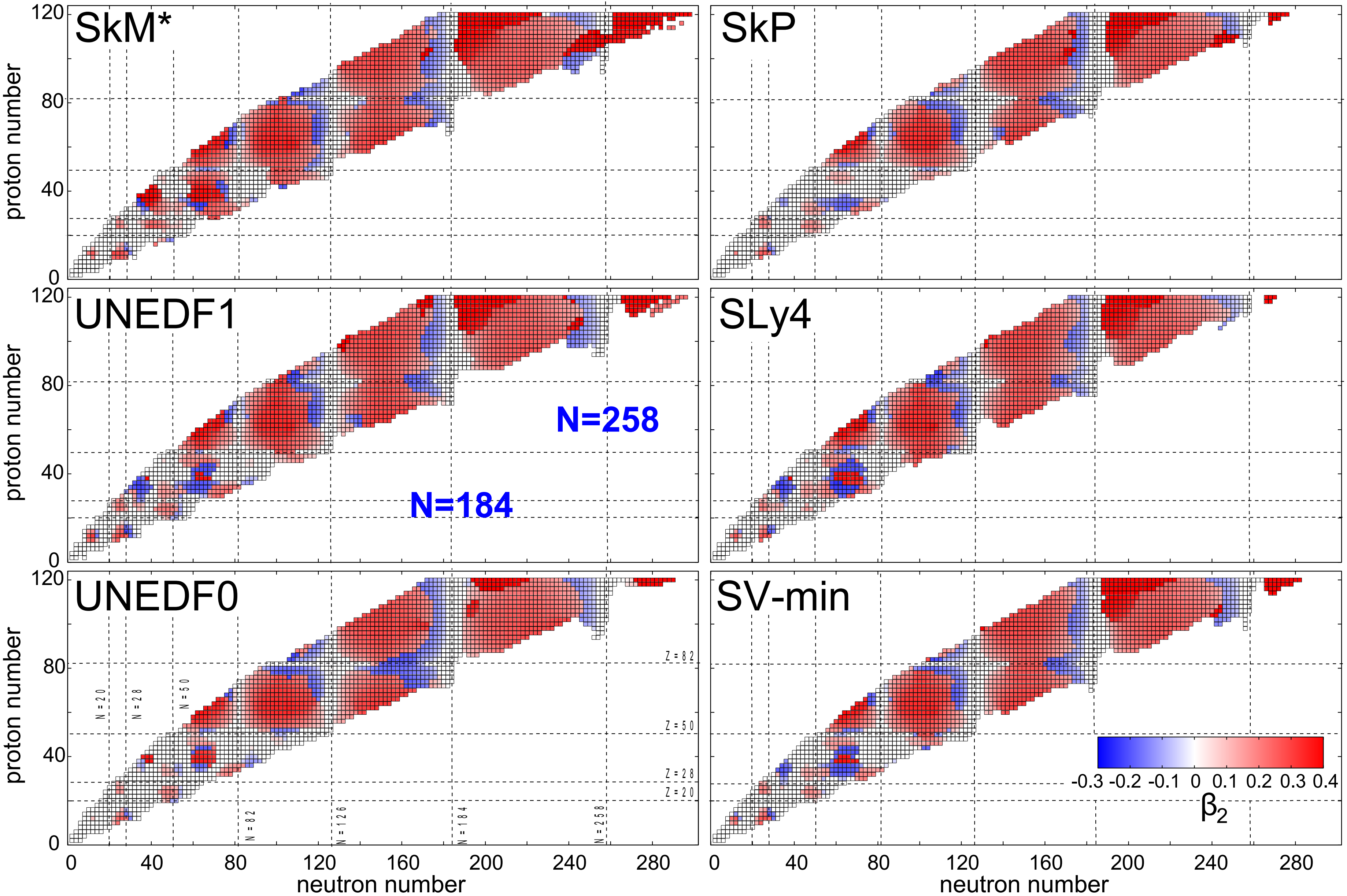


M. Bender & P.-H. Heenen, arXiv:1210.2780

Computed quadrupole ground-state shape deformations

Global behavior shows generic patterns and similar systematic trends

Erler et al., Nature 486, 509 (2012)



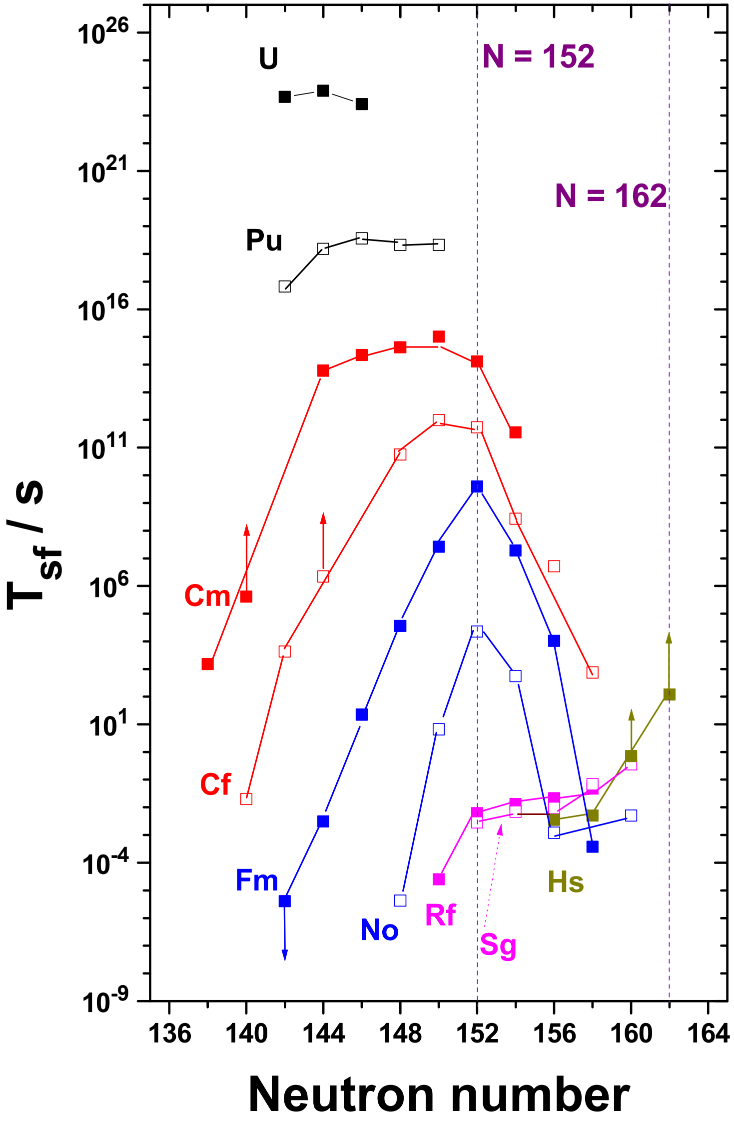
Fission: the major uncertainty

238U lives 4.5 billion years

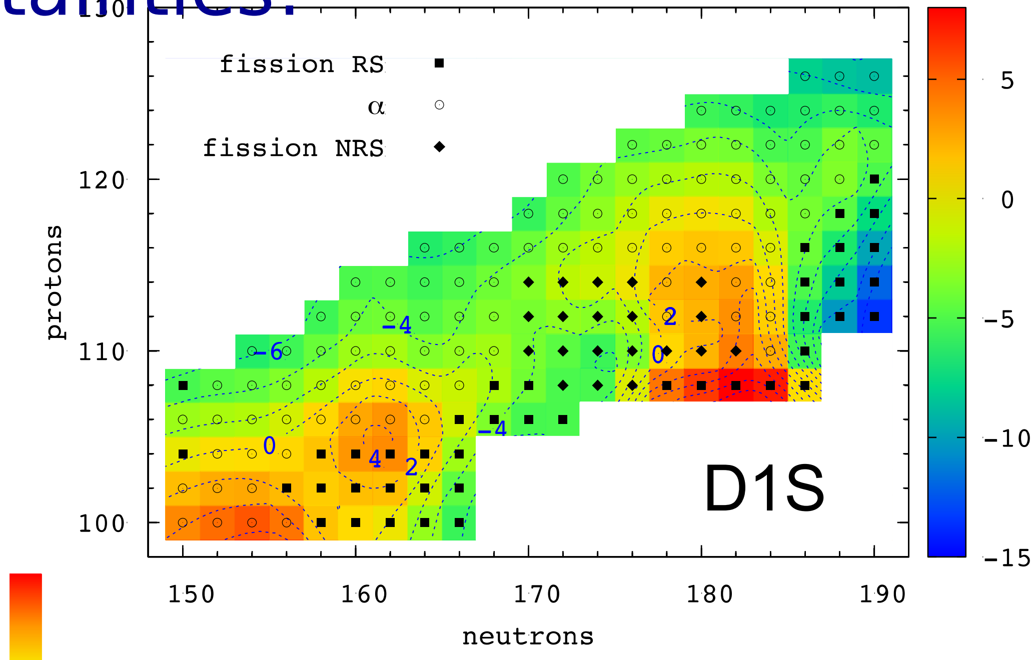
250No fissions after 4.2 µs

A huge span indeed!

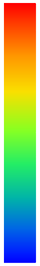
Major theoretical challenge



Spontaneous Fission Lifetimes: huge theoretical uncertainties!



M. Warda and J.L. Egido, Phys. Rev. C 86, 014322



see also: *Spontaneous fission lifetimes from the minimization of self-consistent collective action*, Jhilam Sadhukhan et al., Phys. Rev. C 88, 064314 (2013)

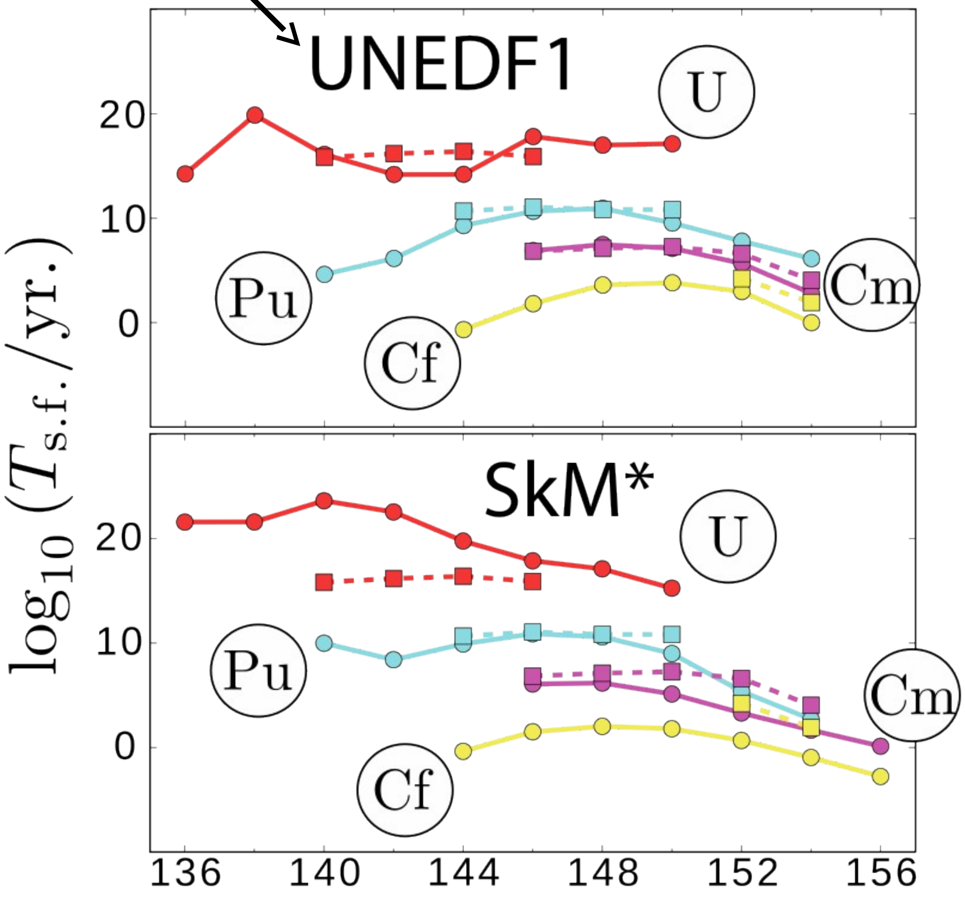
J. Erler et al, Phys. Rev. C 85, 025802 (2012)

Spontaneous Fission Lifetimes

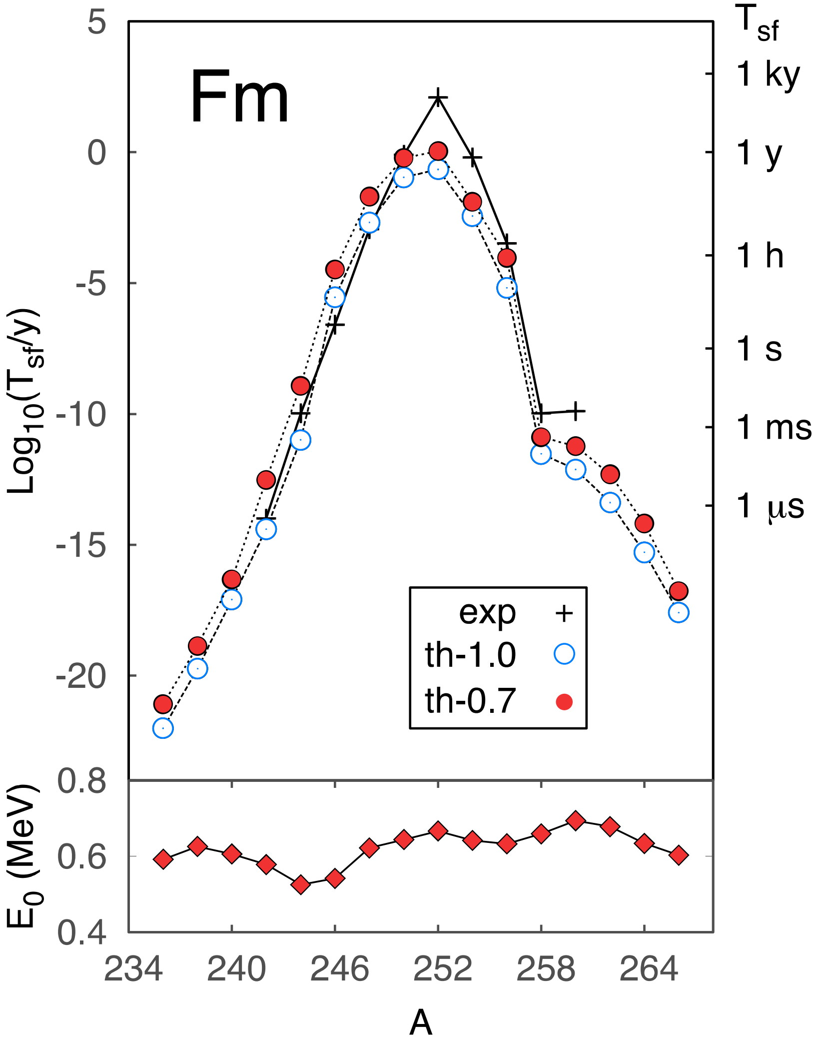
SF fission lifetimes in the actinides

Quality input

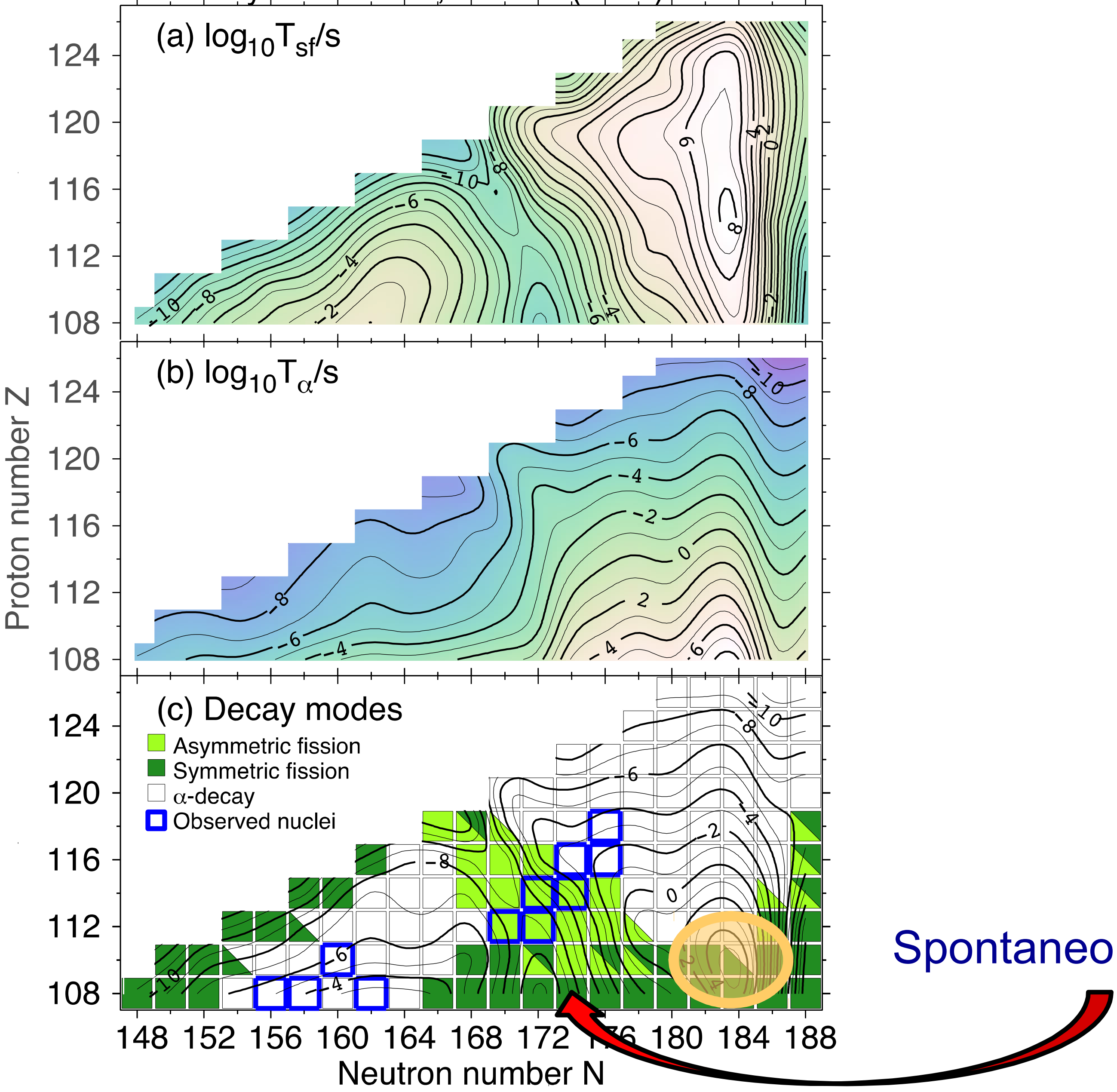
J. McDonnell et al.



A. Staszczak, A. Baran, WN,
Phys. Rev. C 87, 024320 (2013)



A. Staszczak, A. Baran, WN,
Phys. Rev. C 87, 024320 (2013)



Oganessian et al.

Spontaneous fission “Death Valley”

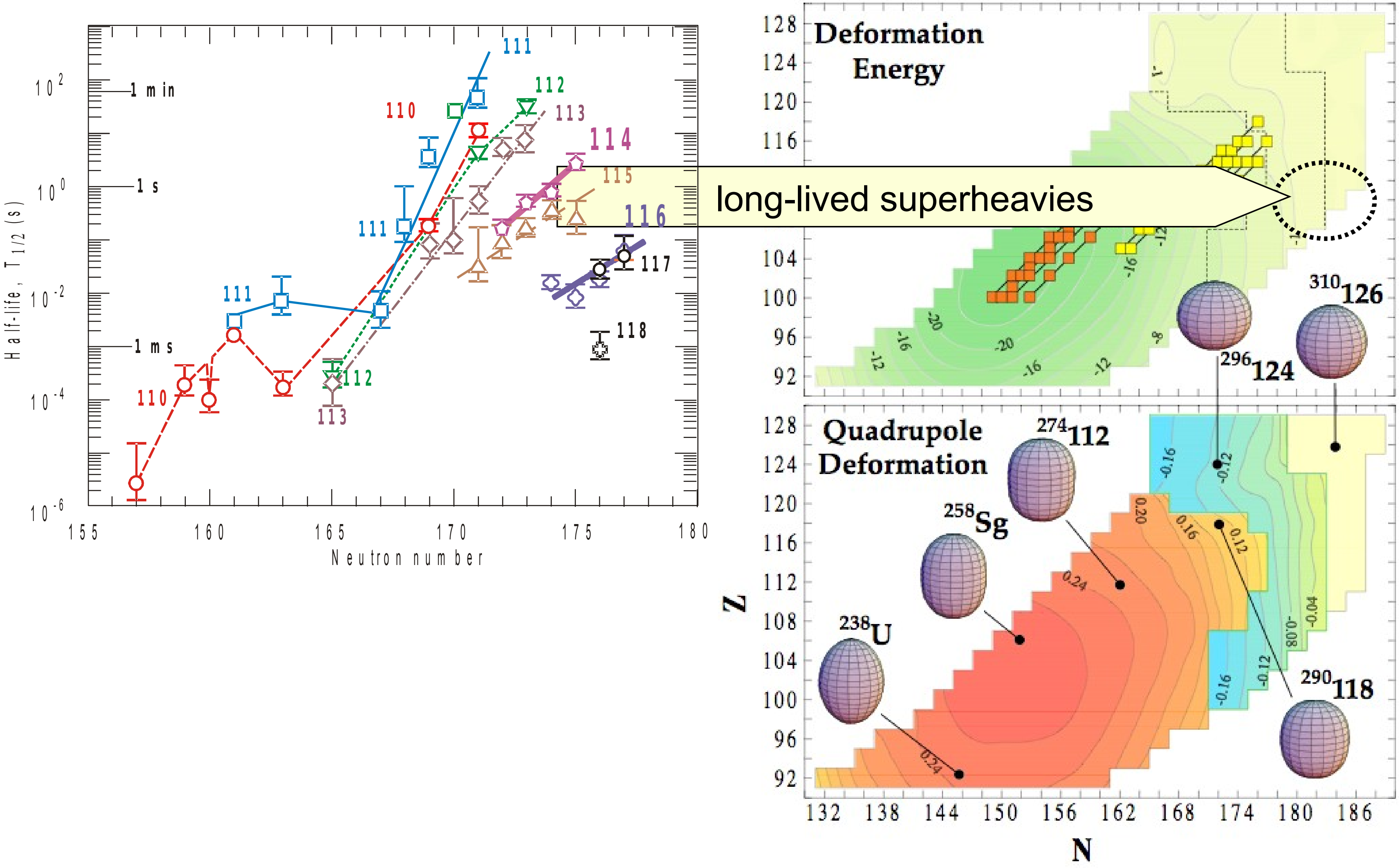
The major challenge: towards N=184

The Holy Grail

How to get there experimentally?

Towards long-lived Superheavy Nuclei

Nature, 433, 705 (2005)

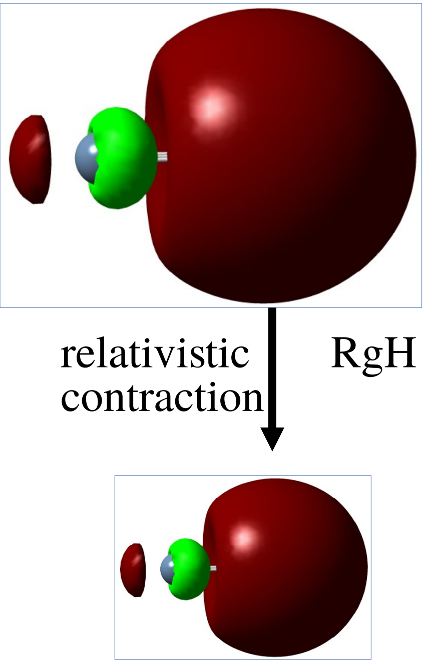


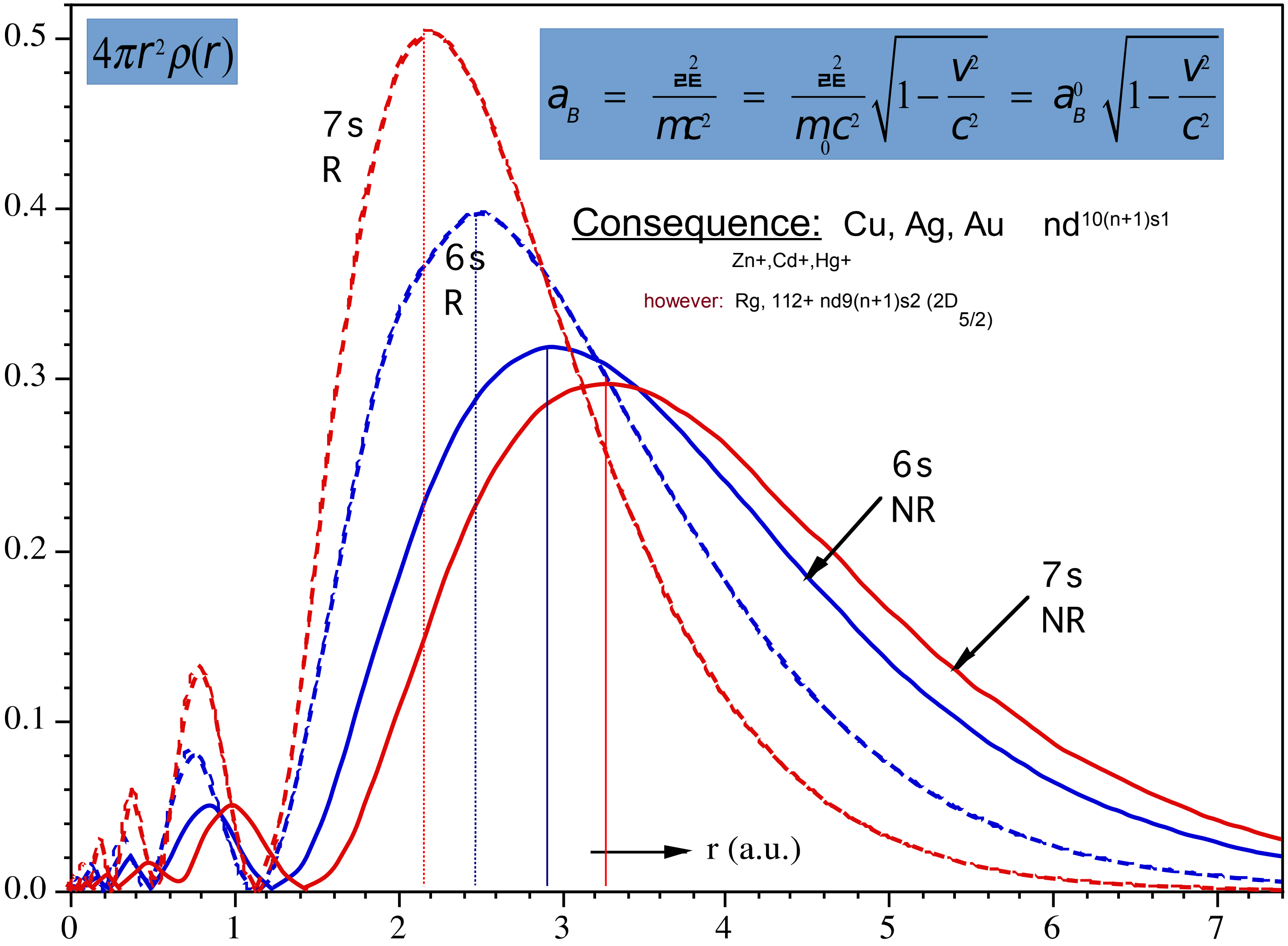
What are chemical properties of superheavy elements?

(after P. Schwerdtfeger)

Would element 137 (feynmanium) really spell the end of the periodic table?

The relativistic 7s contraction in Au and Rg





$$a_B = \frac{\hbar^2}{mc^2} = \frac{\hbar^2}{m_0 c^2}\sqrt{1-\frac{v^2}{c^2}} = a_B^0\sqrt{1-\frac{v^2}{c^2}}$$

Consequence: Cu, Ag, Au $nd^{10(n+1)s1}$

Zn+,Cd+,Hg+

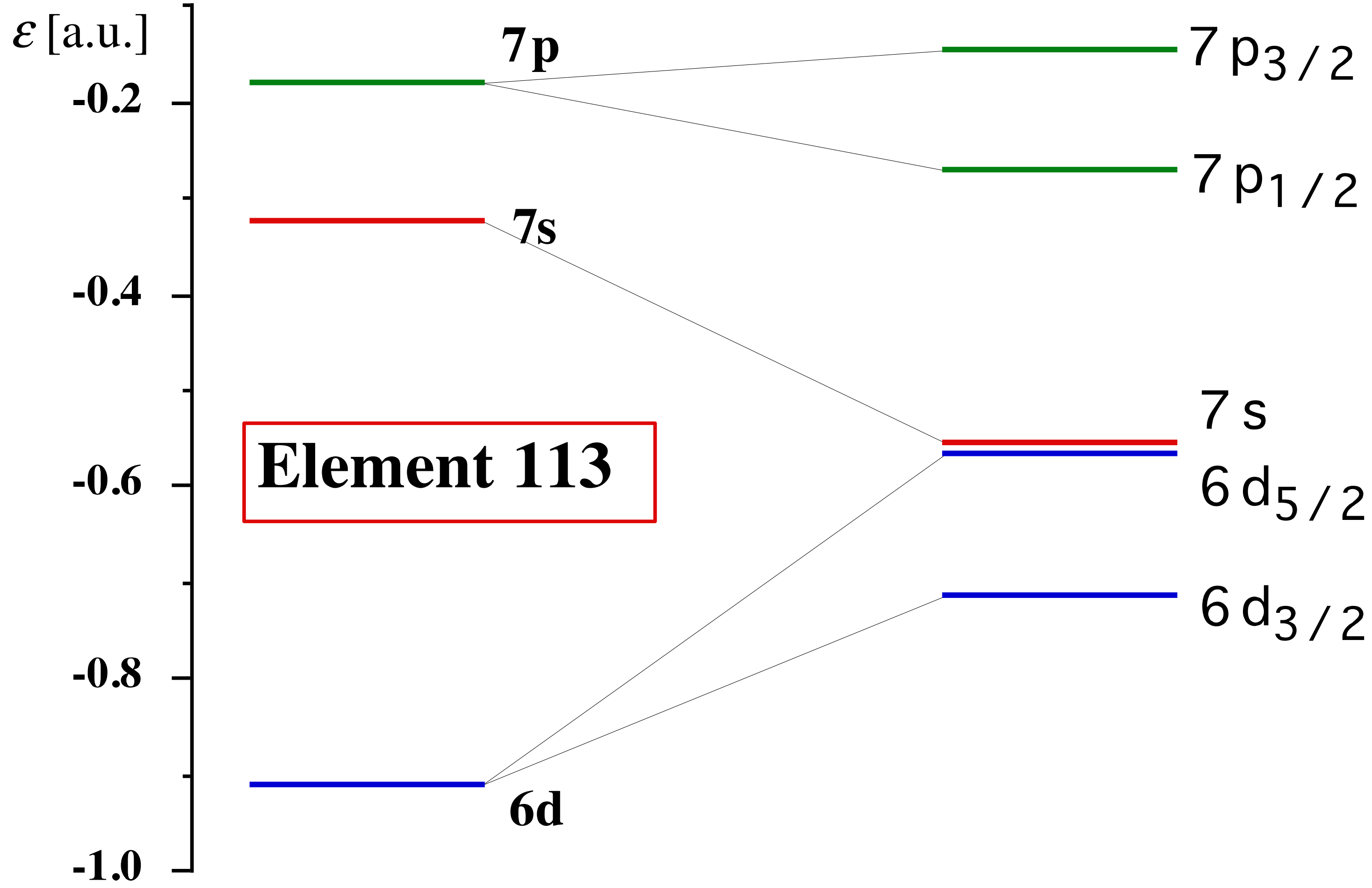
however: Rg, 112+ nd9(n+1)s2 ($2D_{5/2}$)

E. Eliav, U. Kaldor, P. Schwerdtfeger, B. Hess, Y. Ishikawa, *Phys. Rev. Lett.* 73, 3203 (1994).

M. Seth, P. Schwerdtfeger, M. Dolg, K.Faegri, B.A. Hess, U. Kaldor, *Chem. Phys. Lett.* 250, 461 (1996).

Relativistic shell-expansions and spin-orbit

Due to the increased relativistic shielding by the *s*-orbitals, the diffuse $p_{3/2}$ and higher angular momentum orbitals will expand relativistically



C. Thierfelder, P. Schwerdtfeger, A. Koers, A. Borschevsky, B. Fricke, *Phys. Rev. A* 80, 022501-1-10 (2009).

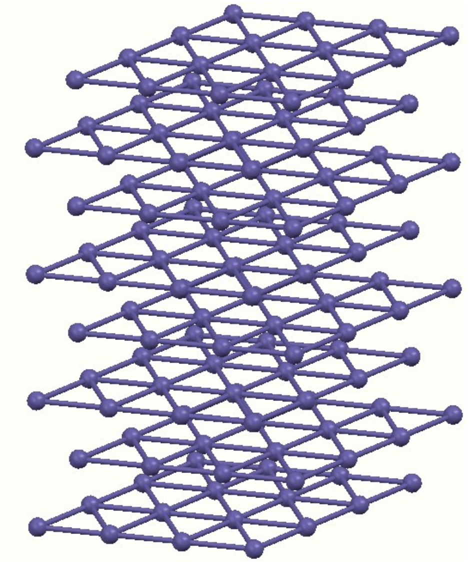
Is Copernicium a Group 12 Metal?

30
Zn
Zinc
65.409
2
8
18
2

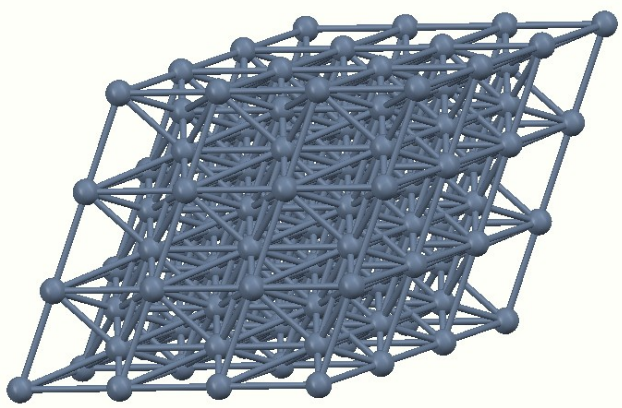
48
Cd
Cadmium
112.411
2
8
18
18
2

80
Hg
Mercury
200.59
2
8
18
32
18
2

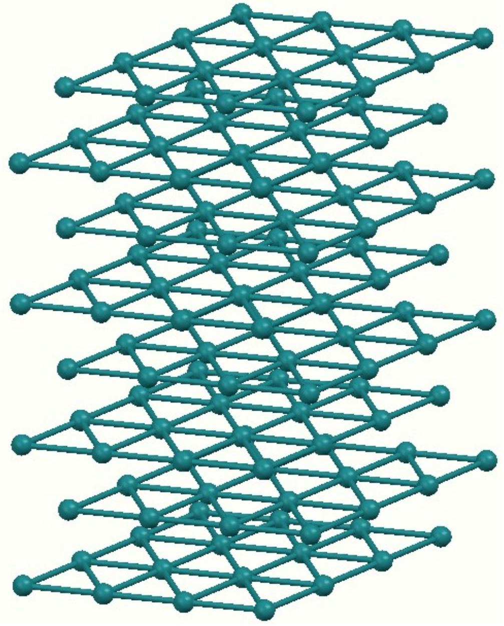
112
Cn
(285)
2
8
18
32
32
18
2



Zn, Cd (*hcp*, *P63/mmc*)



Hg (*rhomb.*, *R-3mr*)

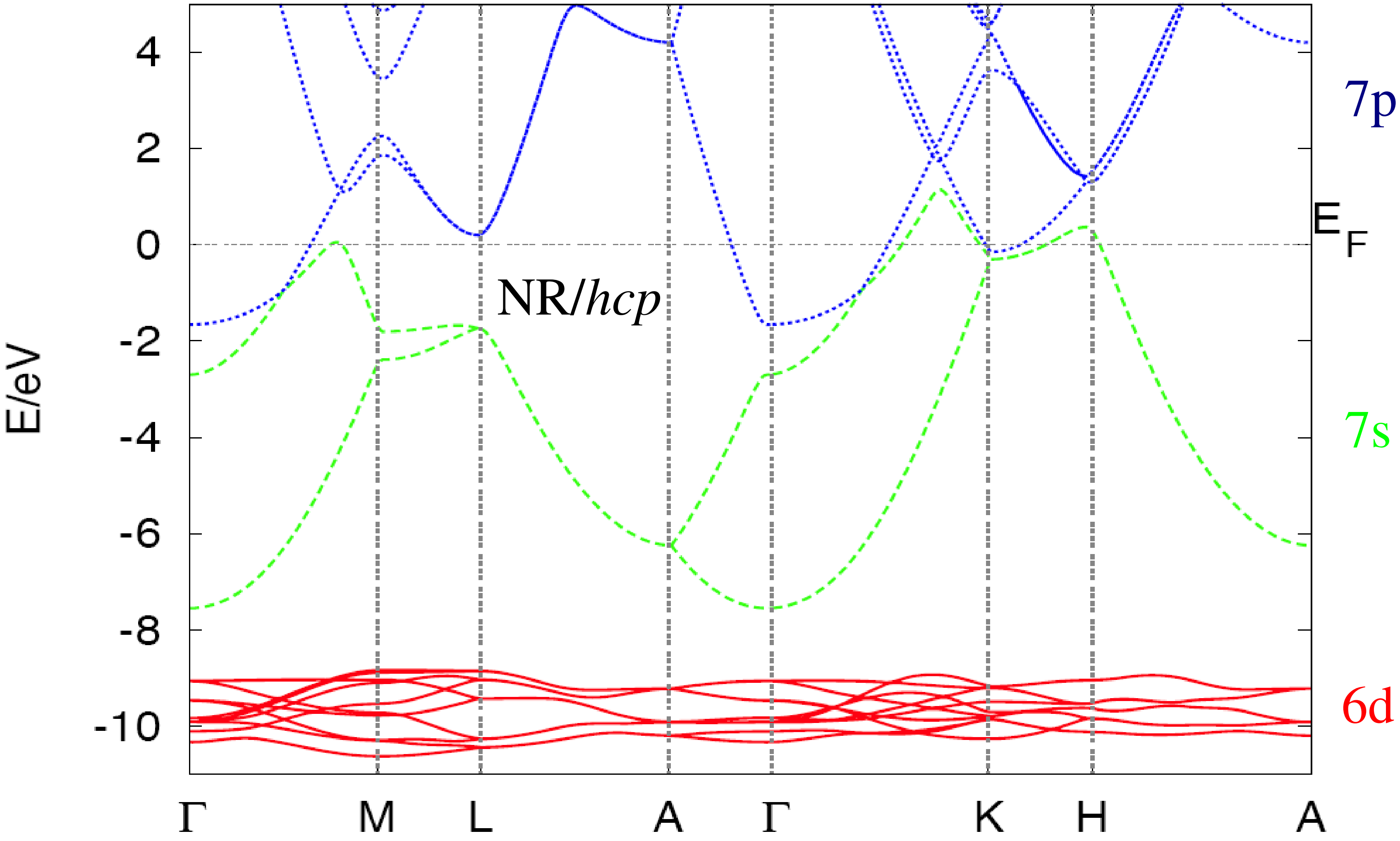


112 (*hcp*, *P63/mmc*)

?

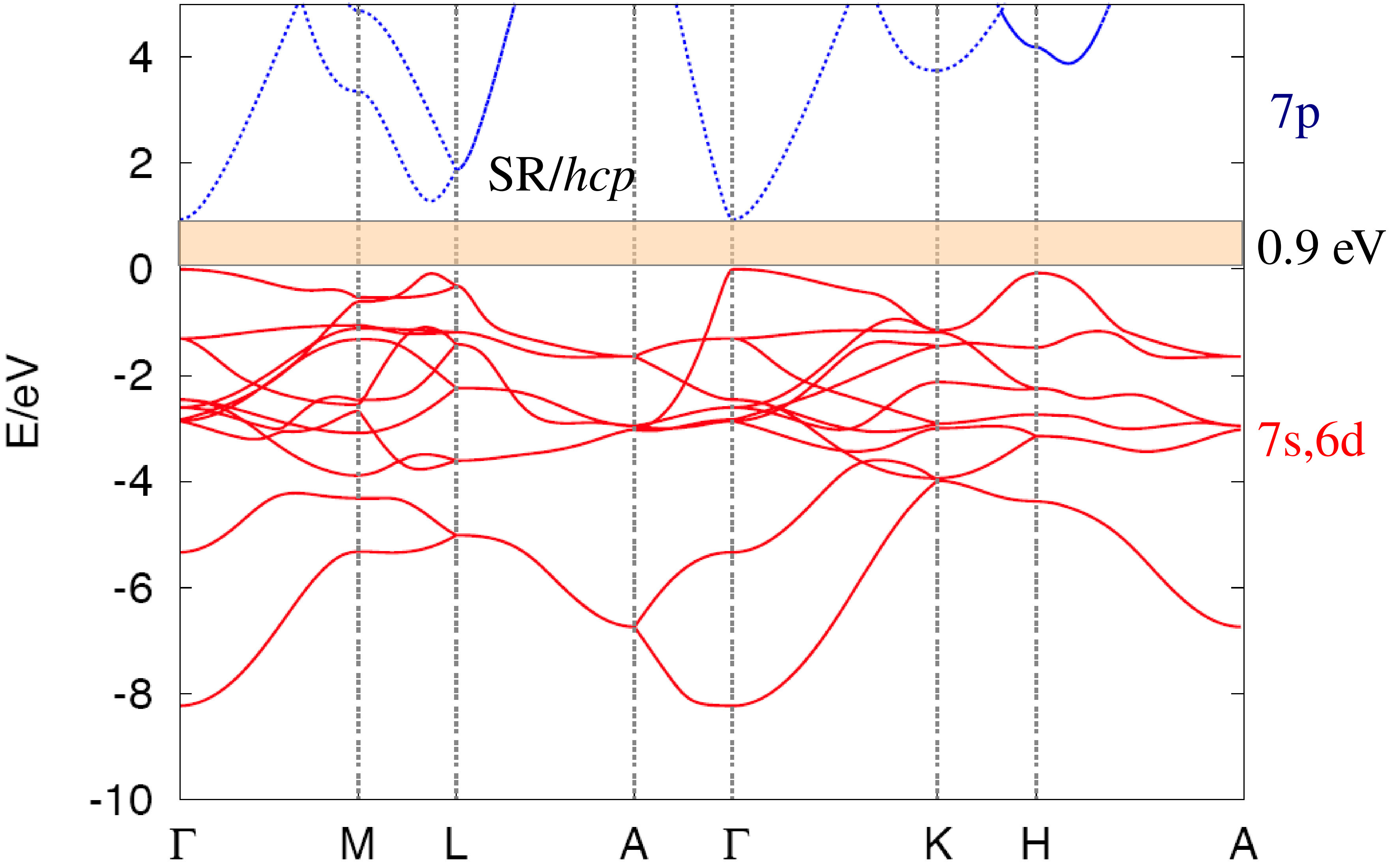
N. Gaston, I. Opahle, H. W. Gäggeler, P. Schwerdtfeger, *Angew. Chem. Int. Ed.* 46, 1663 (2007).

Band Structure of Copernicium



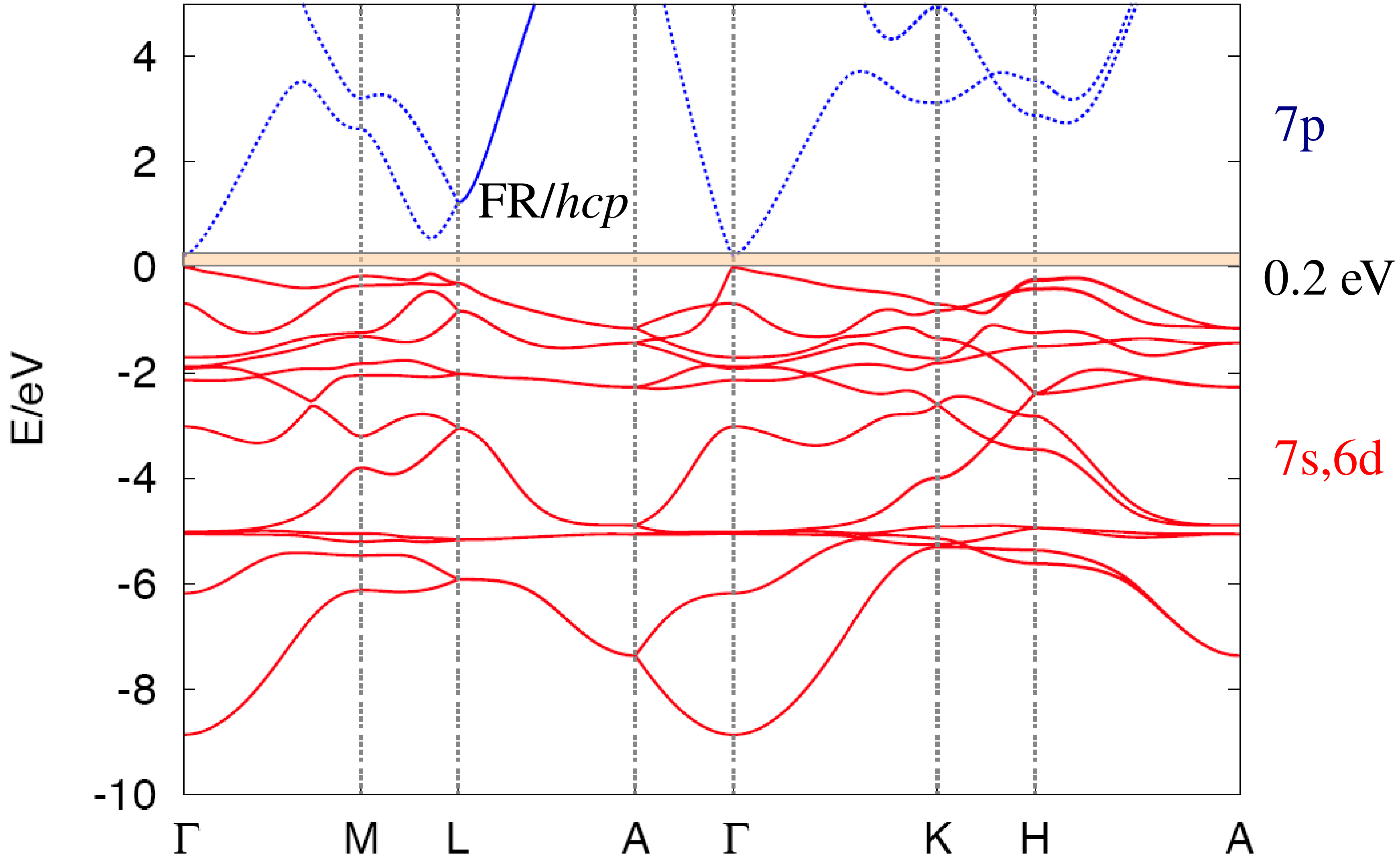
➡ Metal at the nonrelativistic level (as is Zn, Cd and Hg)

Band Structure of Copernicium



➡ Insulator at the scalar relativistic level

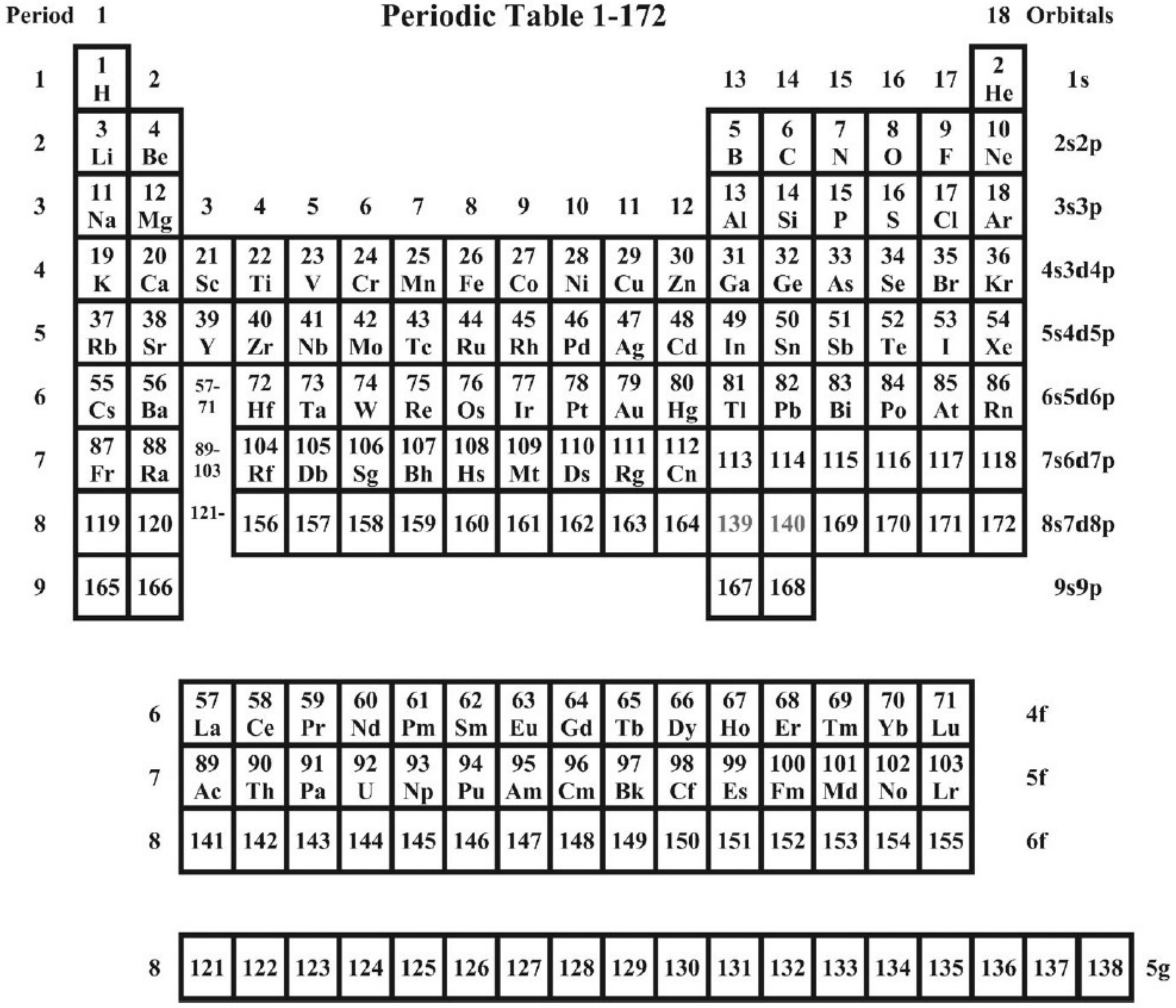
Band Structure of Copernicium



→ Semiconductor at the fully relativistic level (cohesive energy similar to Hg)

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)

$$Z\alpha \to 1$$



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"

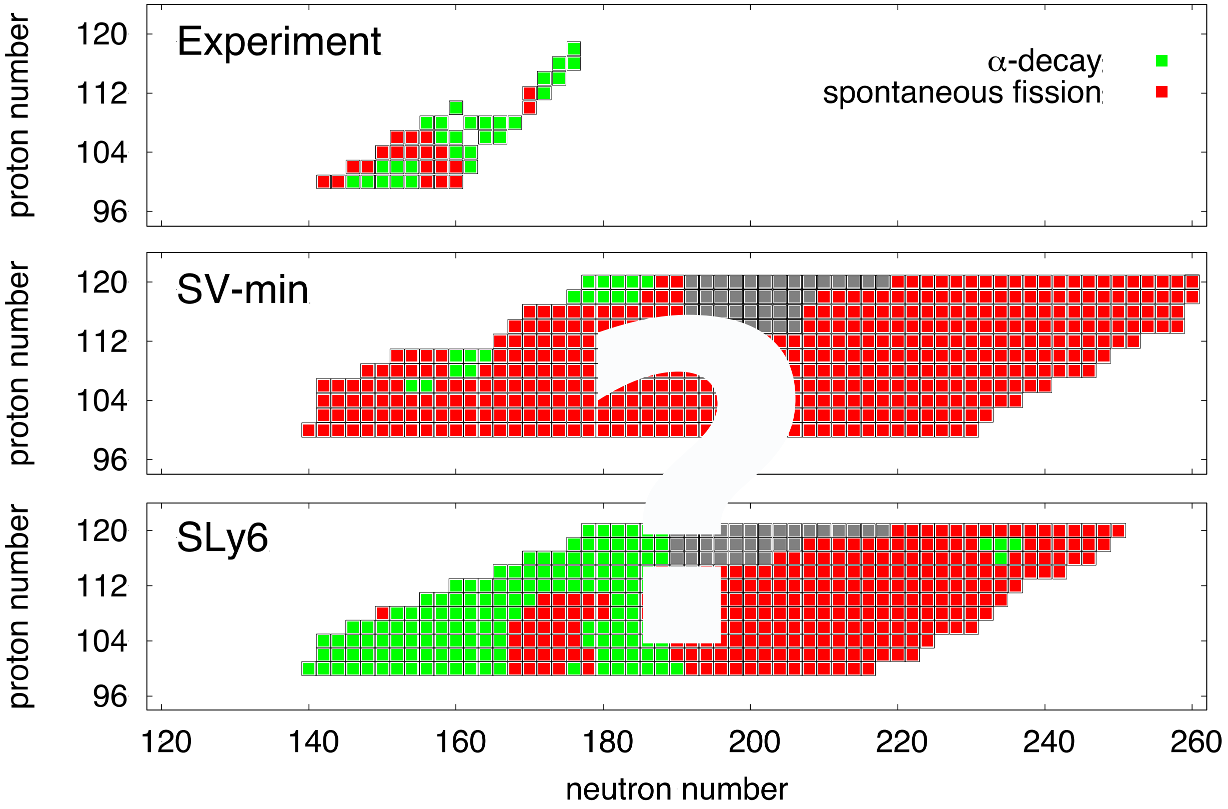
The limit of mass and charge is still undiscovered. We don't know what it looks like and that's the challenge.

Are superheavy nuclei produced in stellar explosions?

Fission of neutron rich nuclei impacts the formation of heavy elements at the final stages of the r-process through the recycling mechanism. The fission recycling is believed to be of particular importance during neutron star mergers where free neutrons of high density are available.

Super-heavy nuclei can be formed in the r-process. But their yields strongly depend on predicted nuclear data and astrophysical scenario.

I.V. Panov et al., A&A 513, A61 (2010).



Fission properties for r-process nuclei

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

N. Nikolov et al., Phys. Rev. C 83, 034305 (2011)

What have we learned so far?

- Elements up to Z=118 do exist
- Their stability is governed by alpha decay and spontaneous fission – consistent with theoretical expectations
- Their half-lives increase with *N* – consistent with theoretical expectations
- Their chemical properties can be investigated

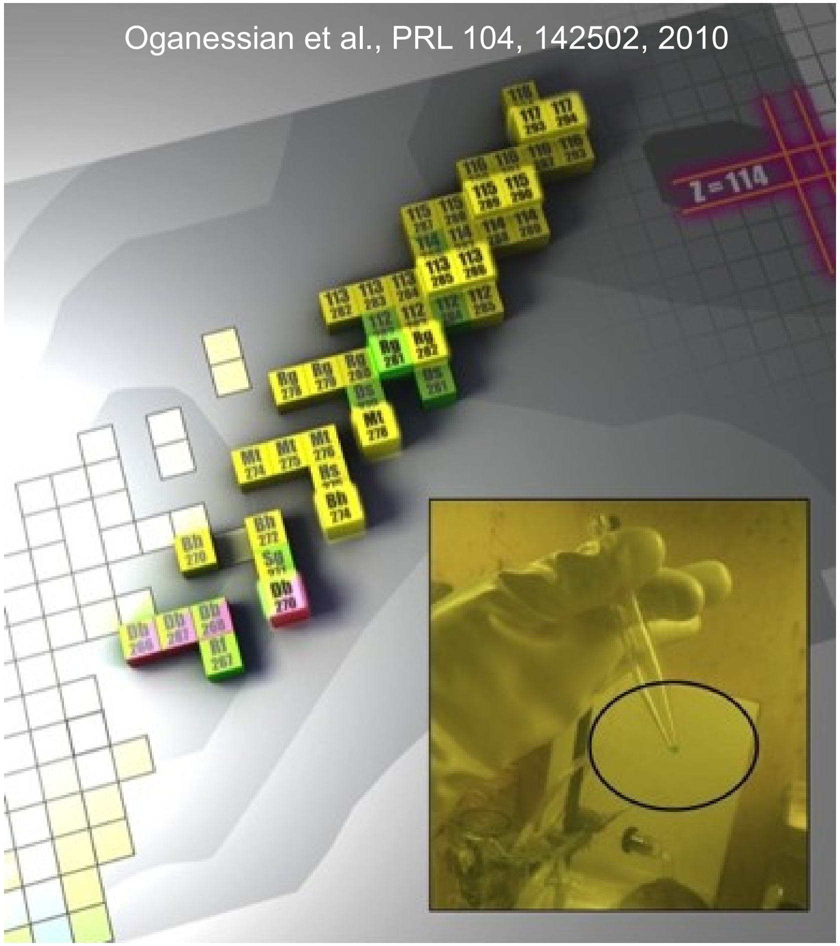
Conclusions

- Cool multi-scale science
- International collaboration
- Importance of basic research

SHE – international collaboration

The superheavy element Z=117 required coordinated collaborative efforts between US and Russia laboratories and nearly 3 years to achieve.

- Production of the berkelium-249 target material, with a short half-life of $T_{1/2}$ = 330 days, required an intense neutron irradiation at the High Flux Isotope at ORNL, chemical separation from other reactor-produced products including californium-252 at ORNL
- Target fabrication in Dimitrovgrad, Russia
- Six months of accelerator bombardment with an intense calcium-48 beam at Dubna
- Analysis of the experimental data was performed independently at Dubna and Lawrence Livermore National Laboratory.


Oganessian et al., PRL 104, 142502, 2010

REC SEP @ SHE CHEM

TASCA

International Cooperation on the TASCA Recoil Separator for Transactinide Chemistry and Physics

Australia: ANU; **China**: Lanzhou; **Finland**: Jyväskylä; **Germany**: GSI, Mainz, Munich; **India**: Kolkata; **Japan**: Niigata, Tokai, RIKEN; **Norway**: Oslo; **Poland**: Warsaw; **Russia**: St. Petersburg; **Sweden**: Göteborg, Lund; **Switzerland**: Bern, PSI; **UK**: Surrey, Liverpool; **USA**: Berkeley, LLNL, ORNL, Tennessee

Conclusions: Importance of basic research

(based on D. Geesaman's IUPAP slides)