Theoretical Models for Superheavy Nuclei - Energy Density Functionals

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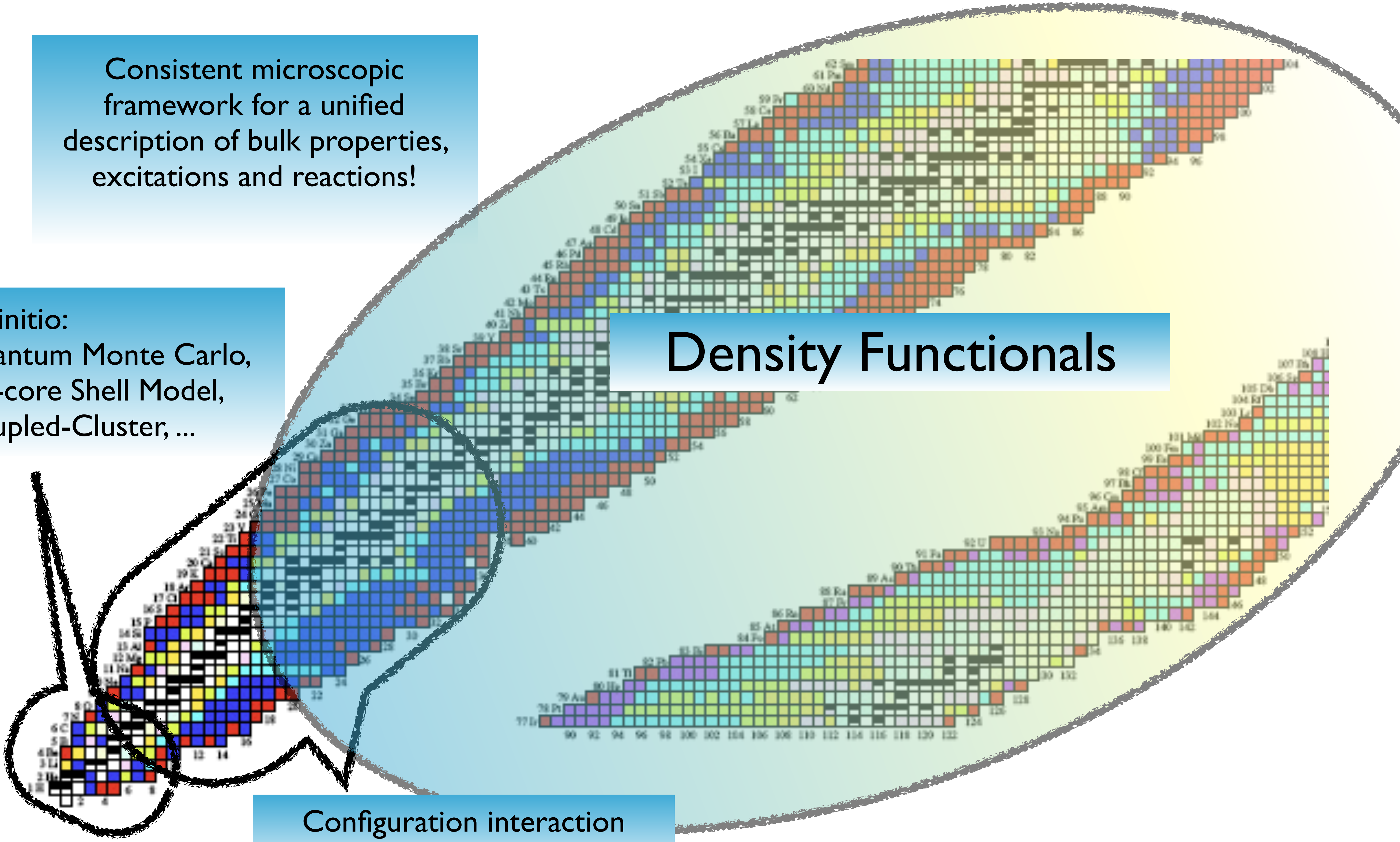
Energy Density Functionals

Consistent microscopic framework for a unified description of bulk properties, excitations and reactions!

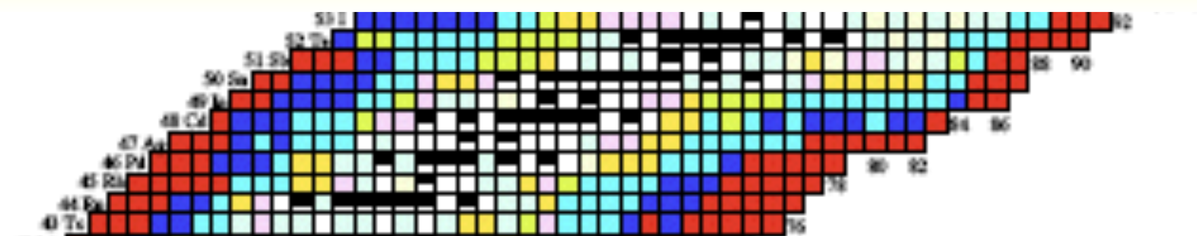


Ab initio:
Quantum Monte Carlo,
No-core Shell Model,
Coupled-Cluster, ...

Configuration interaction
(Interacting Shell-Model)

Energy Density Functionals

✔ the quantum many-body problem is effectively mapped onto a ***one-body problem*** without explicitly involving inter-particle interactions!



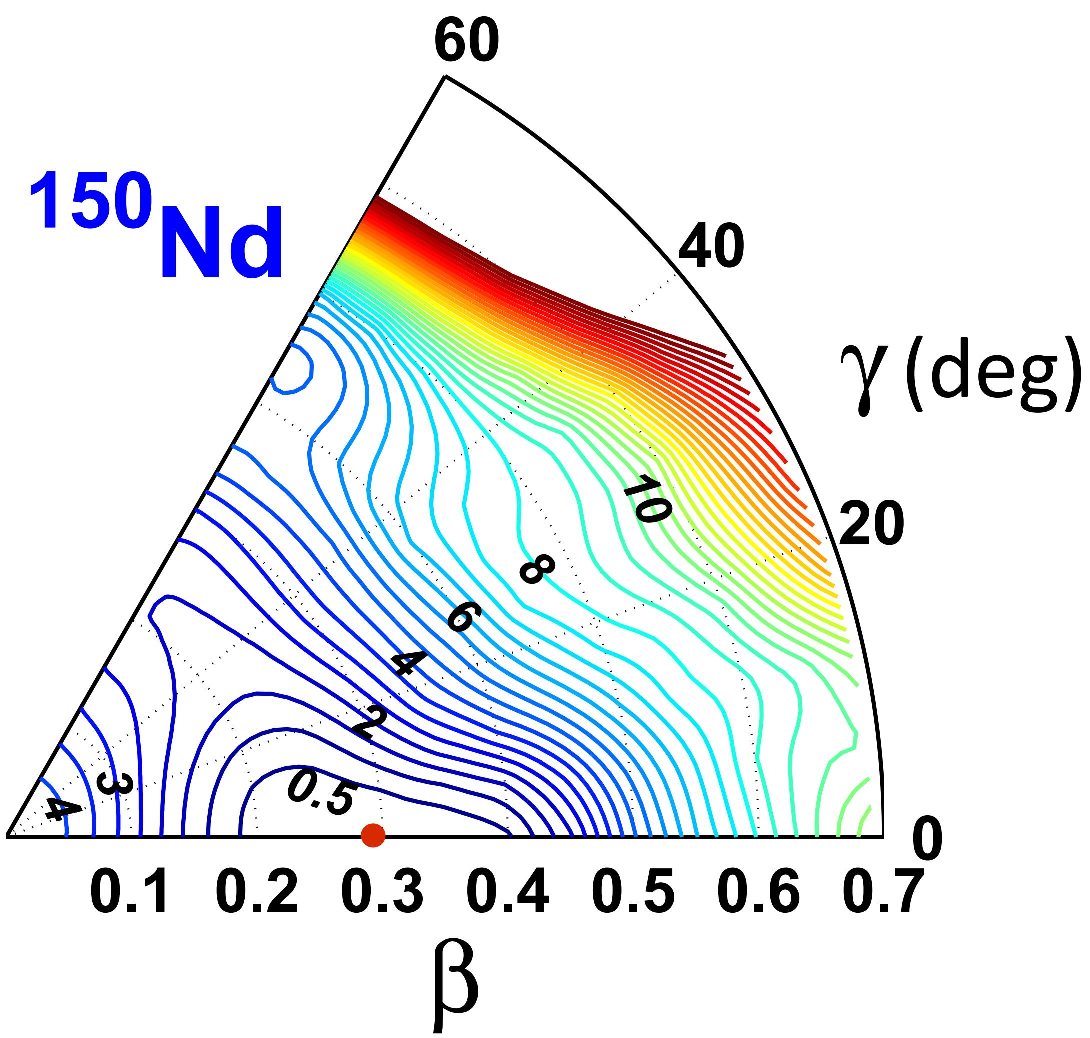
✔ the exact density functional is approximated with ***powers and gradients of ground-state densities and currents.***

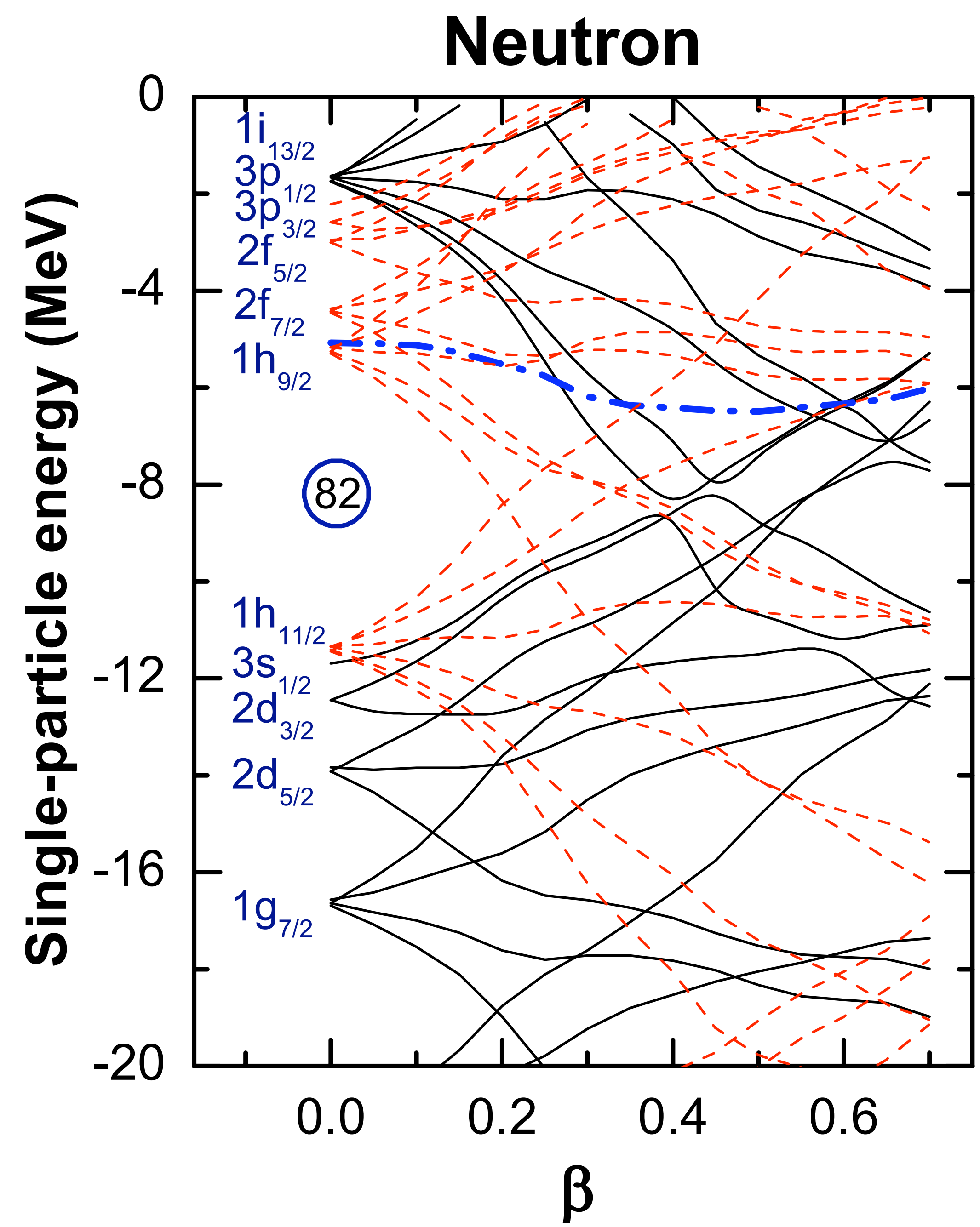
✔ ***universal density functionals*** can be applied to all nuclei throughout the chart of nuclides.

Important for extrapolations to regions far from stability!

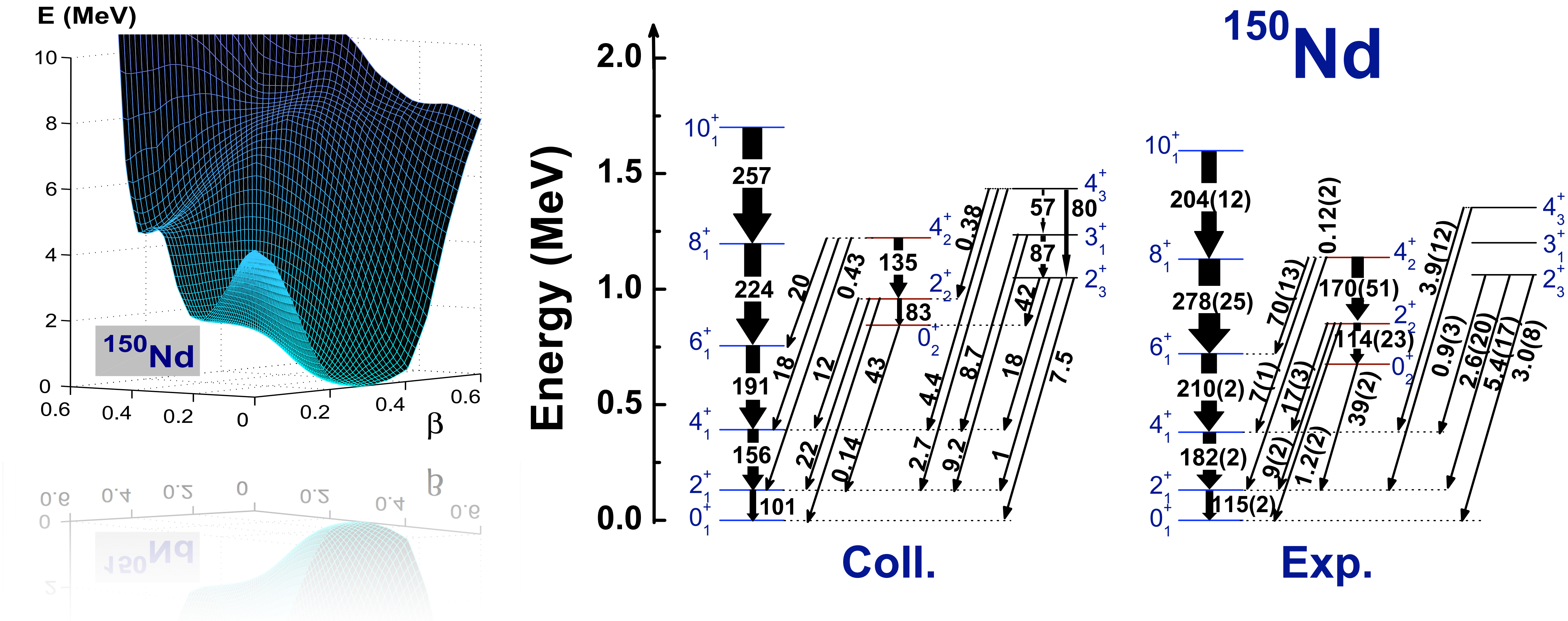
Self-Consistent Mean-Field Models based on EDFs

✔ an intuitive interpretation of mean-field results in terms of ***intrinsic shapes*** and ***single-particle states.***





✔ fully microscopic input for structure models that include collective correlations (RPA, GCM, collective Hamiltonian) ➜ ***spectroscopic properties that can be directly compared to data!***



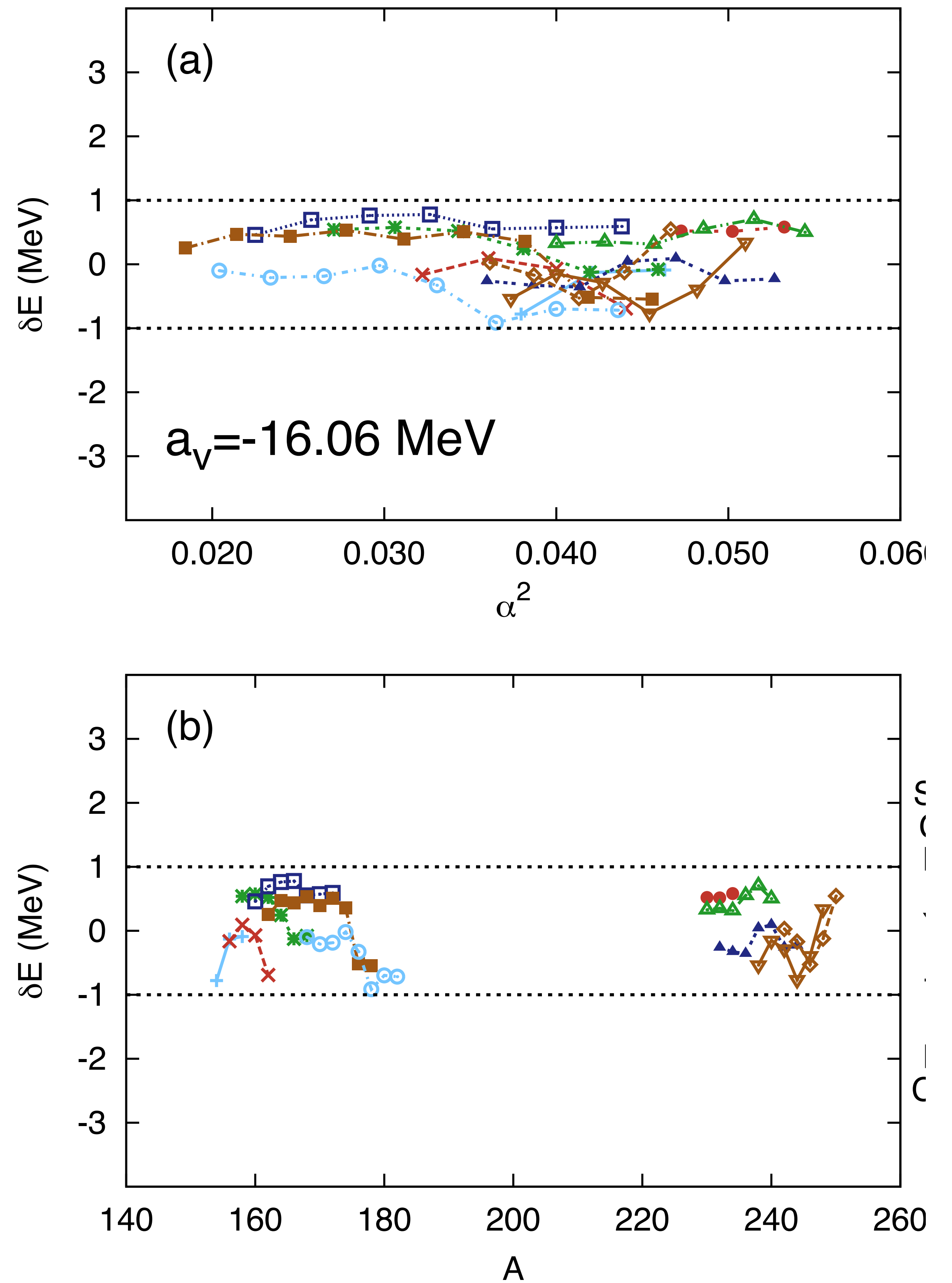
✔ ***full model space*** of occupied states ➜ no distinction between core and valence nucleons, ***no need for effective charges!***

DD-PC1

➠ semi-empirical relativistic energy density functional

➠ based on a (semi-empirical) nuclear matter EOS.

➠ parameters adjusted in self-consistent mean-field calculations of masses of *64* axially deformed nuclei in the mass regions A ~ 150-180 and A ~ 230-250.



T. NIKŠIĆ, D. VRETENAR, AND P. RING
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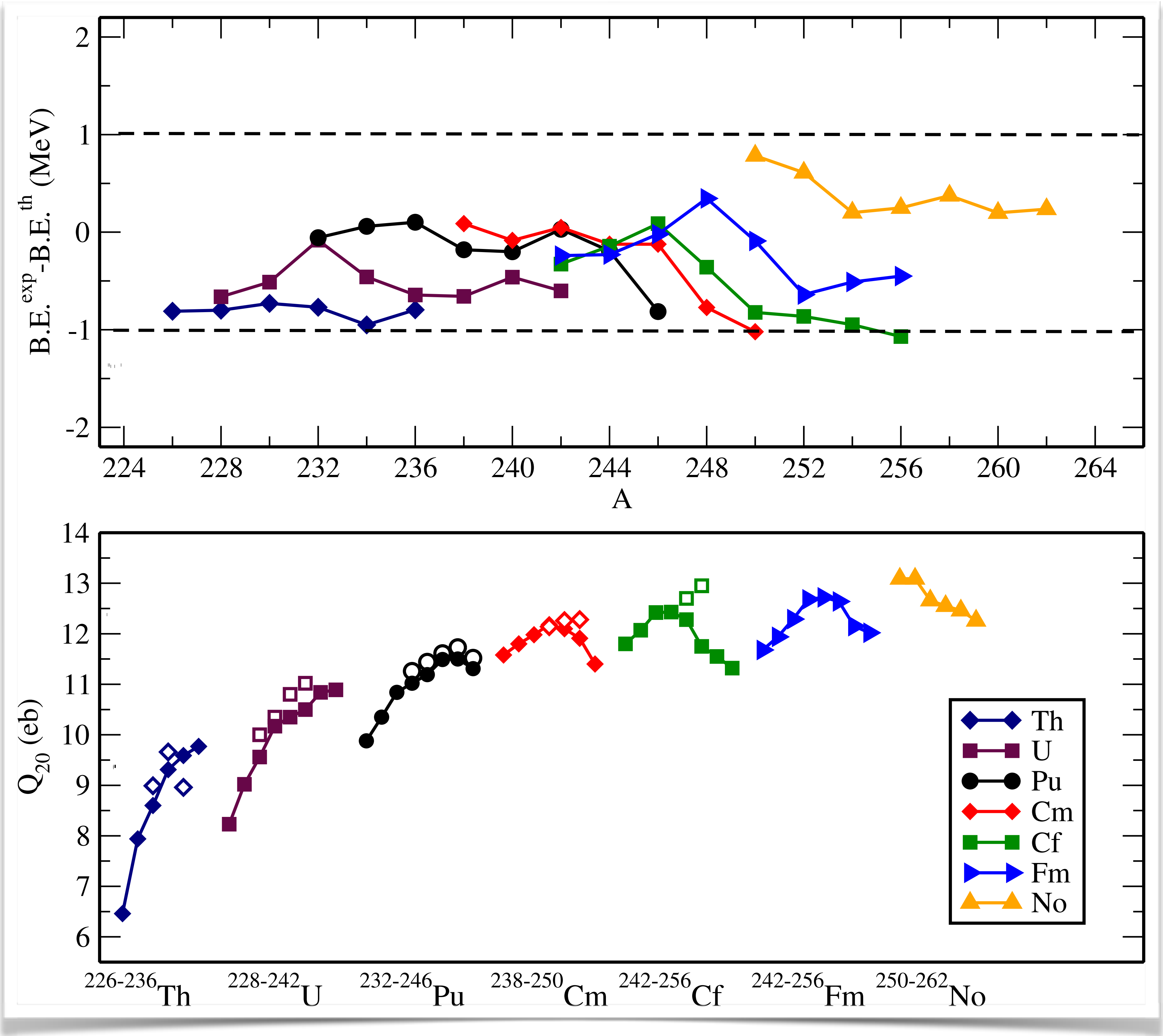
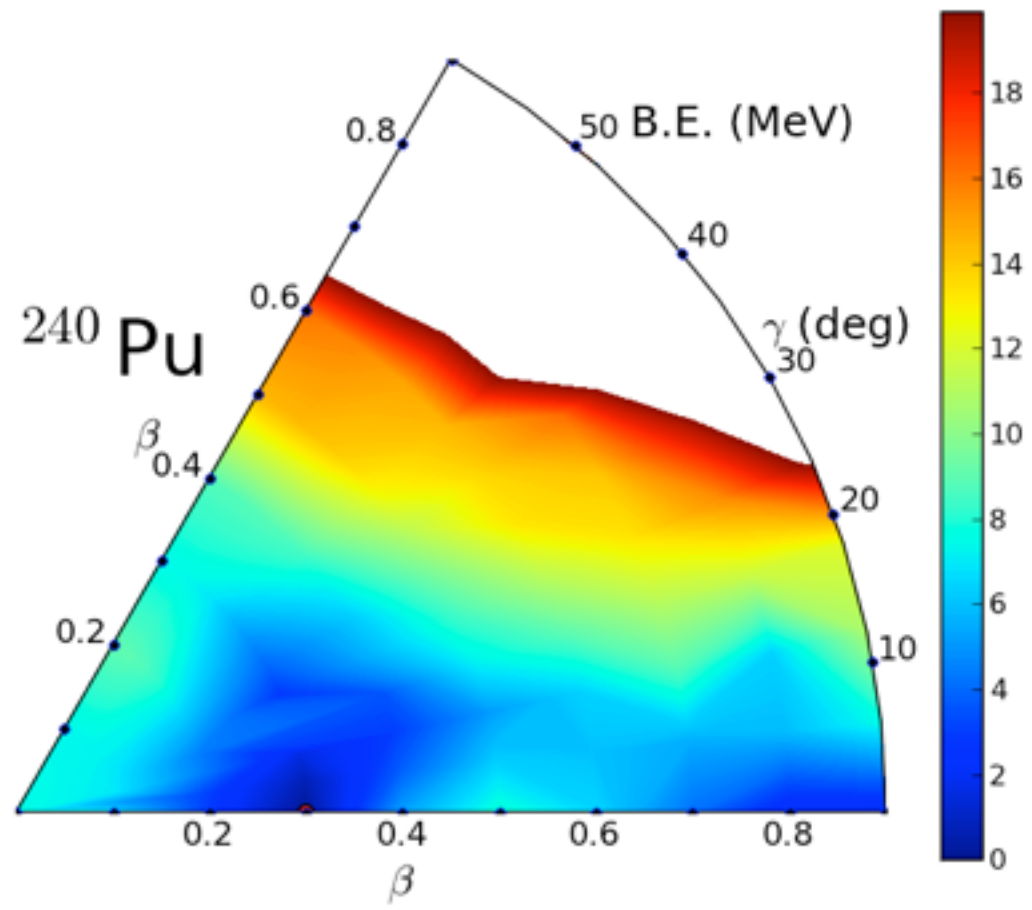
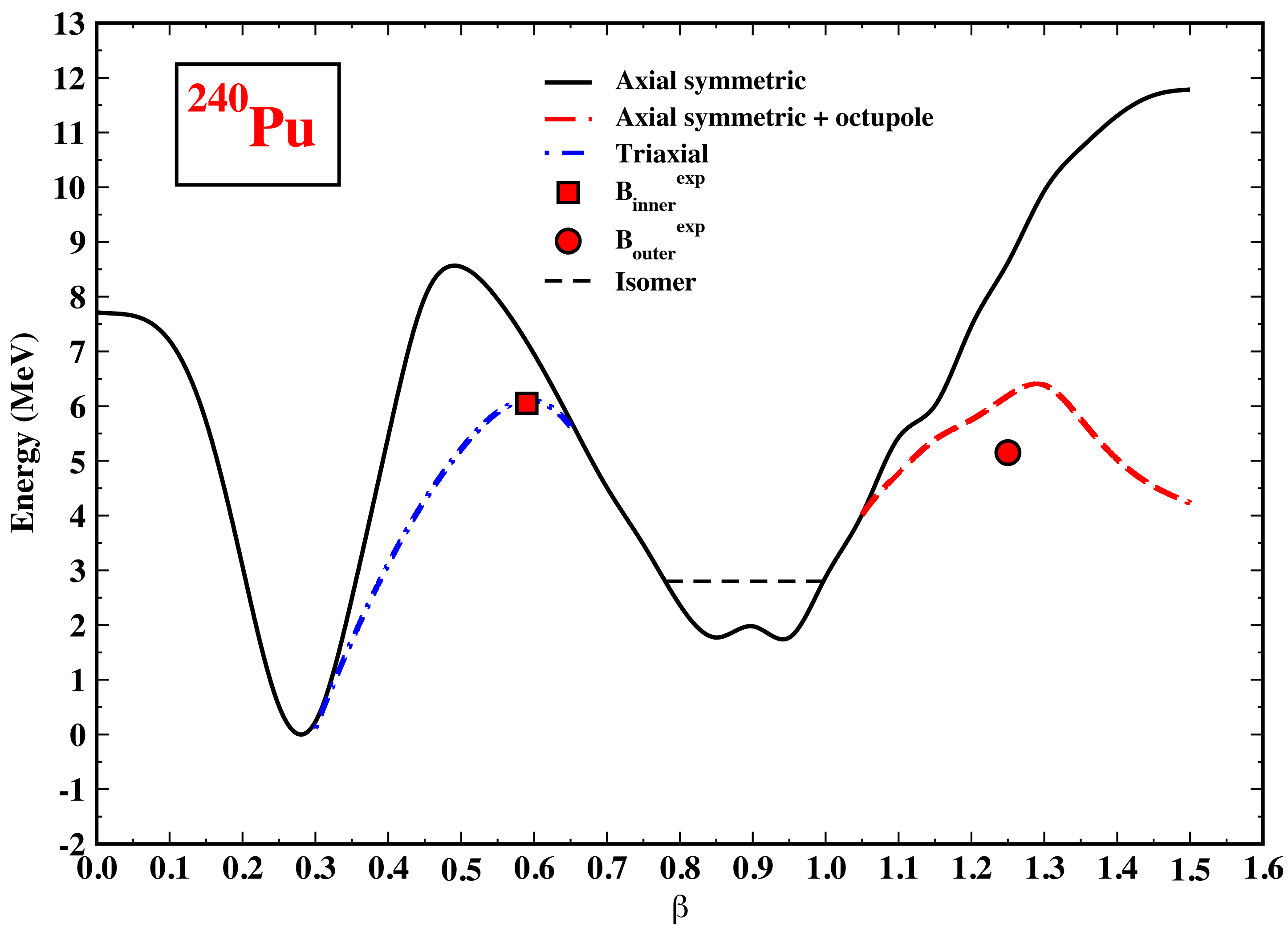
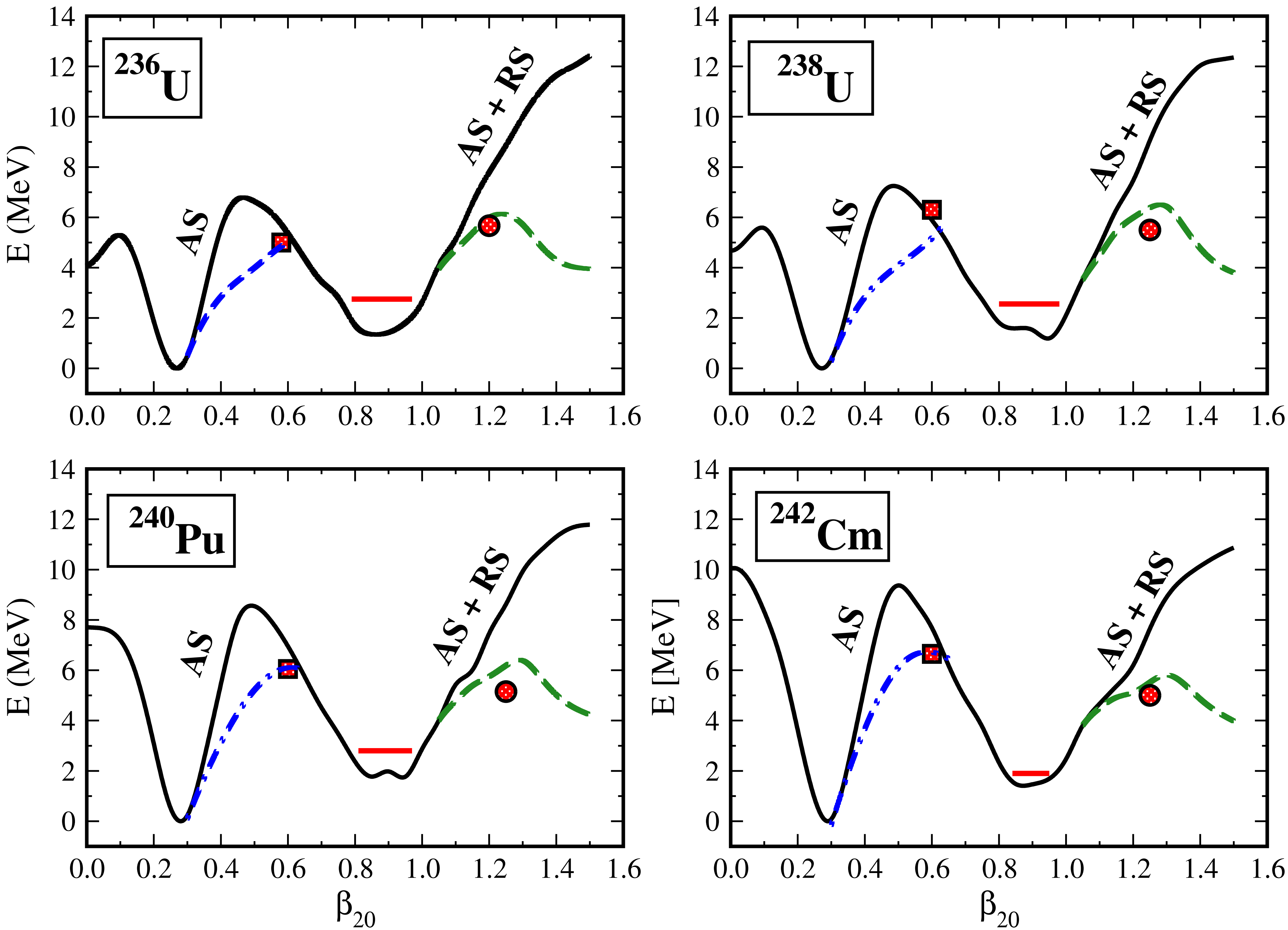
Test: ground-state properties of actinides



Test: "double-humped" fission barriers of actinides

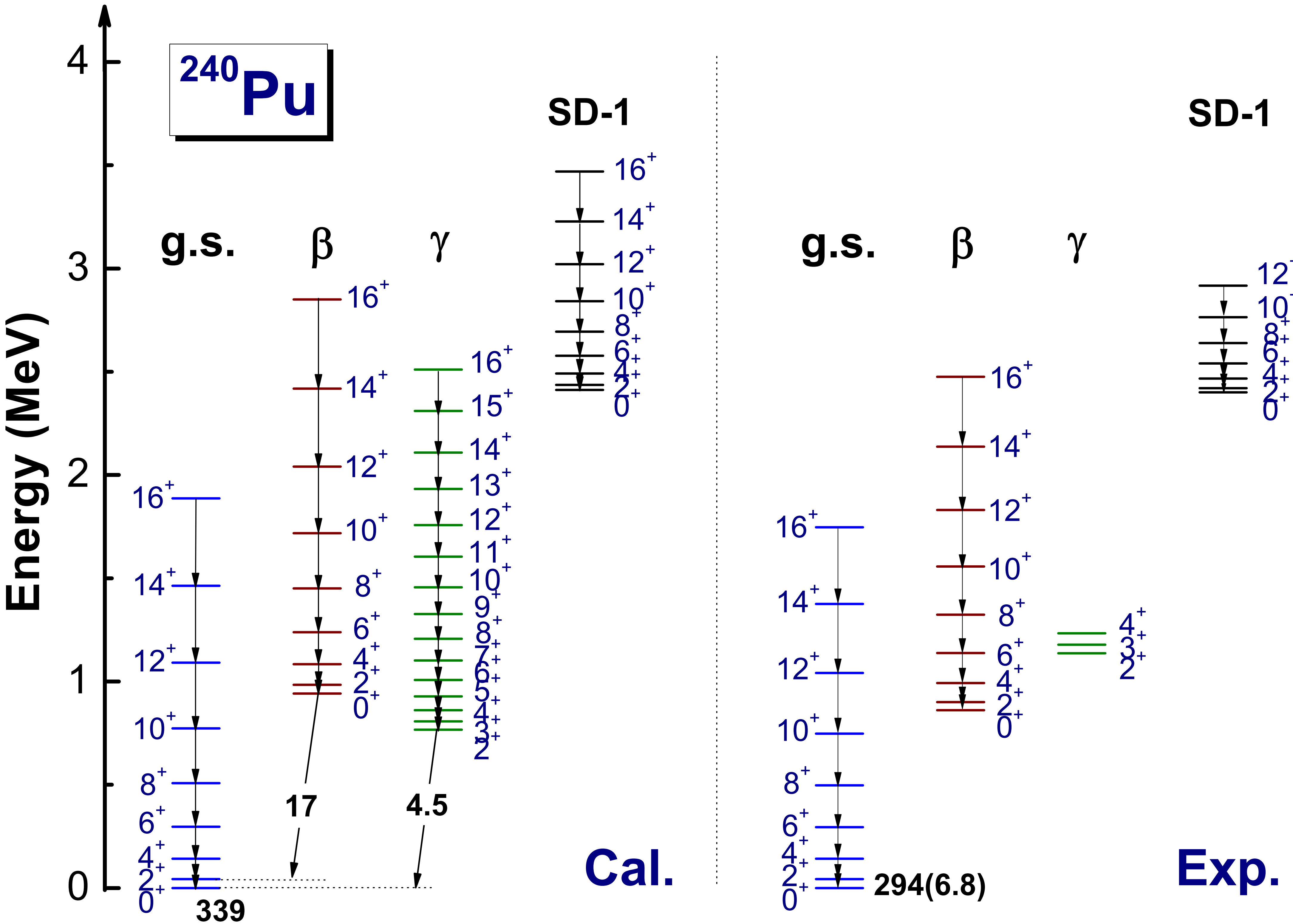






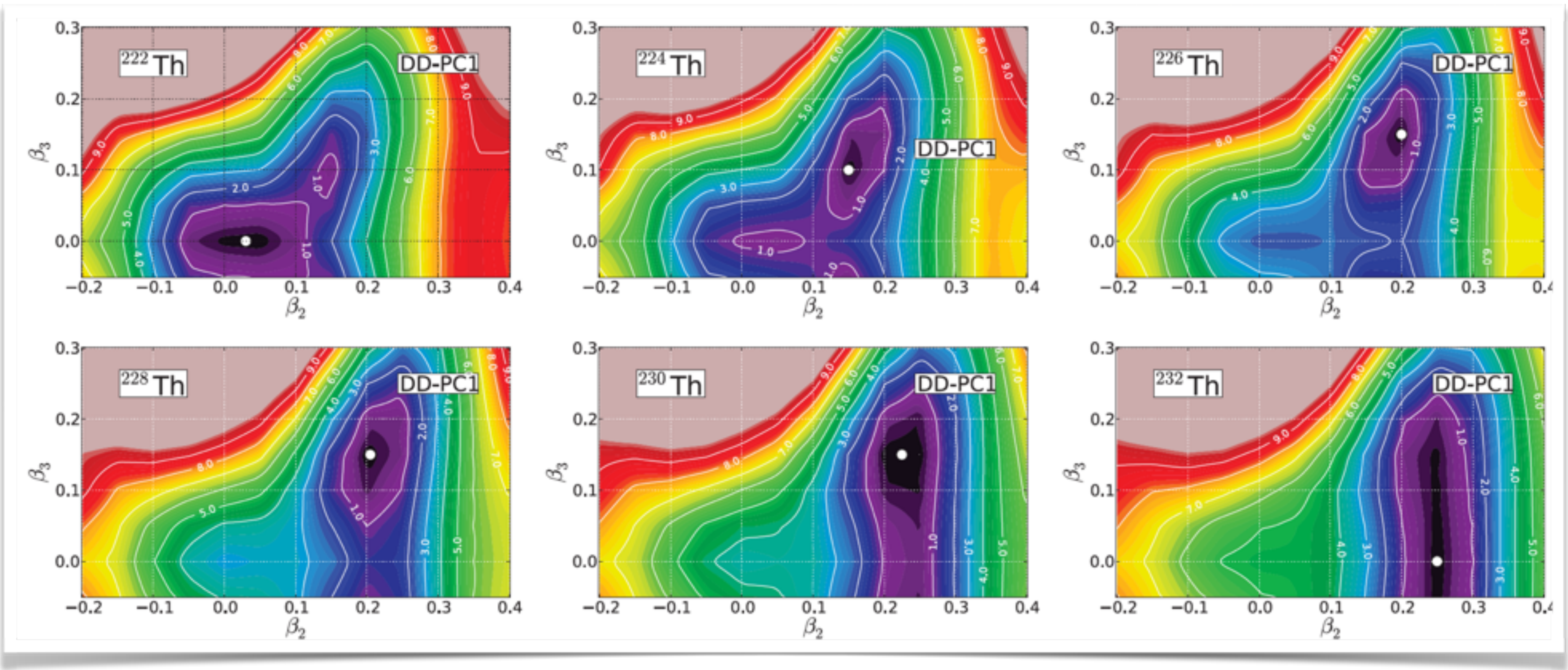
236U
AS
AS + RS
E (MeV)
238U
240Pu
242Cm
E [MeV]
β20
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6
0 2 4 6 8 10 12 14

$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 3.33 \qquad E^{exp}_{4_1^+}/E^{exp}_{2_1^+} = 3.31$$



Quadrupole-octupole shape transitions in actinide nuclei

Axially symmetric deformation energy surfaces of $^{222-232}$Th in the (β_2,β_3) plane:



NOMURA, VRETENAR, NIKŠIĆ, AND LU

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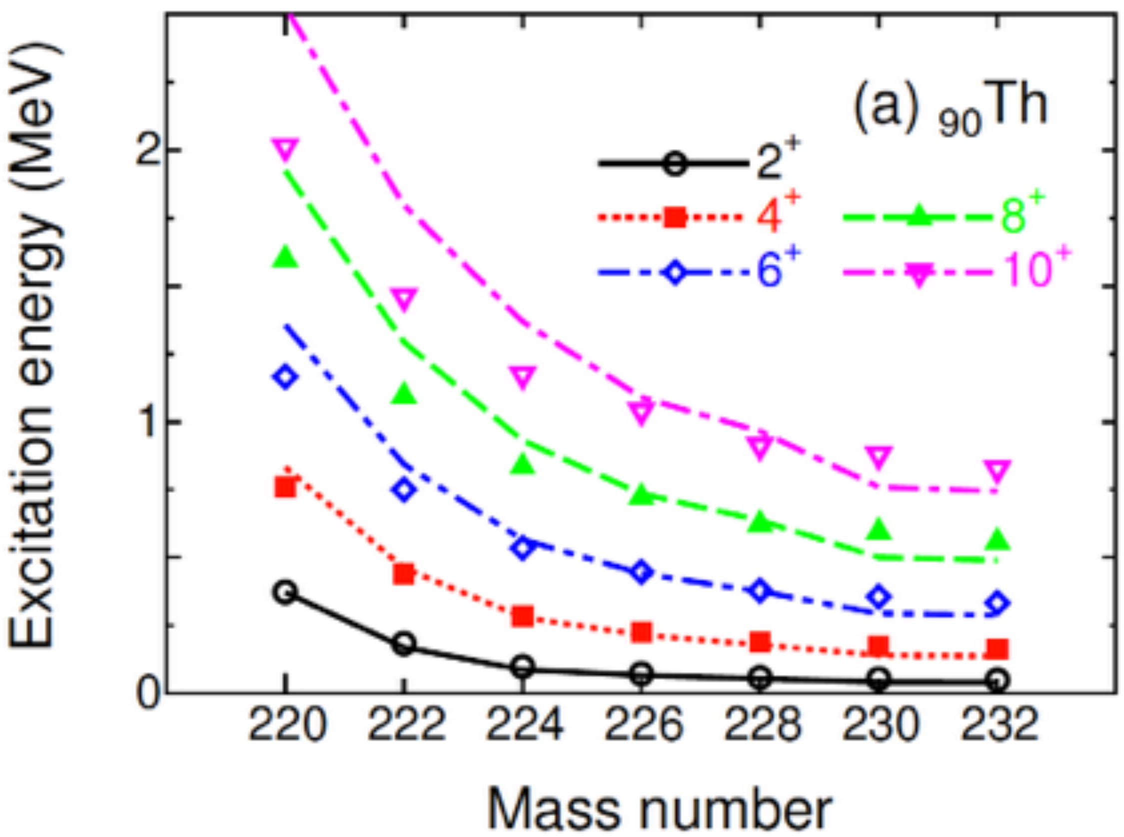
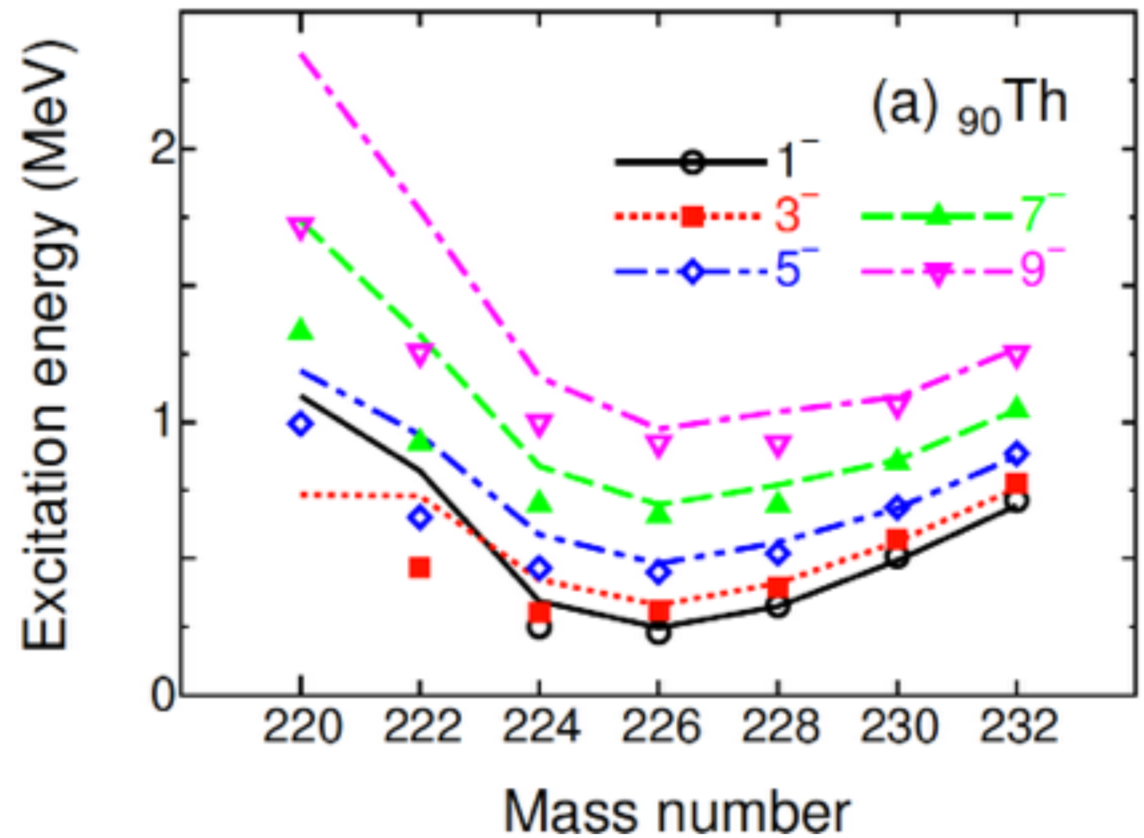
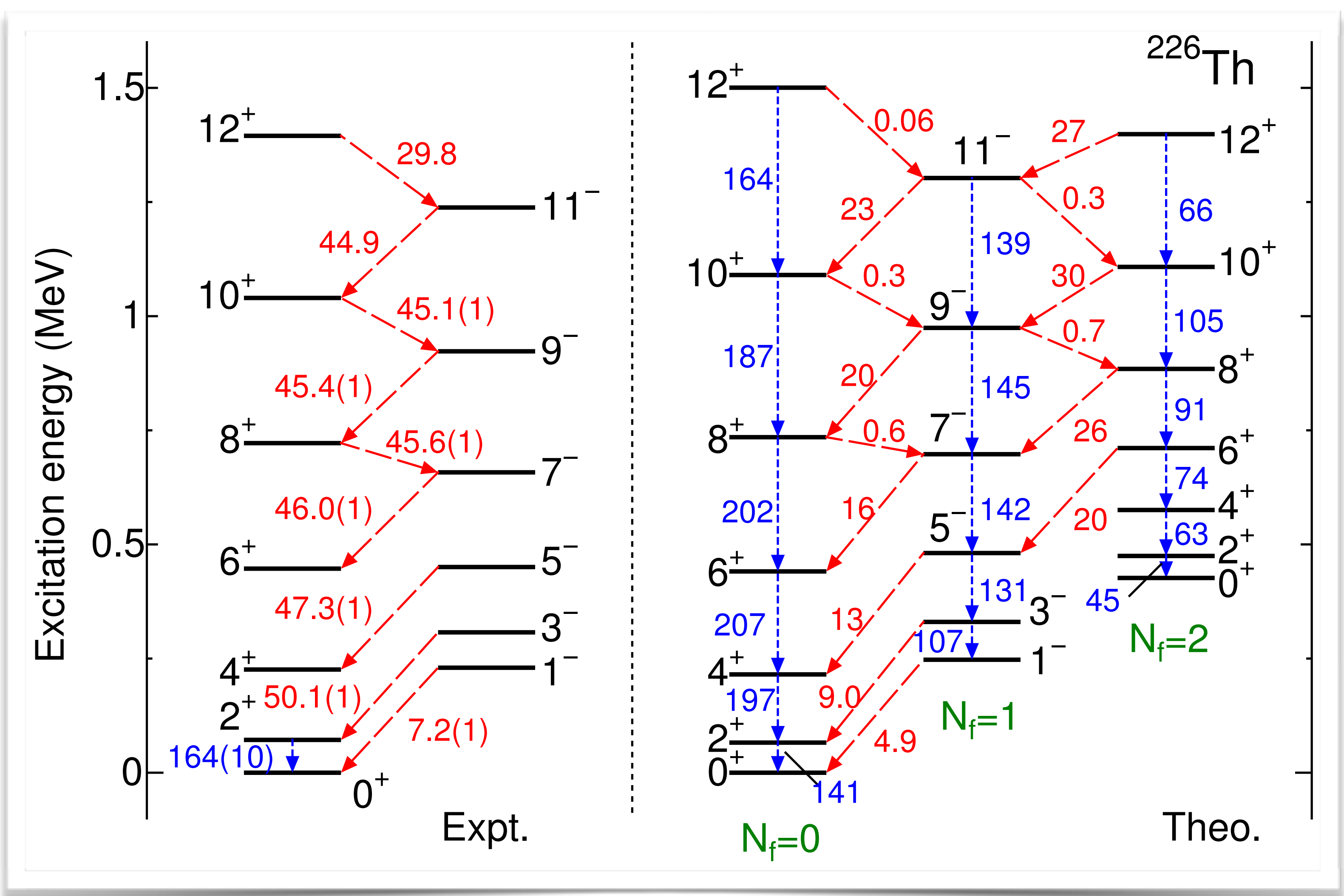


(a) $_{90}$Th
2^+
4^+
6^+
8^+
10^+
Excitation energy (MeV)
0
1
2
220 222 224 226 228 230 232
Mass number



(a) $_{90}$Th
1^-
3^-
5^-
7^-
9^-
Excitation energy (MeV)
0
1
2
220 222 224 226 228 230 232
Mass number



^{226}Th
Excitation energy (MeV)
0
0.5
1
1.5
Expt.
Theo.
$N_f=0$
$N_f=1$
$N_f=2$
12^+ 10^+ 8^+ 6^+ 4^+ 2^+ 0^+
11^- 9^- 7^- 5^- 3^- 1^-
29.8
44.9
45.1(1)
45.4(1)
45.6(1)
46.0(1)
47.3(1)
50.1(1)
7.2(1)
164(10)
0.06
27
164
23
0.3
66
139
0.3
30
105
187
20
0.7
145
0.6
26
91
202
16
142
20
74
63
45
207
13
131
107
197
9.0
4.9
141

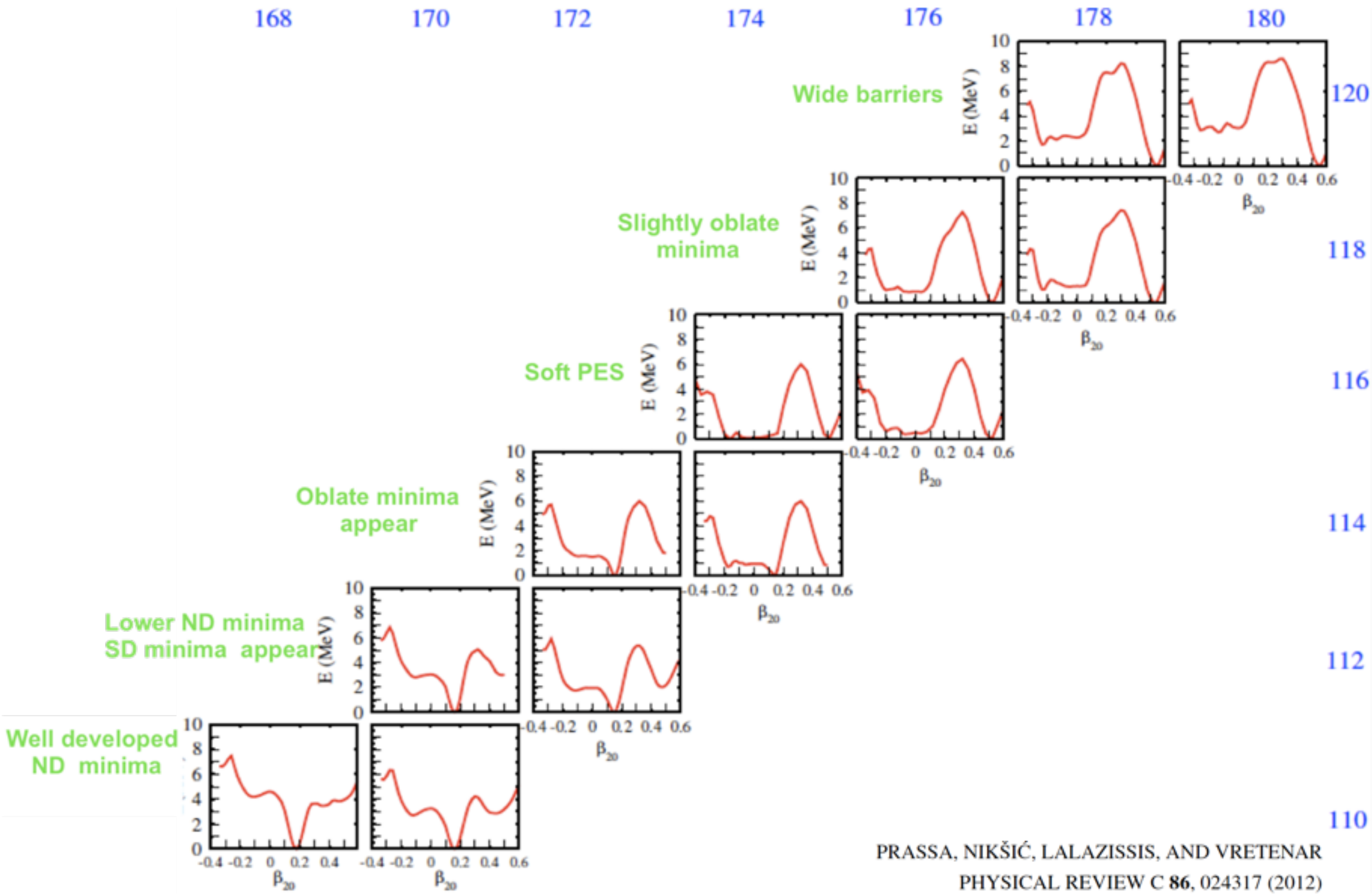
Extrapolation to SHE

EDFs and the corresponding structure models are applied to a region far from those in which their parameters are determined by data ➠ large uncertainty in model predictions?

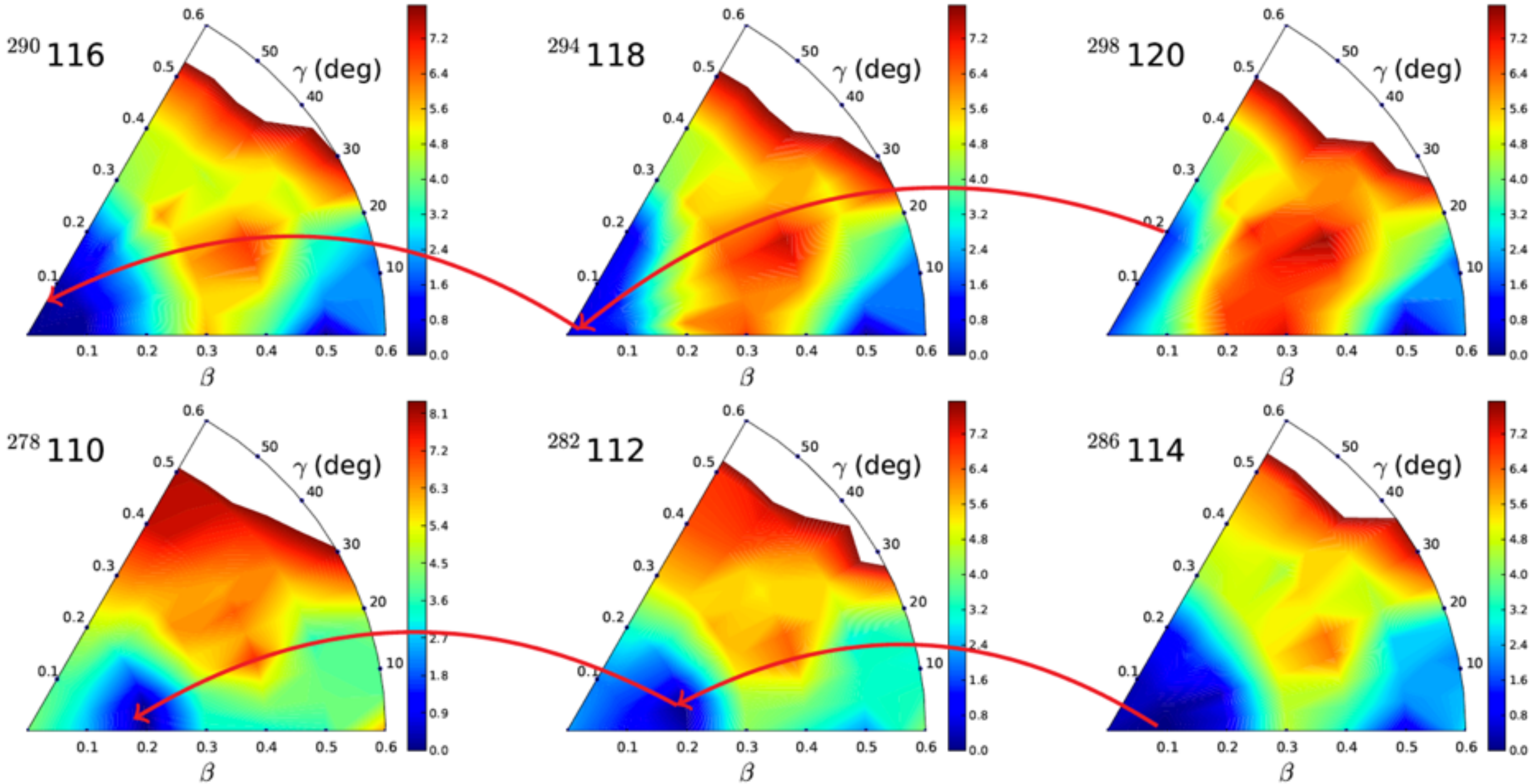
Much higher density of single-particle states close to the Fermi energy ➠ details of the evolution of deformed shells with nucleon number will have more pronounced effects on energy gaps, separation energies, Q_α-values, band-heads in odd-A nuclei, K-isomers …

Much stronger competition between the attractive short-range nuclear interaction and the long-range electrostatic repulsion ➠ pronounced effects on the Coulomb, surface and isovector energies! Fast shape transitions! Exotic shapes!

Shape transitions in superheavy nuclei

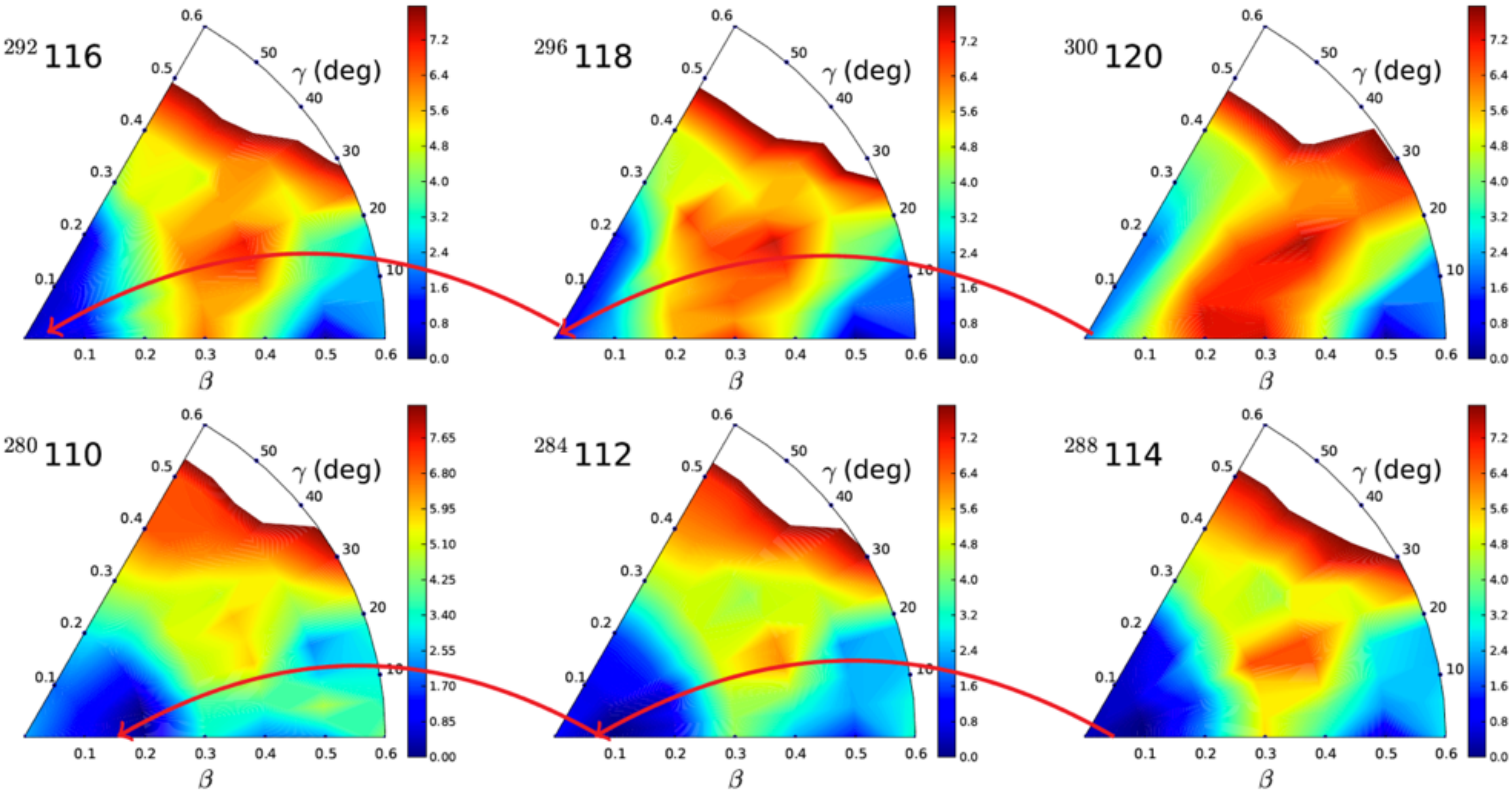


Triaxial shapes in the α-decay chain of $^{298}120$

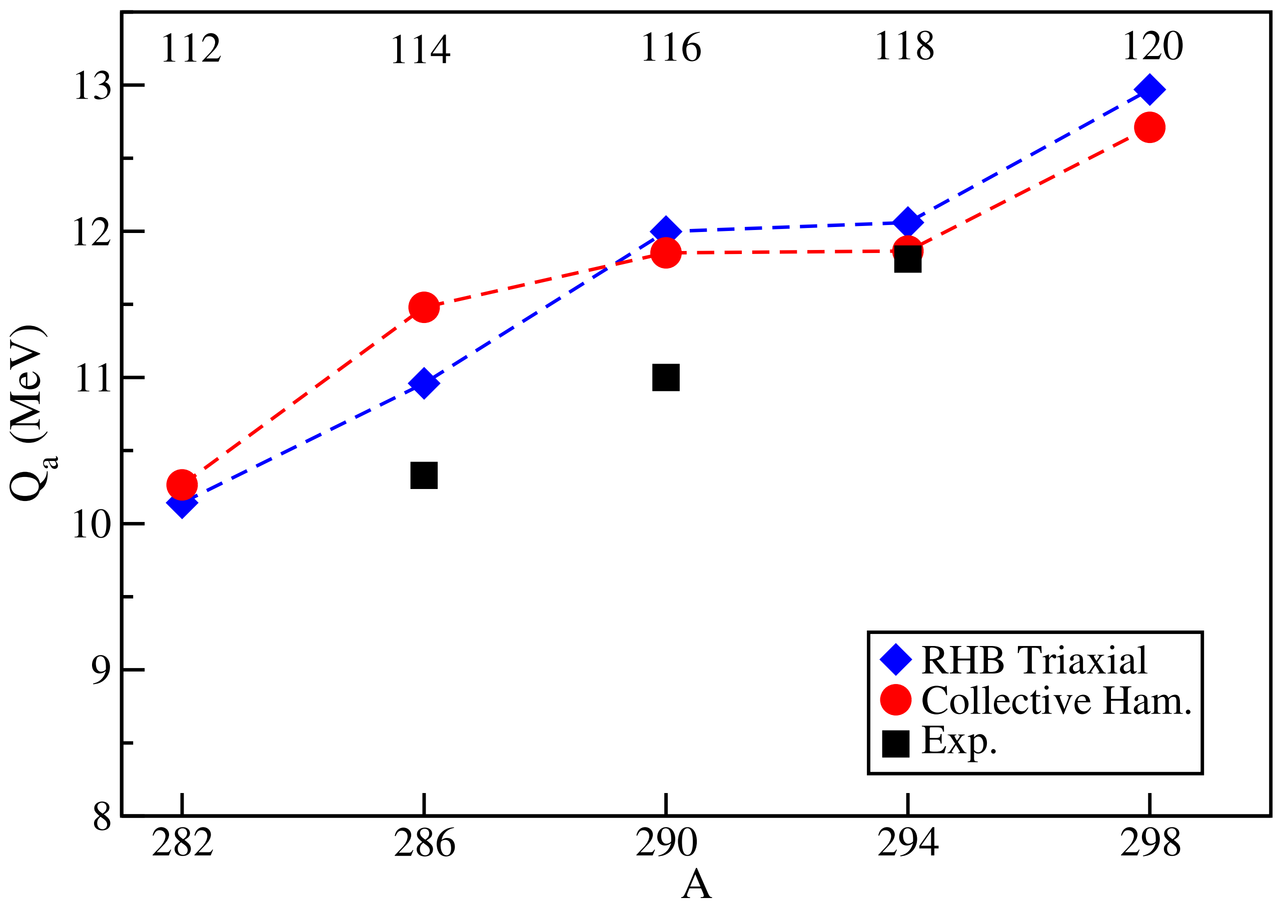


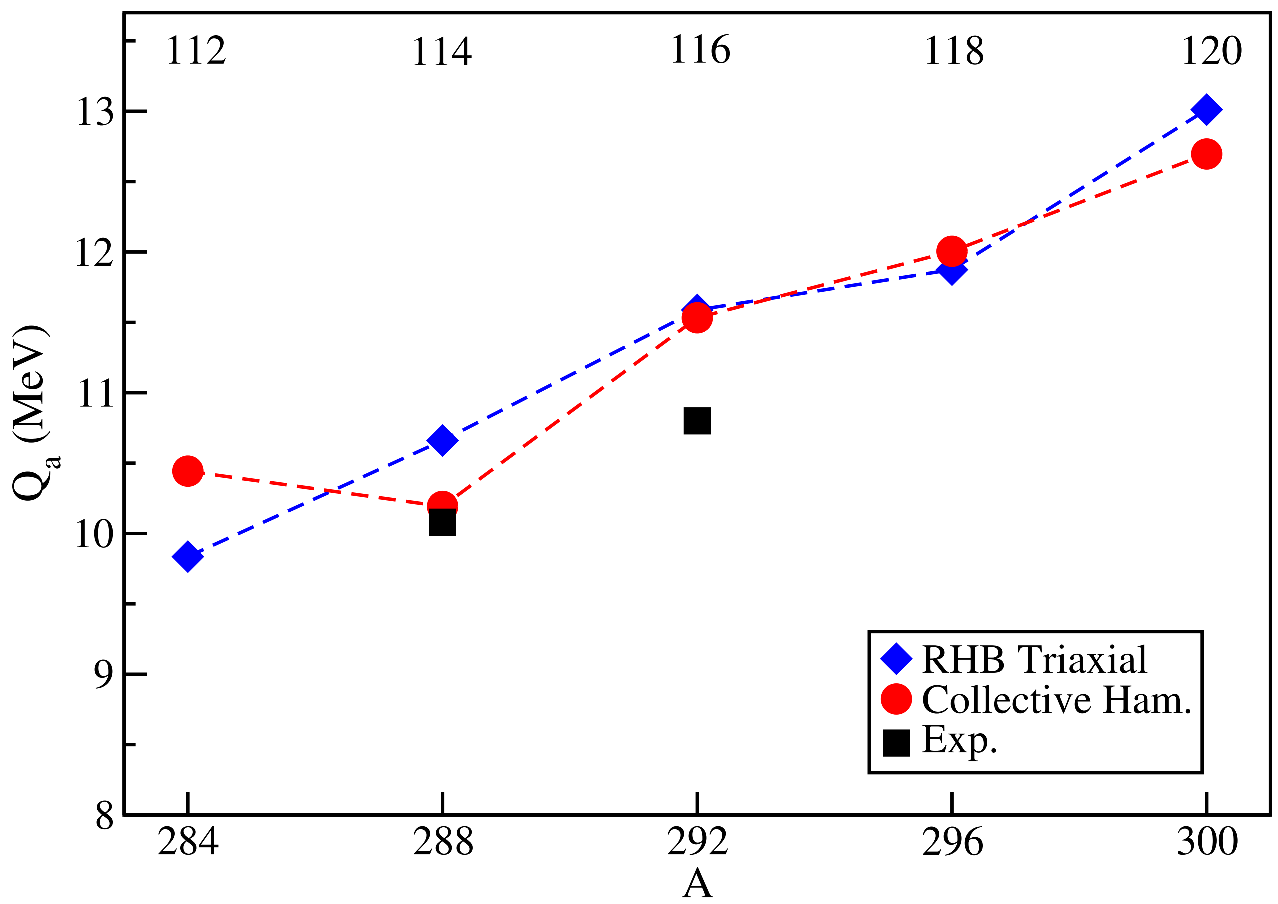
Fluctuations in shape degrees of freedom and configuration mixing ➠ influence on ground-state properties and transitions!

Triaxial shapes in the α-decay chain of $^{300}120$



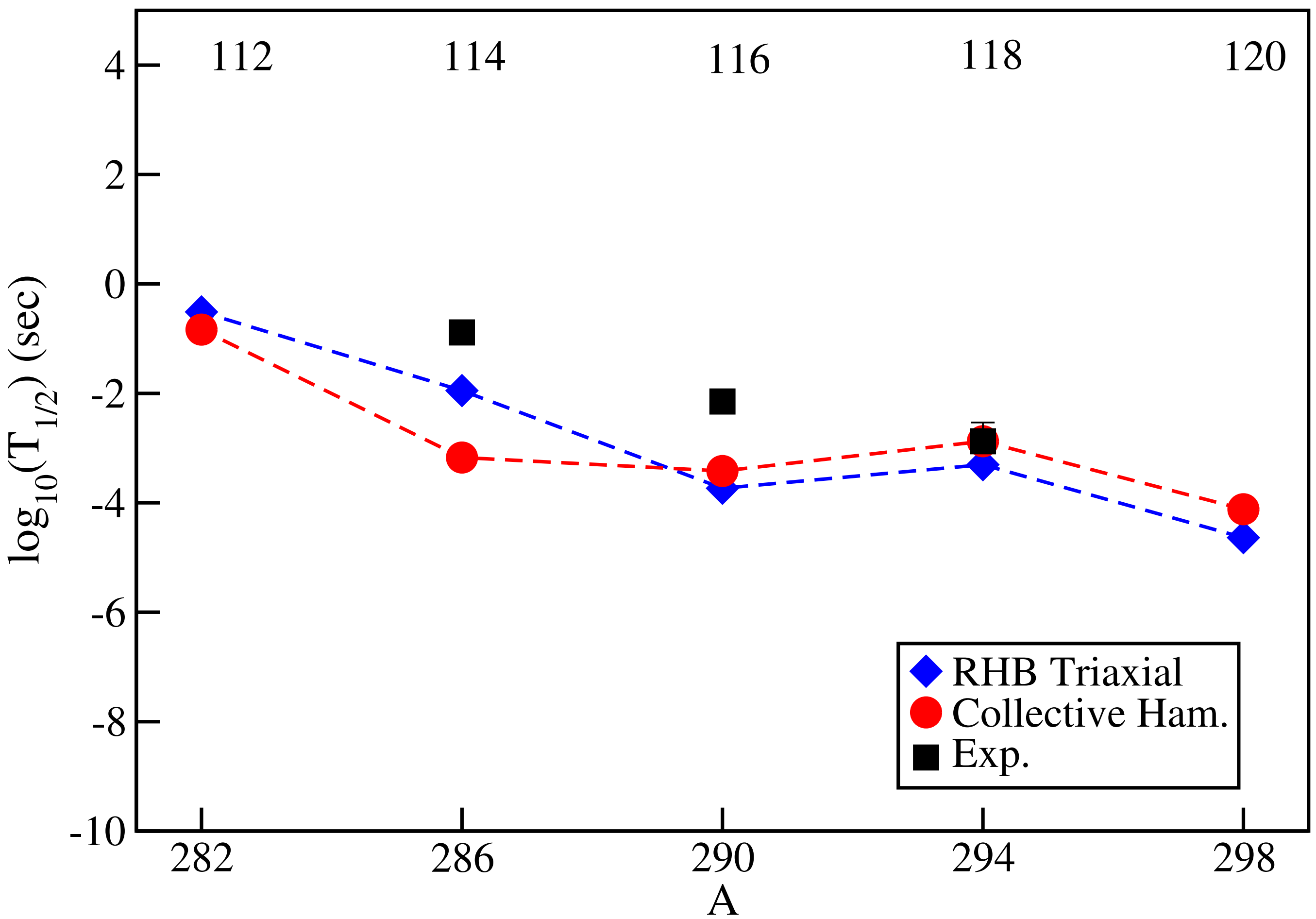
α-decay chains of $^{298}120$ and $^{300}120$

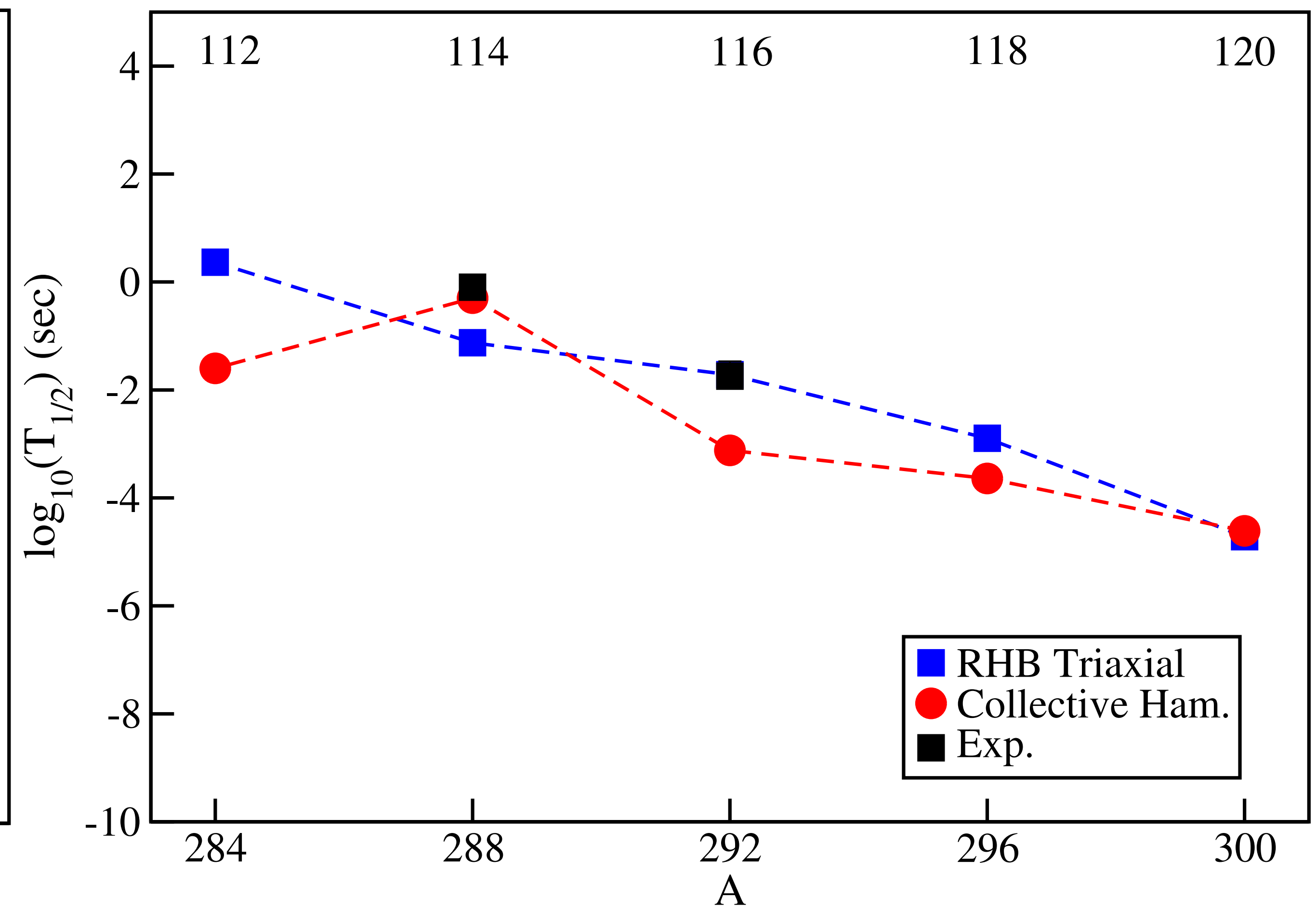




Importance of collective correlations (not included in the EDF) ➠ restoration of symmetries broken at the SCMF level (rotational, particle number) and mixing of configurations with different deformation!

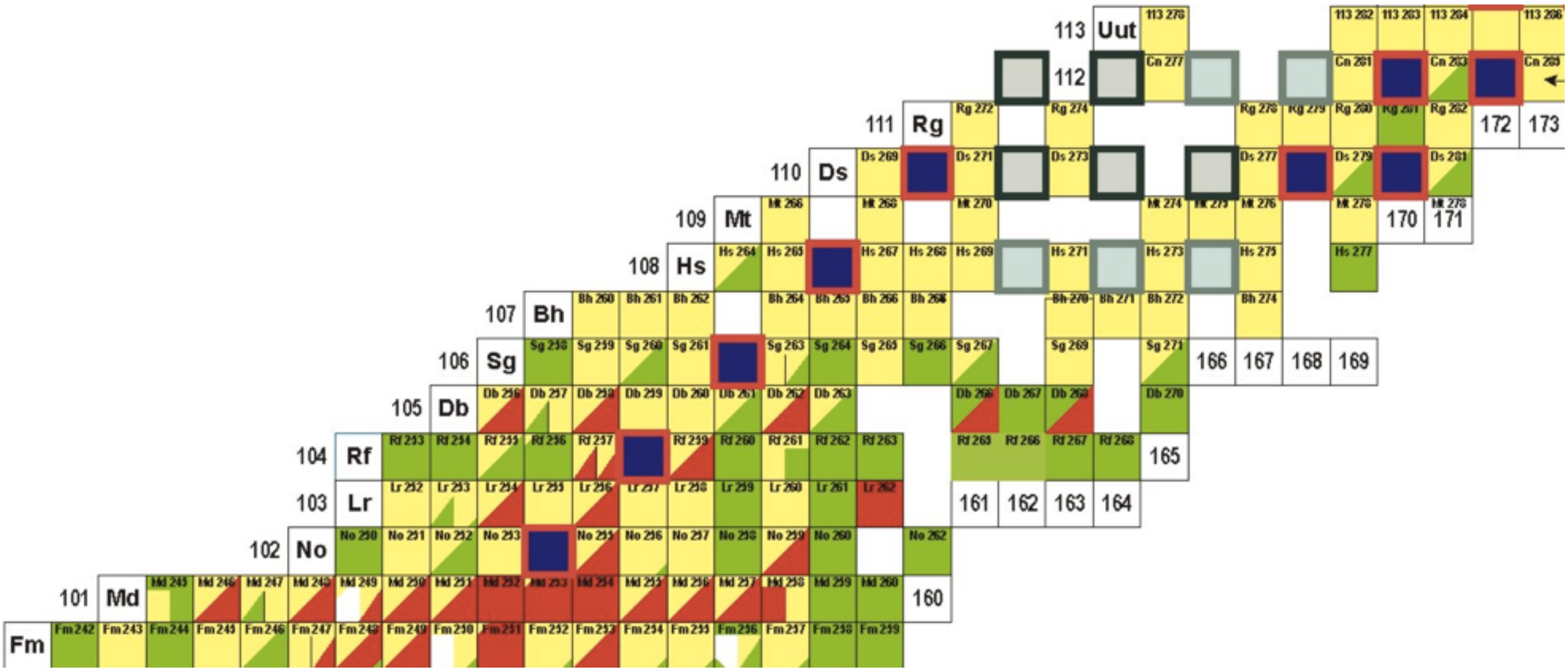
Half-lives in the α-decay chains of $^{298}120$ and $^{300}120$



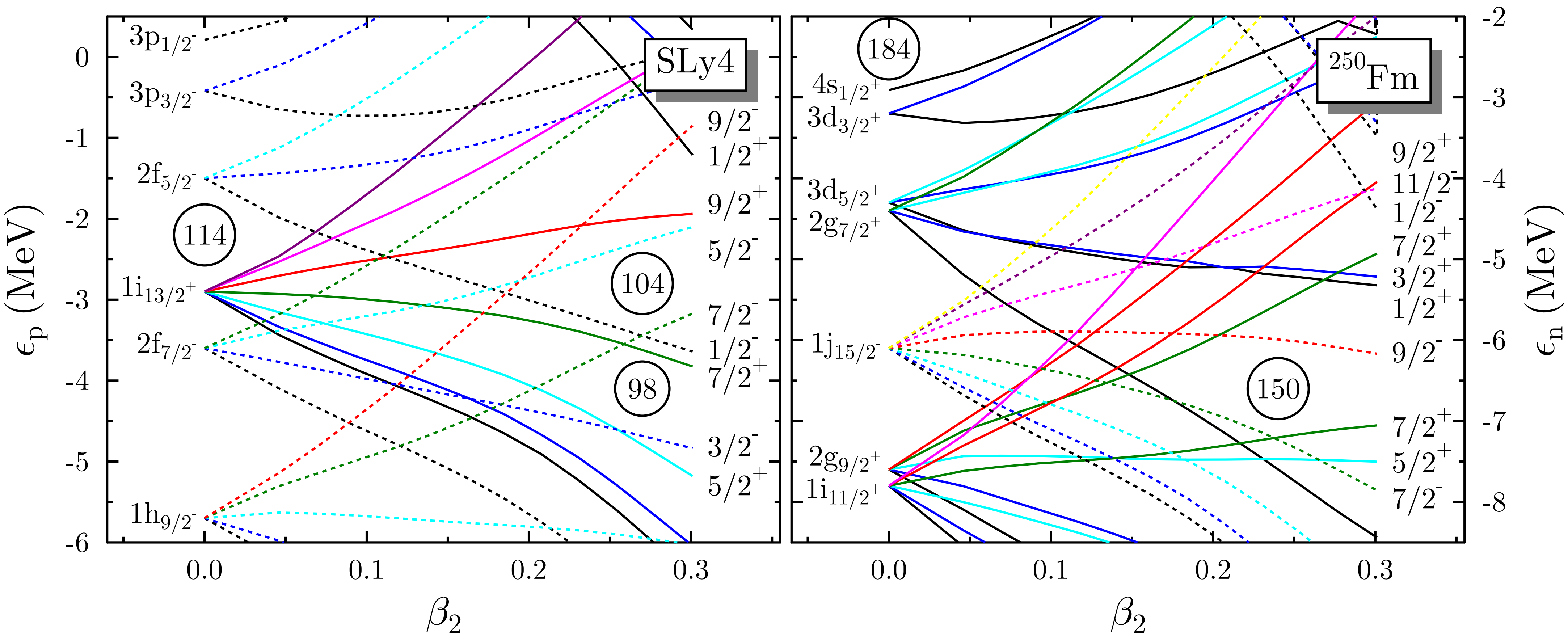


PRASSA, NIKŠIĆ, LALAZISSIS, AND VRETENAR
PHYSICAL REVIEW C **86**, 024317 (2012)

Transactinides



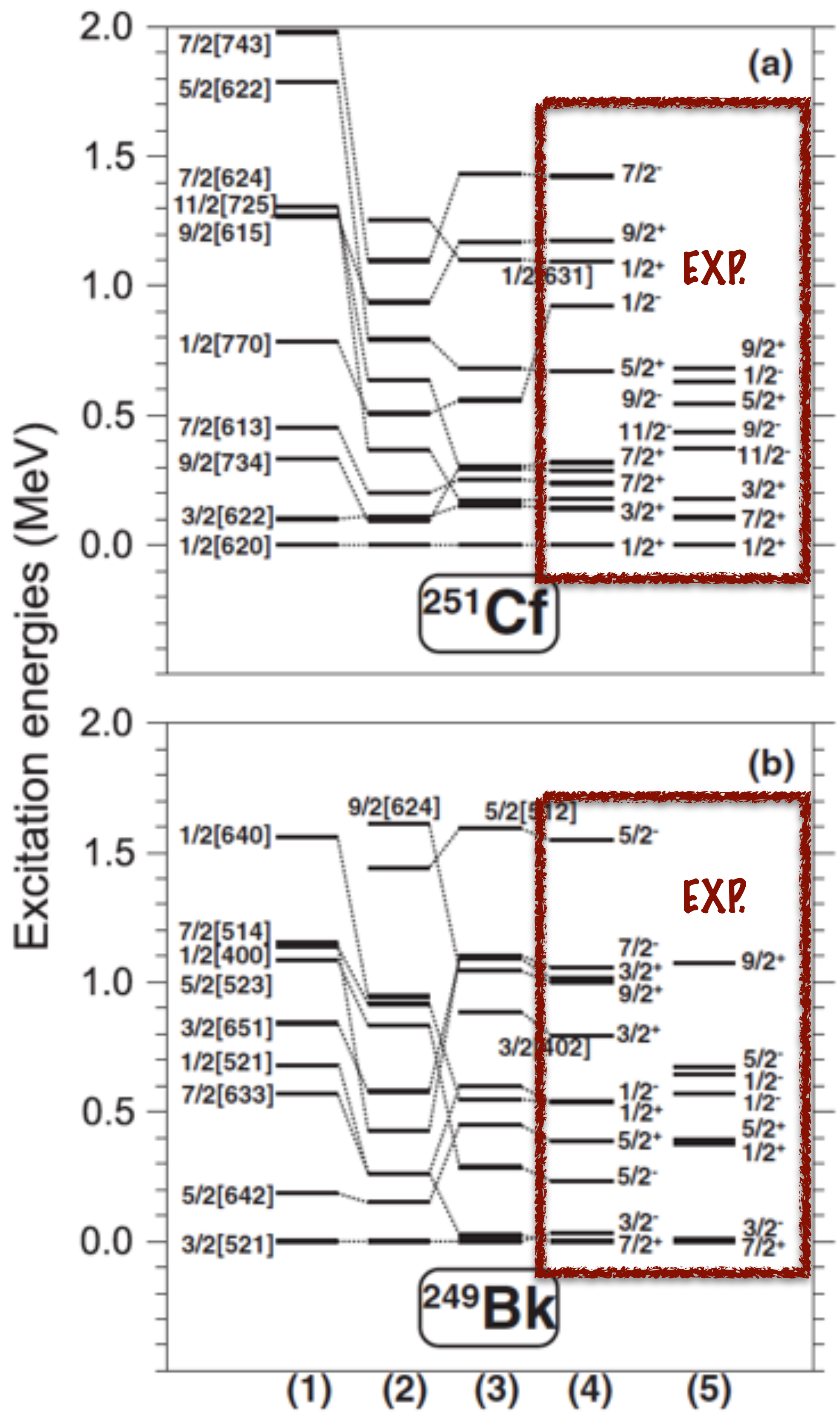
None of the SCMF models based on modern EDFs reproduce the empirical deformed shell closures at N=152 and Z=100, as evidenced by available data (separation energies, Q_α-values, excitation energies of band-heads in odd-A nuclei, excitation energies of high-K isomers).



M. Bender and P.-H. Heenen

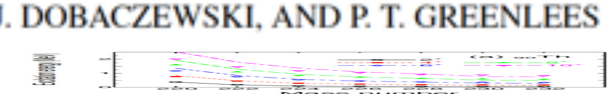
The details of the single-particle spectra depend on the choice of the effective interaction!

➠ an improved description of the single-particle properties and rotational bands in the nobelium region can be obtained by *locally* adjusting the parameters of an EDF to this region of nuclei:



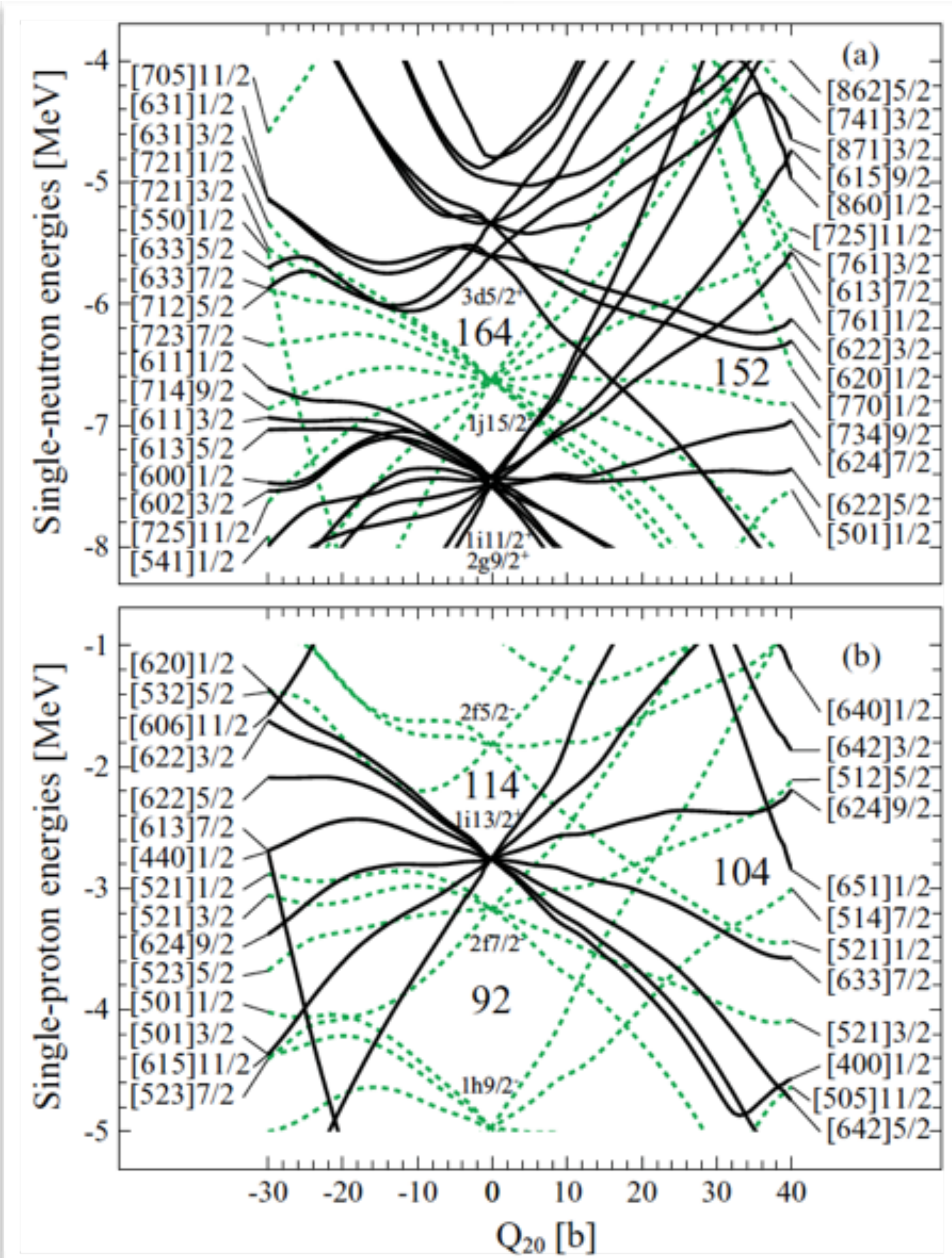
Starting from the Skyrme functional UNEDF1, the spin-orbit coupling constants and pairing strengths are adjusted to odd-even mass staggering and intruder excitation energies in ^{251}Cf and ^{249}Bk.

YUE SHI, J. DOBACZEWSKI, AND P. T. GREENLEES

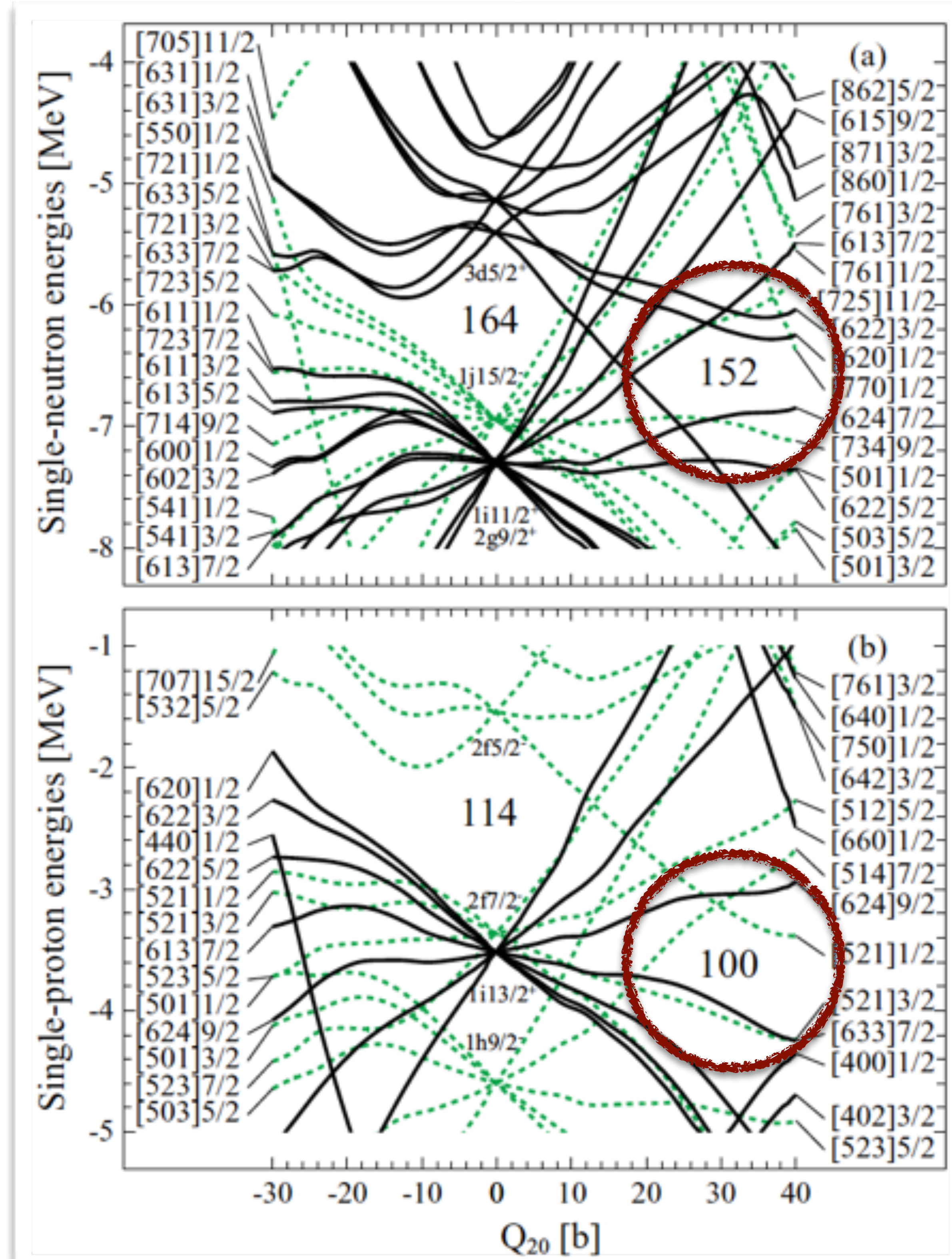


The readjustment of the SO coupling constants → the intruder neutron 1*j*15/2− and proton 1*i*13/2+ spherical shells are shifted down by a few hundred keV with respect to the normal-parity levels.
At deformation of $Q20 \approx 33$ b this opens up the deformed neutron $N = 152$ and proton $Z = 100$ gaps.

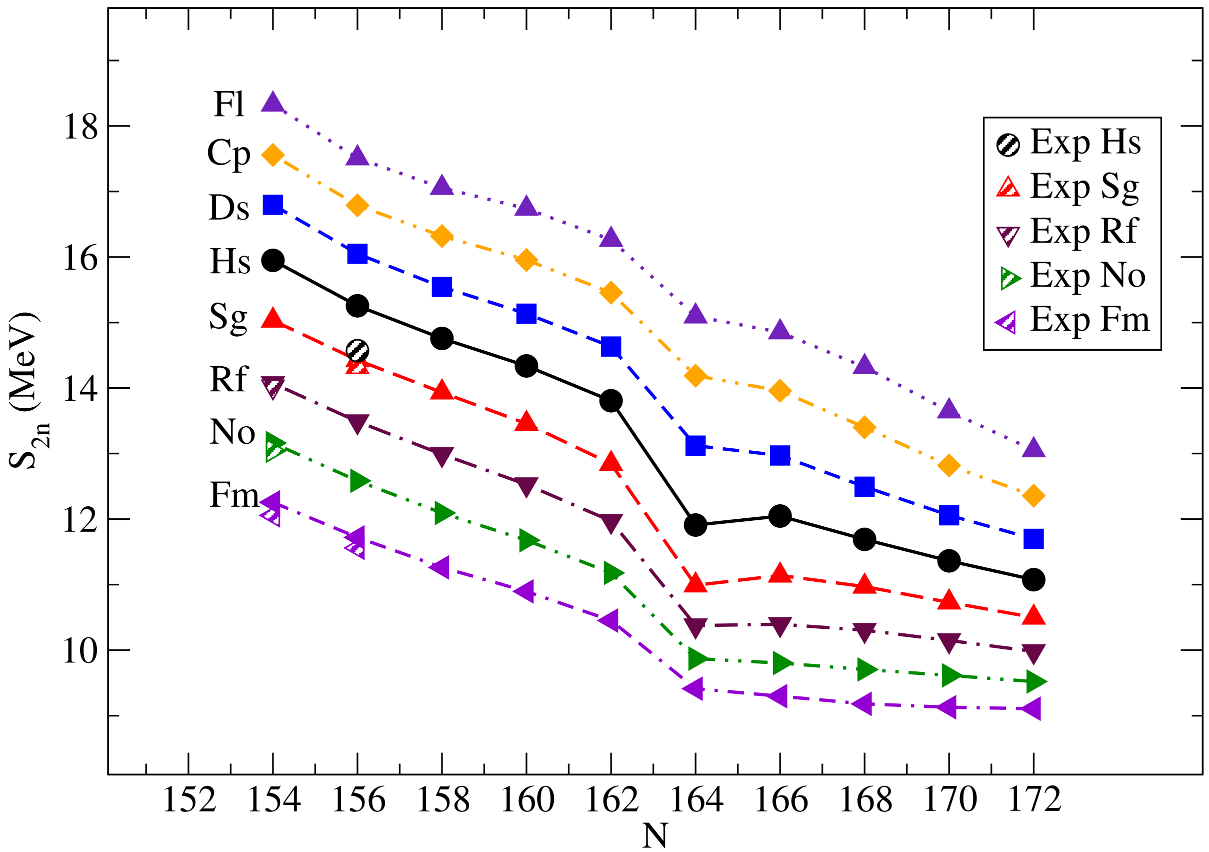
Nilsson diagrams in ^{254}No calculated for the Skyrme EDF UNEDF1.



Nilsson diagrams in ^{254}No calculated for the Skyrme EDF UNEDF1^{SO}.

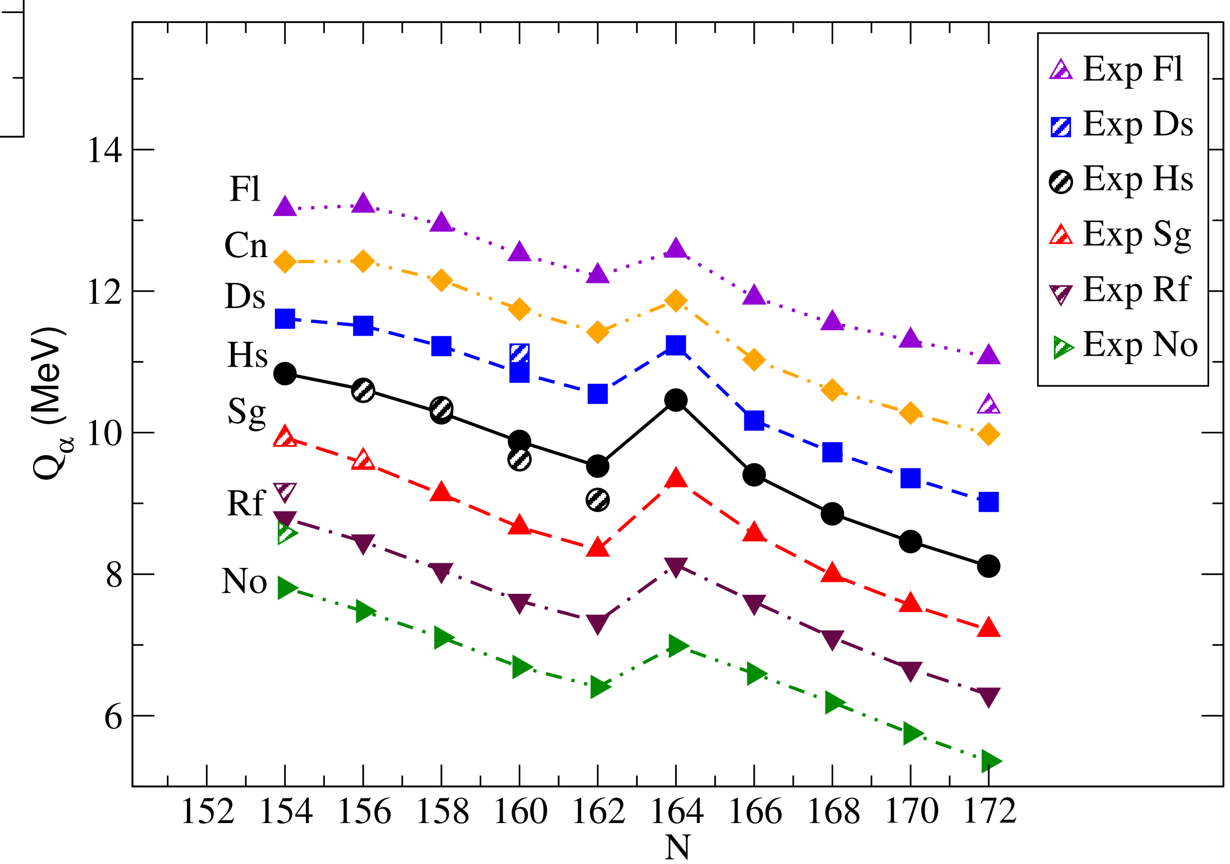


Transactinides



2n separation energies

Qα values



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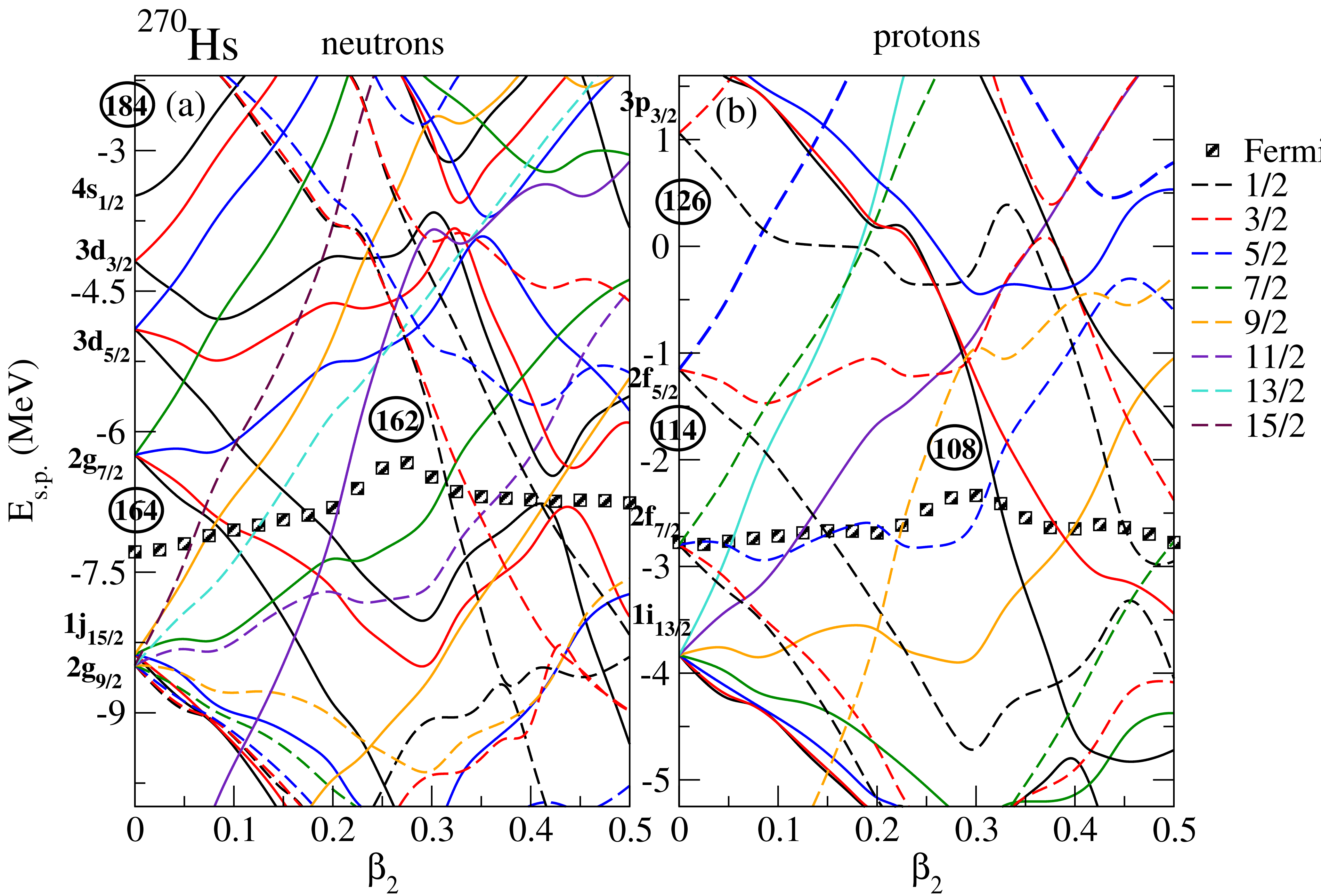
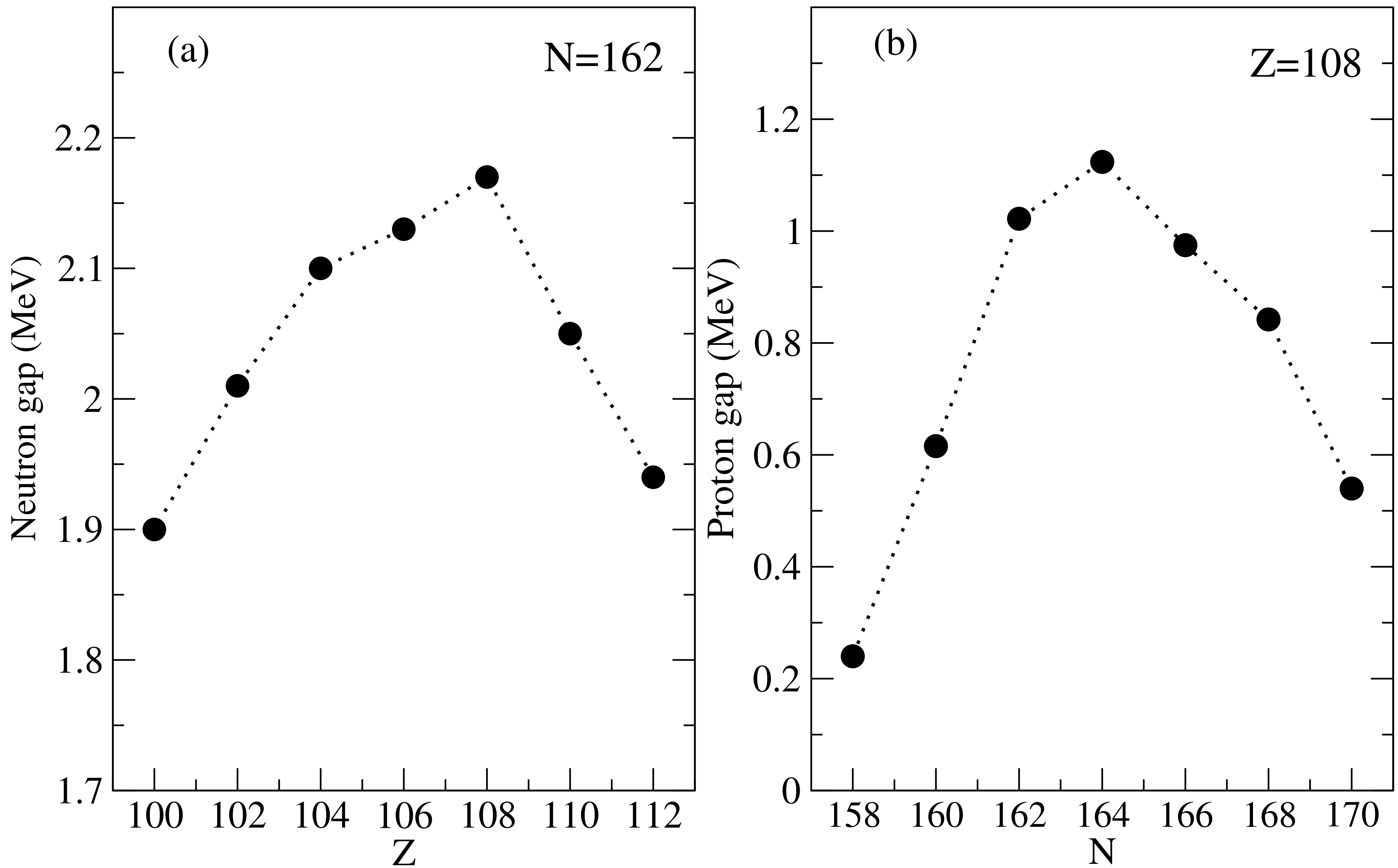
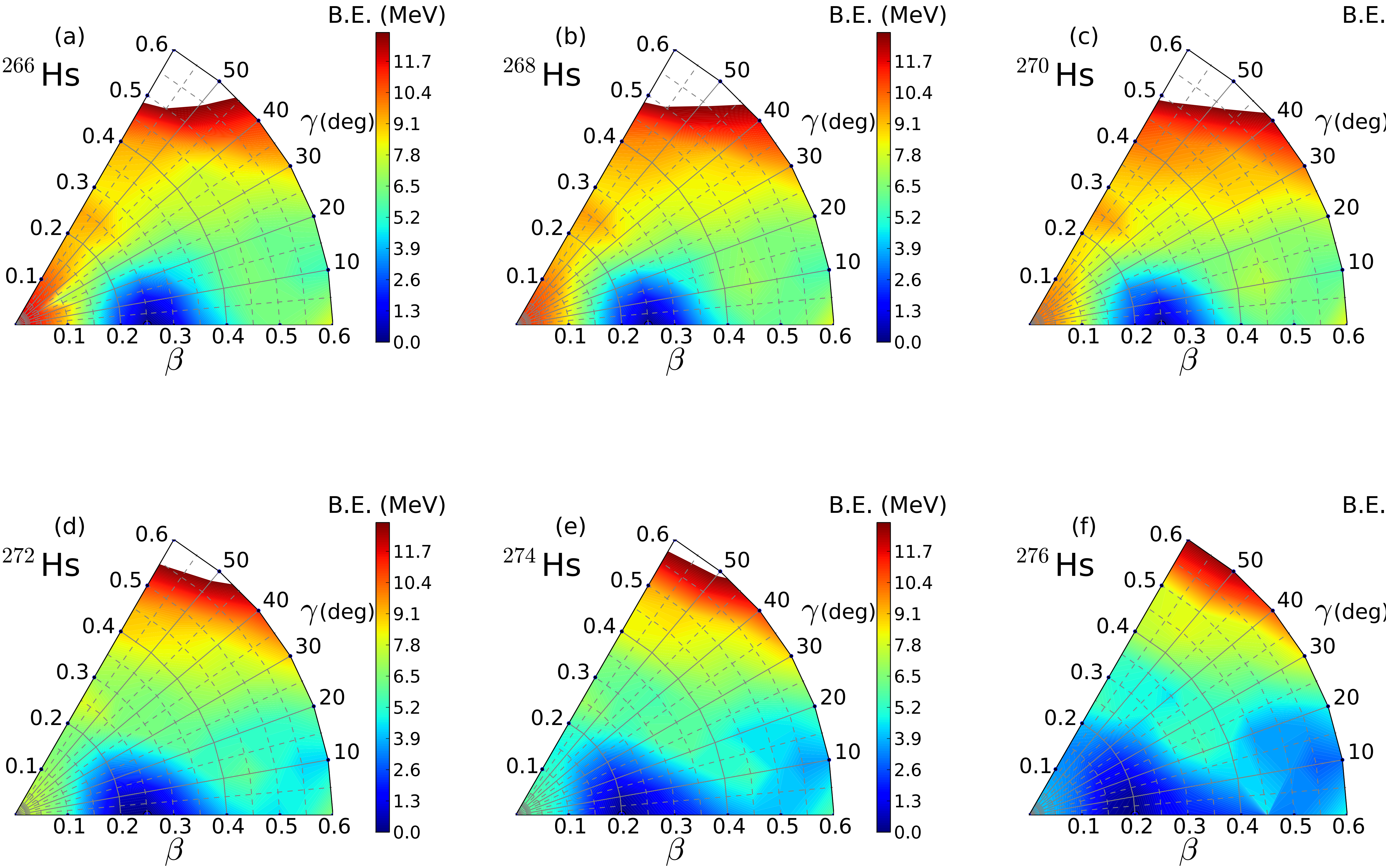
Energy gaps are small! Shape stabilisation depends on how fast the shell structures vary with deformation!



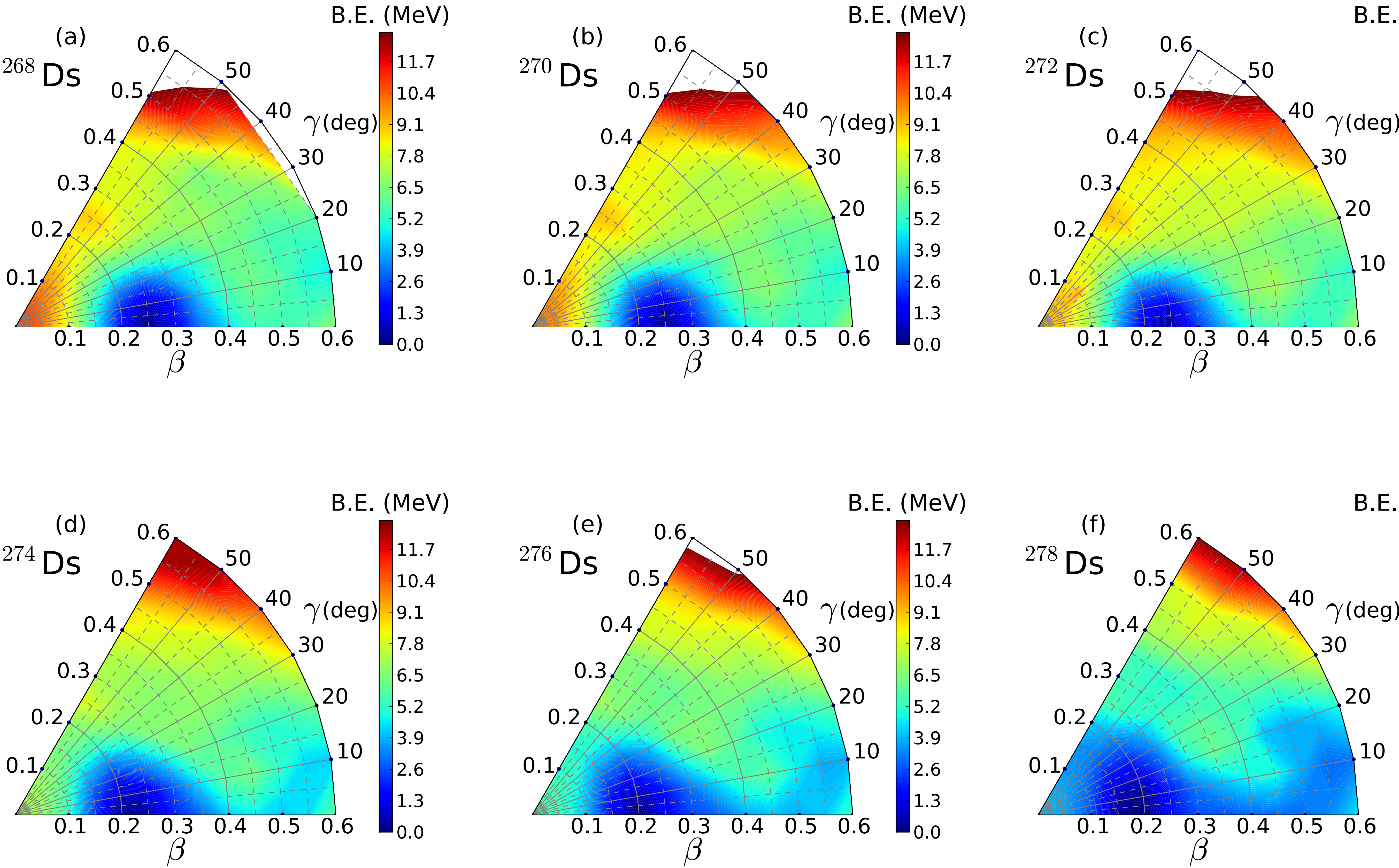
Neutron and proton shell gaps



^{270}Hs ➠ deformed “doubly magic” nucleus

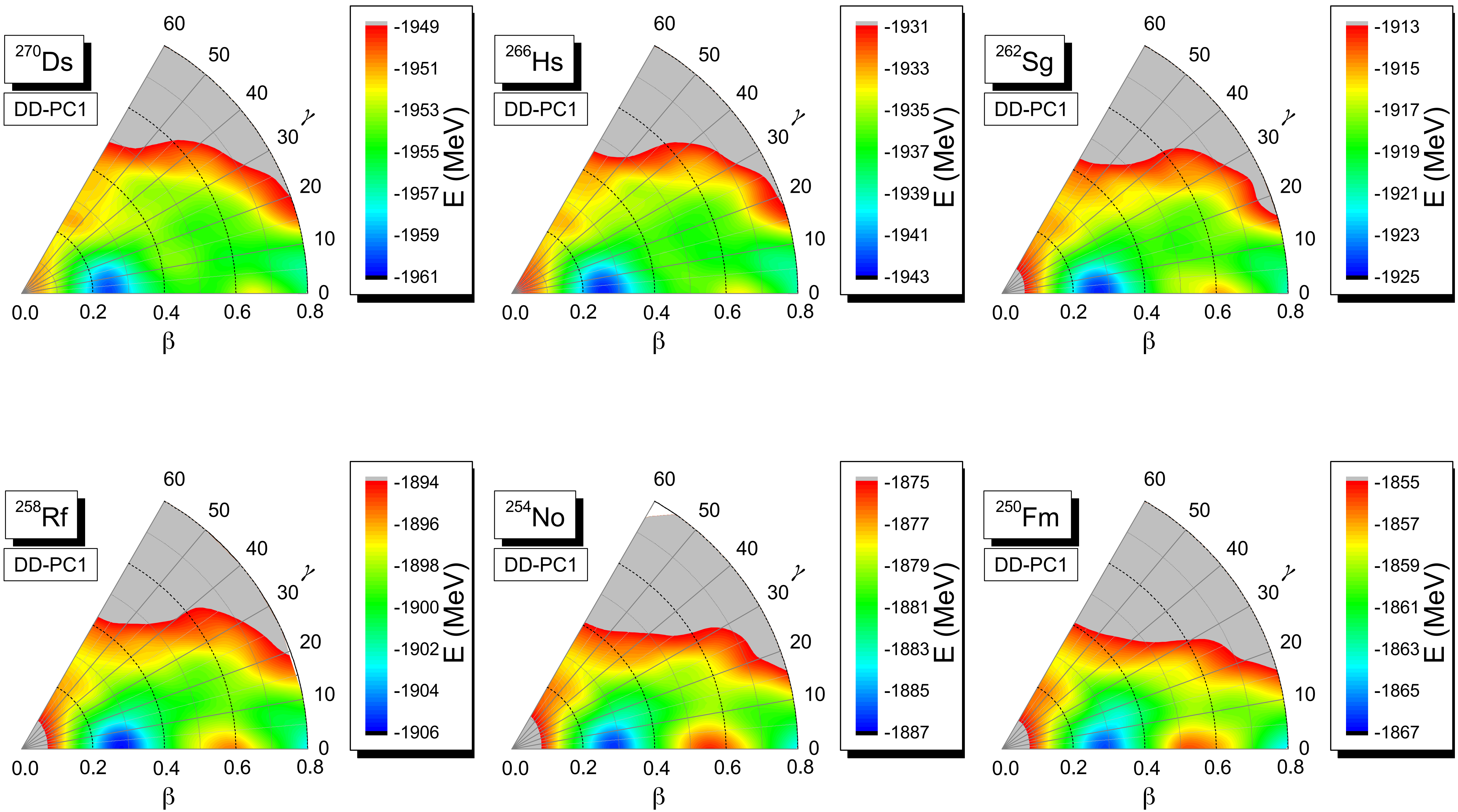


(a) ^{266}Hs
(b) ^{268}Hs
(c) ^{270}Hs
(d) ^{272}Hs
(e) ^{274}Hs
(f) ^{276}Hs
B.E. (MeV)
0.0 1.3 2.6 3.9 5.2 6.5 7.8 9.1 10.4 11.7
γ(deg)
10 20 30 40 50
β
0.1 0.2 0.3 0.4 0.5 0.6

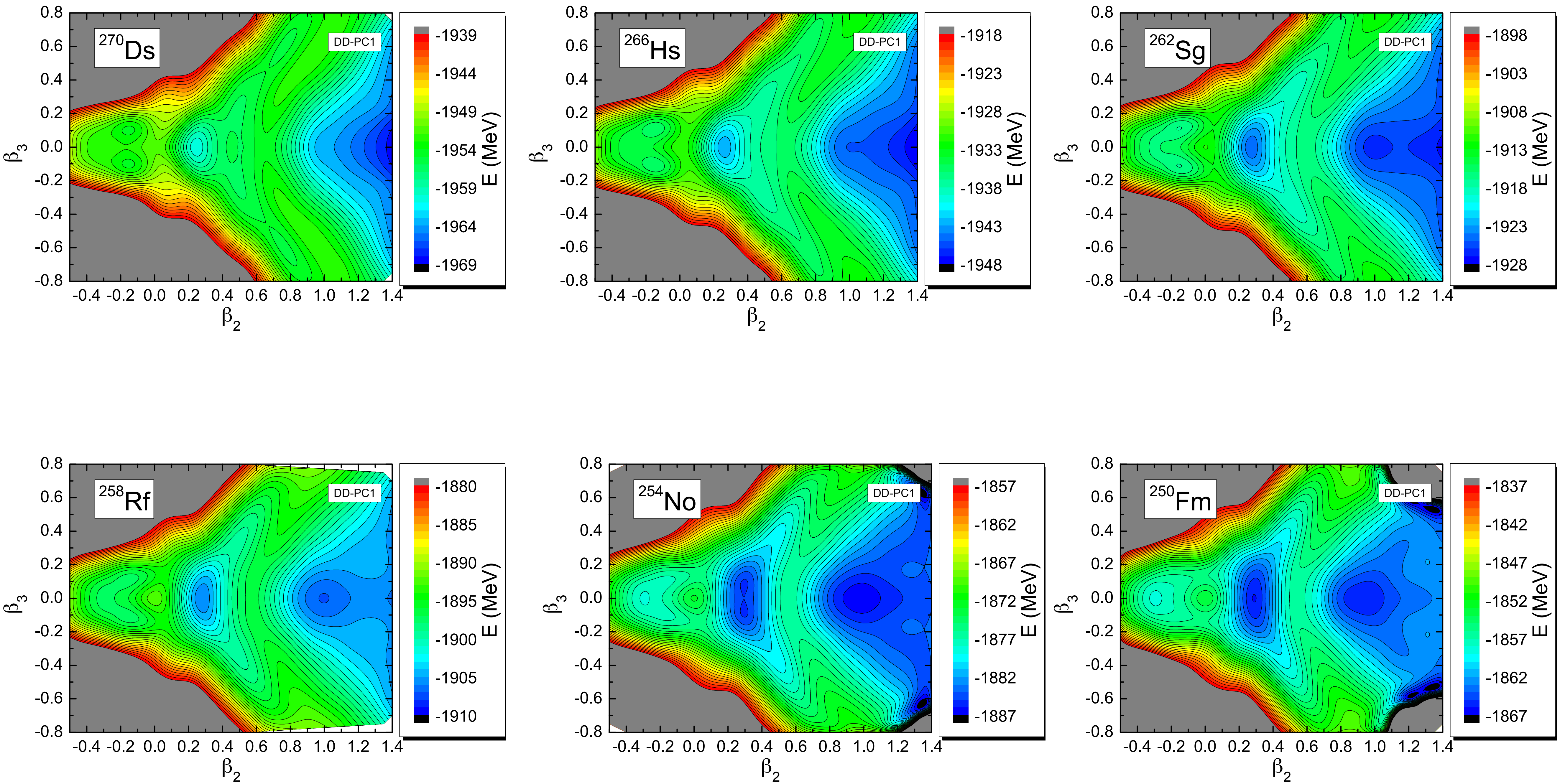


(a)
^{268}Ds
(b)
^{270}Ds
(c)
^{272}Ds
(d)
^{274}Ds
(e)
^{276}Ds
(f)
^{278}Ds
B.E. (MeV)
γ(deg)
β
0.1 0.2 0.3 0.4 0.5 0.6
10 20 30 40 50
0.0 1.3 2.6 3.9 5.2 6.5 7.8 9.1 10.4 11.7

^{270}Ds α-decay chain

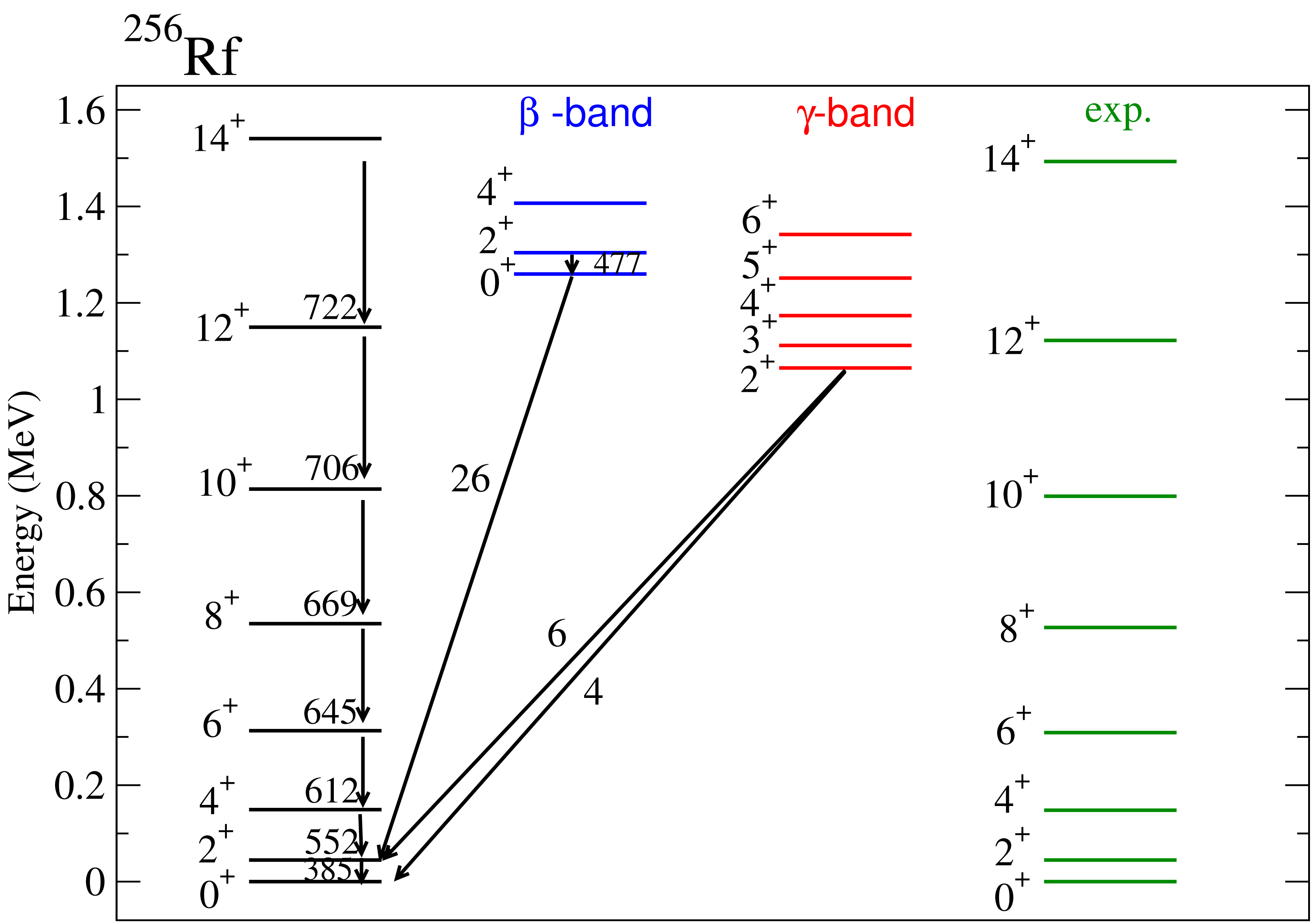


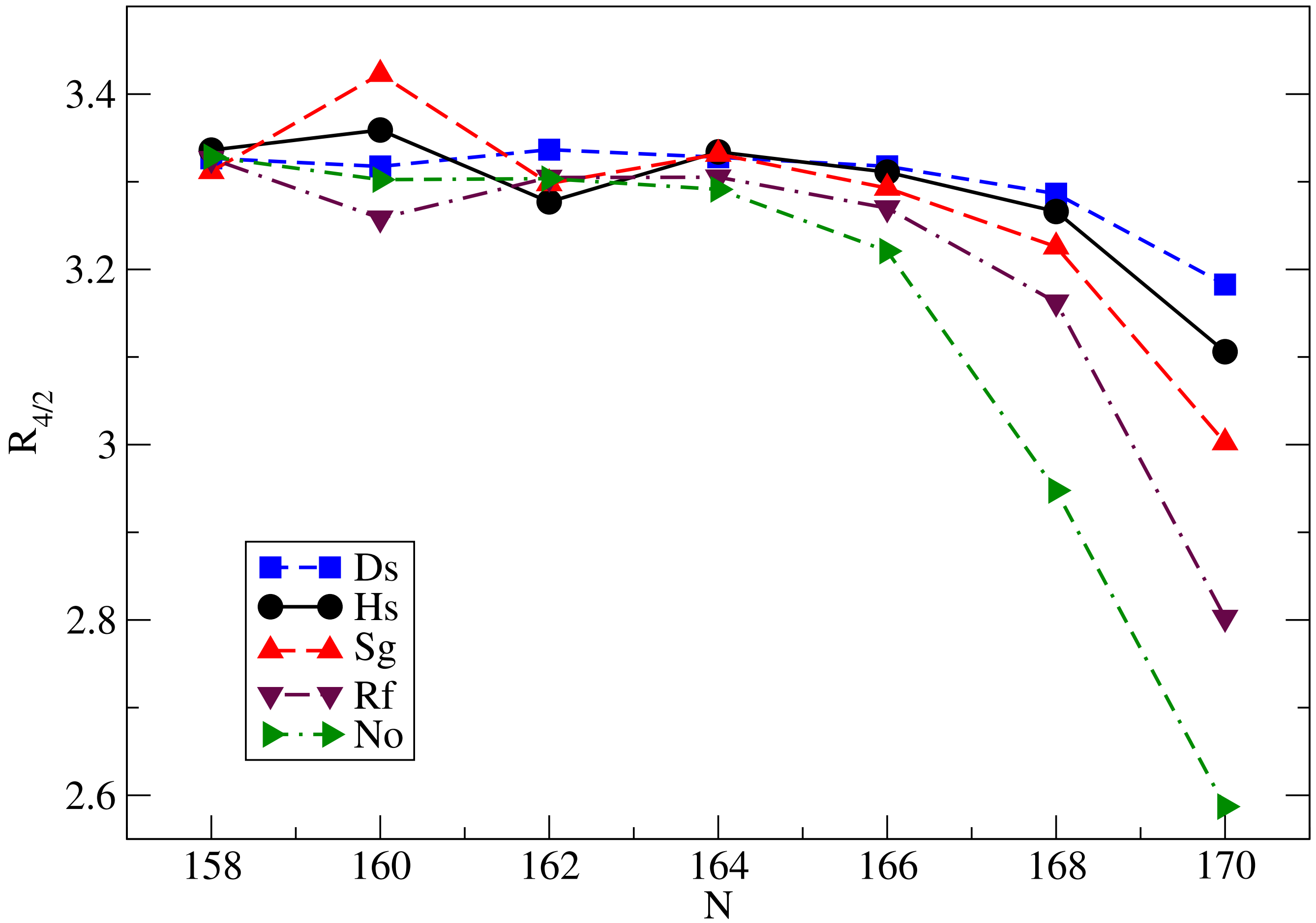
^{270}Ds α-decay chain



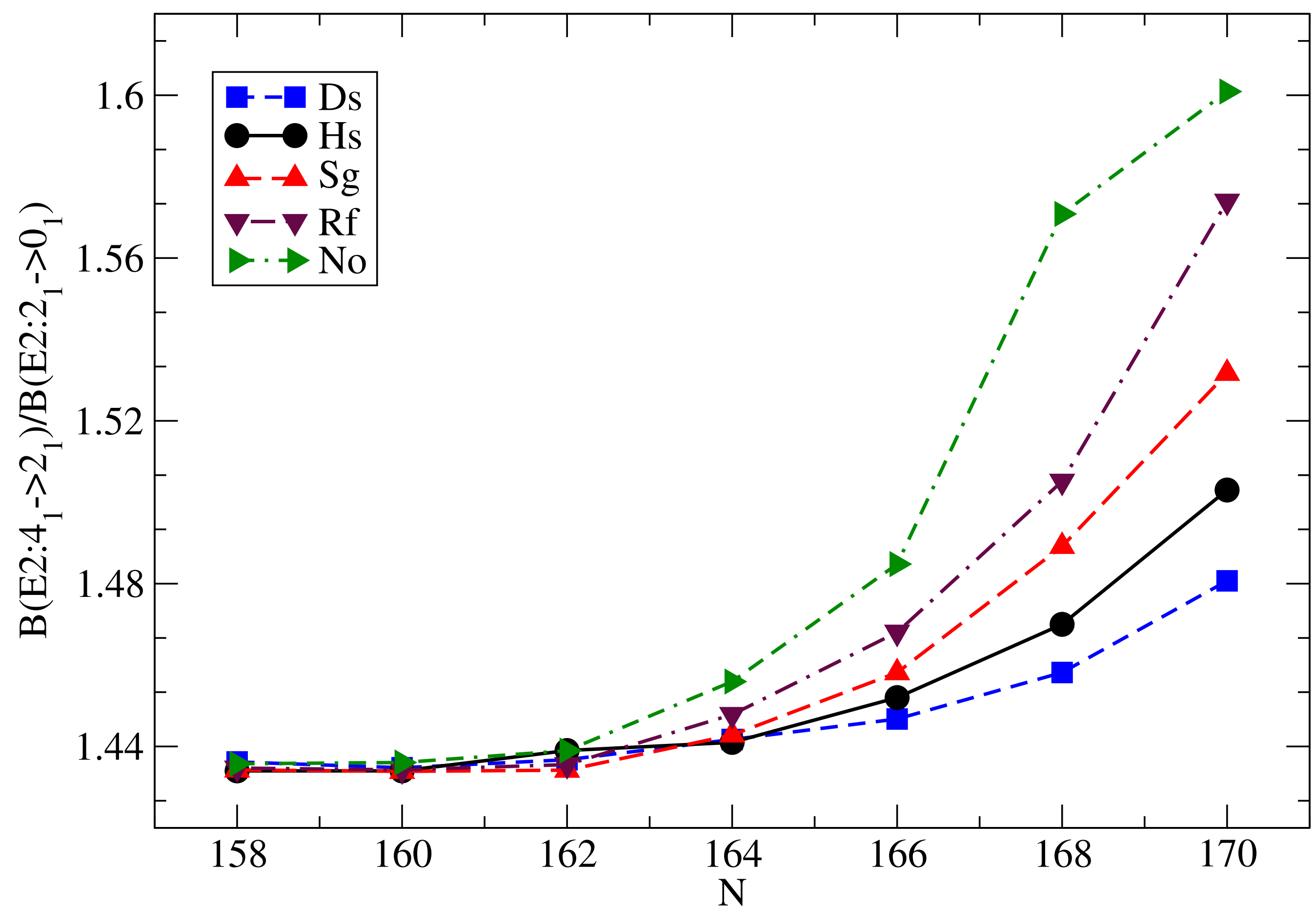
Collective states

Low-energy spectrum of ^{256}Rf calculated with the collective Hamiltonian based on DD-PC1.

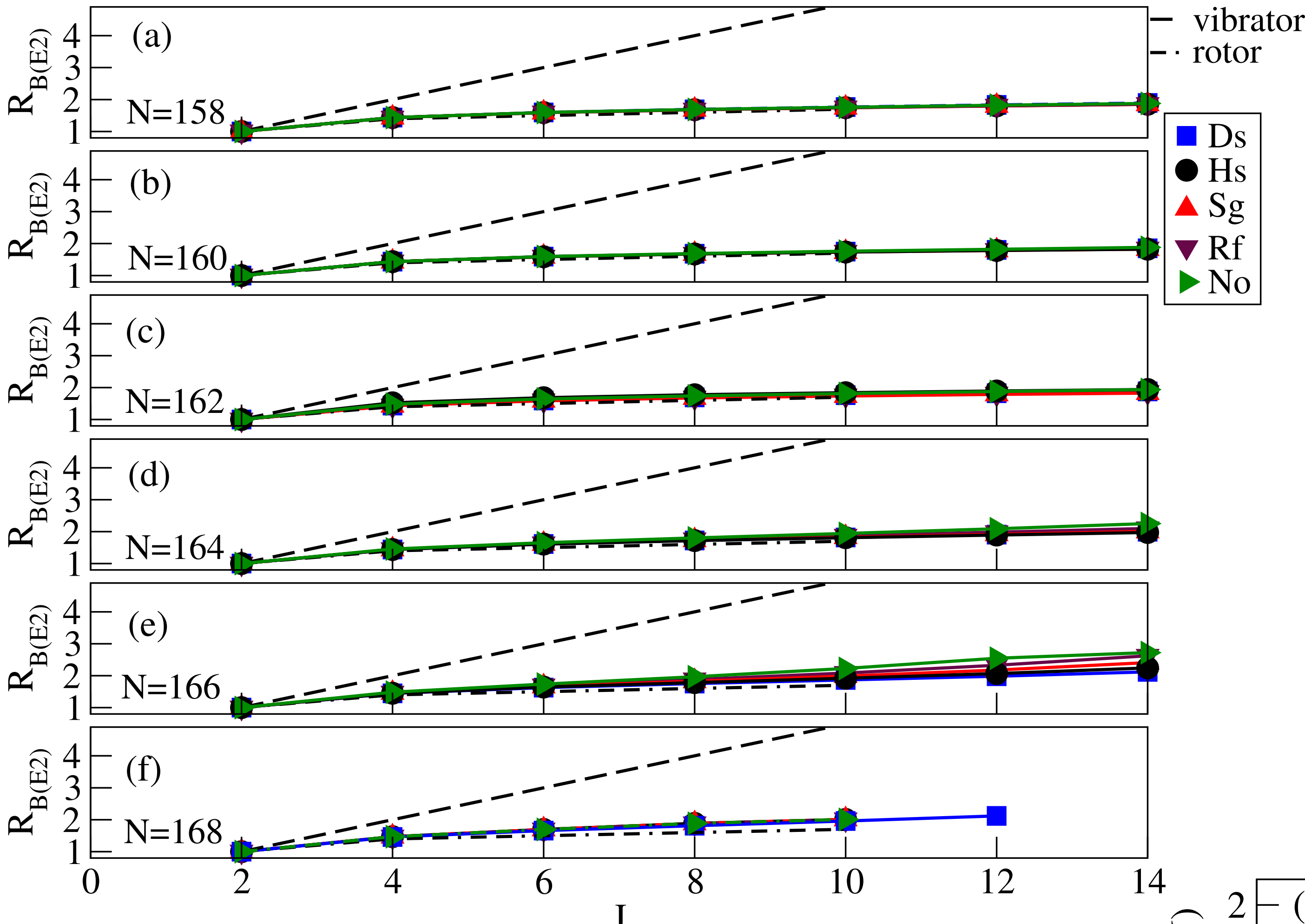




The ratio R4/2 of excitation energies of the yrast states 4^+_1 and 2^+_1 as a function of the neutron number for the isotopic chains of No, Rf, Sg, Hs and Ds.

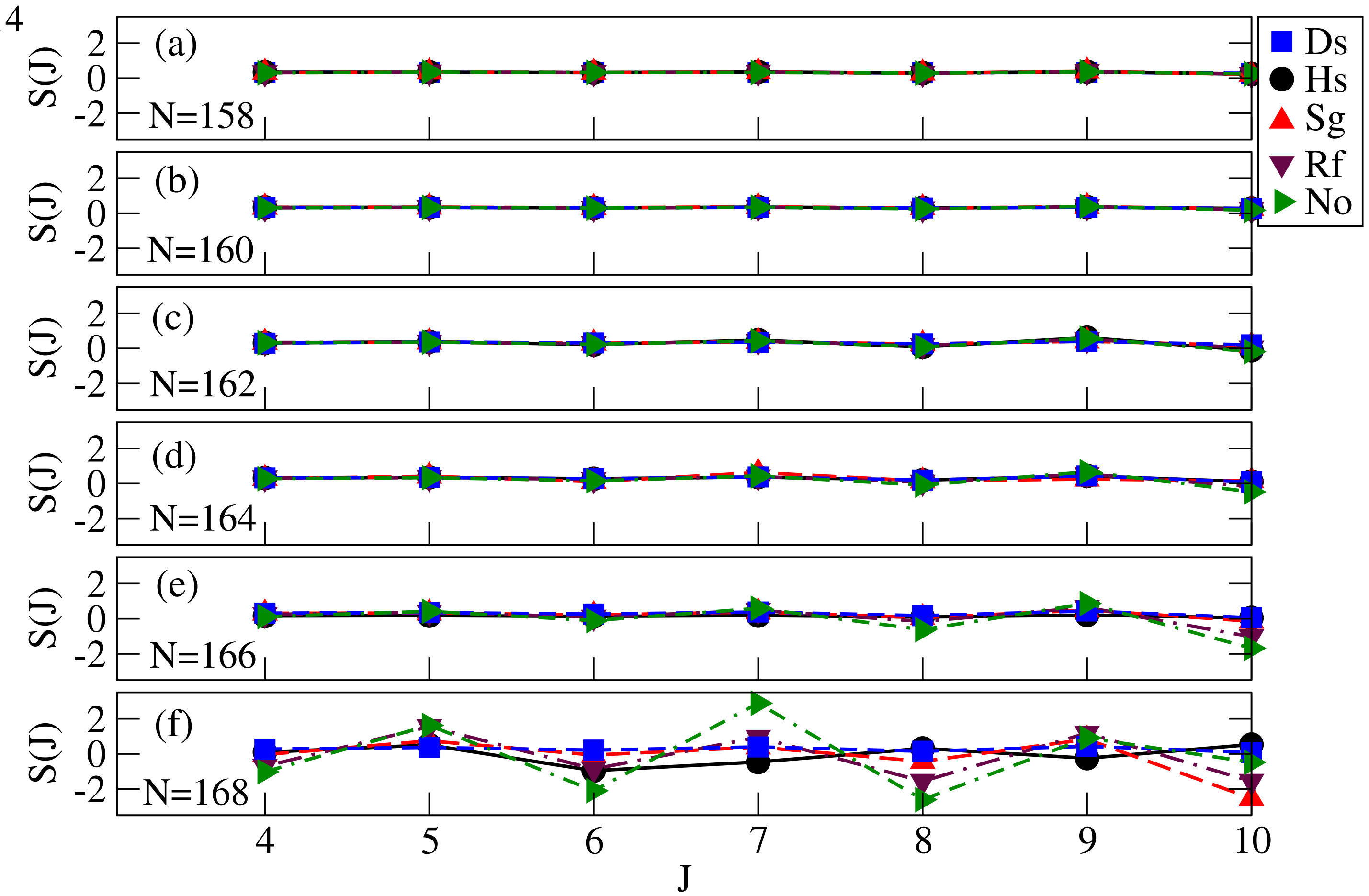


The ratio of reduced transition probabilities $B(E2; 4^+_1 \rightarrow 2^+_1) / B(E2; 2^+_1 \rightarrow 0^+_1)$ as a function of the neutron number.



B(E2) values for transition between yrast states, normalized to B(E2; $2^+_1 \rightarrow 0^+_1$), in the N= 158, 160, 162, 164, 166 and 168 isotones of No, Rf, Sg, Hs and Ds.

Staggering in the γ-bands of No, Rf, Sg, Hs and Ds with N= 158 − 166.



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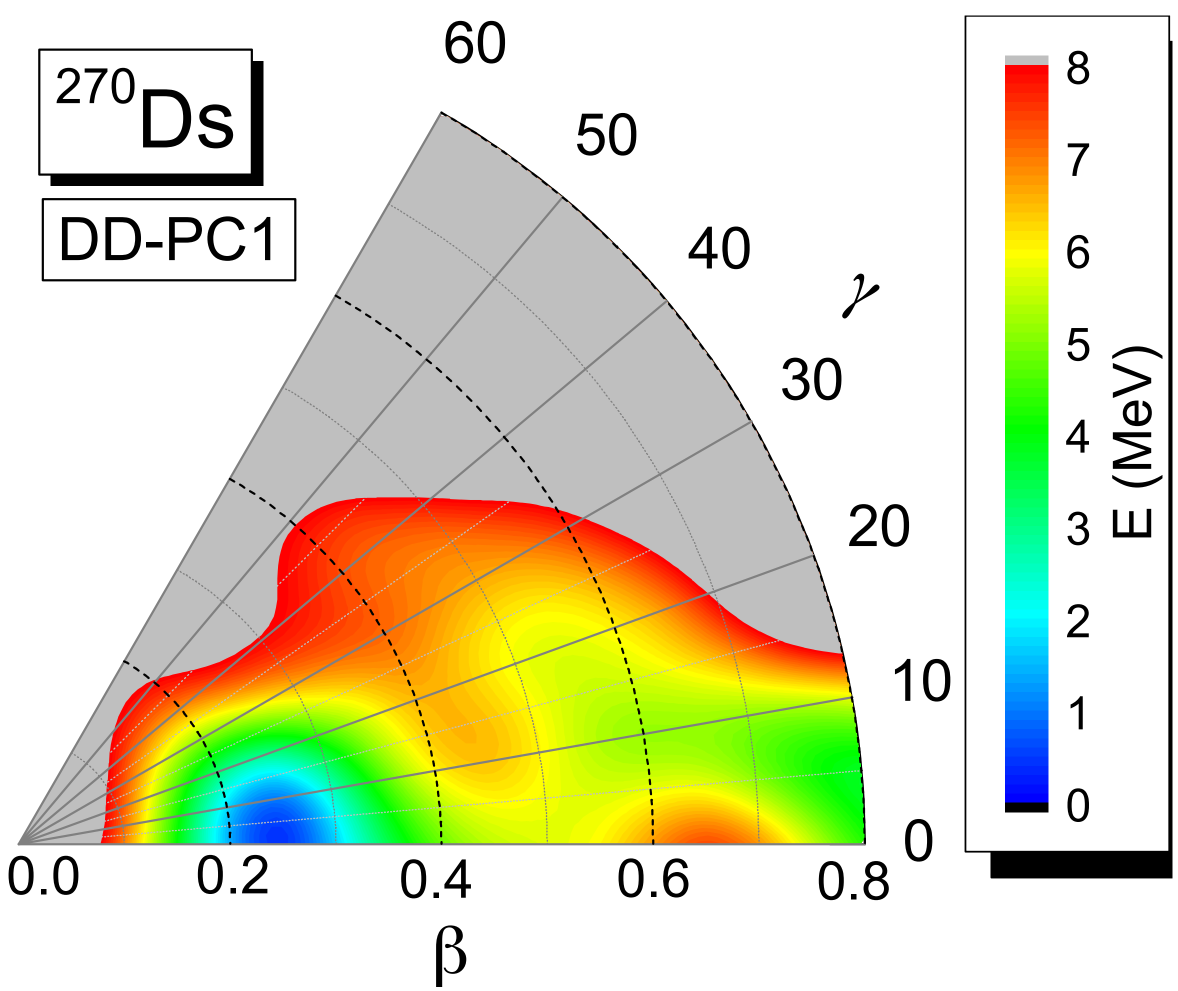
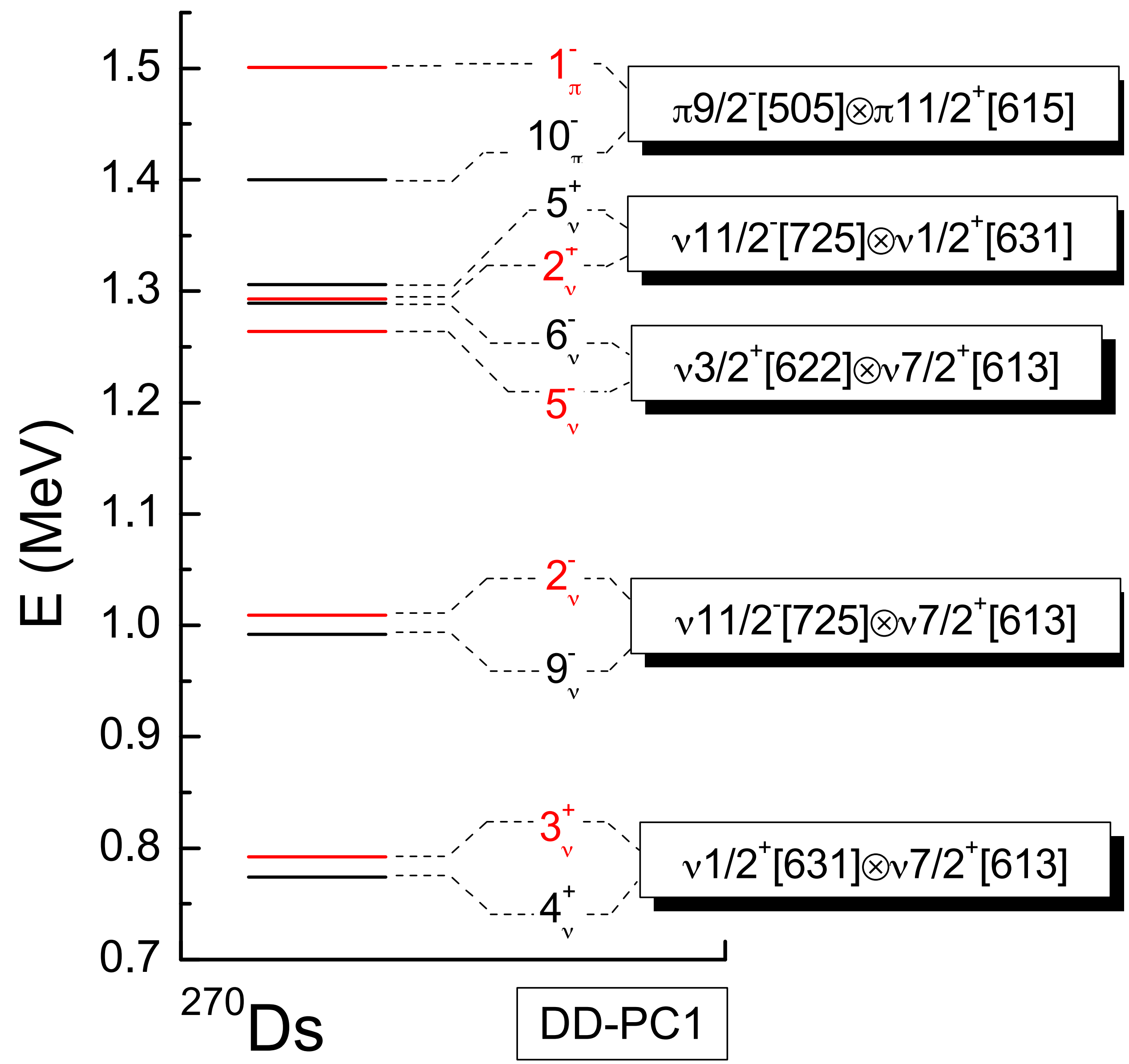
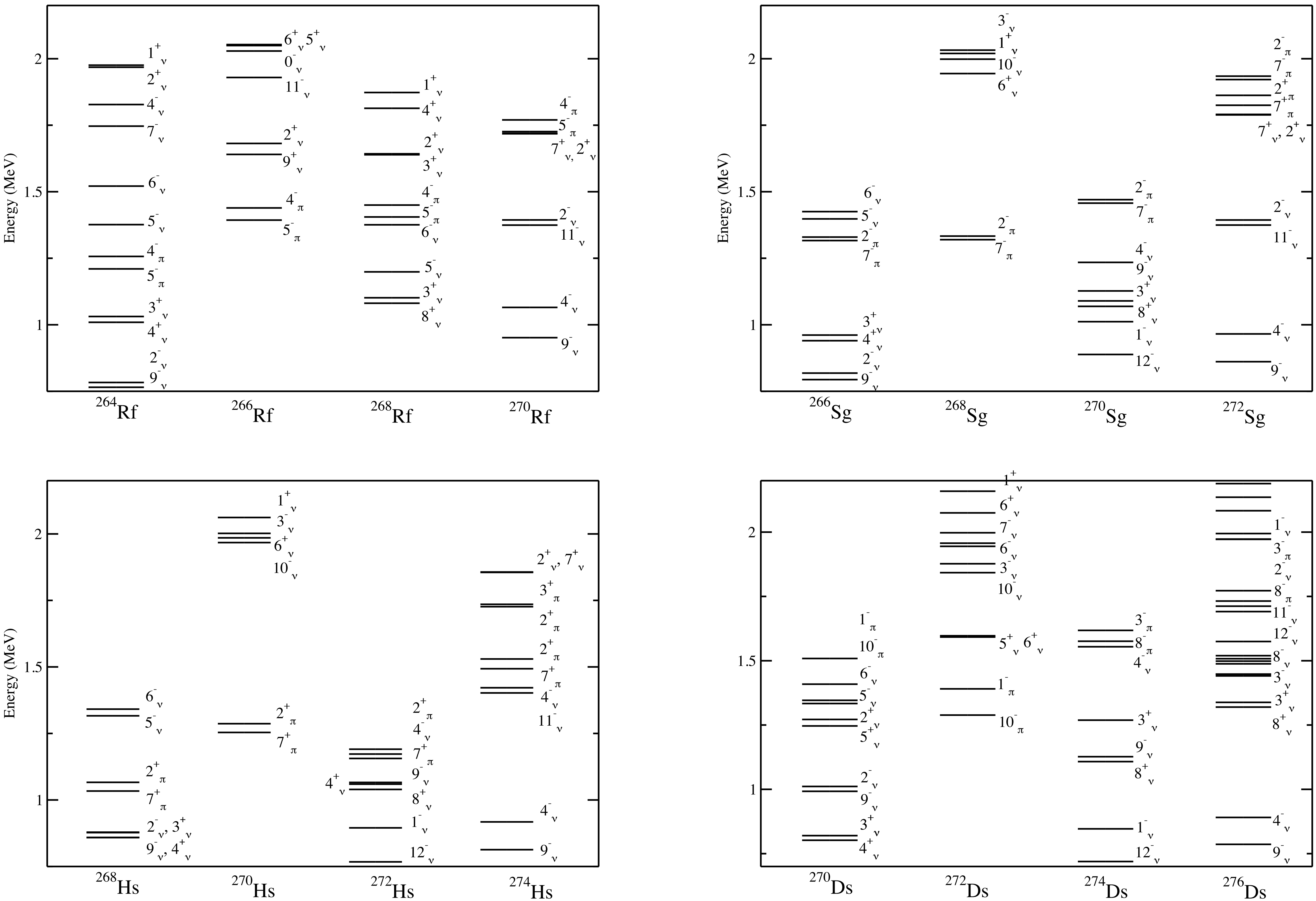
Two-quasiparticle isomers

Axially deformed nuclei ➠ two-quasiparticle K-isomers





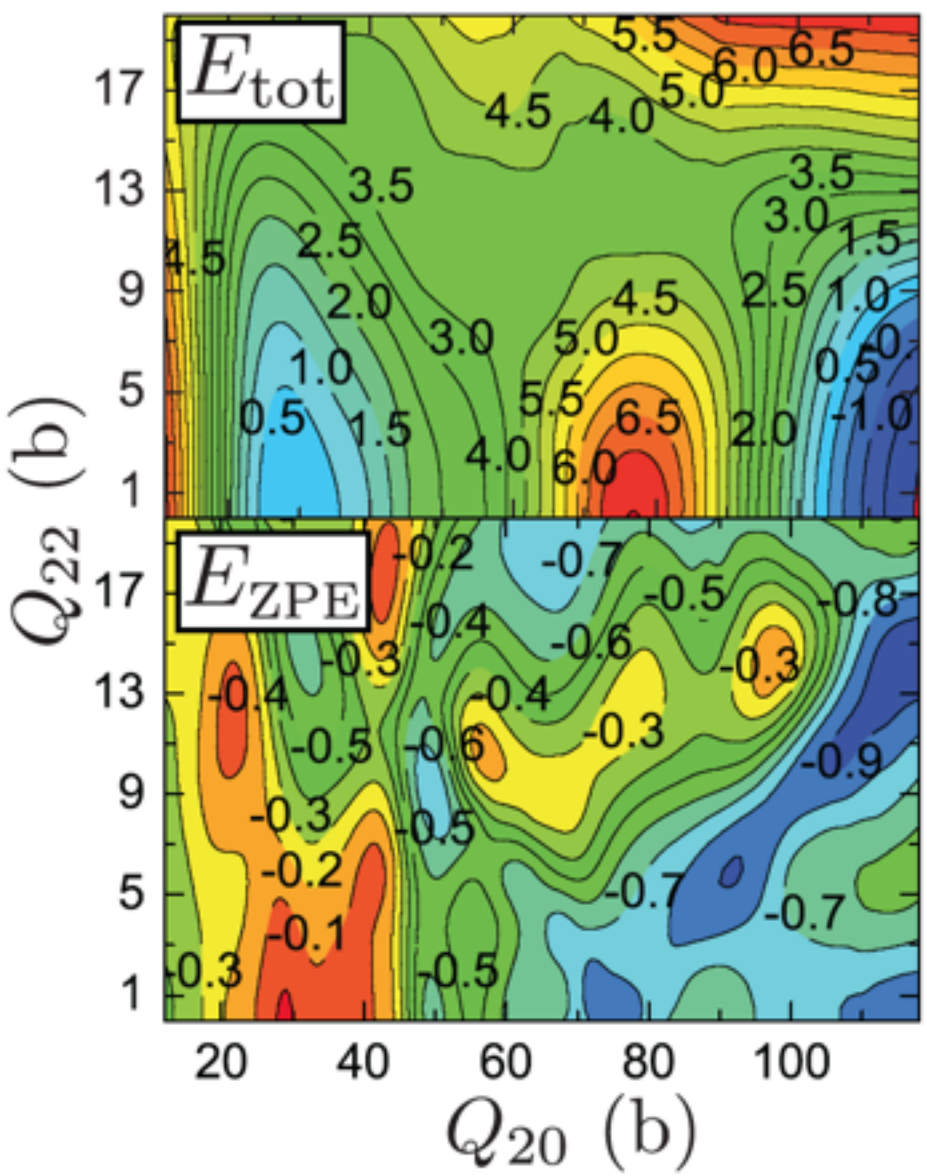
High-excitation energy of K-isomers ➠ evidence for axially deformed shell-closure



Spontaneous fission

… penetration probability: $$P = (1 + \exp[2S(L)])^{-1}$$

⇒ fission action integral: $$S(L) = \int_{s_{in}}^{s_{out}} \frac{1}{\hbar}\sqrt{2\mathcal{M}_{eff}(s)(V_{eff}(s) - E_0)}\, ds$$



The inertia tensor and collective potential calculated in the SCMF approach based on a microscopic energy density functional.

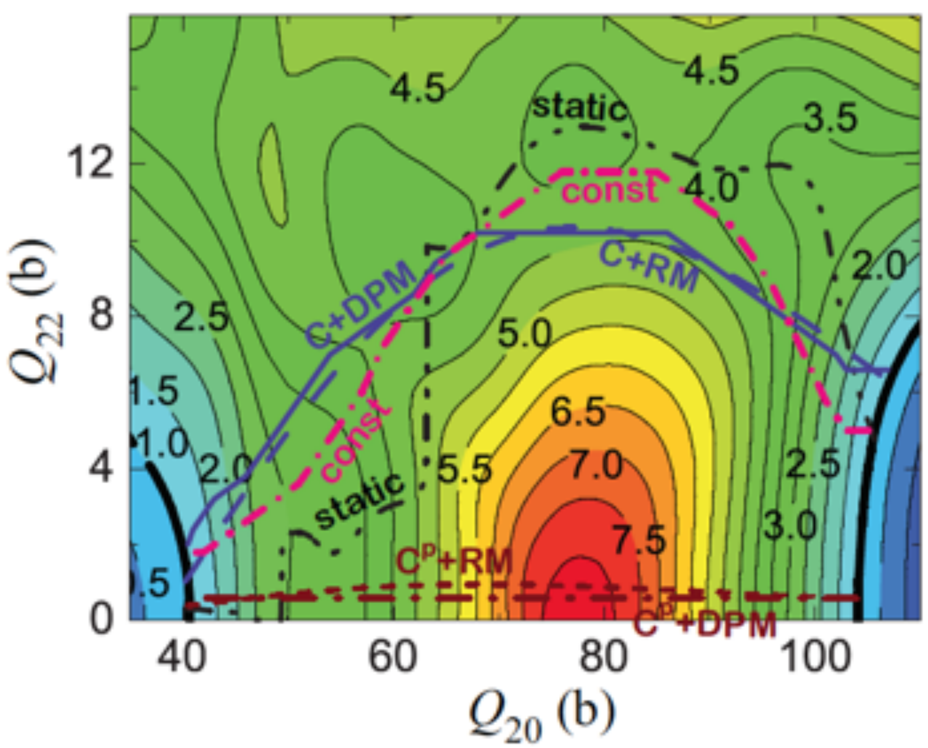
Symmetric fission of ^{264}Fm.

Total HFB deformation energy surface and the zero-point energy correction.

JHILAM SADHUKHAN *et al.*

PHYSICAL REVIEW C **88**, 064314 (2013)

The predicted SF path strongly depends on the choice of the collective inertia!



Values of the action integral and half-lives for different SF paths.

Path	$S(L)$	$\log_{10}(T_{1/2}/\text{yr})$
Static + $\mathcal{M}^{C}$	23.4	−7.7
Static + $\mathcal{M}^{C^P}$	20.8	−10.0
DPM + $\mathcal{M}^{C}$	19.1	−11.4
RM + $\mathcal{M}^{C}$	18.9	−11.6
DPM + $\mathcal{M}^{C^P}$	16.8	−13.4
RM + $\mathcal{M}^{C^P}$	16.8	−13.4

➡ calculation of the full ATDHFB inertia tensor!
➡ dynamical effects caused by the competition between triaxial and reflection asymmetric degrees of freedom, and pairing.

Nuclear Energy Density Functional Framework

✔ unified microscopic description of the structure of stable and nuclei far from stability, and extrapolations toward the region of superheavy nuclei.

✔ when extended to take into account collective correlations, EDFs describe deformations, shape-coexistence and shape transition phenomena associated with shell evolution. Separation energies, Q_α-values, excitation energies of band-heads in odd-A nuclei, excitation energies of high-K isomers, rotational spectra and moments of inertia.

✔ Time-dependent NDFT ➠ LACM, spontaneous fission dynamics