EDF calculation of shapes and barriers: mean field and beyond

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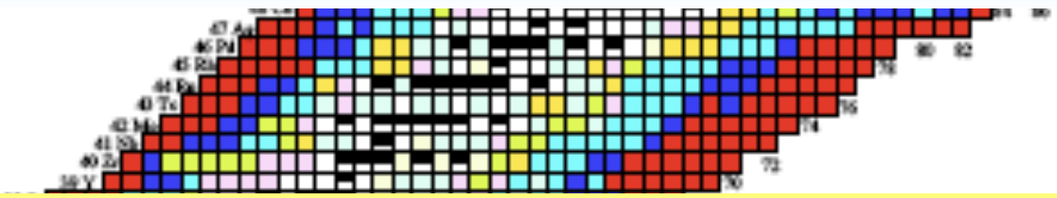
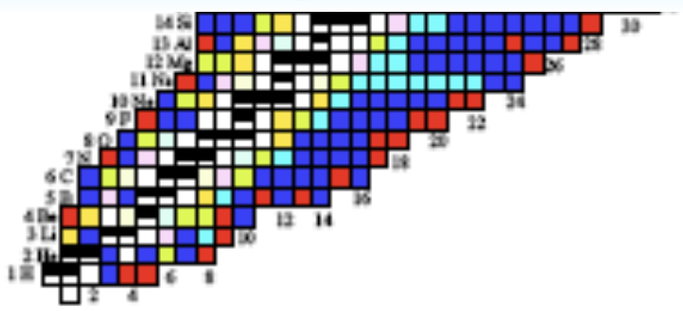
Relativistic Energy Density Functionals

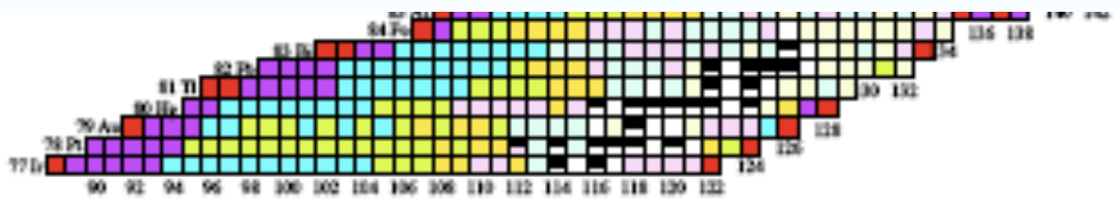
✔ natural inclusion of the ***spin degree of freedom*** (spin-orbit potential with empirical strength).



✔ unique parameterization of ***time-odd components*** (currents) of the nuclear mean-field.

✔ the distinction between scalar and vector self-energies leads to a natural ***saturation mechanism for nuclear matter.***





Relativistic energy density functionals:

The elementary building blocks are two-fermion terms of the general type:

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \qquad \mathcal{O}_\tau \in \{1, \tau_i\} \qquad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

... isoscalar and isovector four-currents and scalar densities:

$$\begin{aligned}
j_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\psi_k \ , \\
\vec{j}_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\vec{\tau}\psi_k \ , \\
\rho_S &= \langle\phi_0|\overline{\psi}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\psi_k \ , \\
\vec{\rho}_S &= \langle\phi_0|\overline{\psi}\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\vec{\tau}\psi_k
\end{aligned}$$

where $|\phi_0\rangle$ is the nuclear ground state.

⇒ build four-fermion (contact) interaction terms in the various isospace-space channels:

isoscalar-scalar:	$(\bar{\psi}\psi)^2$
isoscalar-vector:	$(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)$
isovector-scalar:	$(\bar{\psi}\vec{\tau}\psi)\cdot(\bar{\psi}\vec{\tau}\psi)$
isovector-vector:	$(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi)$

Empirical ground-state properties of finite nuclei can only determine a small set of parameters in the expansion of an effective Lagrangian in powers of fields and their derivatives.

Already at lowest order one finds more parameters than can be uniquely determined from data.

⇒ effective Lagrangian:

$$
\begin{aligned}
\mathcal{L} \quad = \quad & \bar{\psi}(i\gamma\cdot\partial - m)\psi \\
& -\frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\
& -\frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\
& -\frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma\cdot A\frac{(1-\tau_3)}{2}\psi
\end{aligned}
$$

$$
\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} \quad (i \equiv S, V, TV) \quad x = \rho/\rho_{sat}
$$

Hartree

correlations

Only one isovector term and one gradient term can be constrained by data.

Semi-phenomenological functionals

... start from a favorite microscopic nuclear matter EOS.

... the parameters of the functional are fine-tuned to data of finite nuclei.

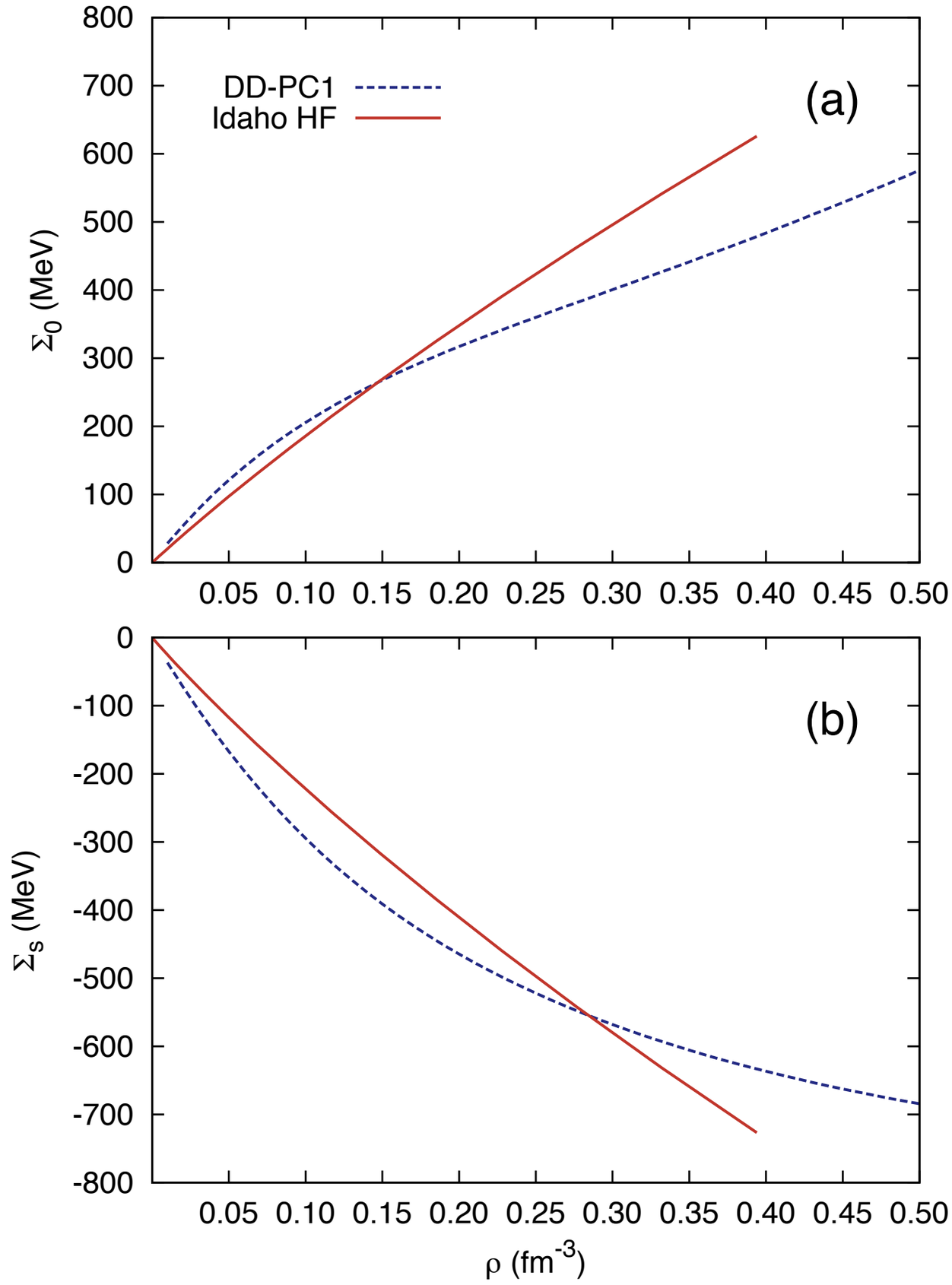
DD-PC1

... starts from microscopic nucleon self-energies in nuclear matter.

... 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.

Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter.

Starting approximation: Hartree-Fock self-energies calculated from the Idaho N^3LO NN-potential.



... calculated masses of finite nuclei are primarily sensitive to the three leading terms in the empirical mass formula:

$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

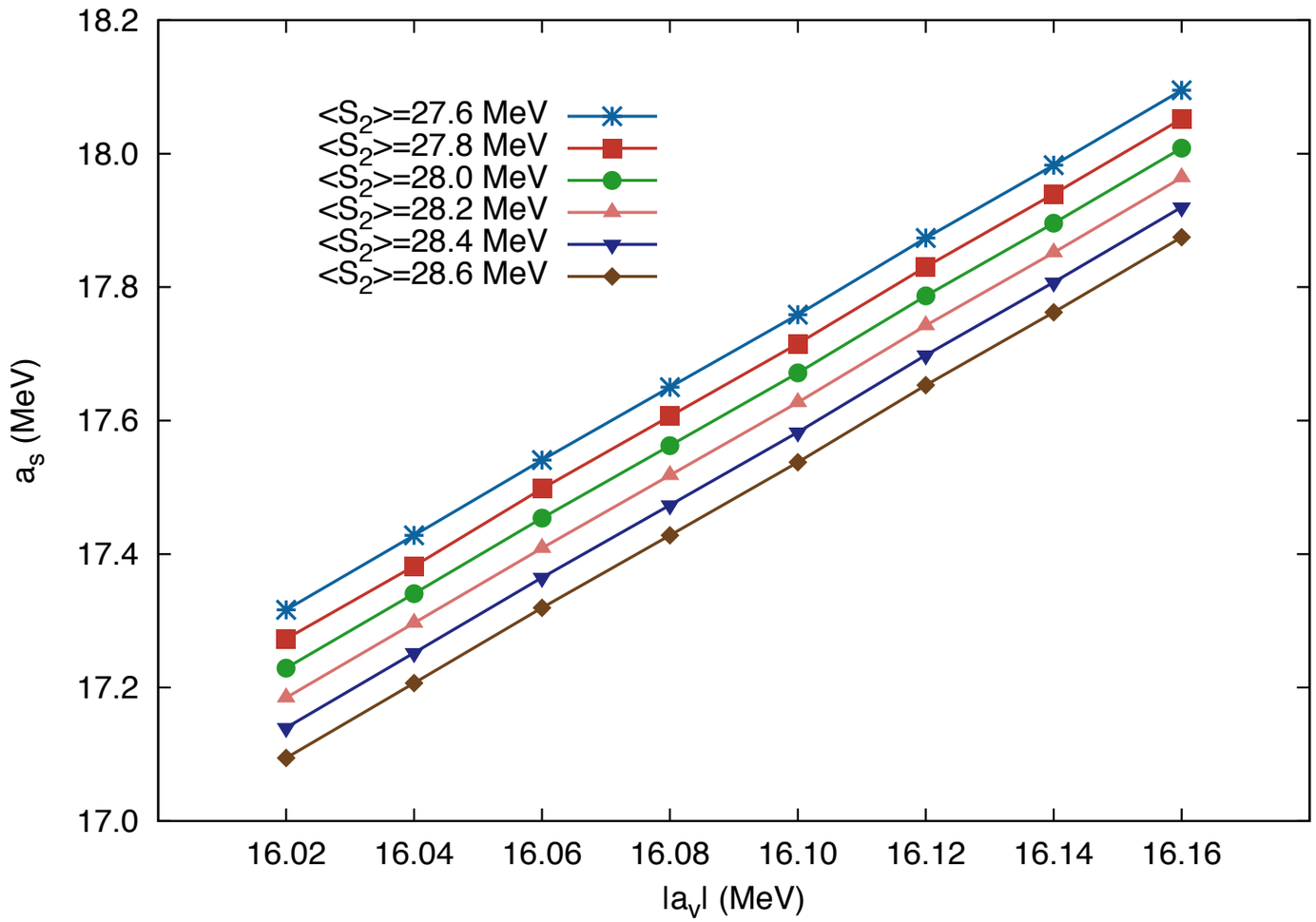
... generate families of effective interactions characterized by different values of a_v, a_s and a_4, and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

Deformed nuclei

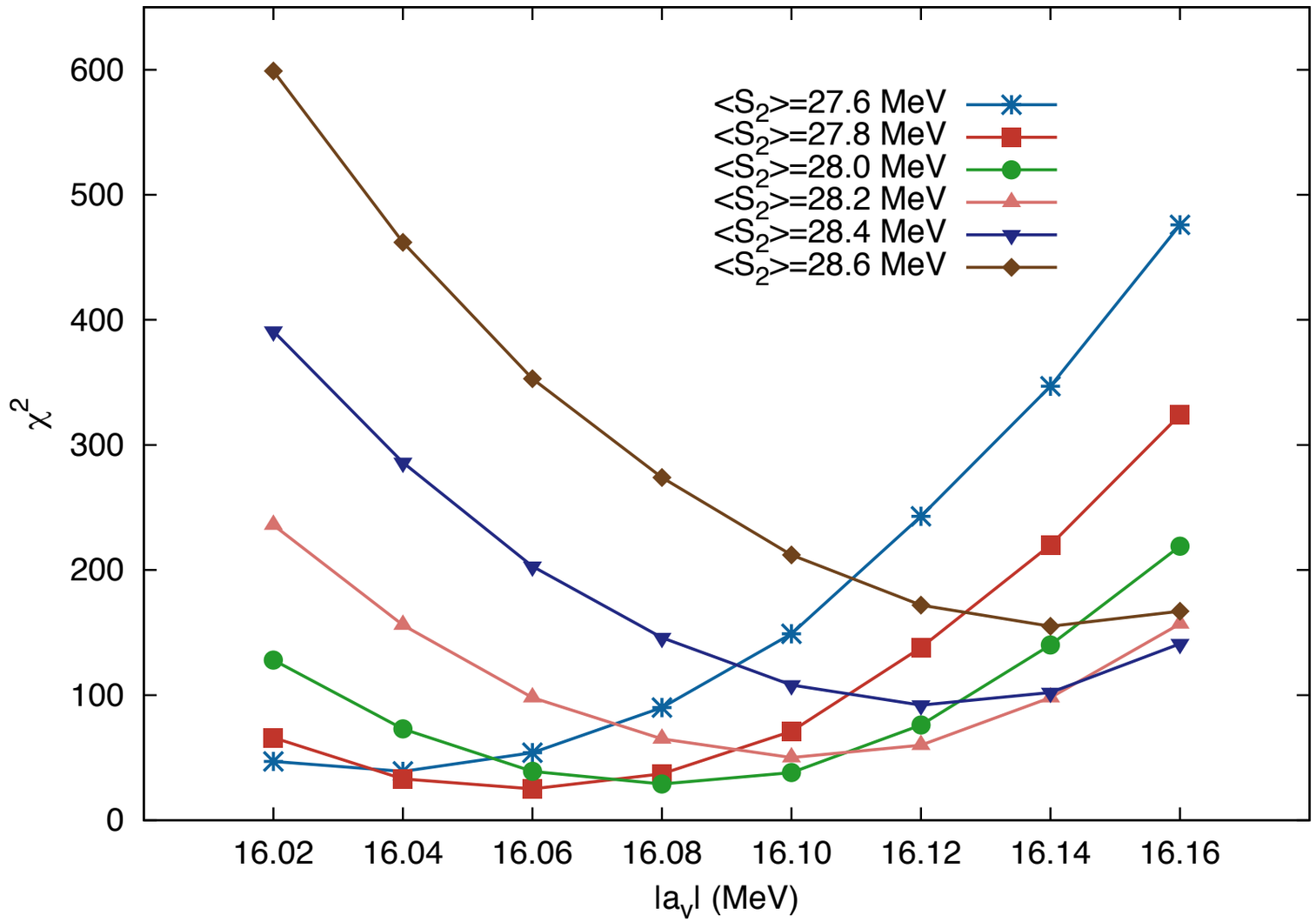
Binding energies used to adjust the parameters of the functional:

Z	62	64	66	68	70	72	90	92	94	96	98
N_{min}	92	92	92	92	92	72	140	138	138	142	144
N_{max}	96	98	102	104	108	110	144	148	150	152	152

Surface energies of semi-infinite nuclear matter that minimize the deviation of the calculated binding energies from data.

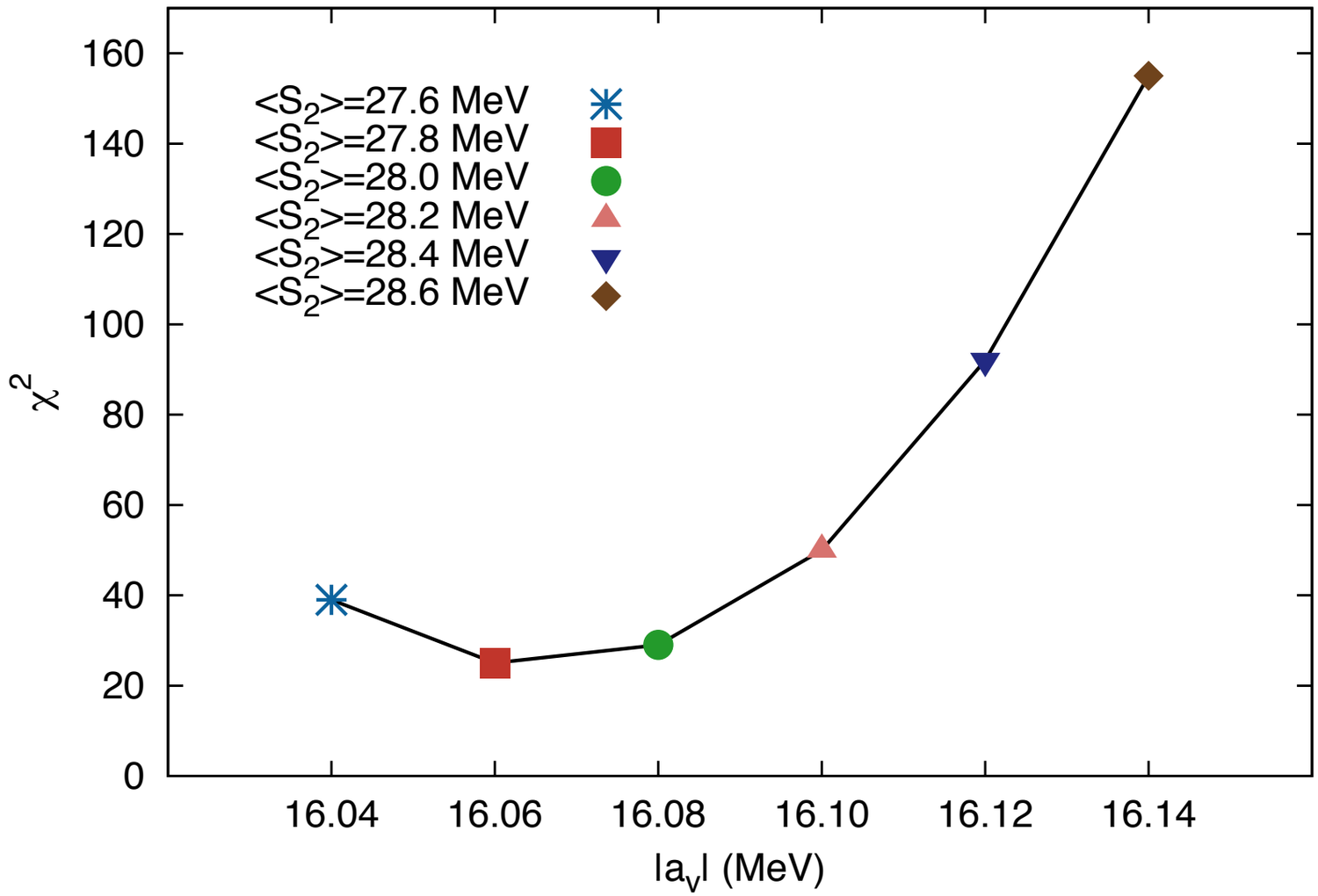


... 48 parameterizations of the energy density functional:



For each value $\langle S_2 \rangle$ of the symmetry energy, there is a unique combination of volume and surface energies that minimizes χ^2!

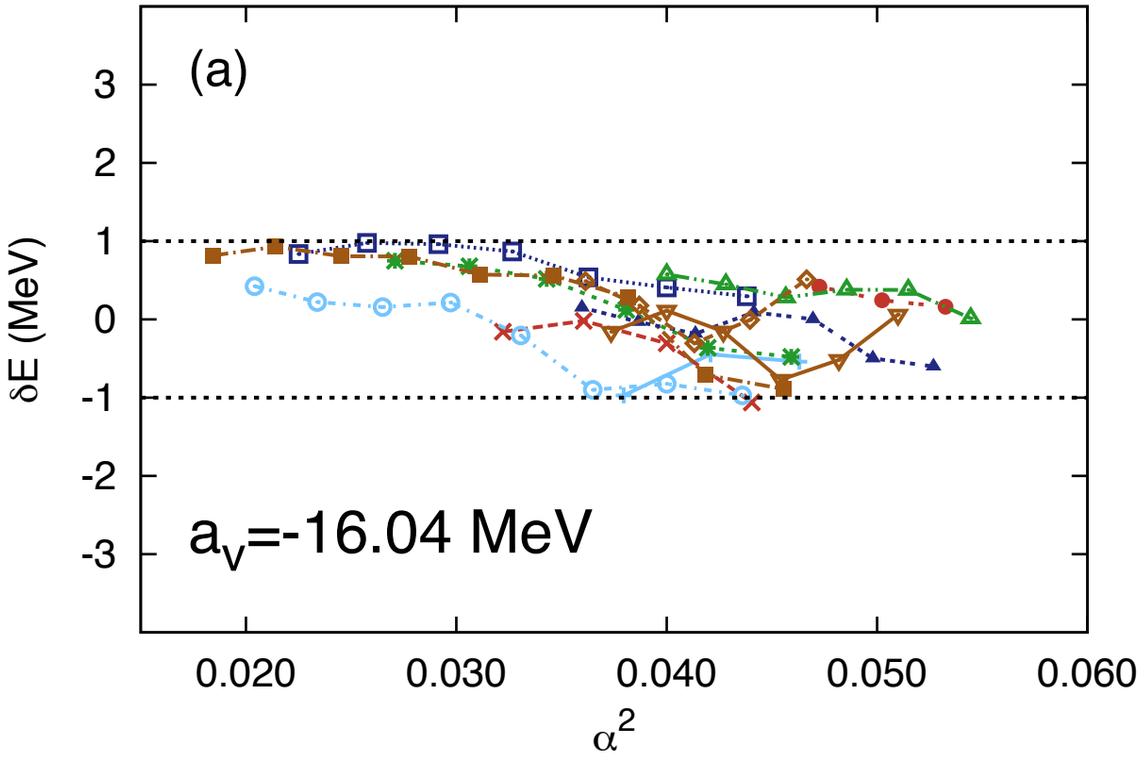
The minimum χ^2-deviation of the theoretical binding energies from data, as a function of the volume energy coefficient:

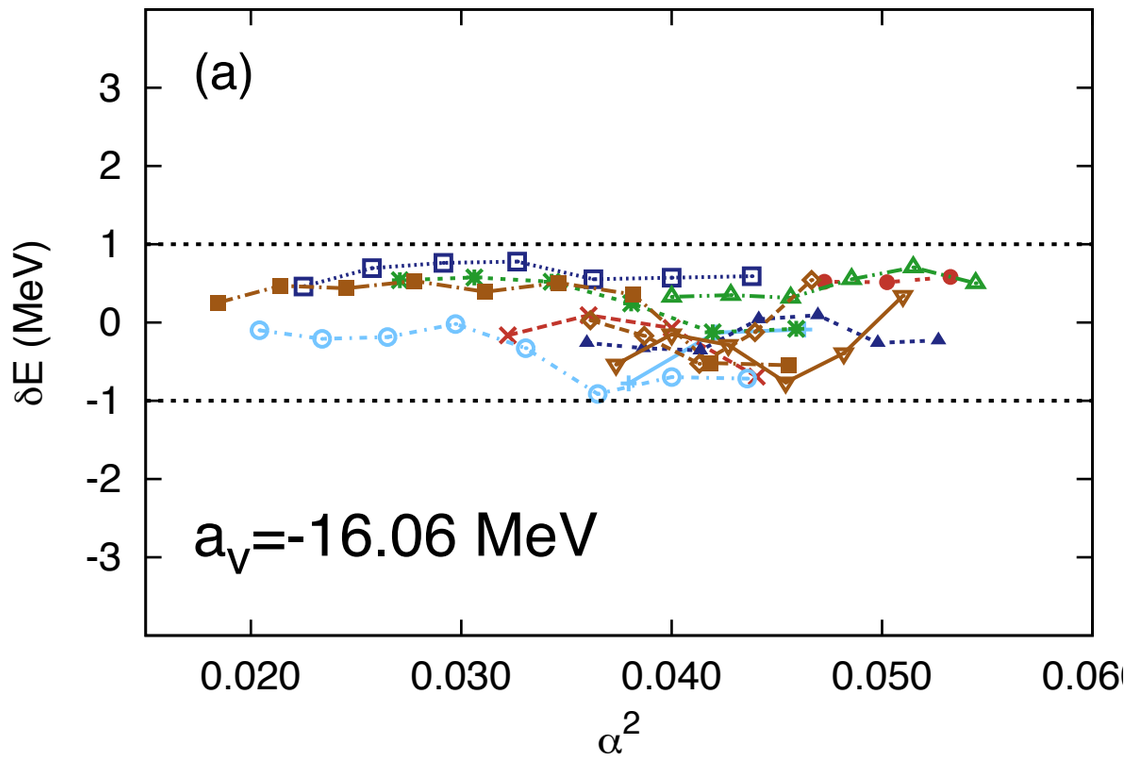


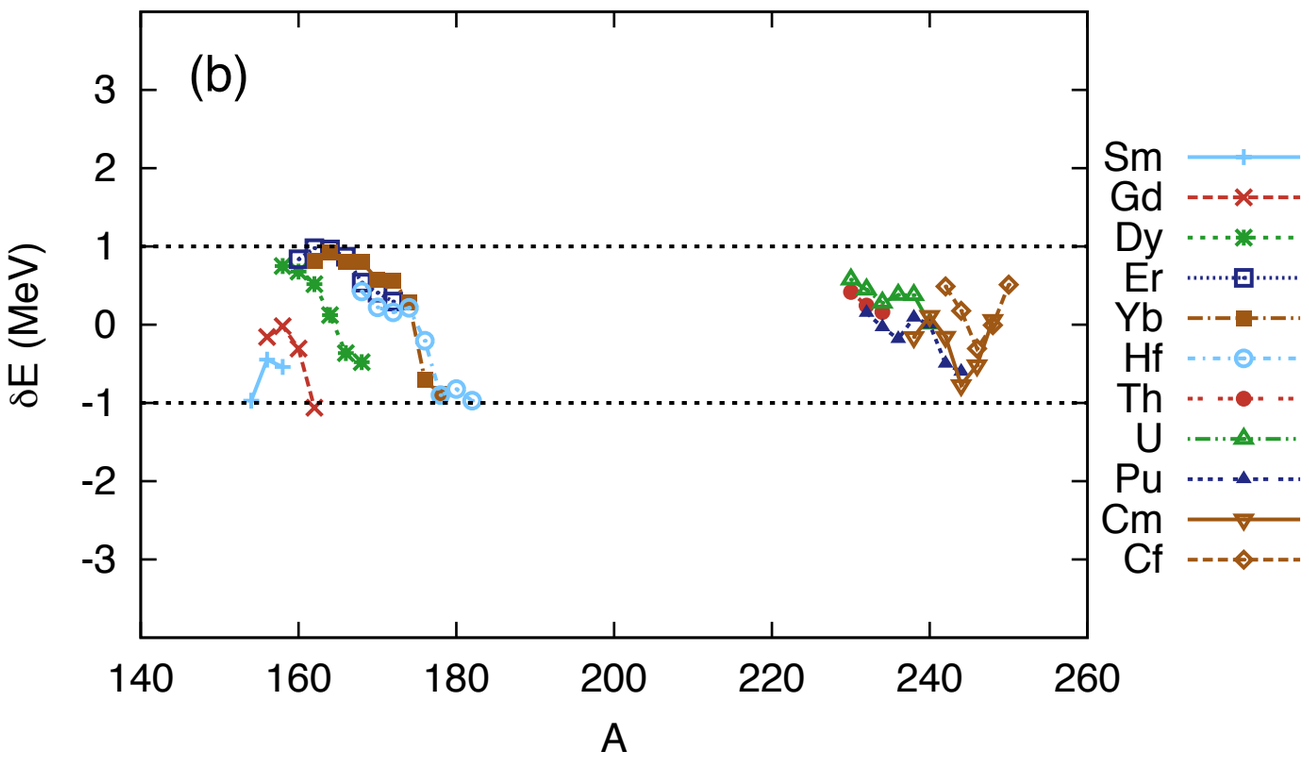
Absolute minimum:

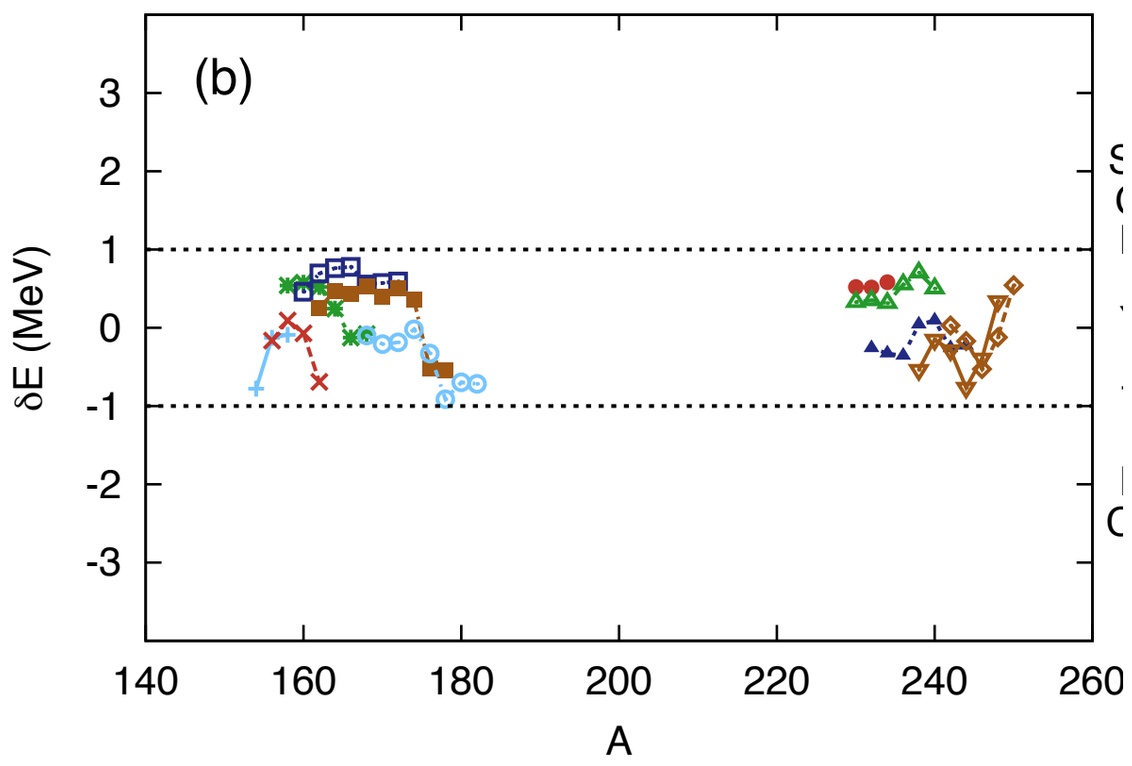
$$a_v = -16.06 \text{ MeV} \quad \langle S_2 \rangle = 27.8 \text{ MeV} \quad a_s = 17.498 \text{ MeV}$$

Absolute deviations of the calculated binding energies from data for 64 axially deformed nuclei:

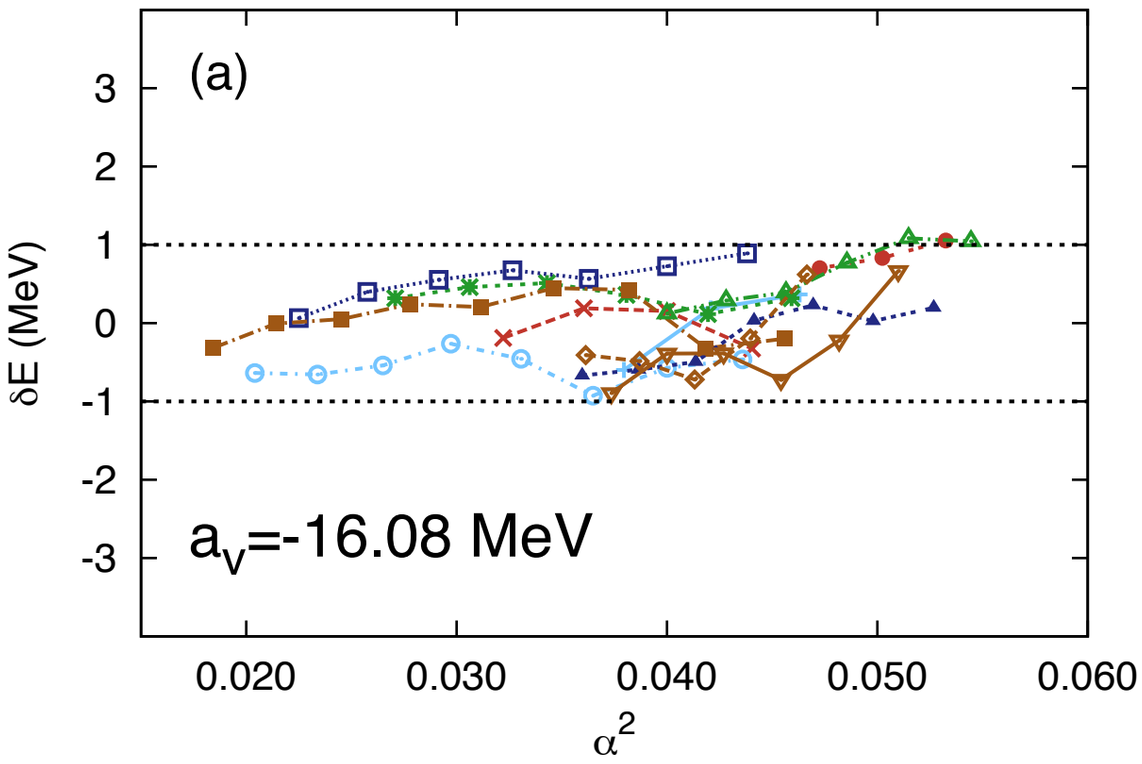


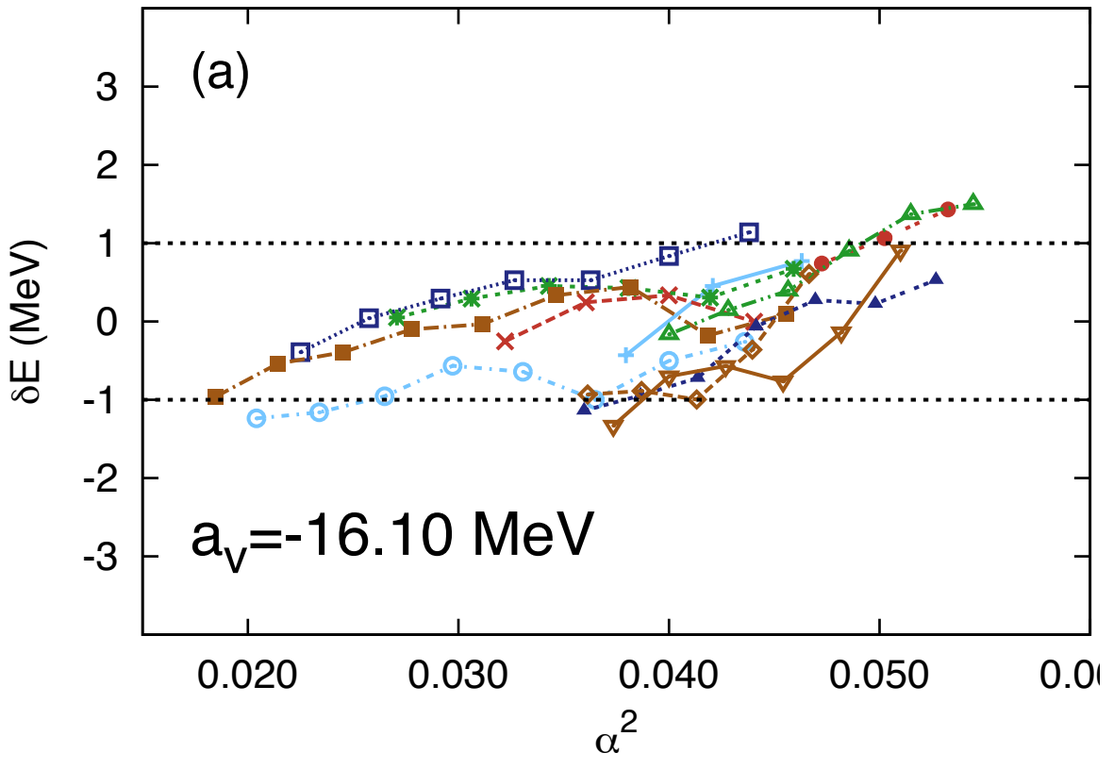


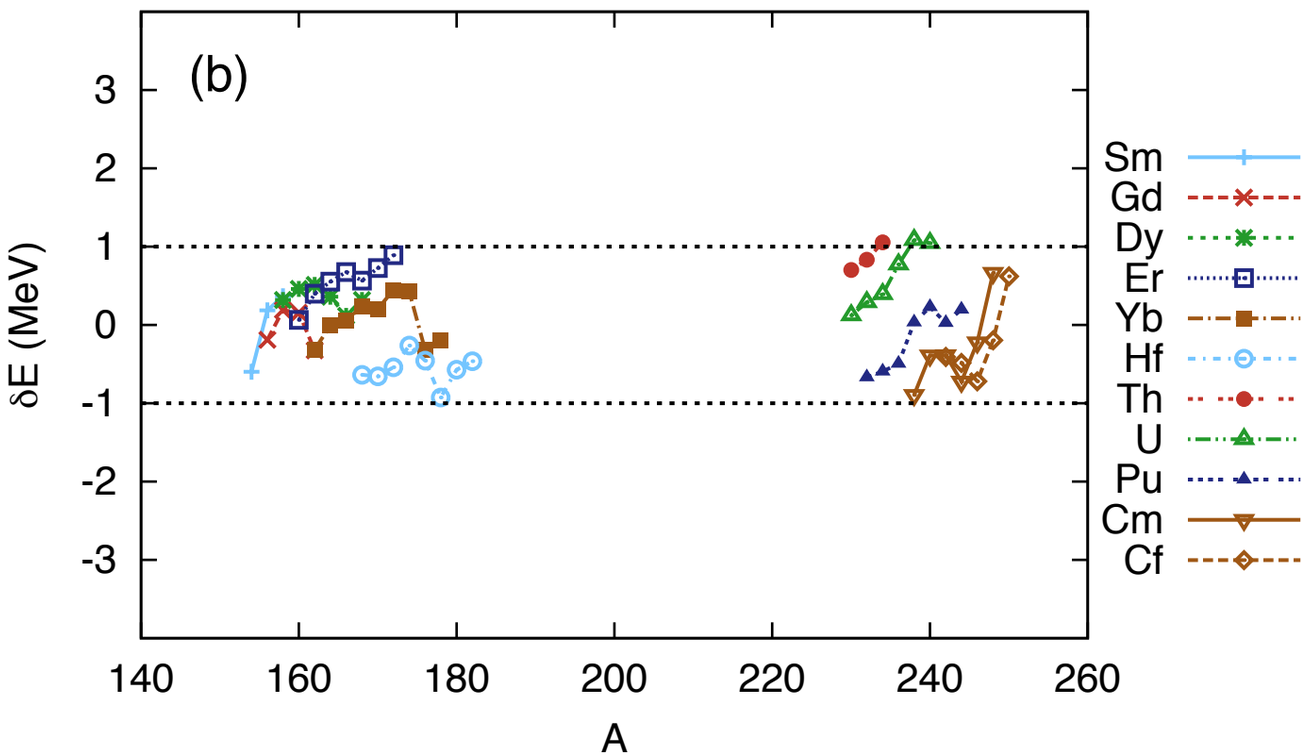


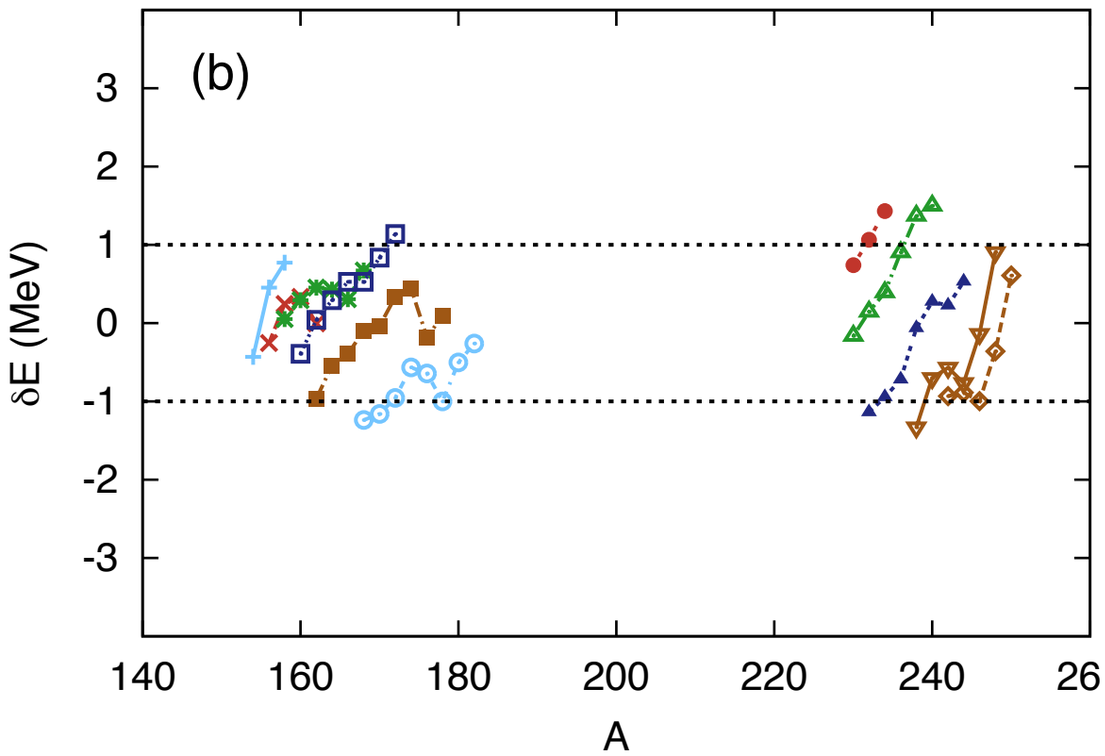


$$\alpha^2 = \frac{(N-Z)^2}{A^2}$$









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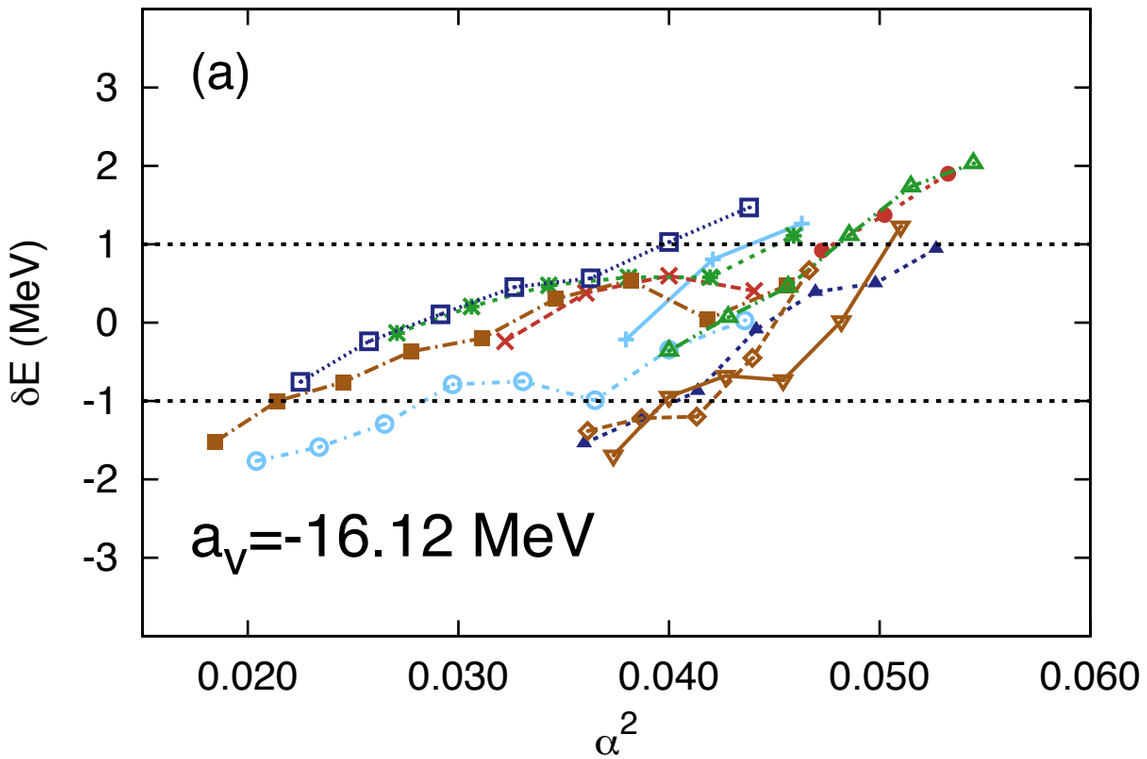
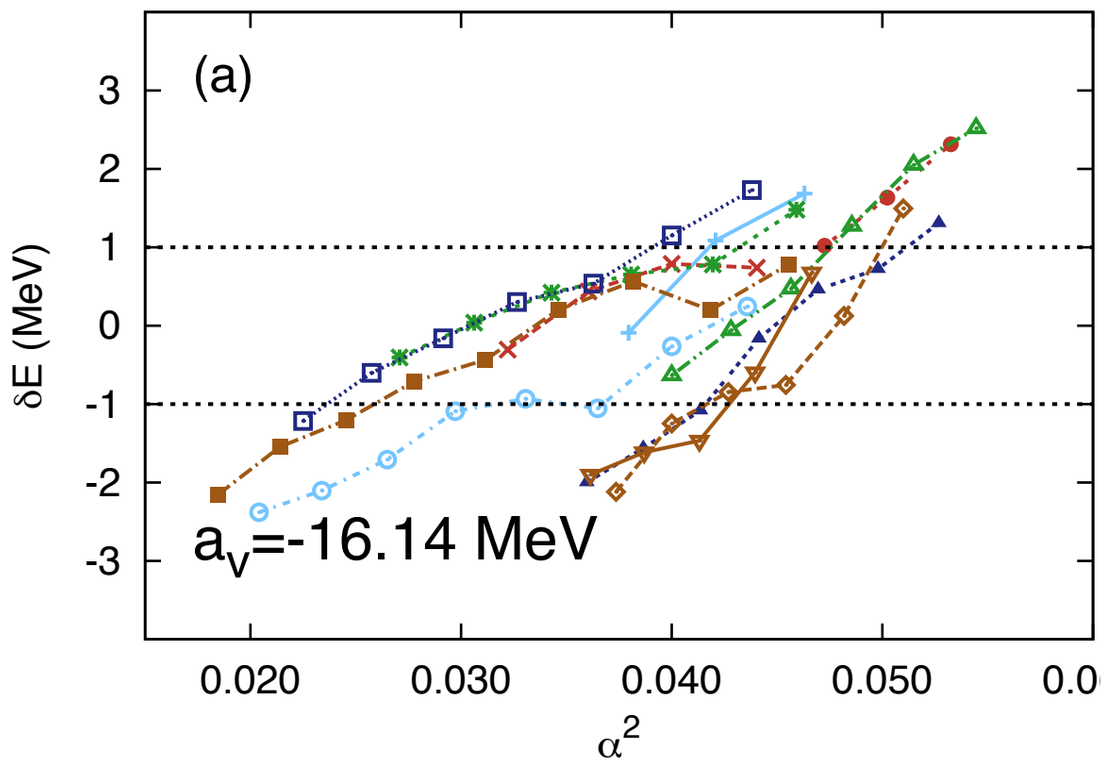
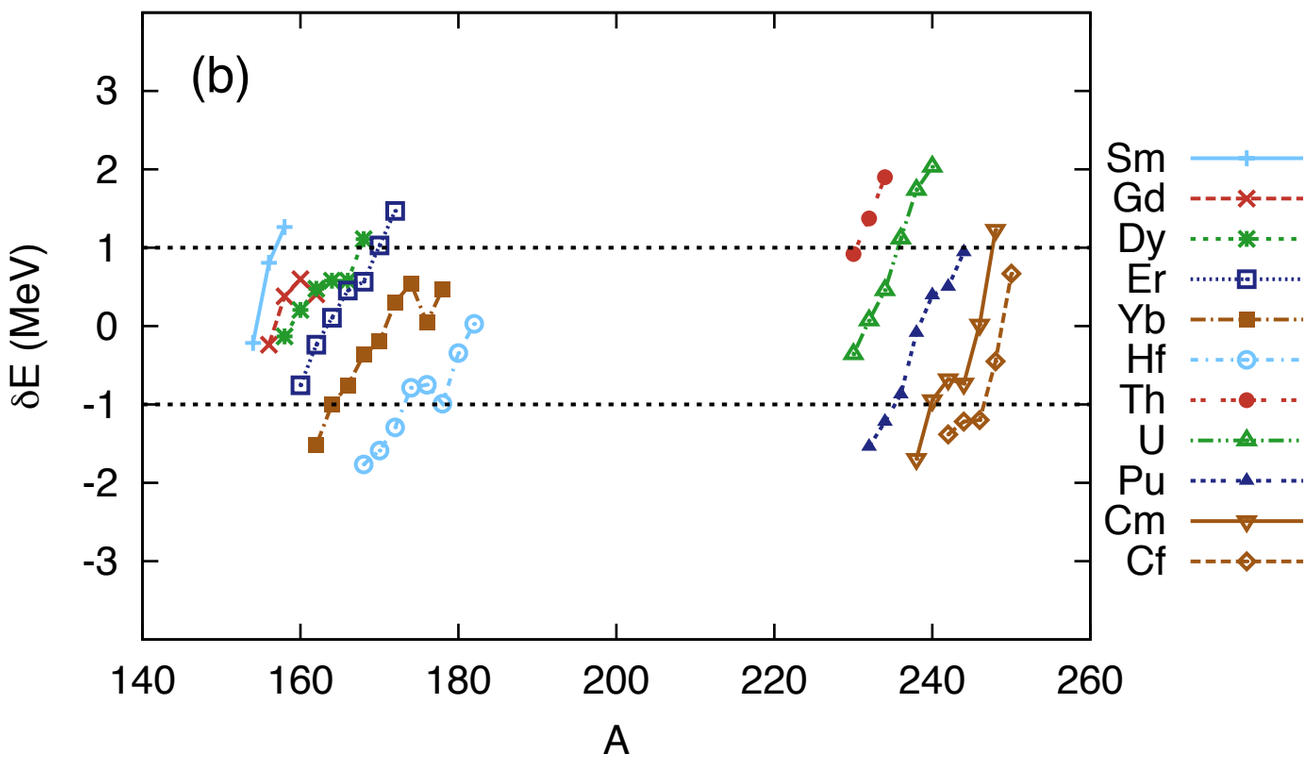
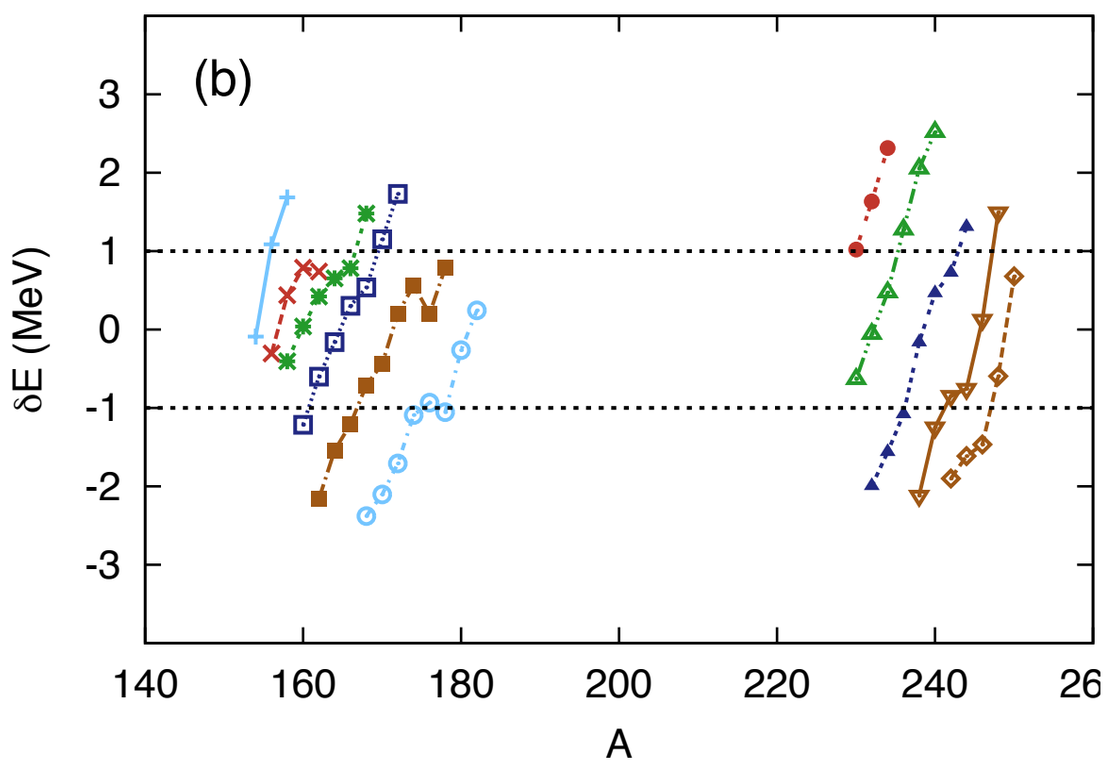
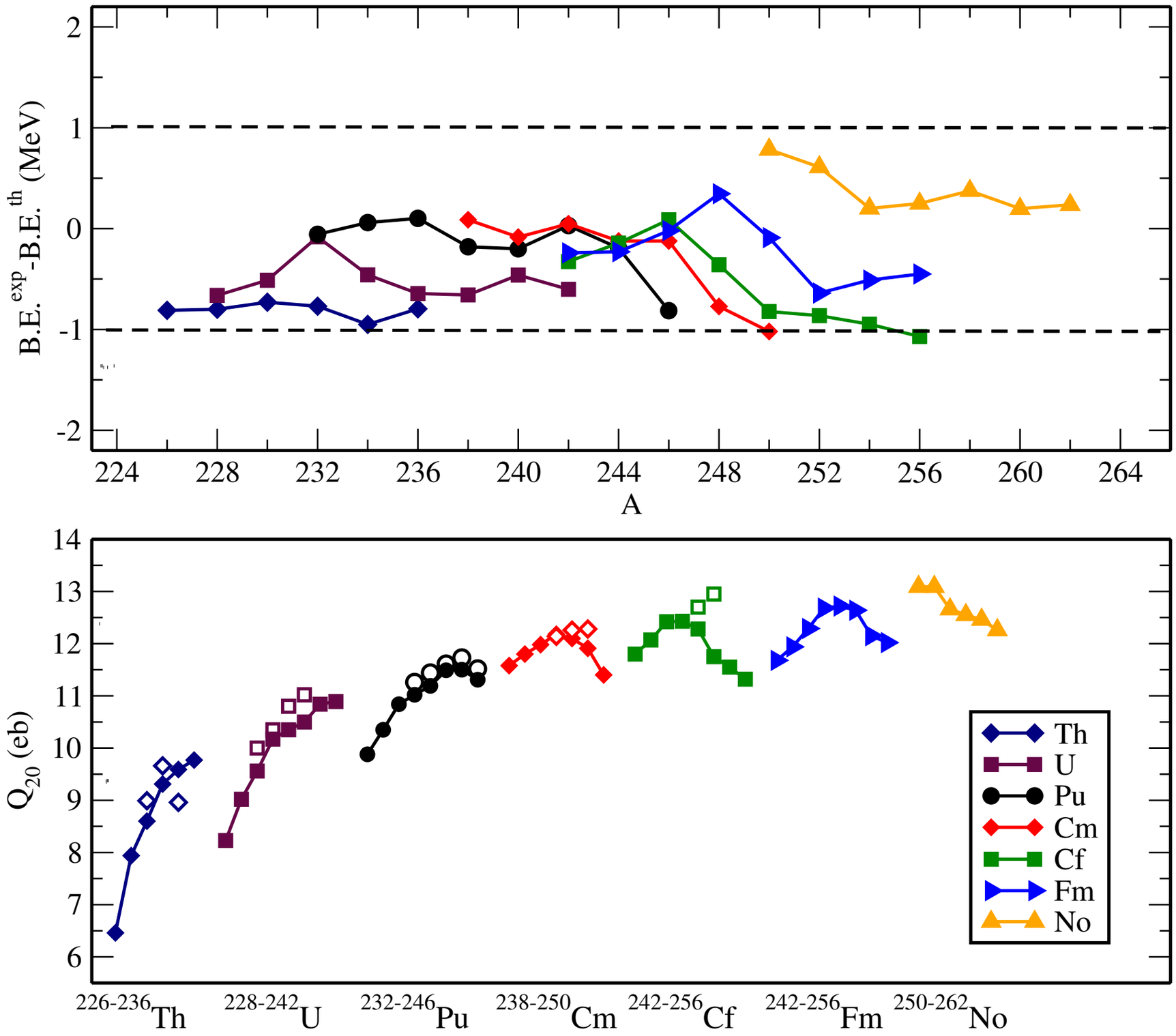




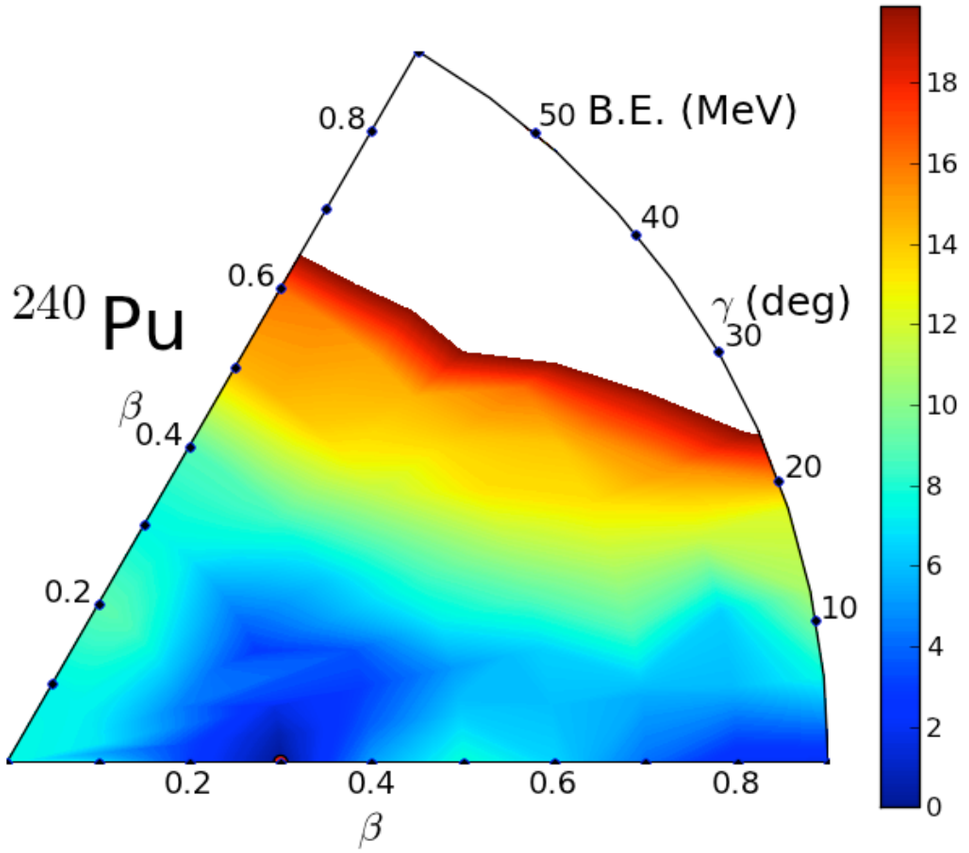


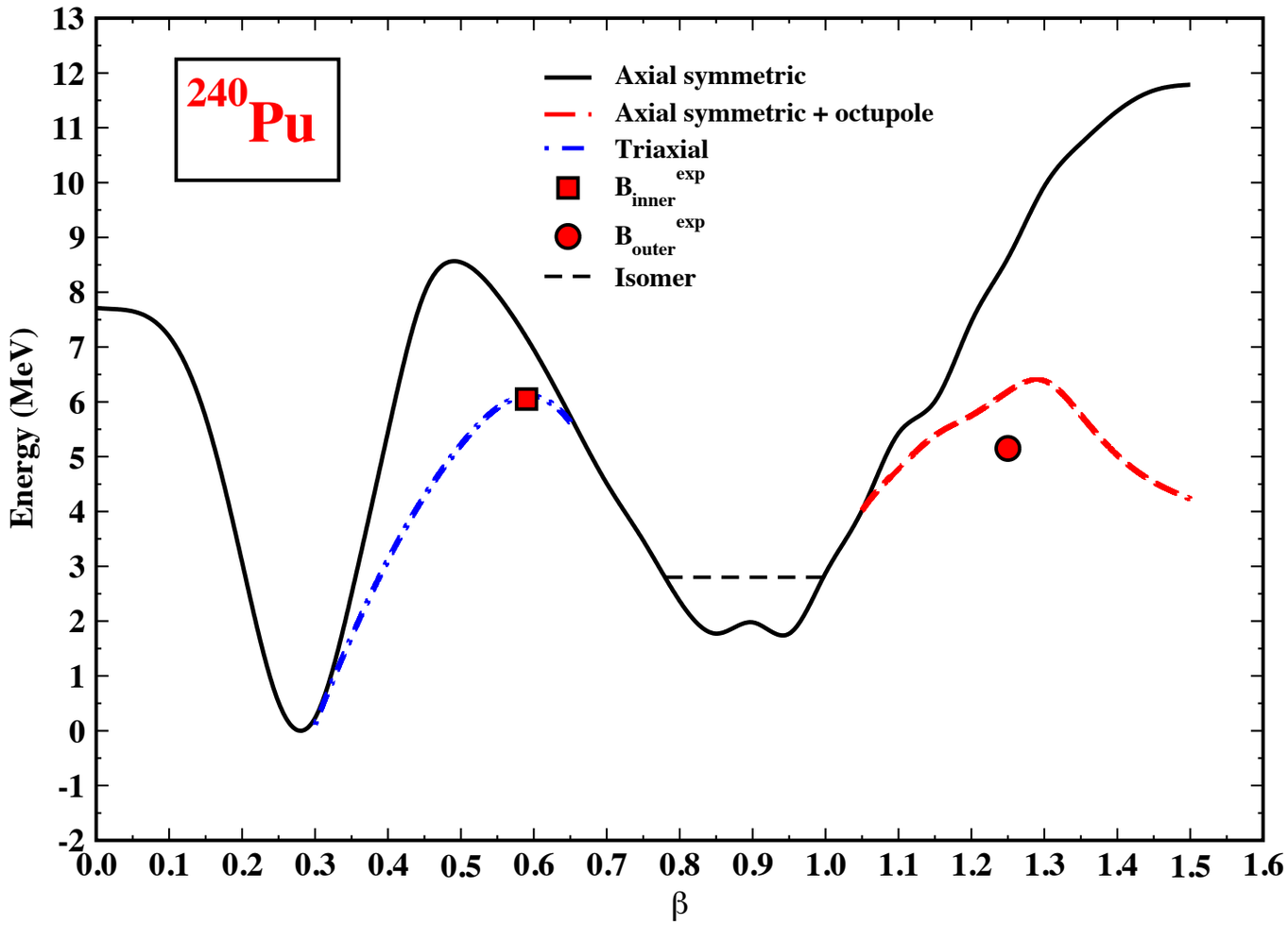


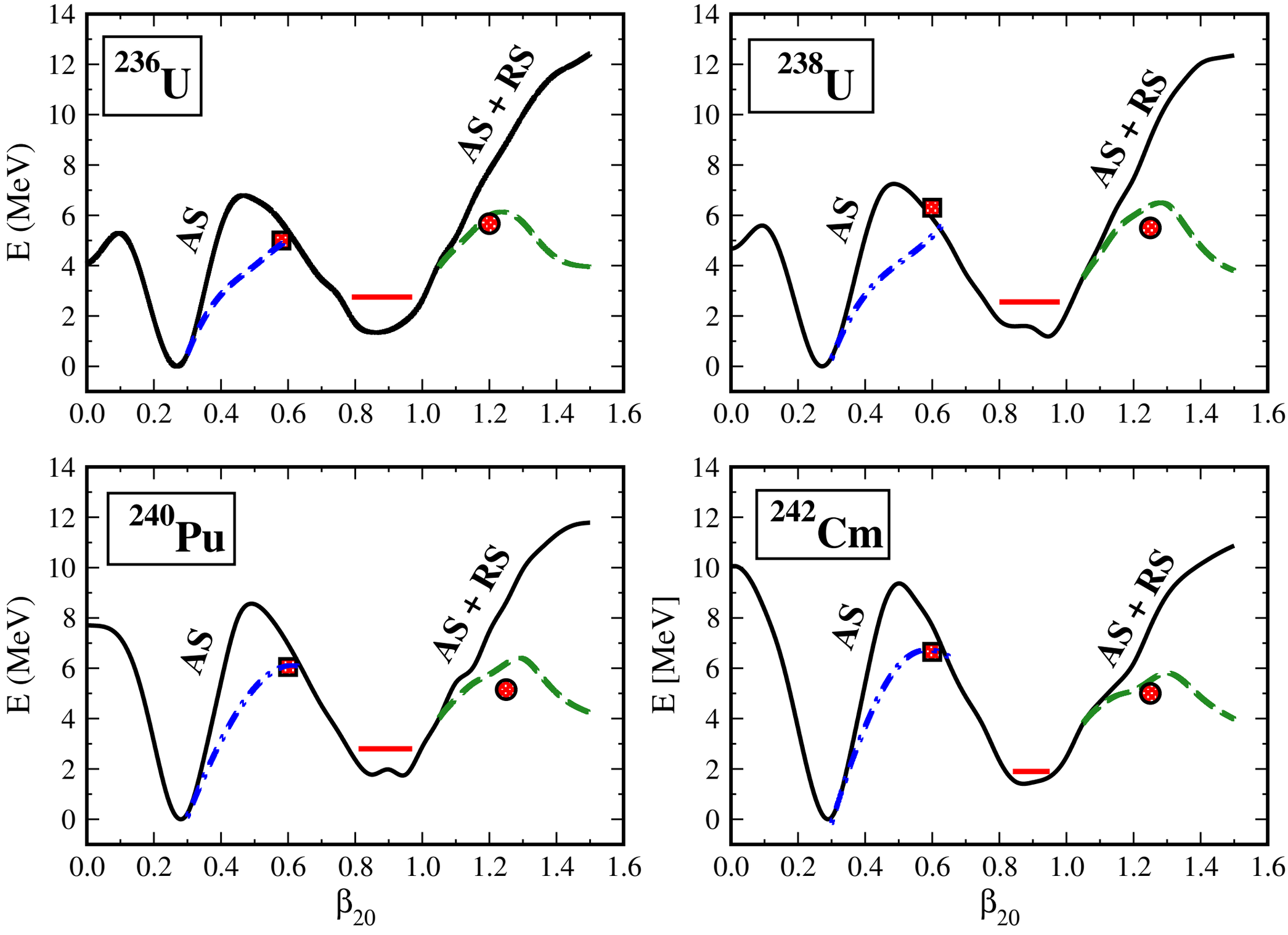
Test: ground-state properties of actinides

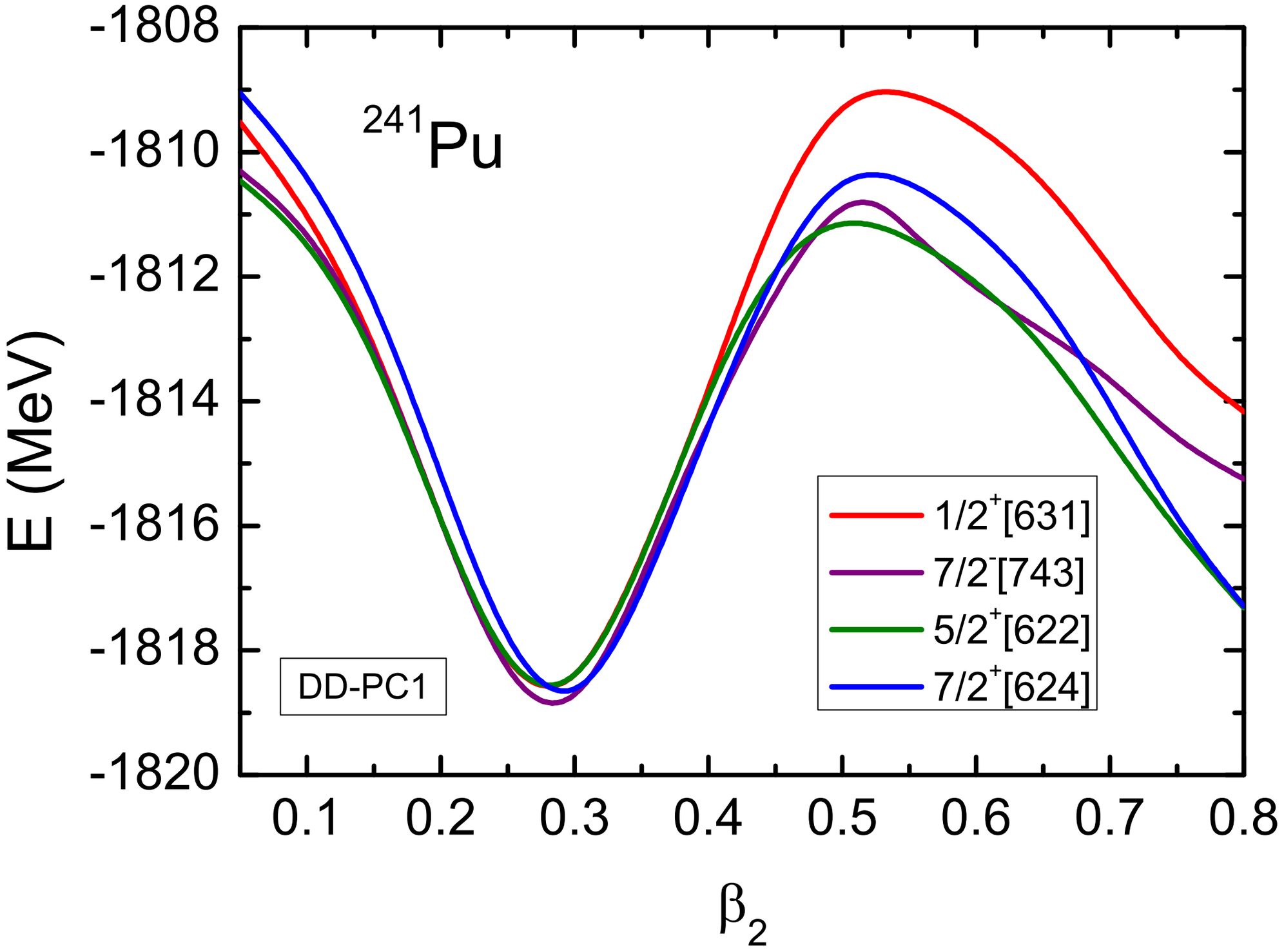


Test: "double-humped" fission barriers of actinides

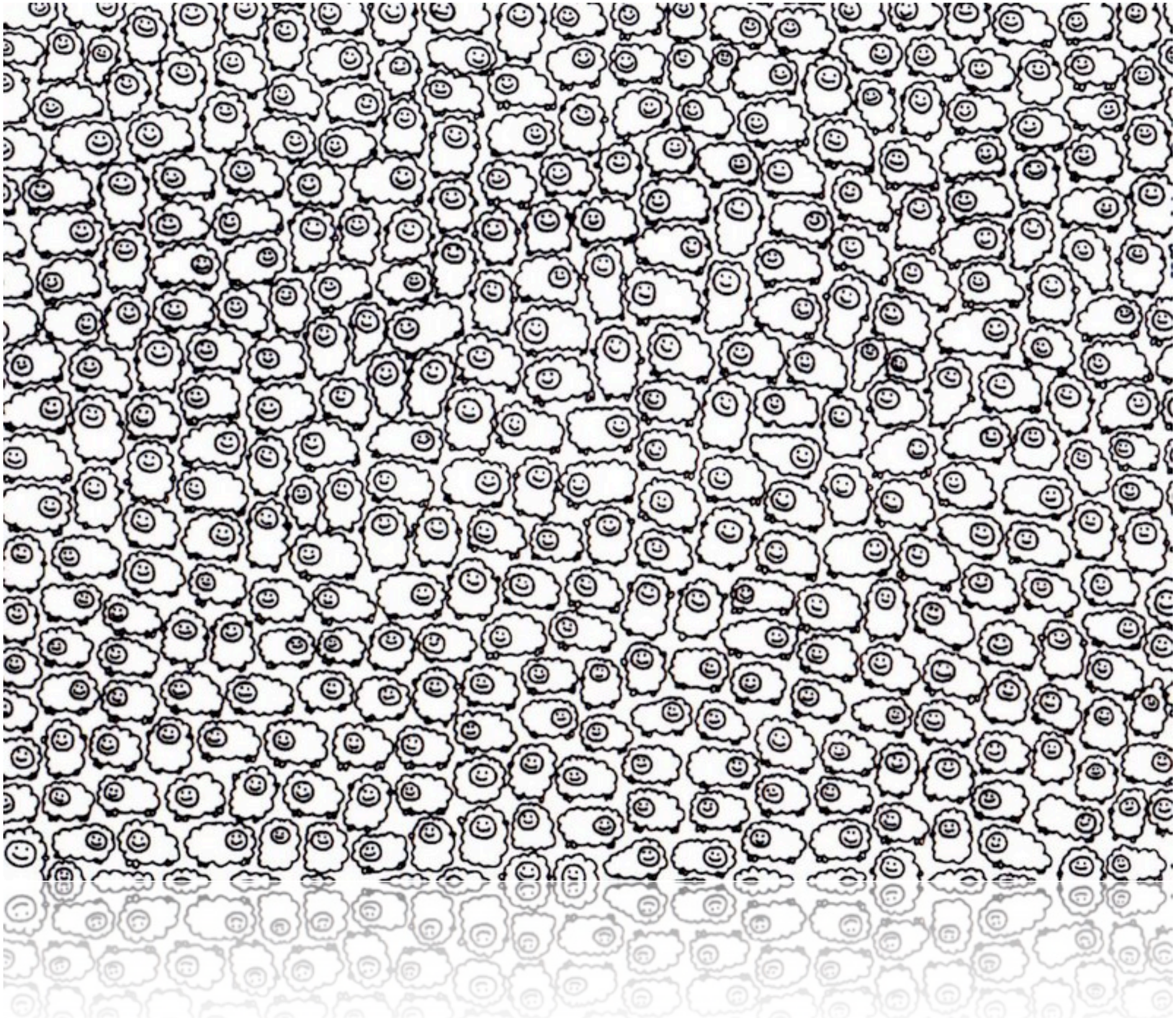





236U
238U
240Pu
242Cm
AS
AS + RS
E (MeV)
E [MeV]
β20


^{241}Pu
DD-PC1
1/2$^+$[631]
7/2$^-$[743]
5/2$^+$[622]
7/2$^+$[624]
E (MeV)
-1808
-1810
-1812
-1814
-1816
-1818
-1820
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
β$_2$

Collective correlations



Five-dimensional collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

$$H_{\rm coll} = \mathcal{T}_{\rm vib}(\beta,\gamma) + \mathcal{T}_{\rm rot}(\beta,\gamma,\Omega) + \mathcal{V}_{\rm coll}(\beta,\gamma)$$

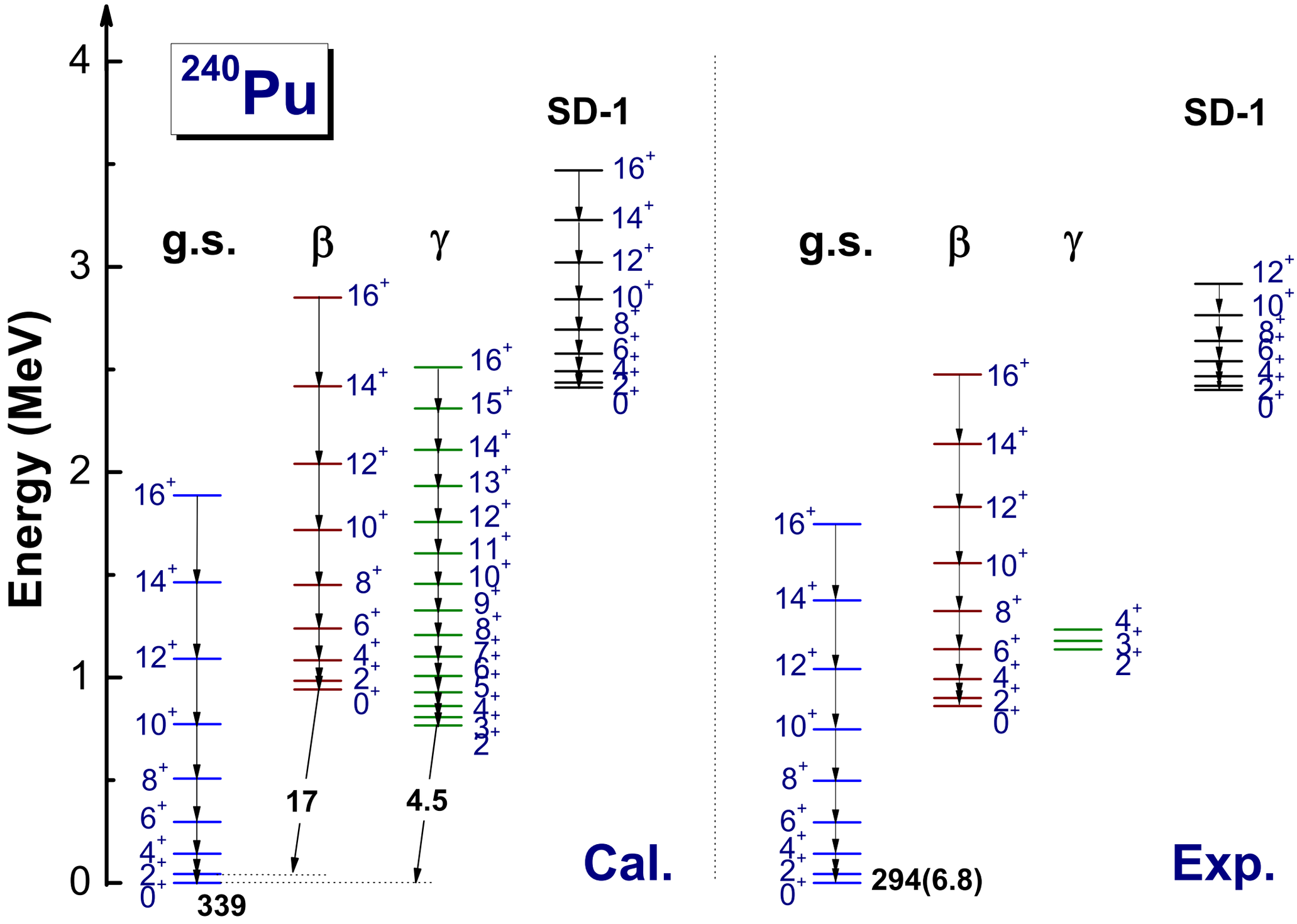
$$\mathcal{T}_{\rm vib} = \frac{1}{2} B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

$$\mathcal{T}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3} \mathcal{I}_k \omega_k^2$$

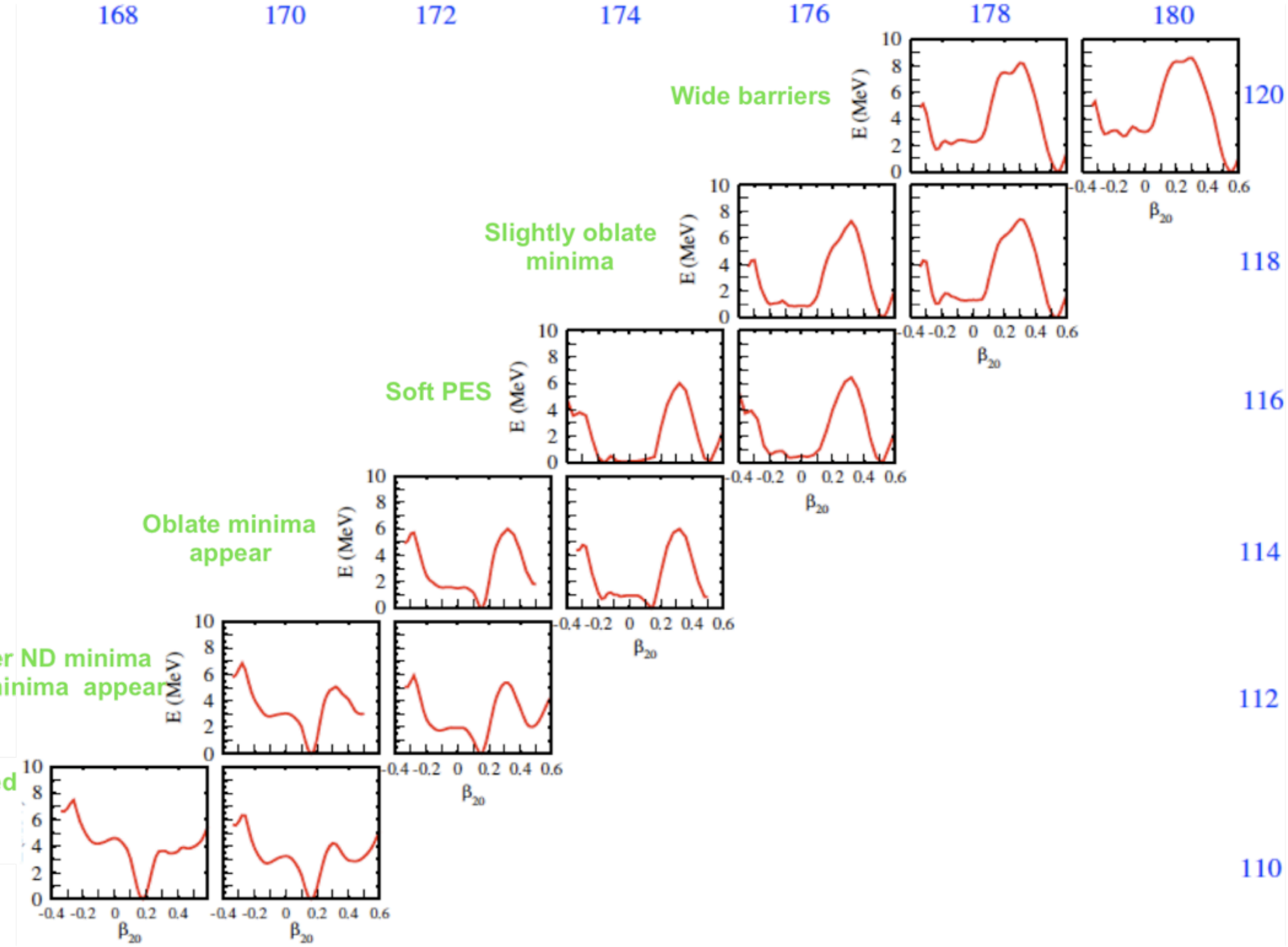
The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ: the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k.

$E^{th}_{4^+_1}/E^{th}_{2^+_1} = 3.33$

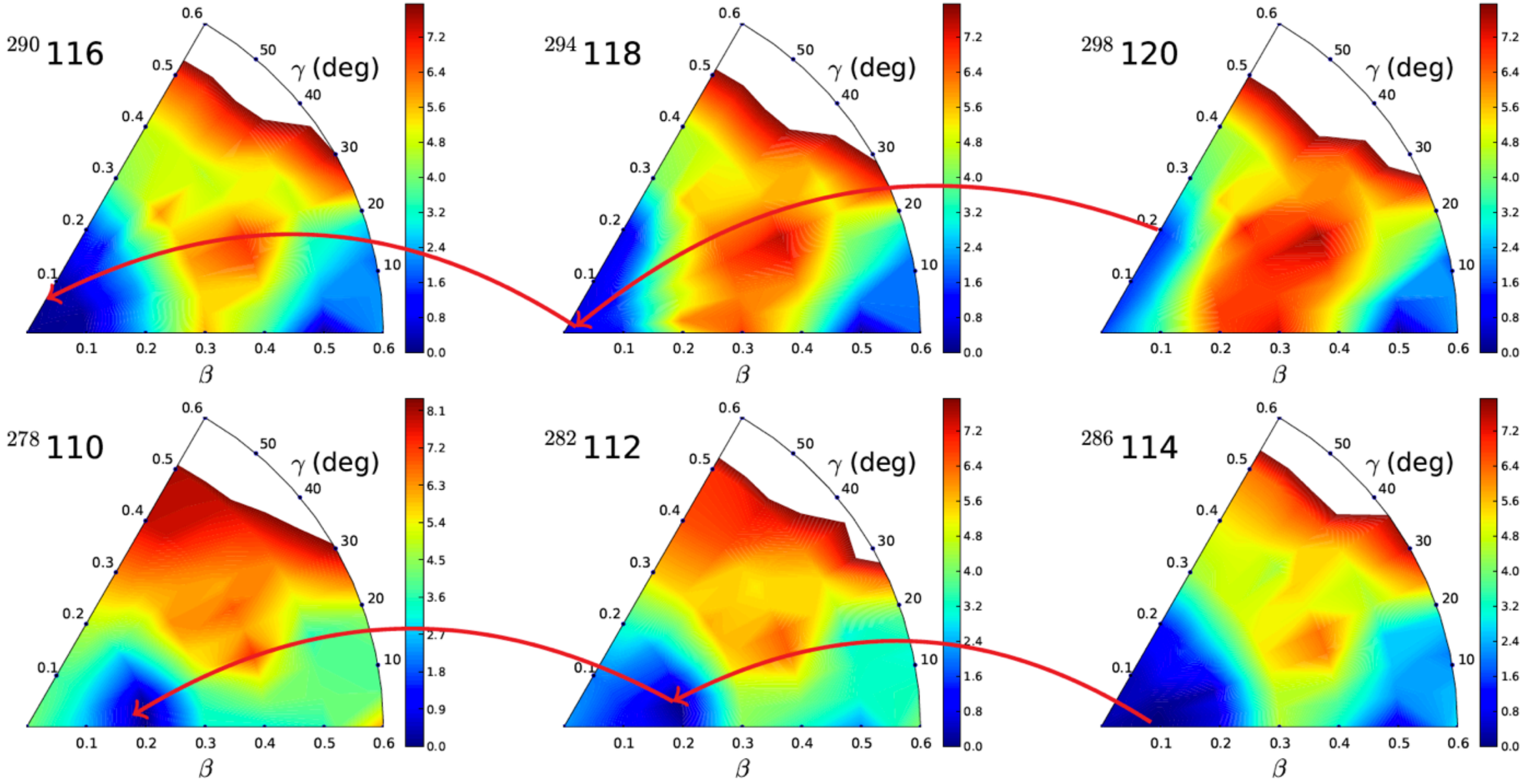
$E^{exp}_{4^+_1}/E^{exp}_{2^+_1} = 3.31$



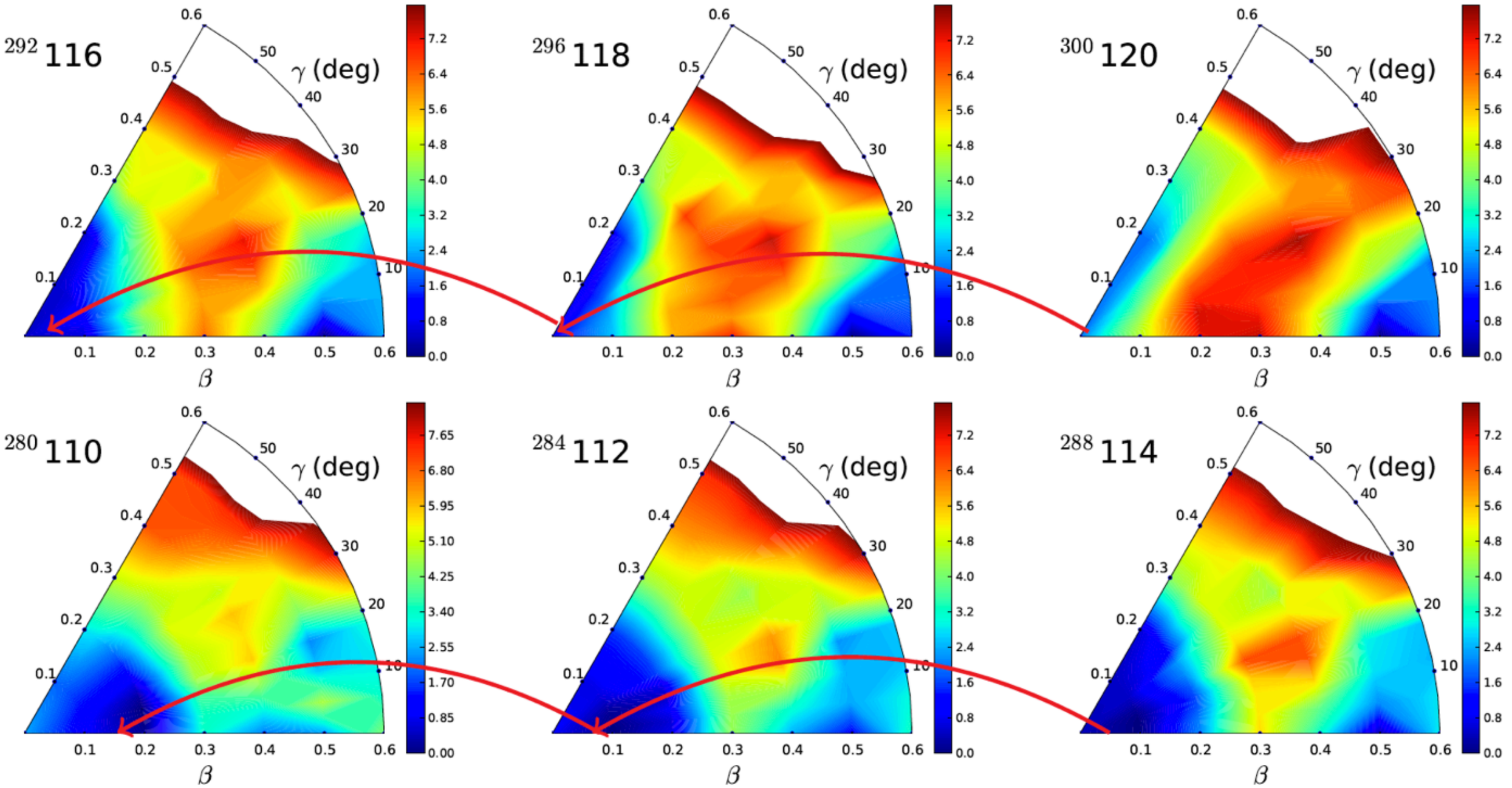
Shape transitions in superheavy nuclei



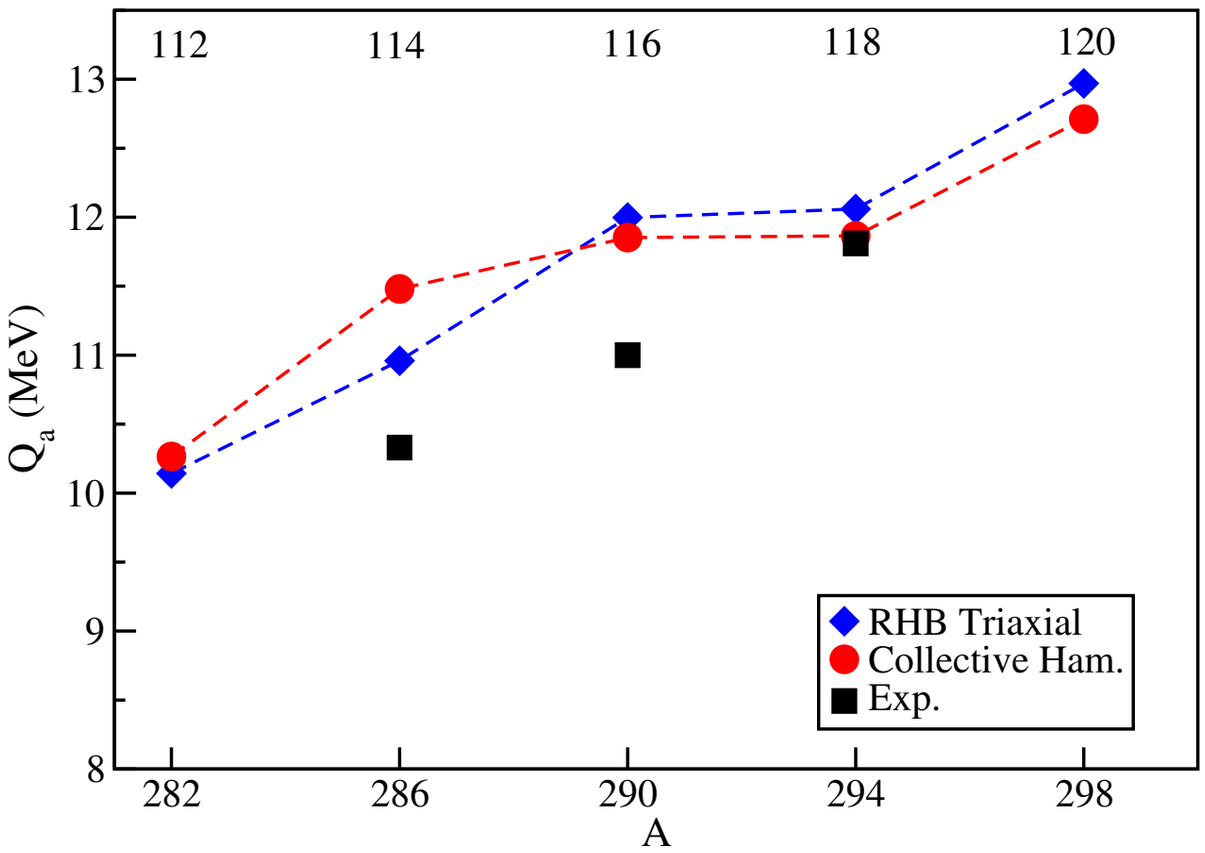
Triaxial shapes in the α-decay chain of $^{298}120$

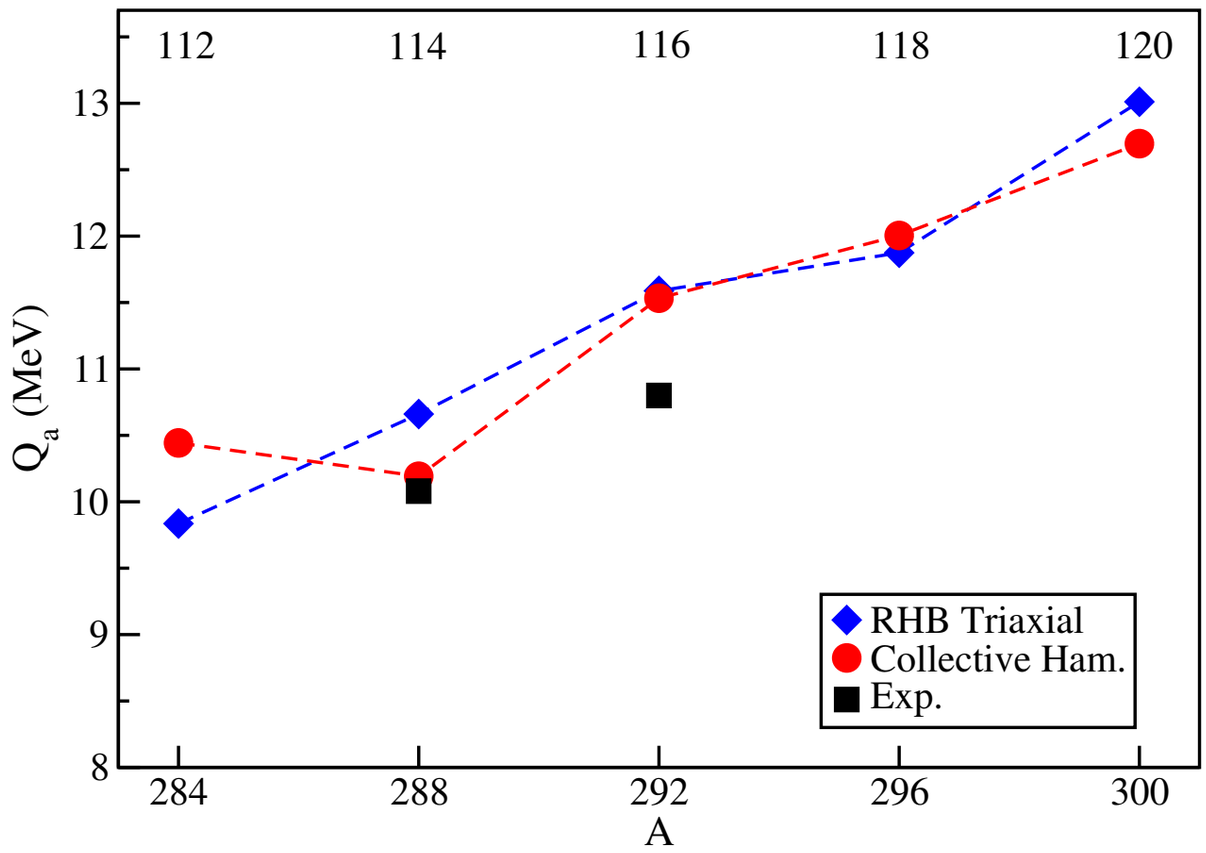


Triaxial shapes in the α-decay chain of $^{300}120$

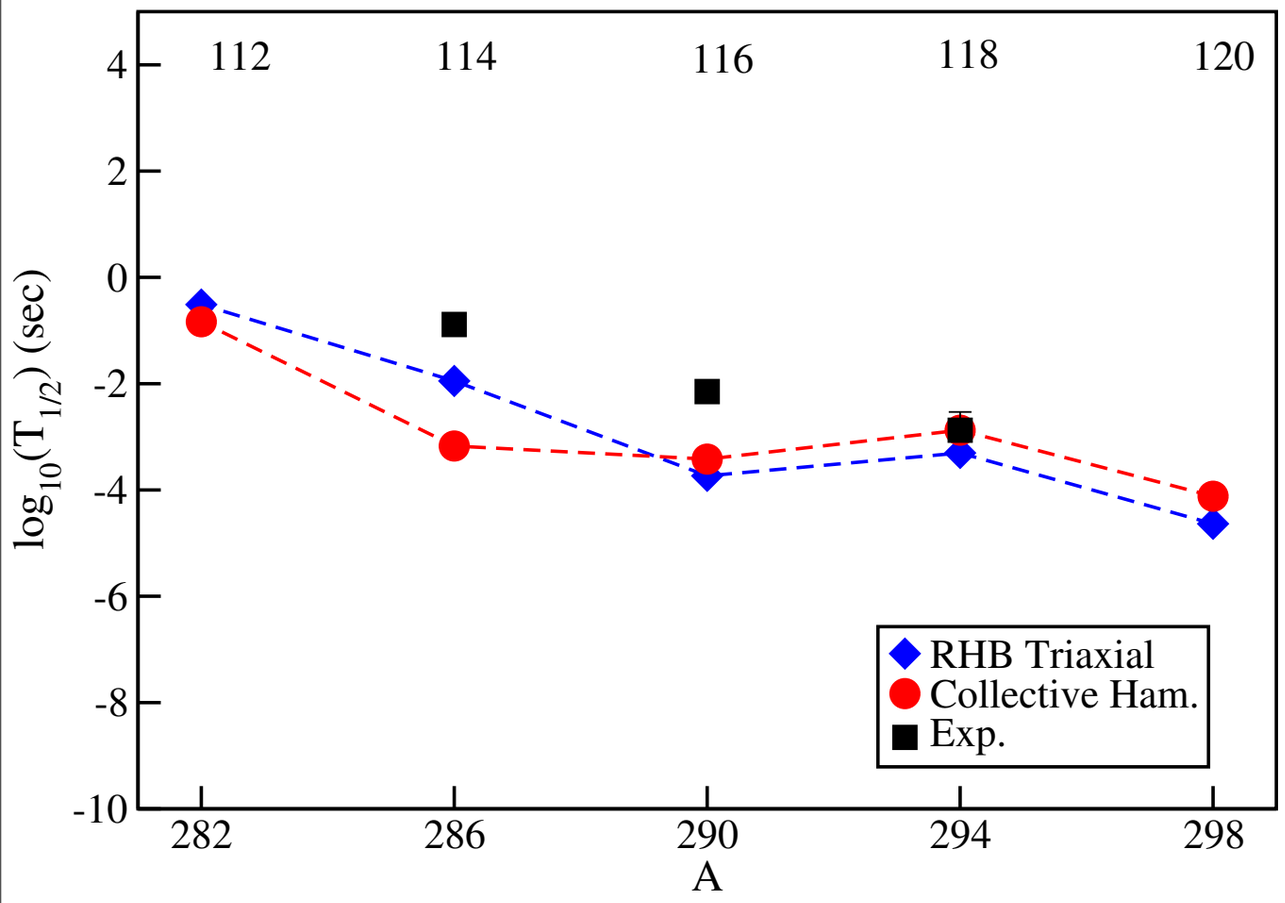


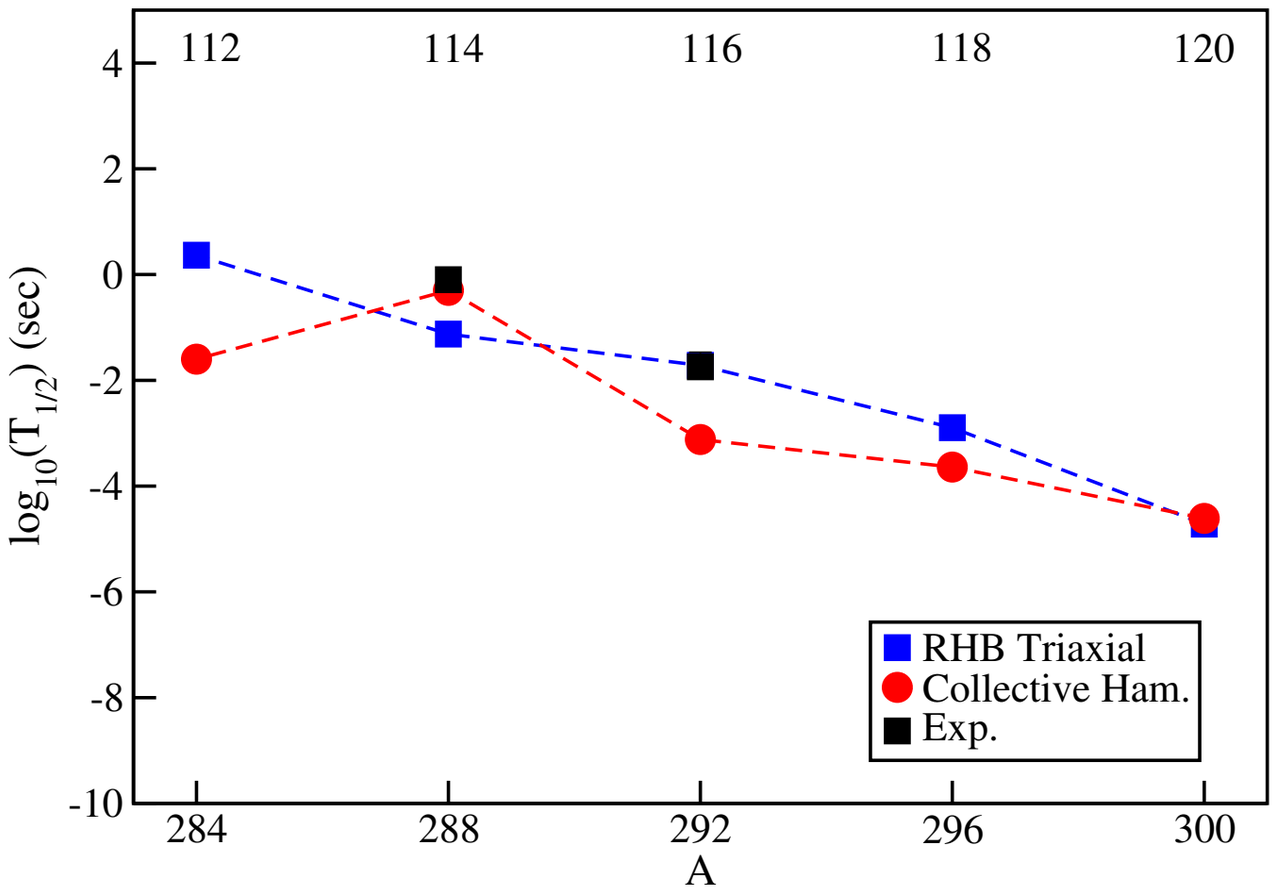
α-decay chains of $^{298}120$ and $^{300}120$



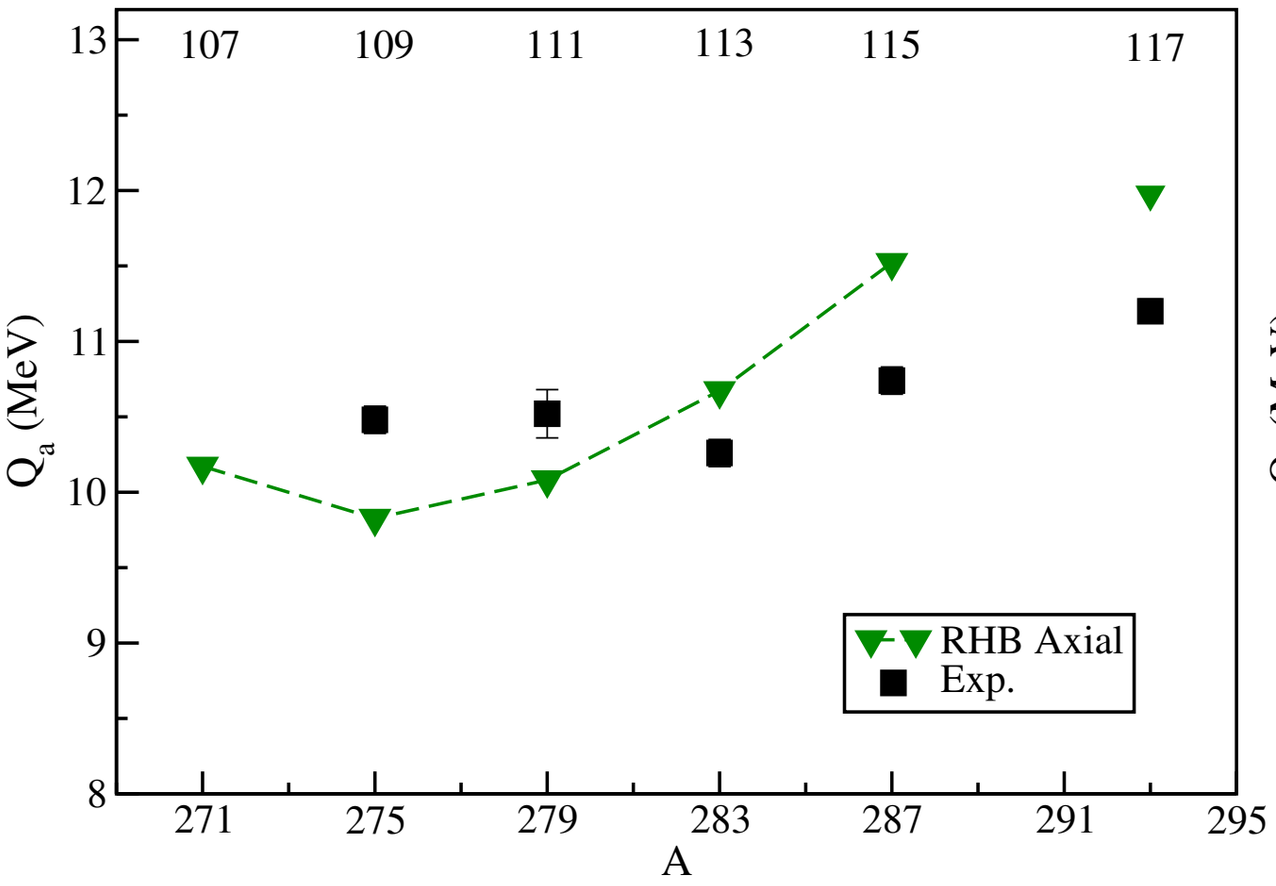


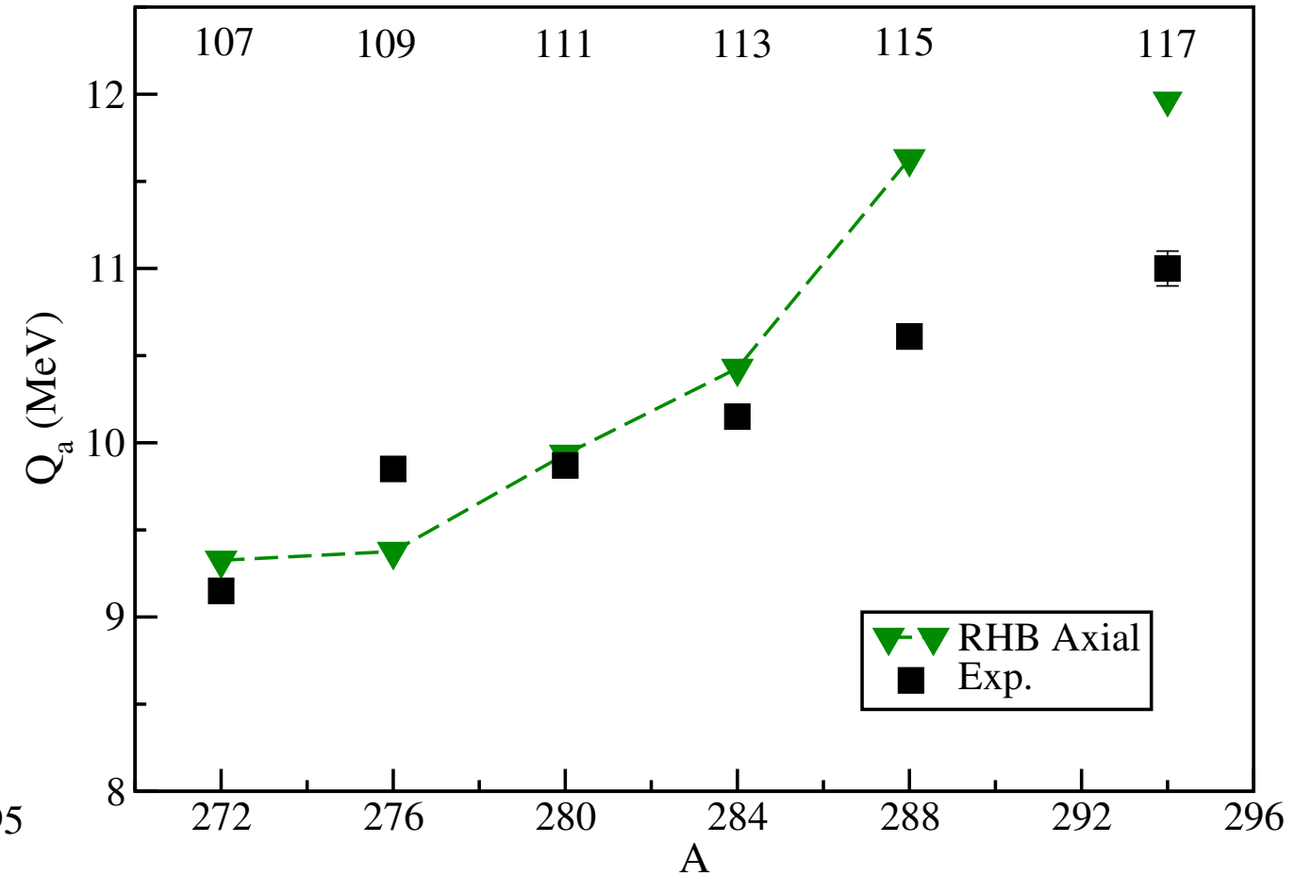
Half-lives in the α-decay chains of $^{298}120$ and $^{300}120$



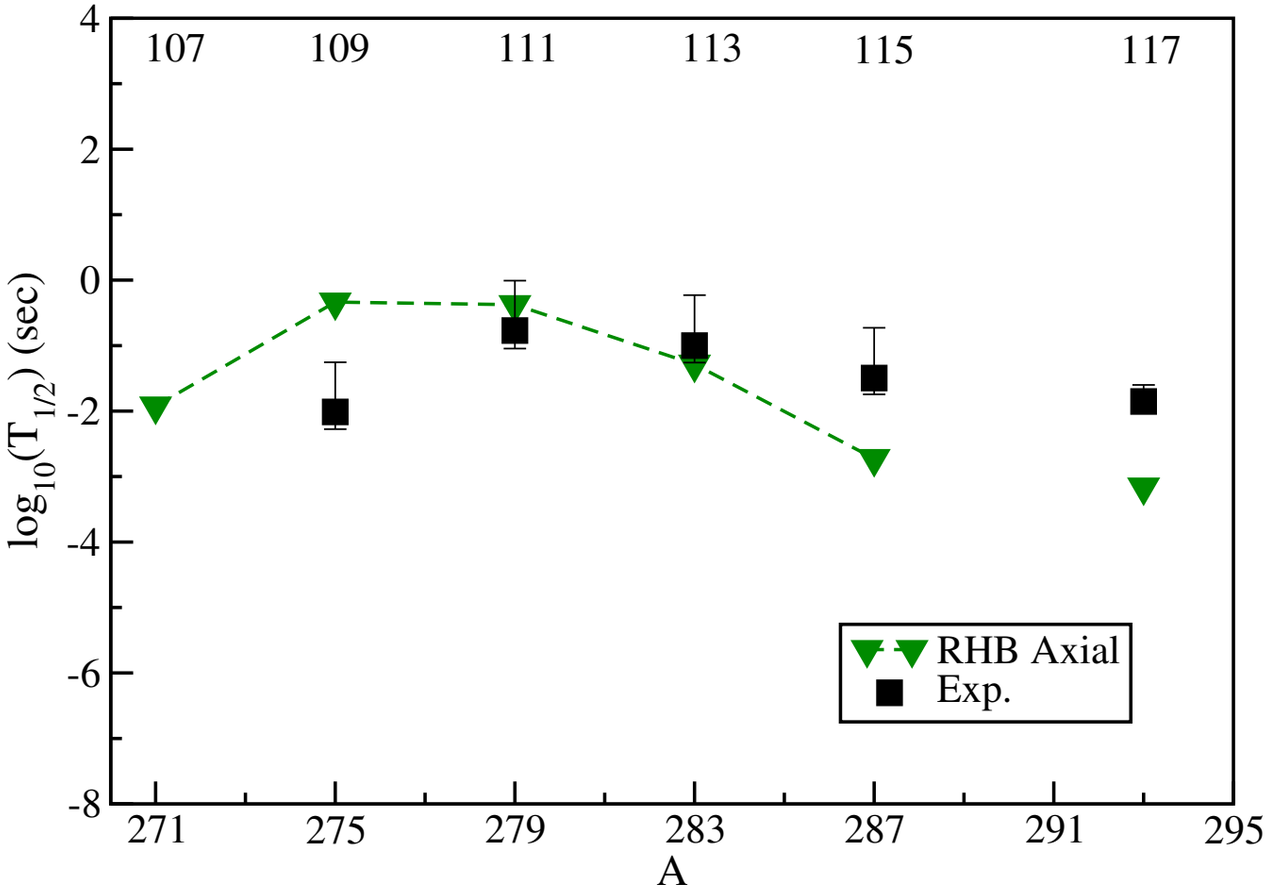


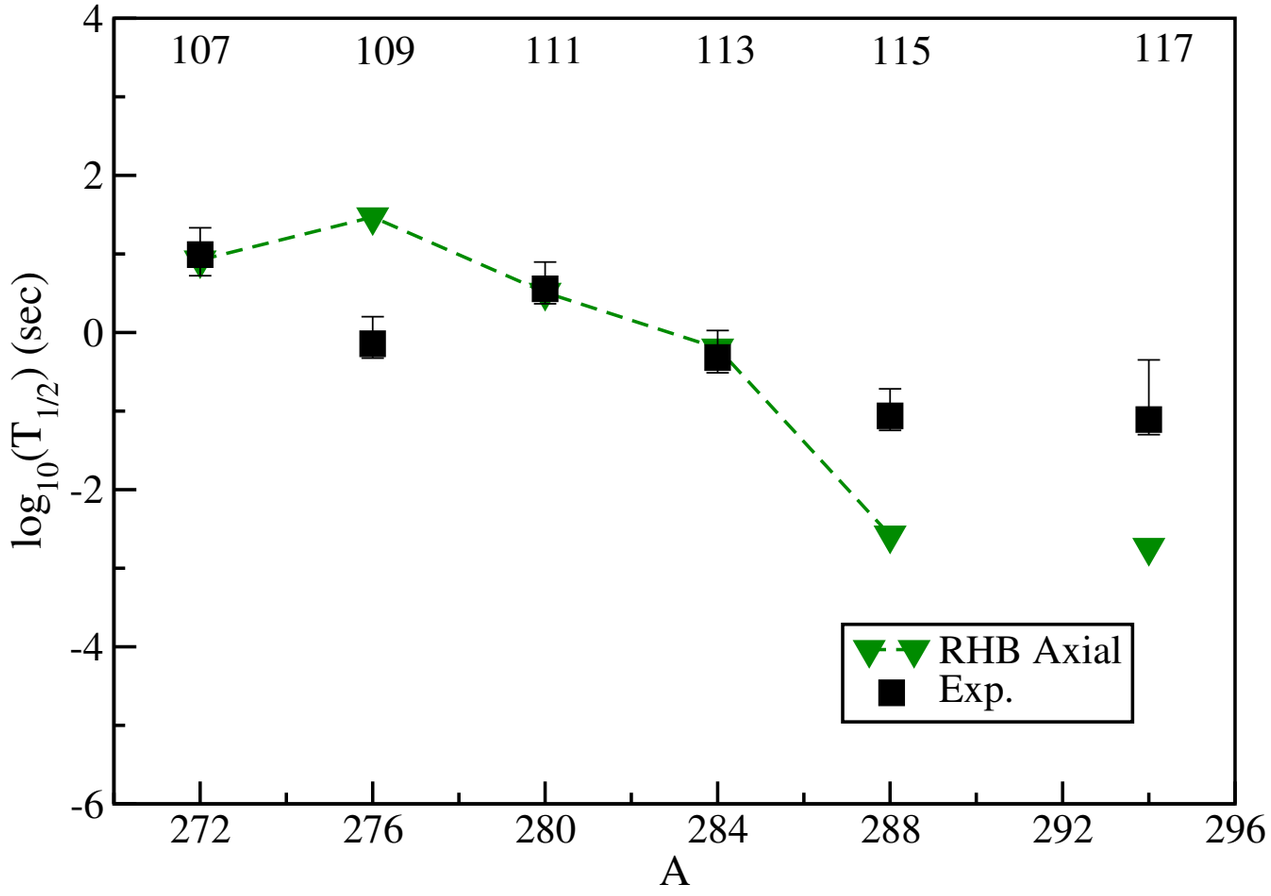
α-decay chains of $^{287}115$ and $^{288}115$



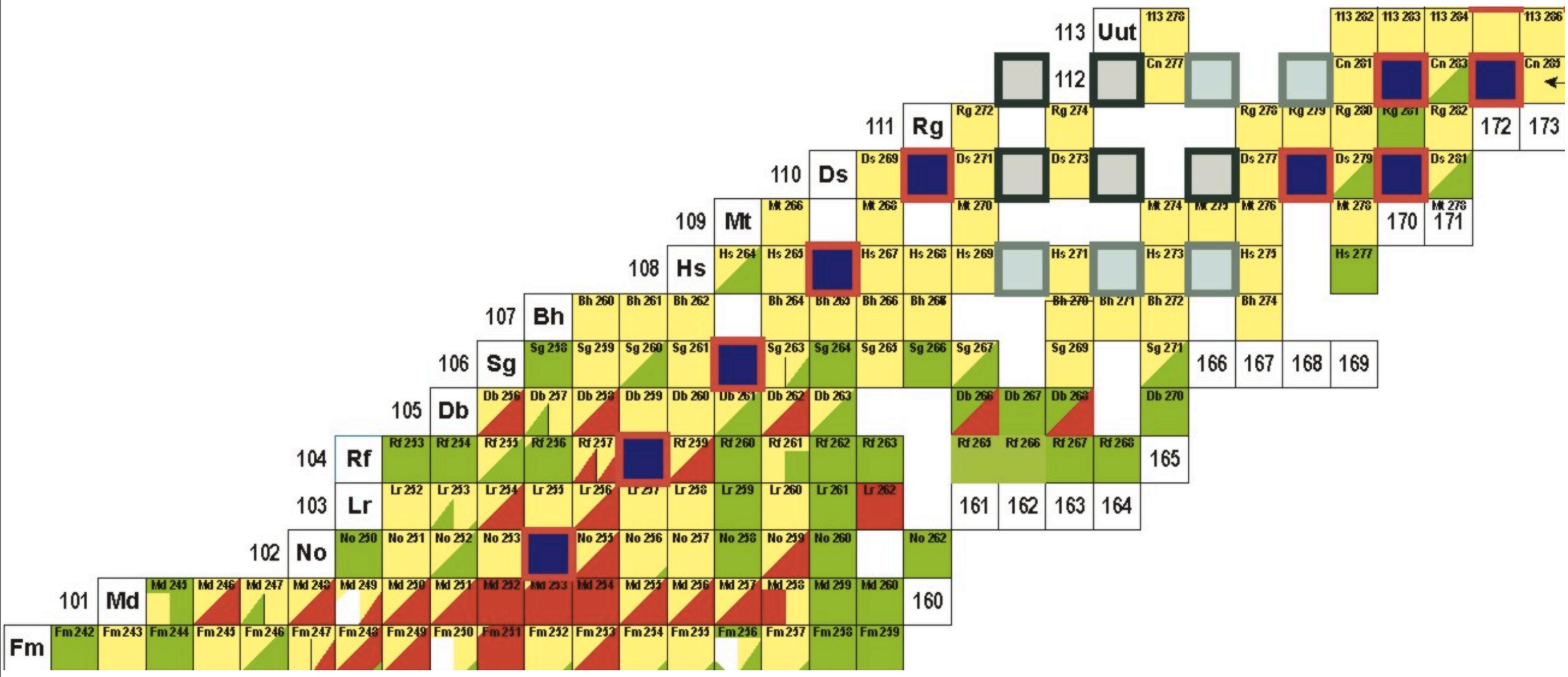


Half-lives in the α-decay chains of $^{287}115$ and $^{288}115$

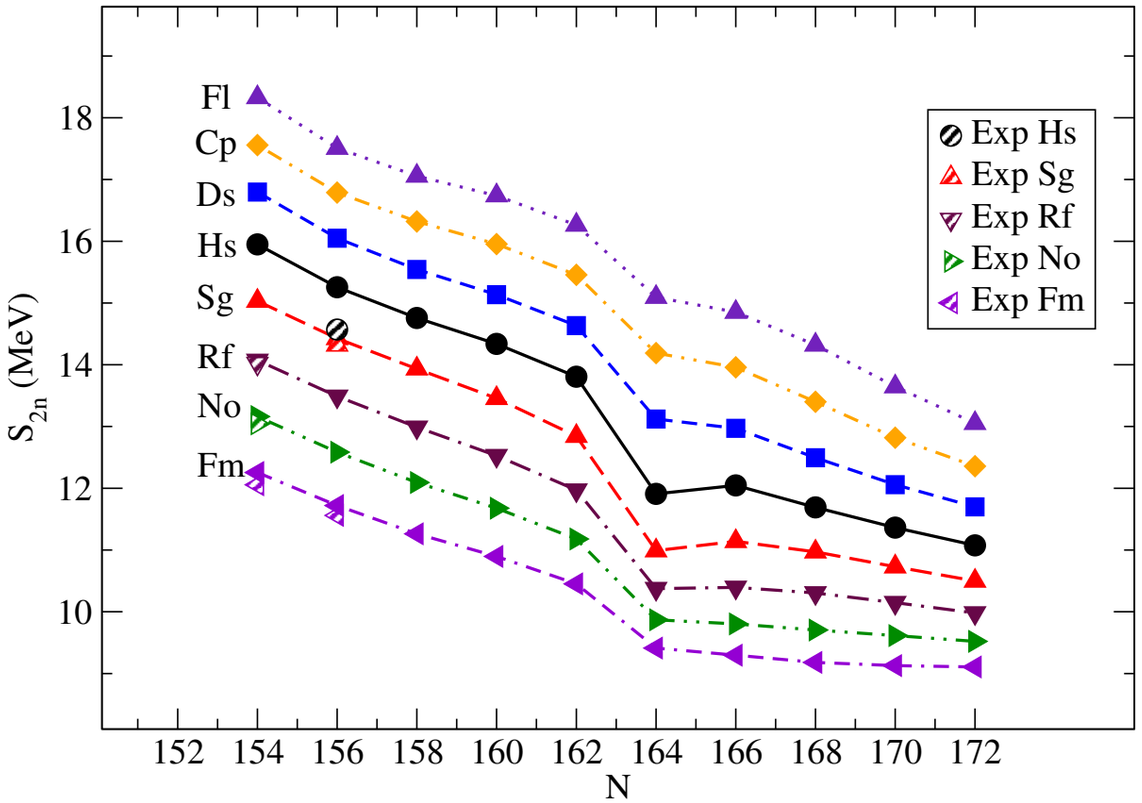




Transactinides

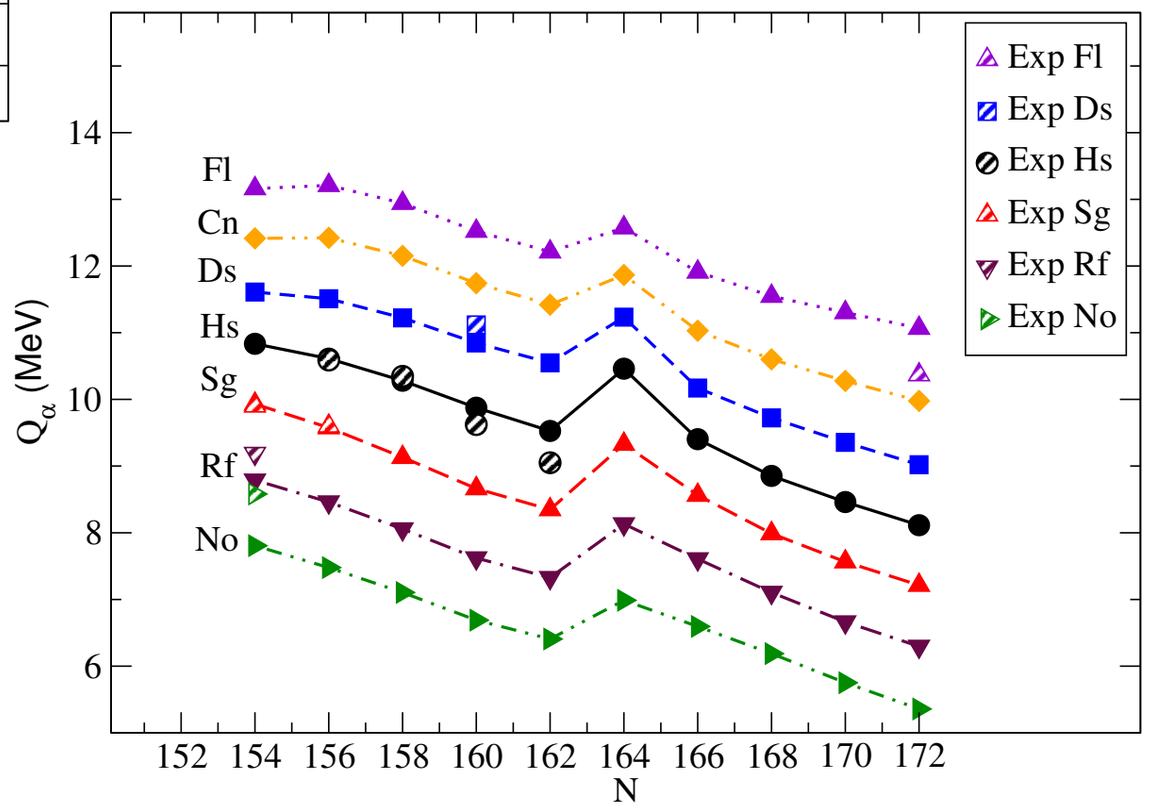


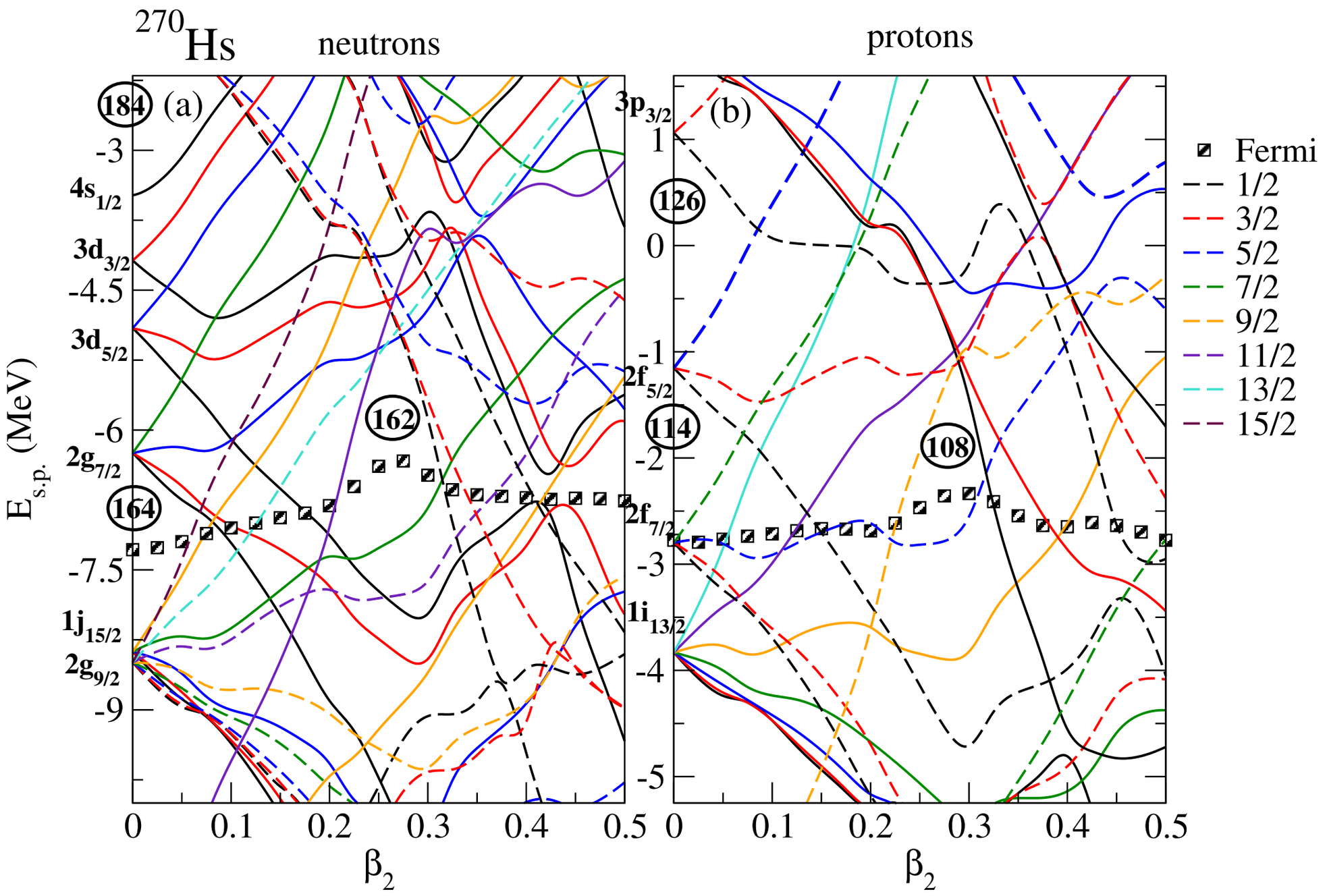
Transactinides



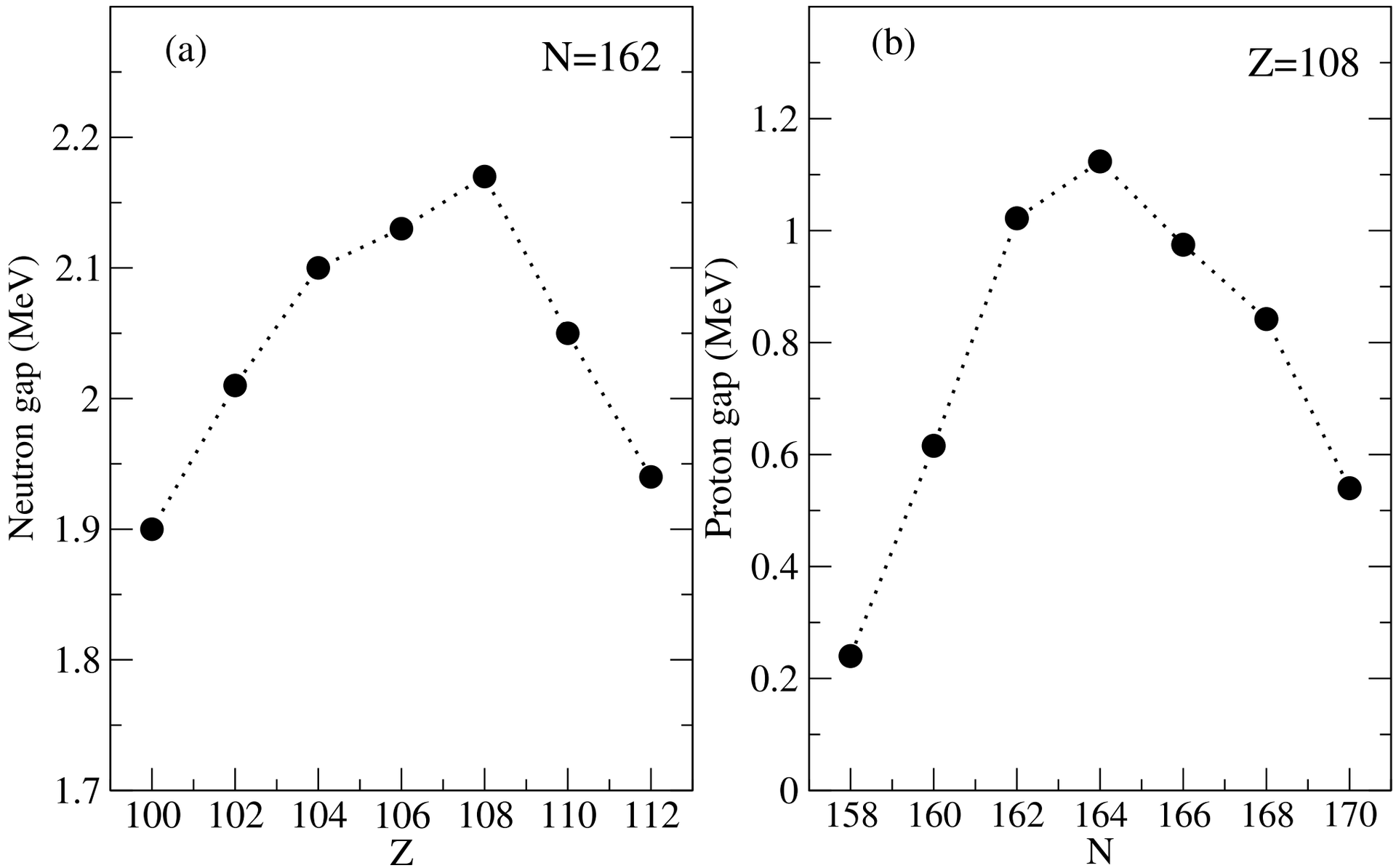
2n separation energies

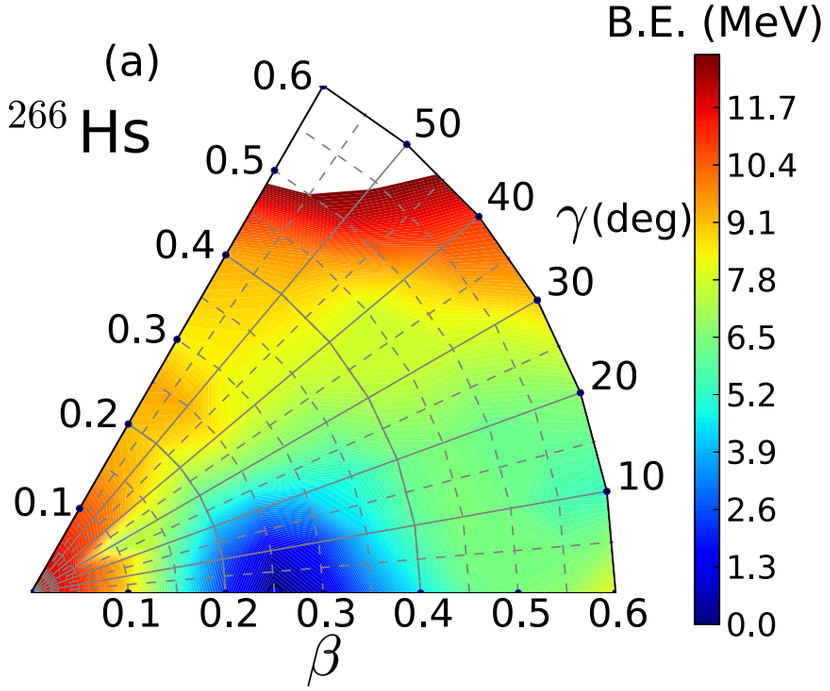
Qα values

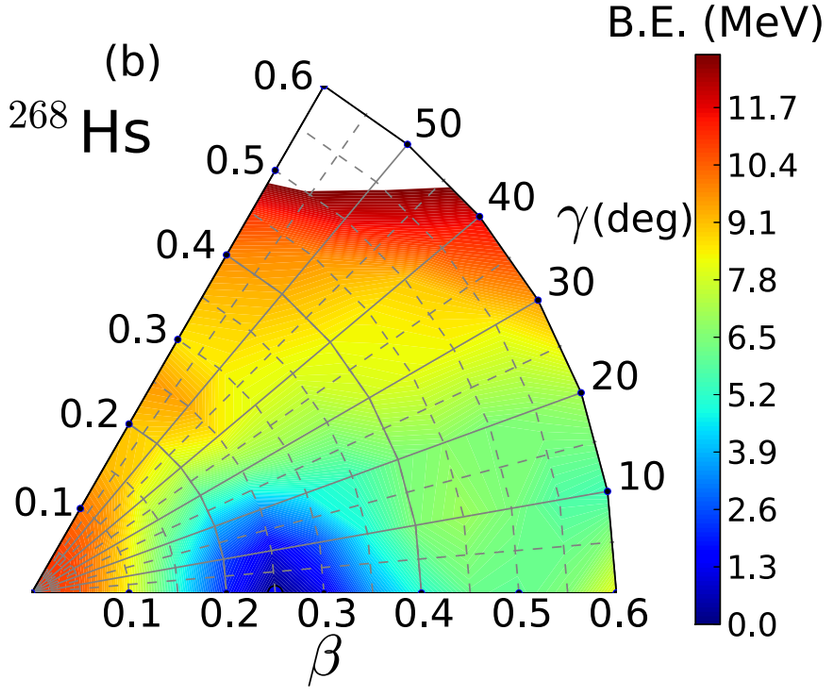


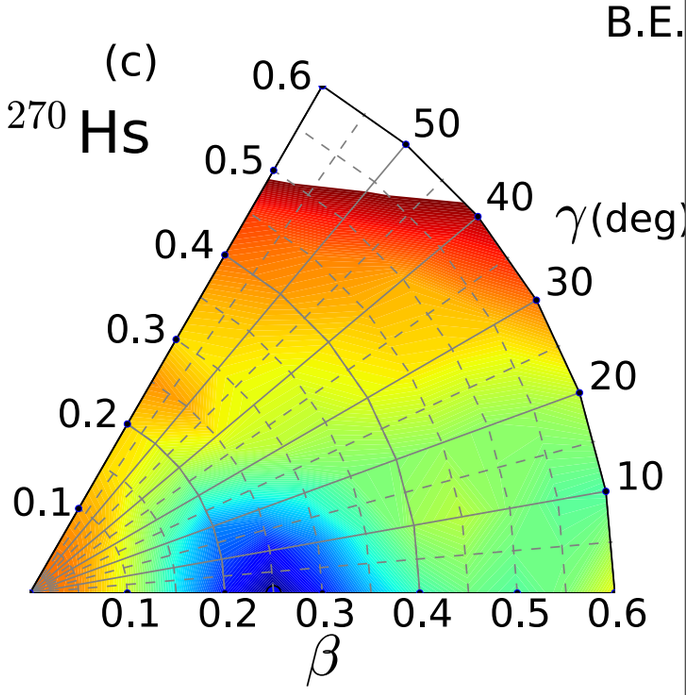

^{270}Hs
neutrons
protons
(a)
(b)
184
162
164
126
114
108
$4s_{1/2}$
$3d_{3/2}$
$3d_{5/2}$
$2g_{7/2}$
$1j_{15/2}$
$2g_{9/2}$
$3p_{3/2}$
$2f_{5/2}$
$2f_{7/2}$
$1i_{13/2}$
$E_{s.p.}$ (MeV)
β_2
Fermi
1/2
3/2
5/2
7/2
9/2
11/2
13/2
15/2

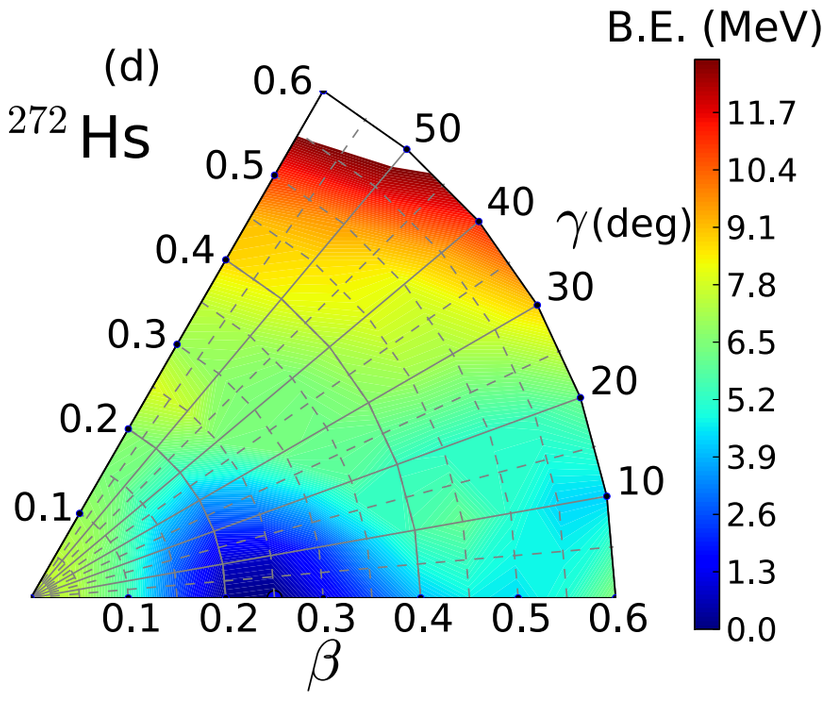
Neutron and proton shell gaps

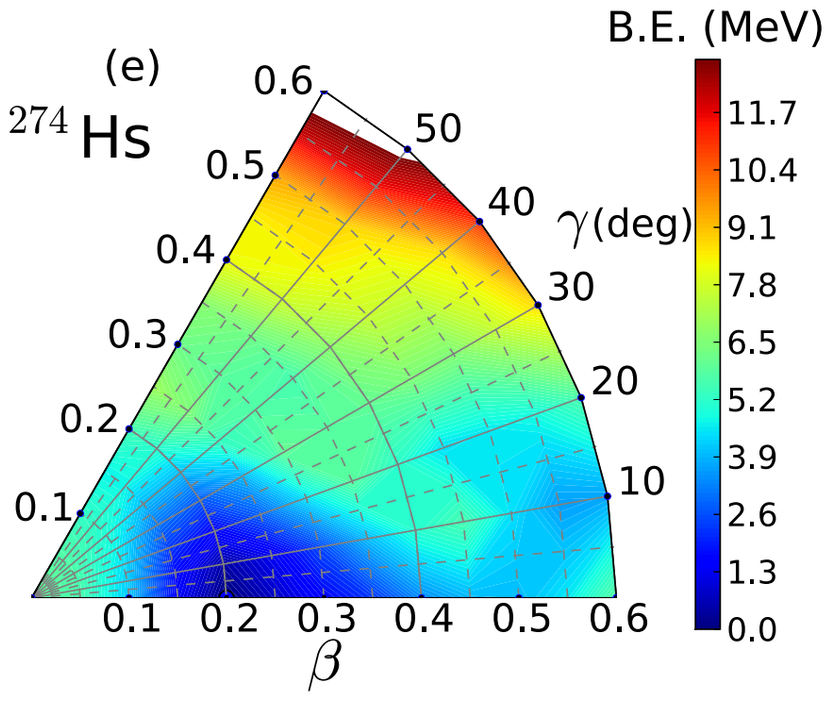


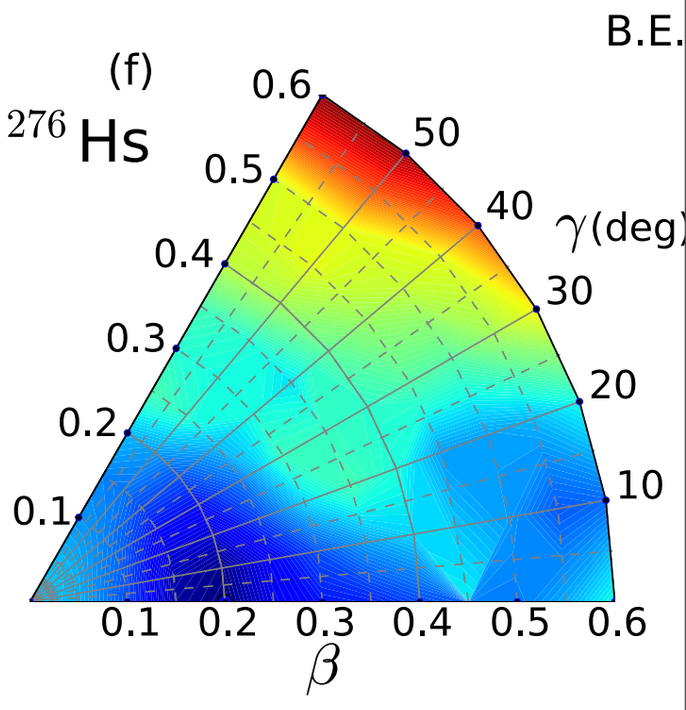

(a)
^{266}Hs
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

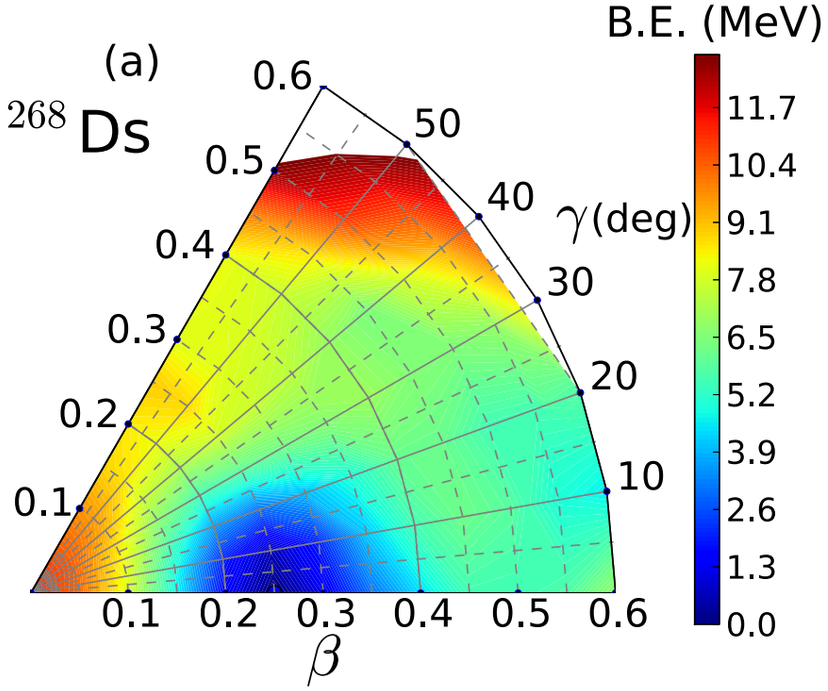

(b)
^{268}Hs
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

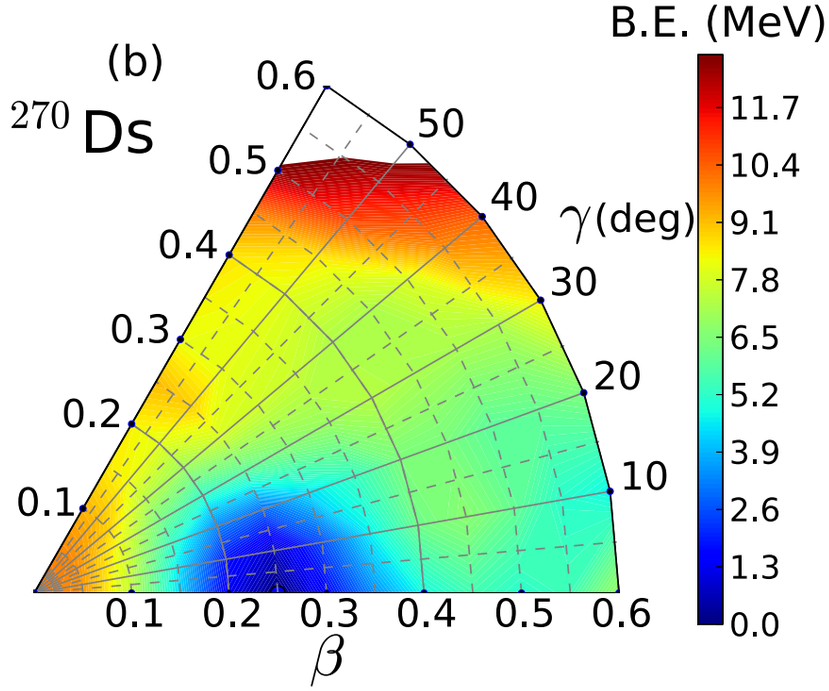

(c)
^{270}Hs
B.E.
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

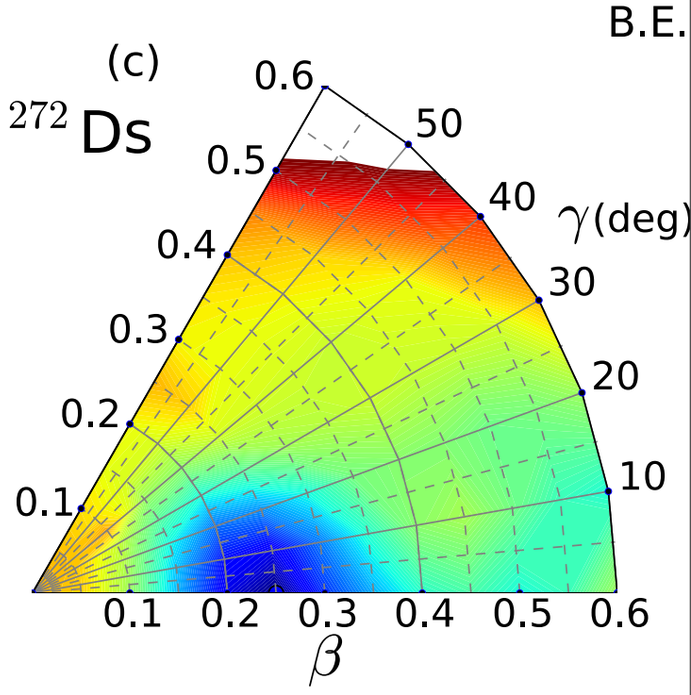

(d)
^{272}Hs
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

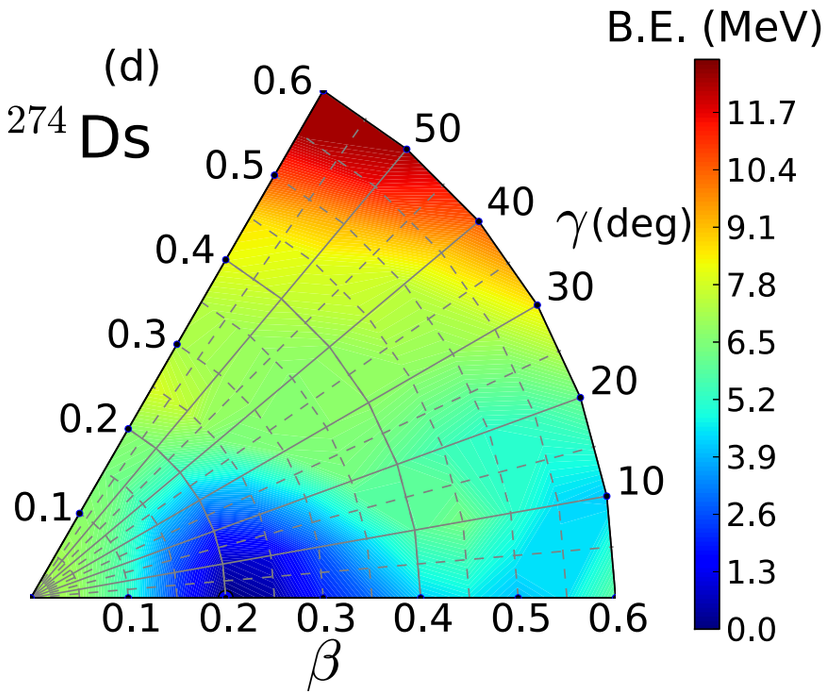

(e)
^{274}Hs
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

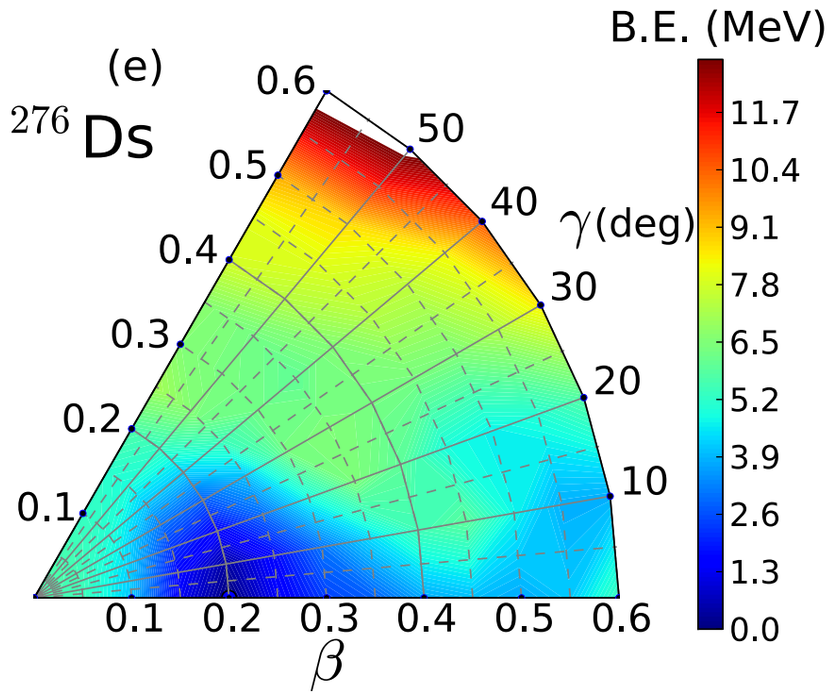

(f)
^{276}Hs
B.E.
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

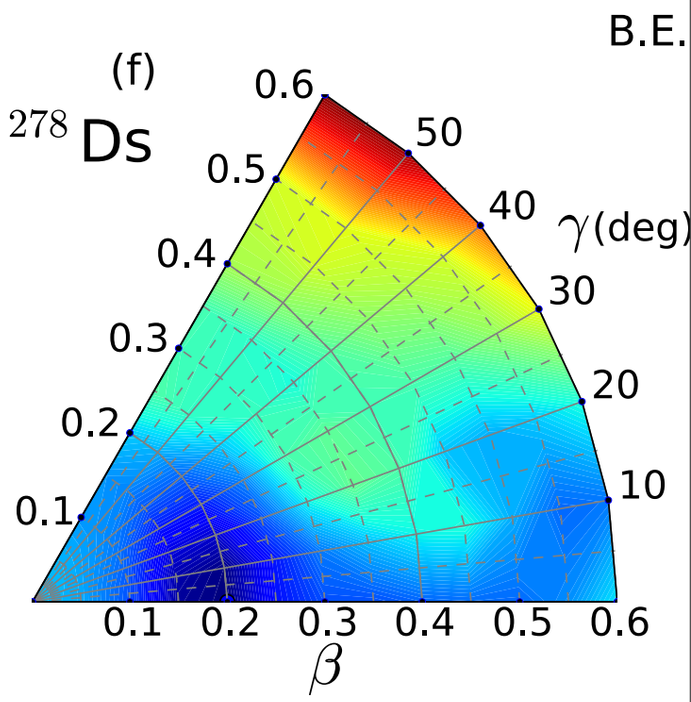

(a)
^{268}Ds
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β


(b)
^{270}Ds
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

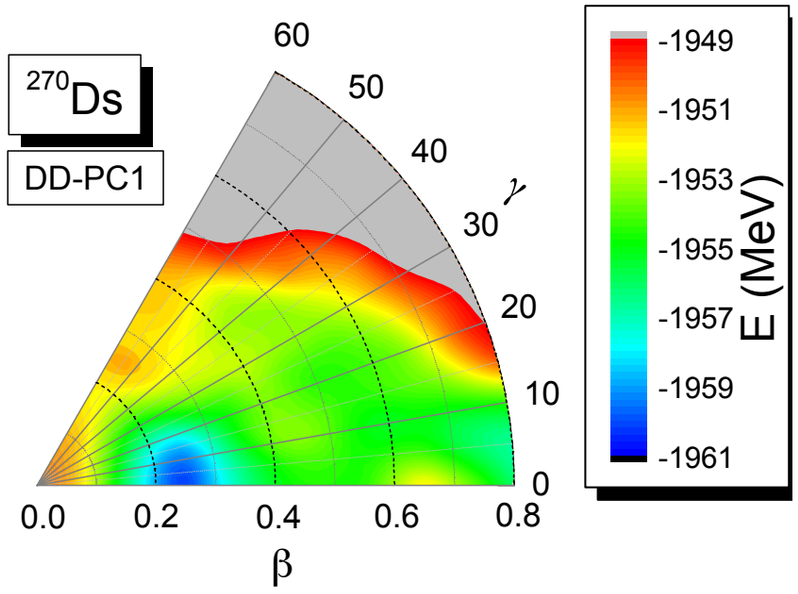

(c)
^{272}Ds
B.E.
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

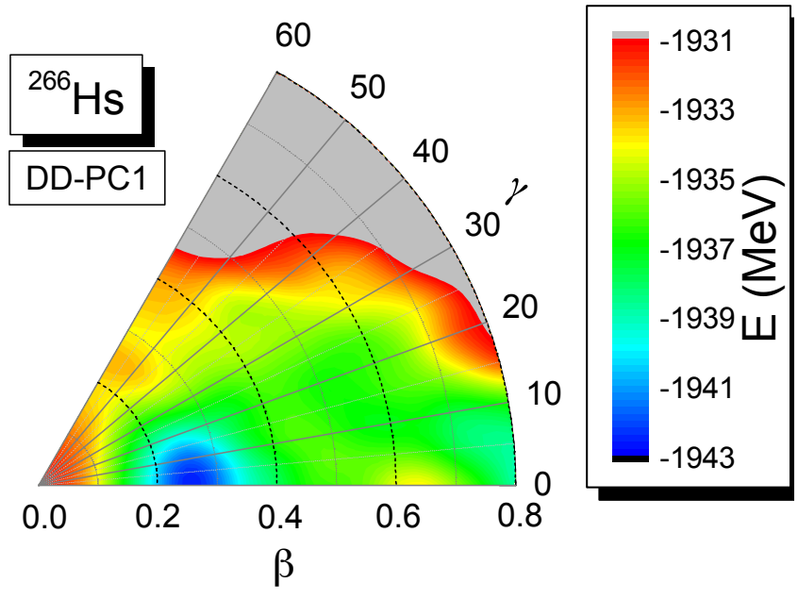

(d)
^{274}Ds
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

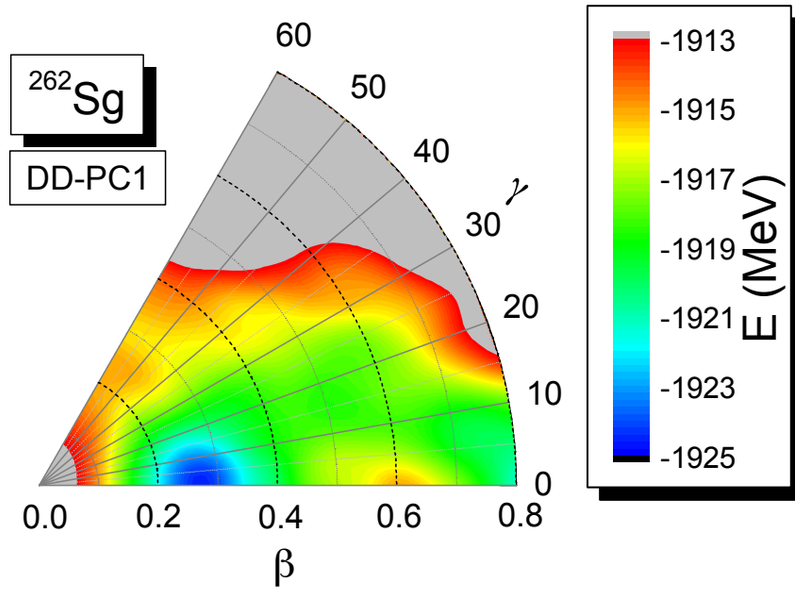

(e)
^{276}Ds
B.E. (MeV)
11.7
10.4
9.1
7.8
6.5
5.2
3.9
2.6
1.3
0.0
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

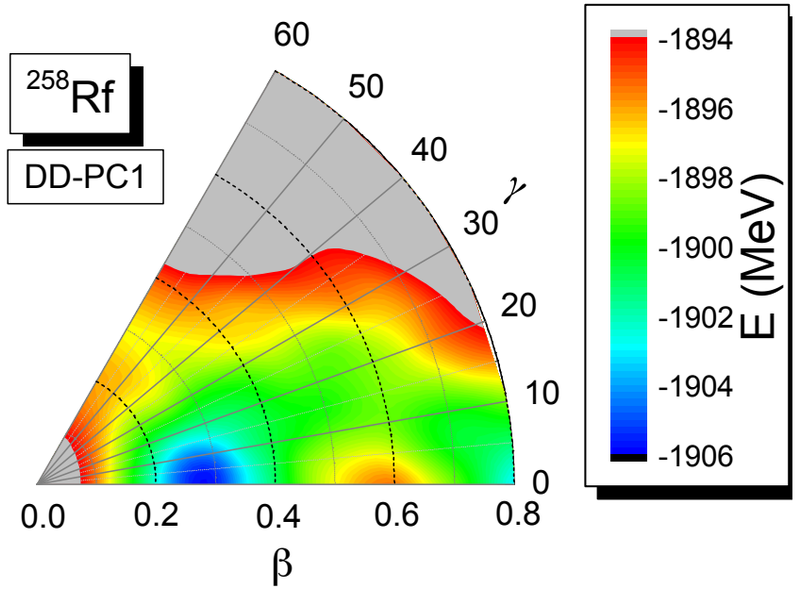

(f)
^{278}Ds
B.E.
γ(deg)
50
40
30
20
10
0.6
0.5
0.4
0.3
0.2
0.1
0.1 0.2 0.3 0.4 0.5 0.6
β

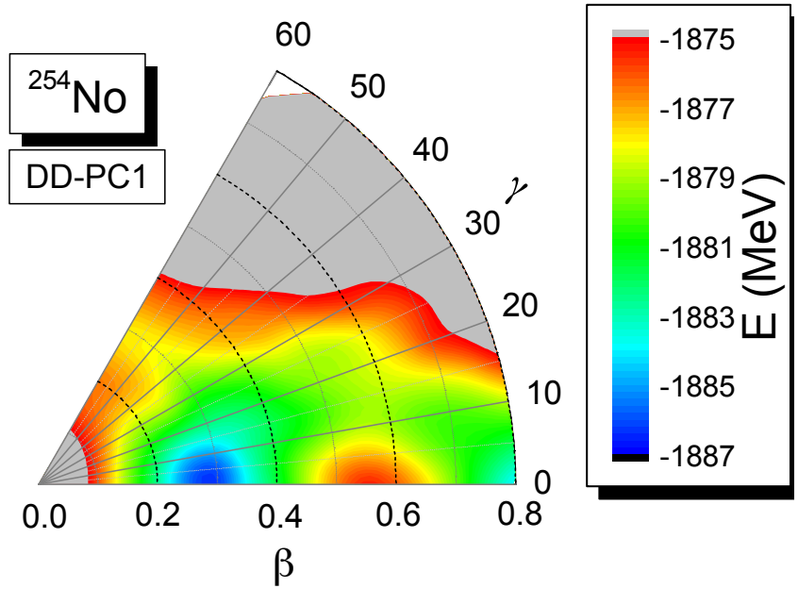
^{270}Ds α-decay chain

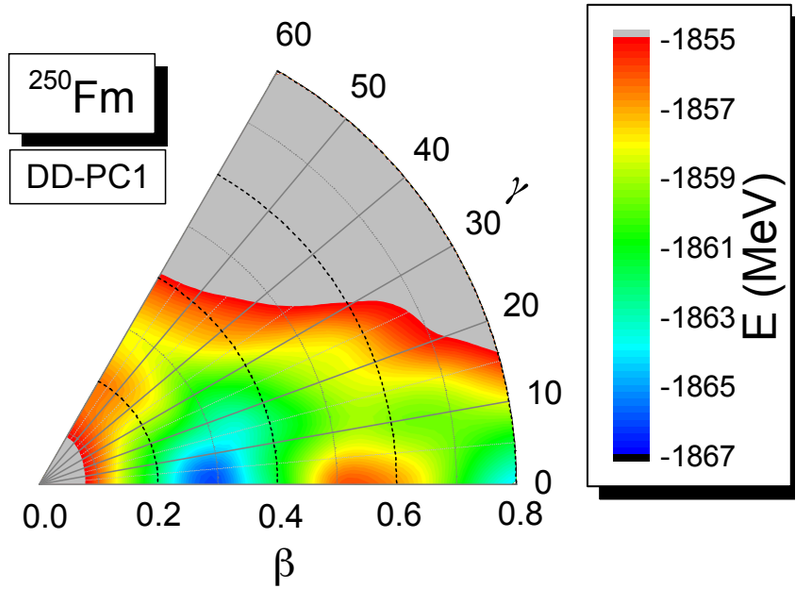




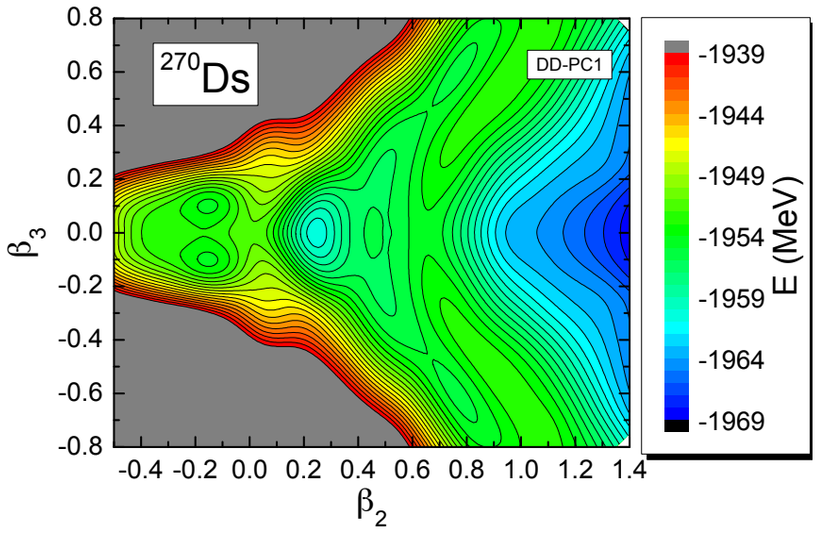


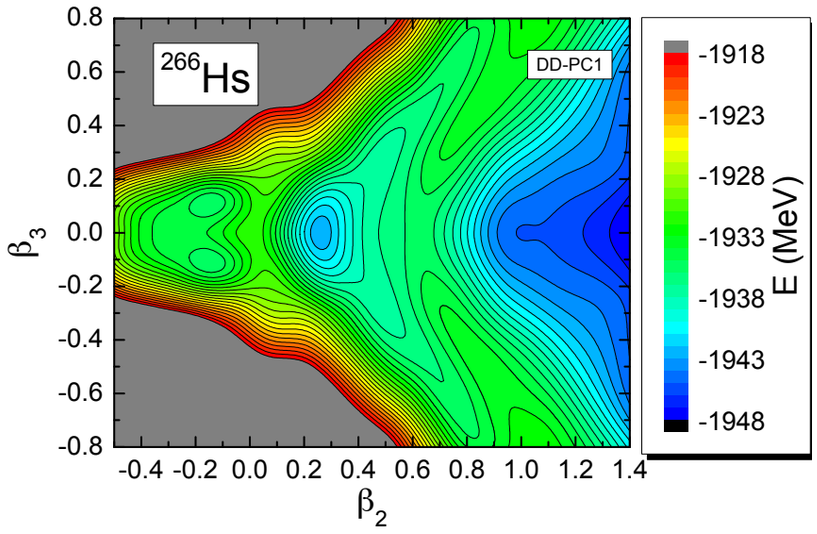


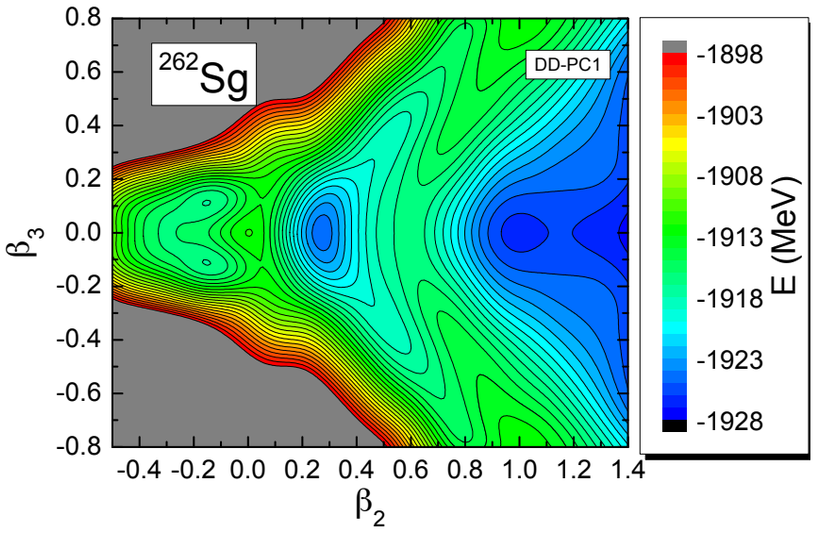


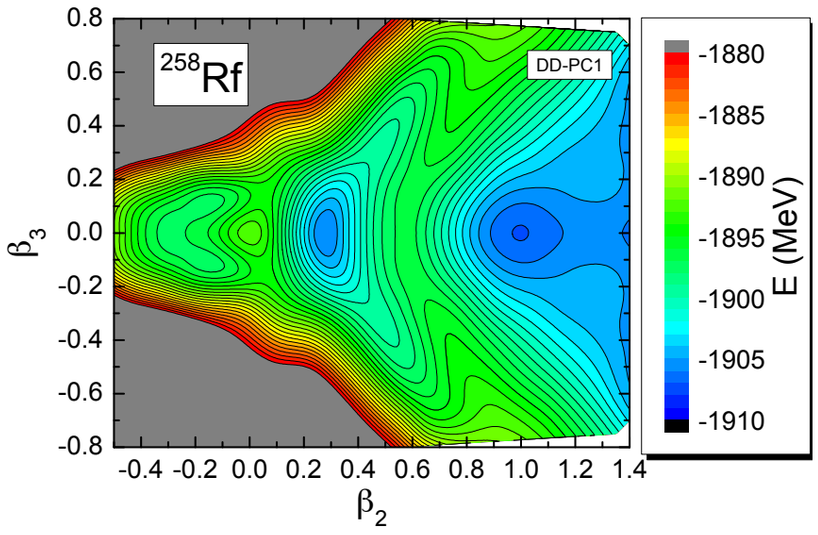


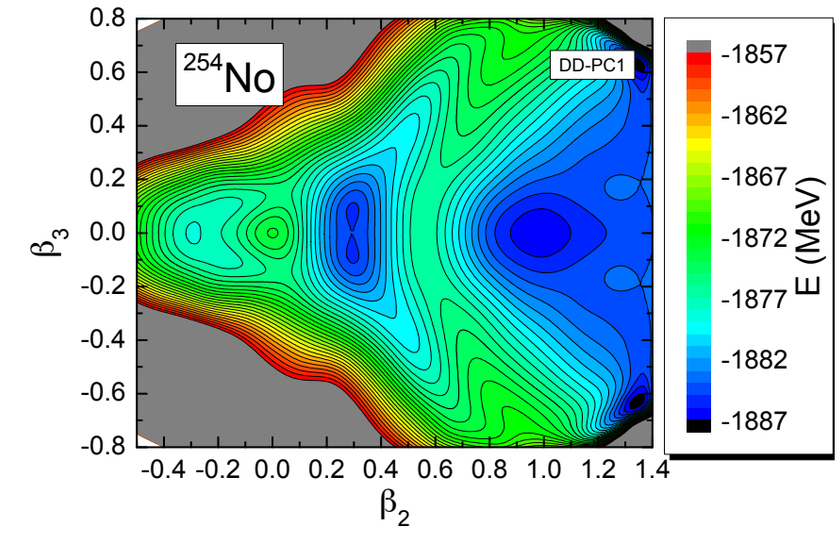
^{270}Ds α-decay chain

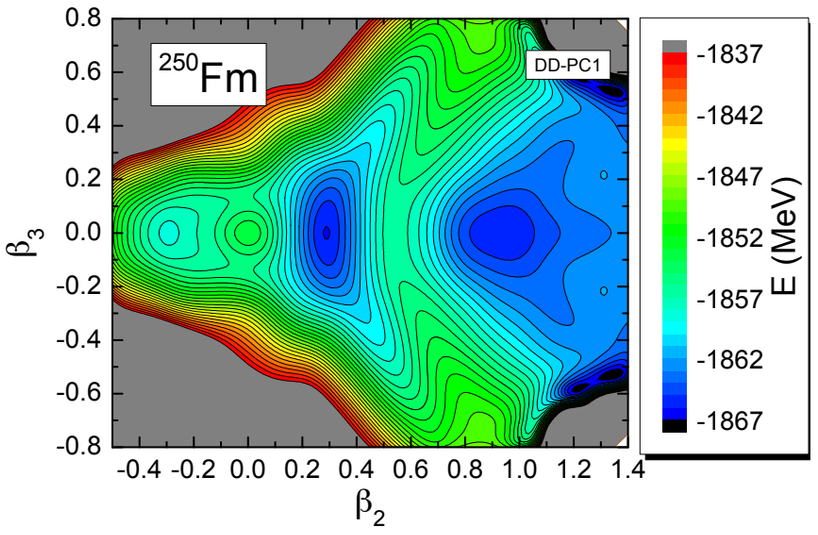




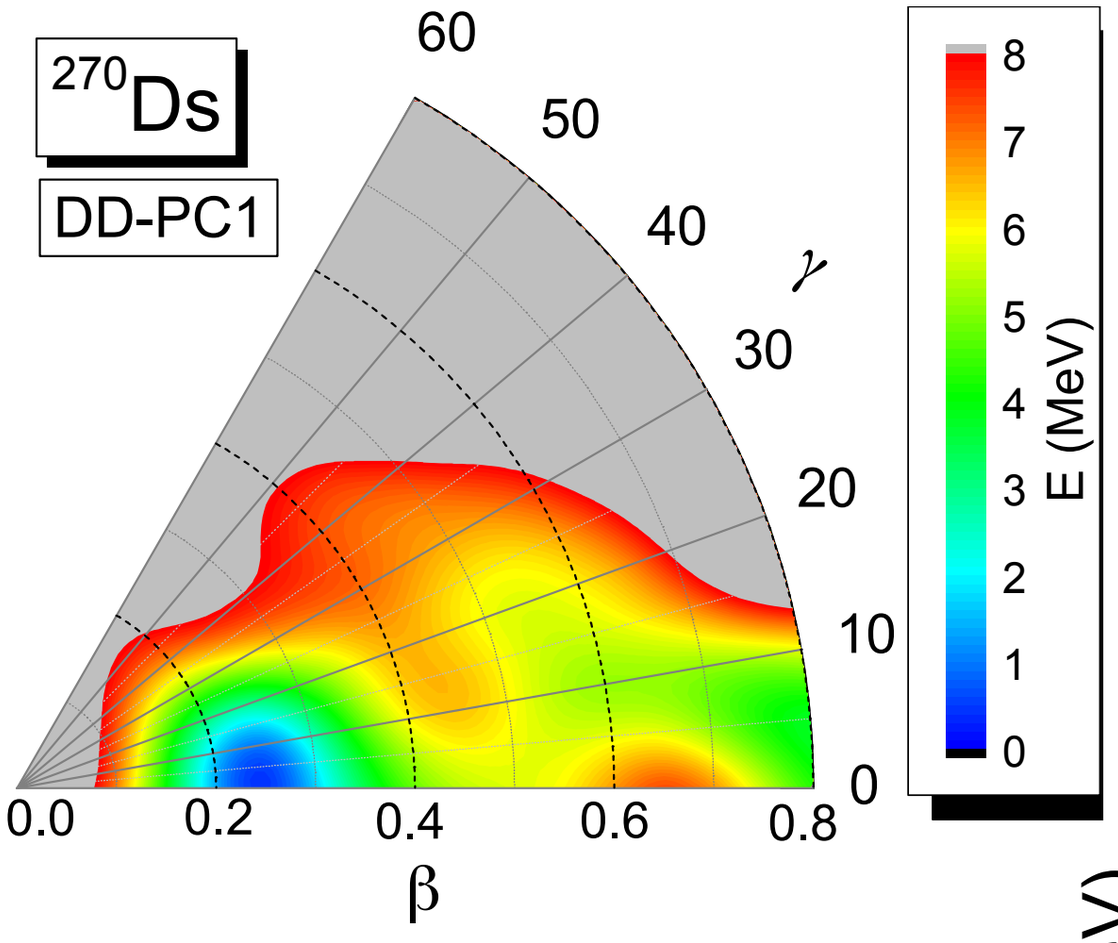


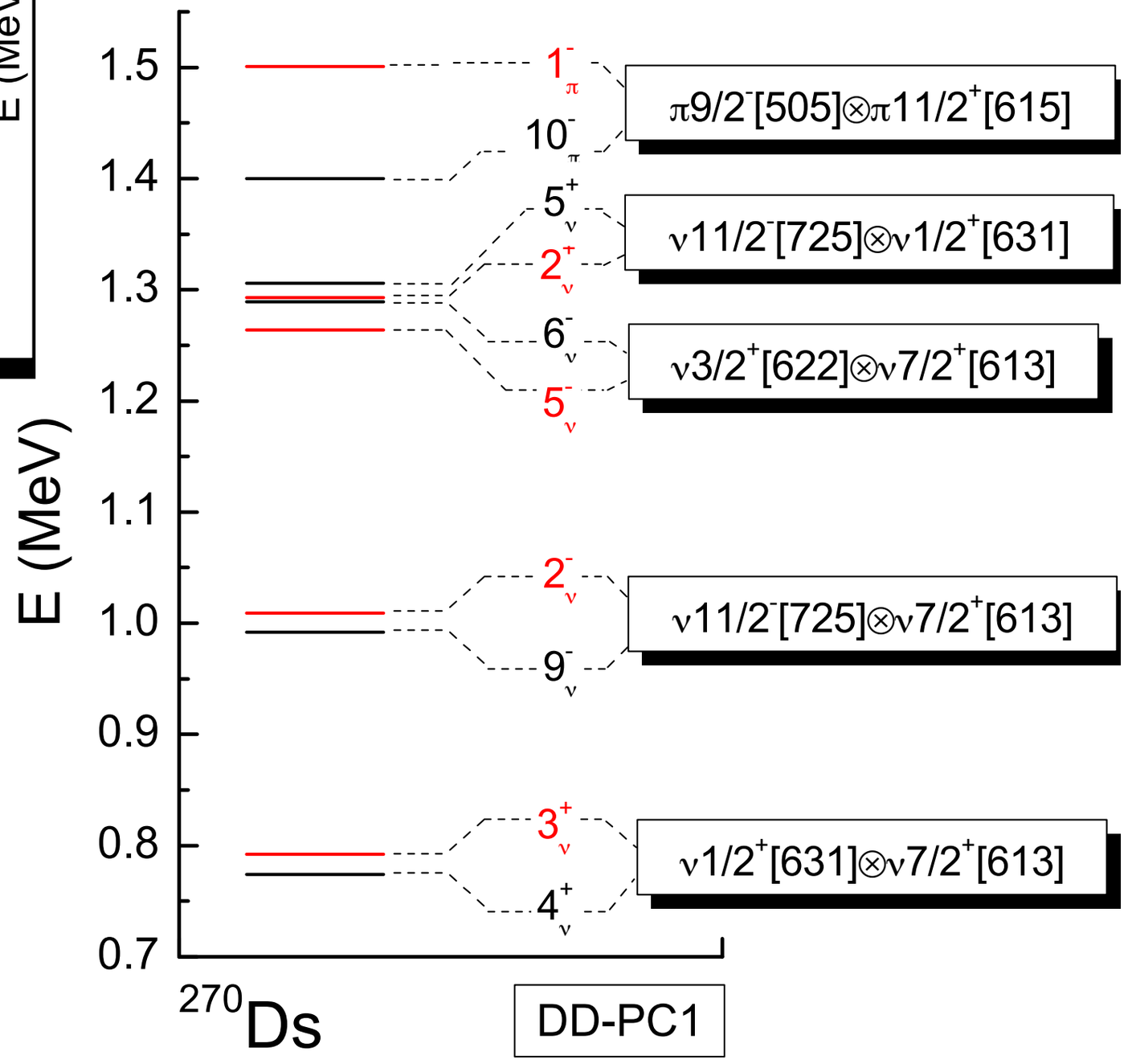




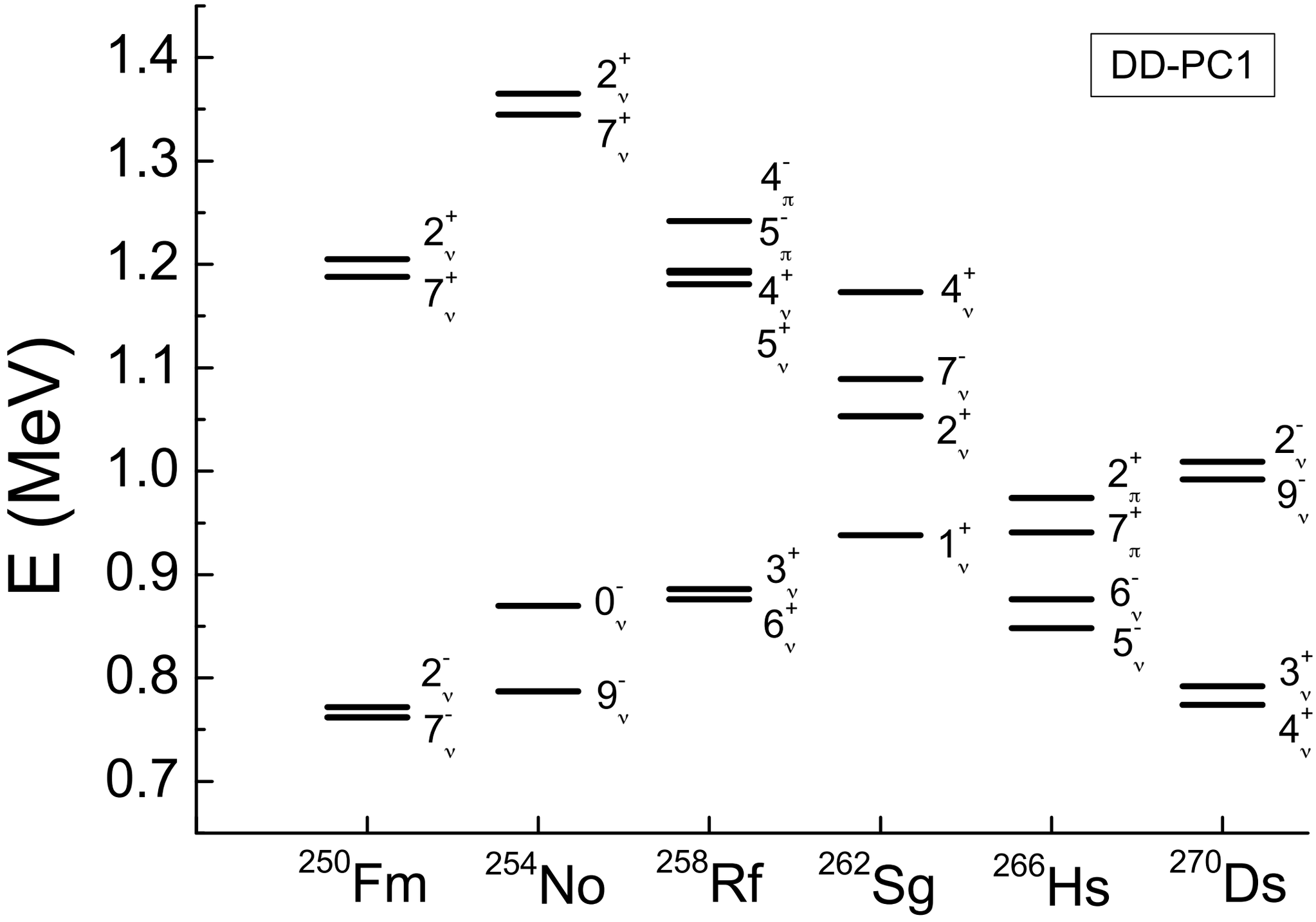


High-K isomers



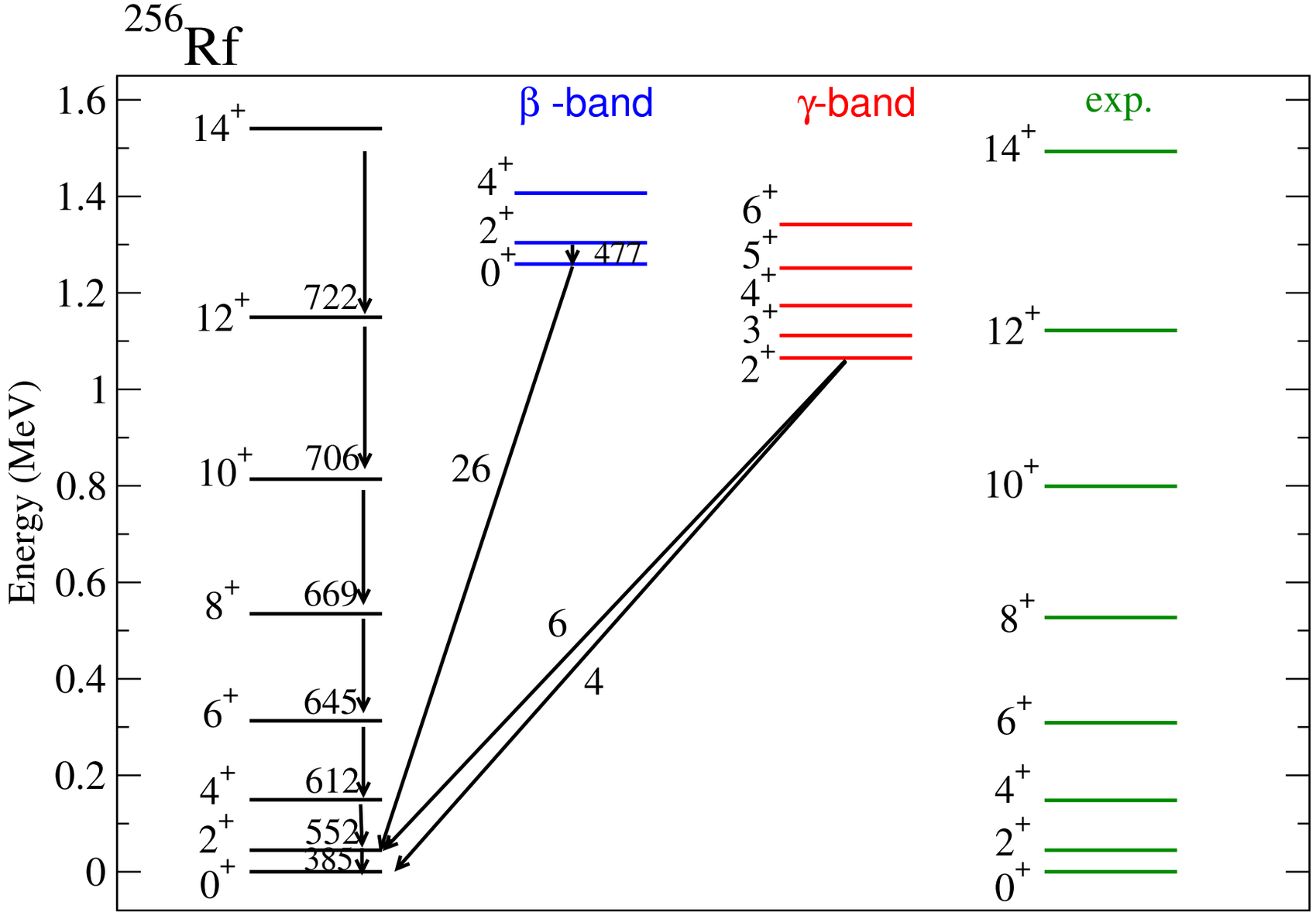


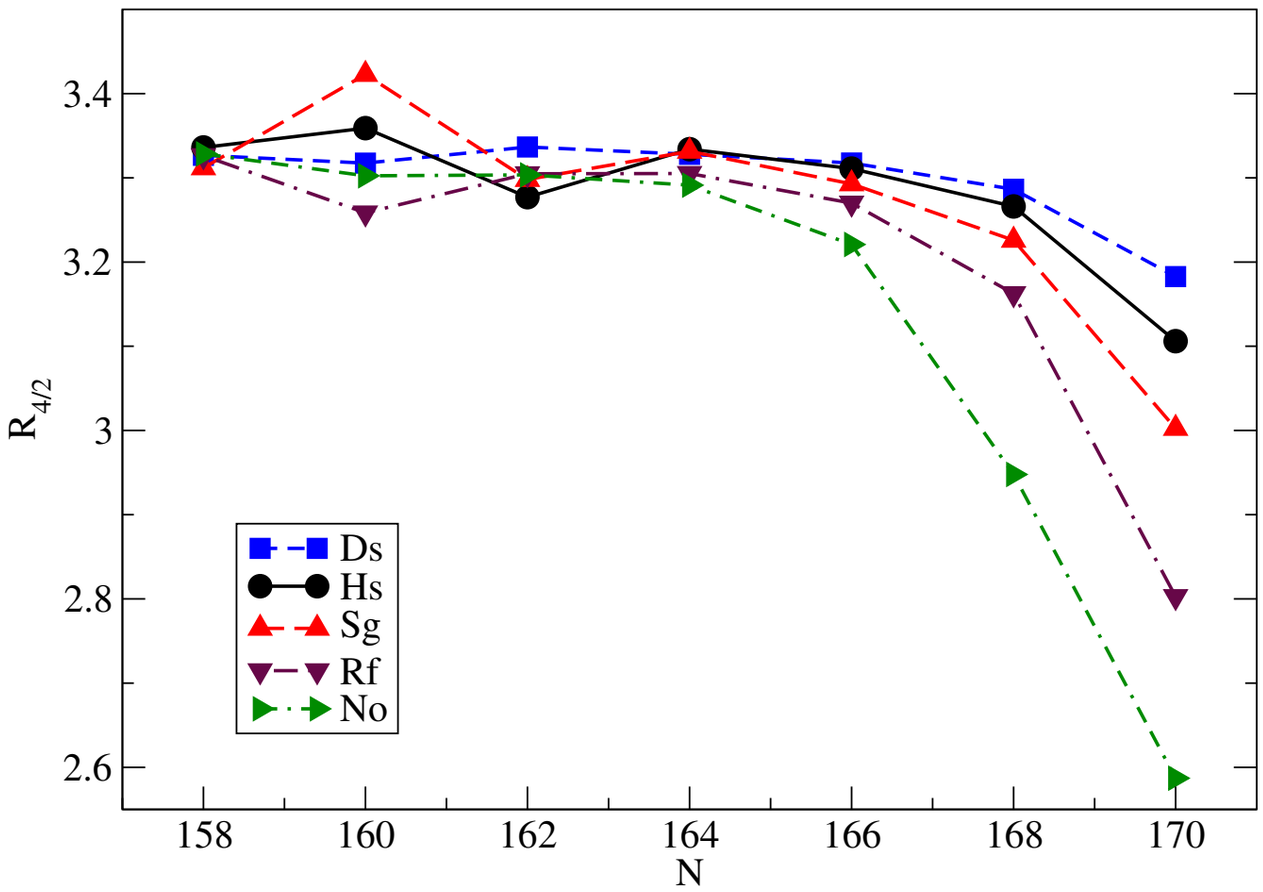
High-K isomers



Collective states

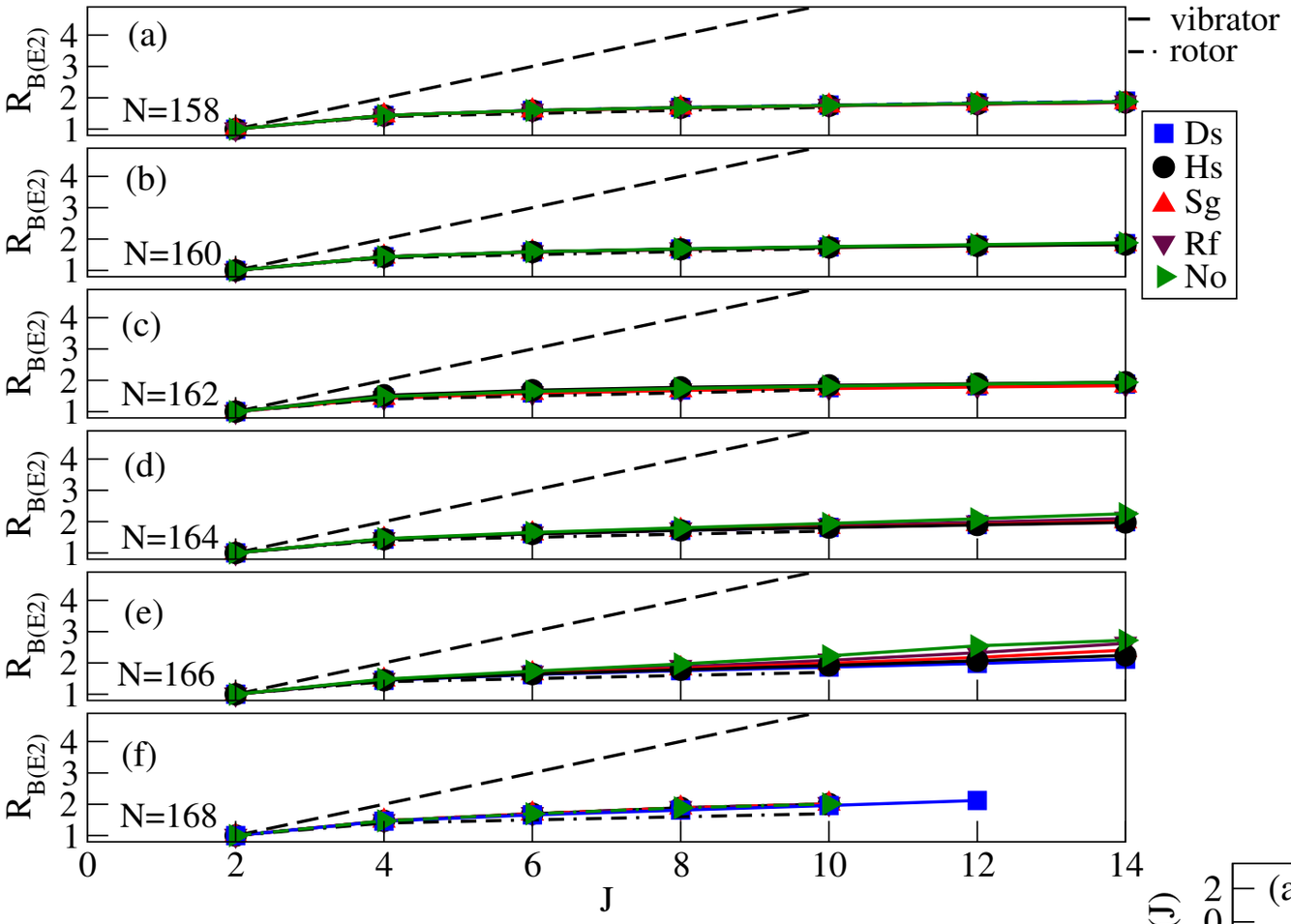
Low-energy spectrum of ^{256}Rf calculated with the collective Hamiltonian based on DD-PC1



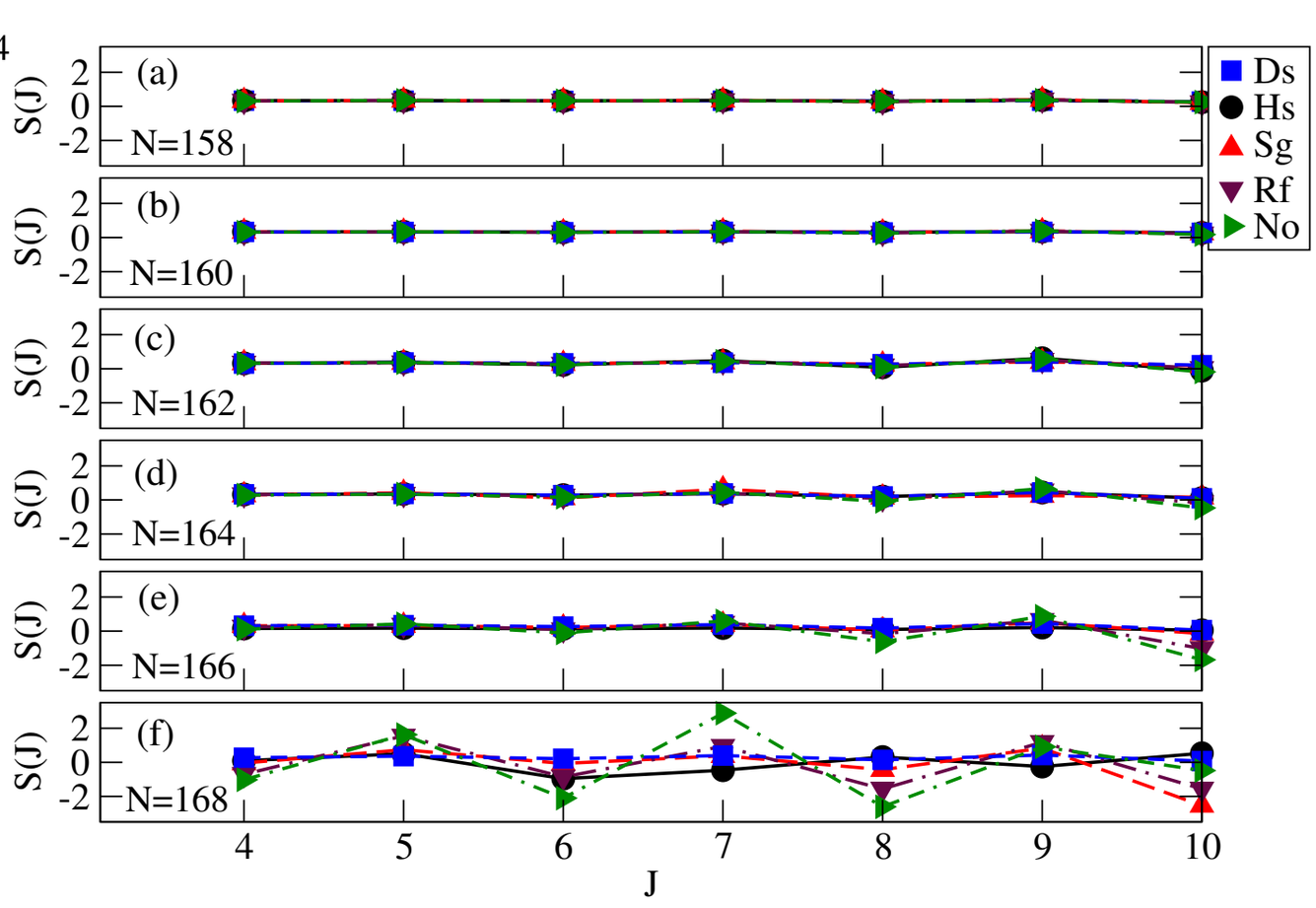


The ratio R4/2 of excitation energies of the yrast states 4^+_1 and 2^+_1 as a function of the neutron number for the isotopic chains of No, Rf, Sg, Hs and Ds.

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.

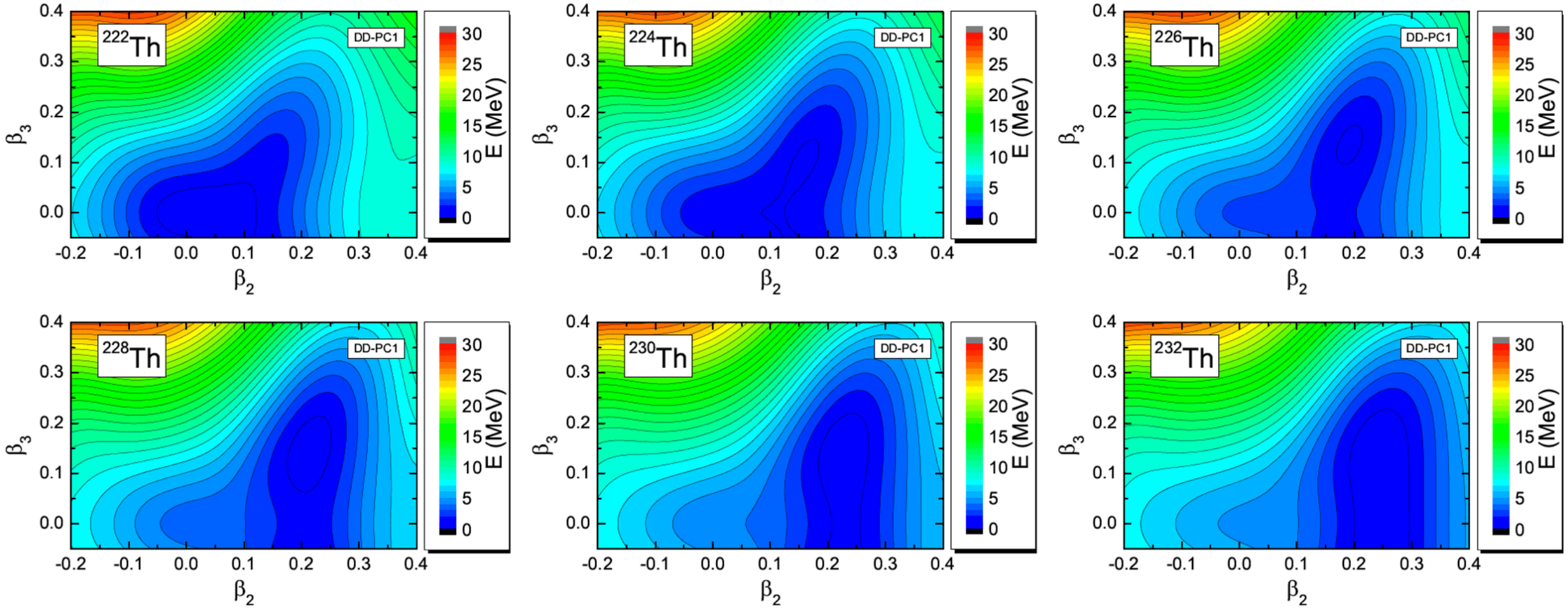


B(E2) values for transition between yrast states, normalized to B(E2; $2^+_1 \rightarrow 0^+_1$), in the N= 158, 160, 162, 164, 166 and 168 isotones of No, Rf, Sg, Hs and Ds.



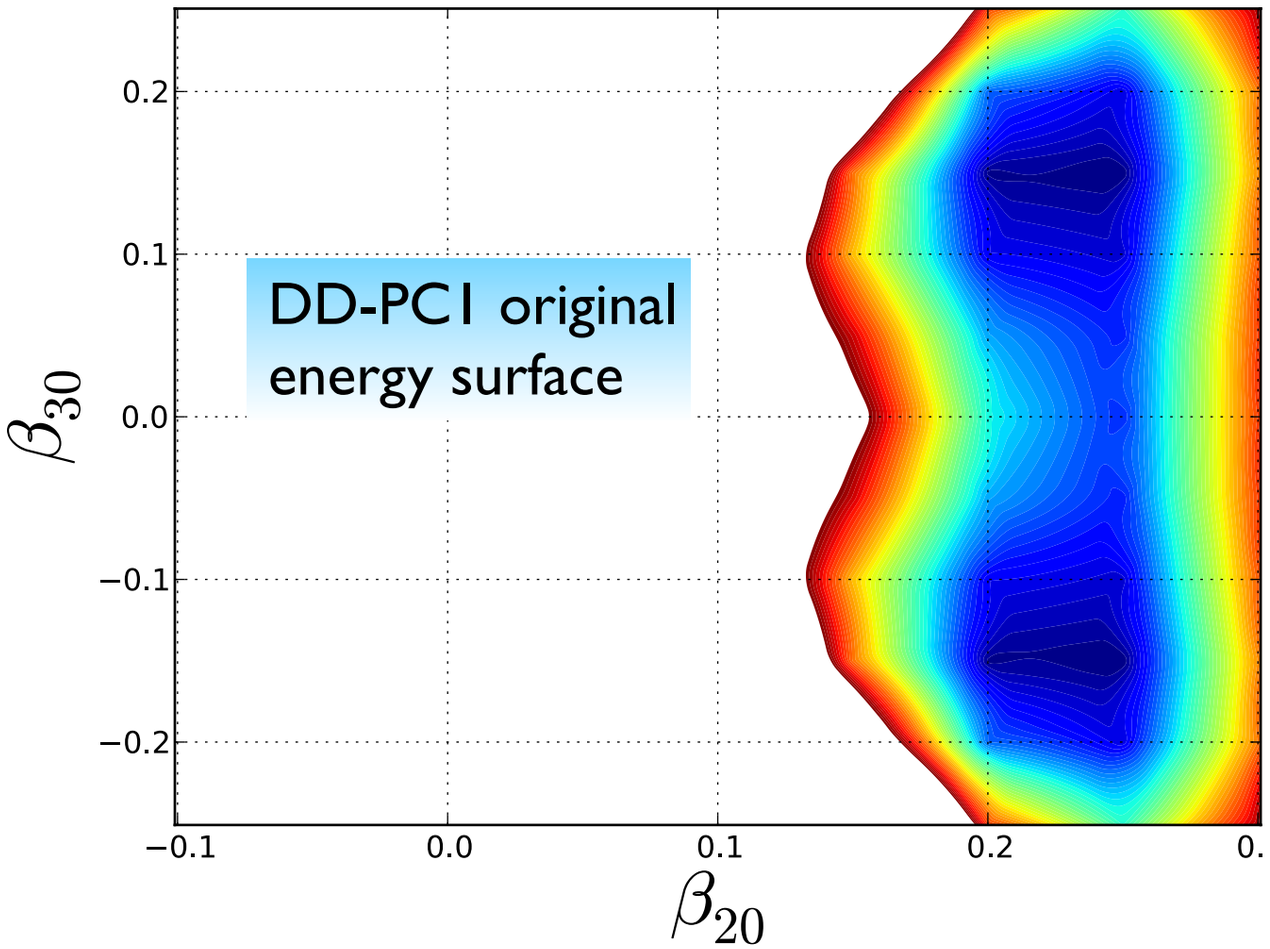
Staggering in the γ-bands of No, Rf, Sg, Hs and Ds with N= 158 − 166.

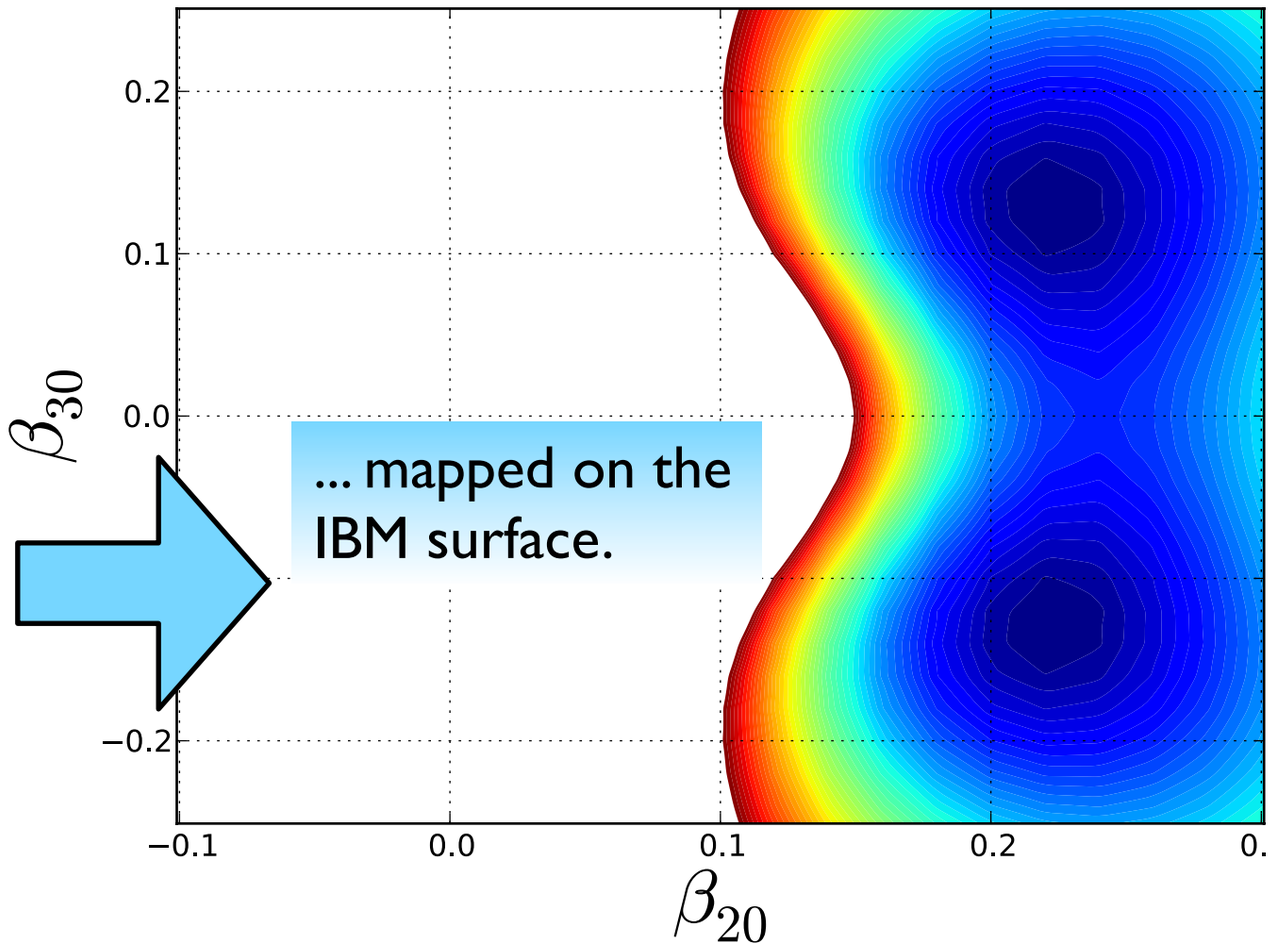
Octupole shape transitions in Th isotopes



Spectroscopic properties ⇒ quadrupole-octupole *sdf*-IBM Hamiltonian

$$\hat{H} = \epsilon_d \hat{n}_d + \epsilon_f \hat{n}_f + \kappa_2 \hat{Q} \cdot \hat{Q} + \alpha \hat{L}_d \cdot \hat{L}_d + \kappa_3 : \hat{V}_3^\dagger \cdot \hat{V}_3 :$$

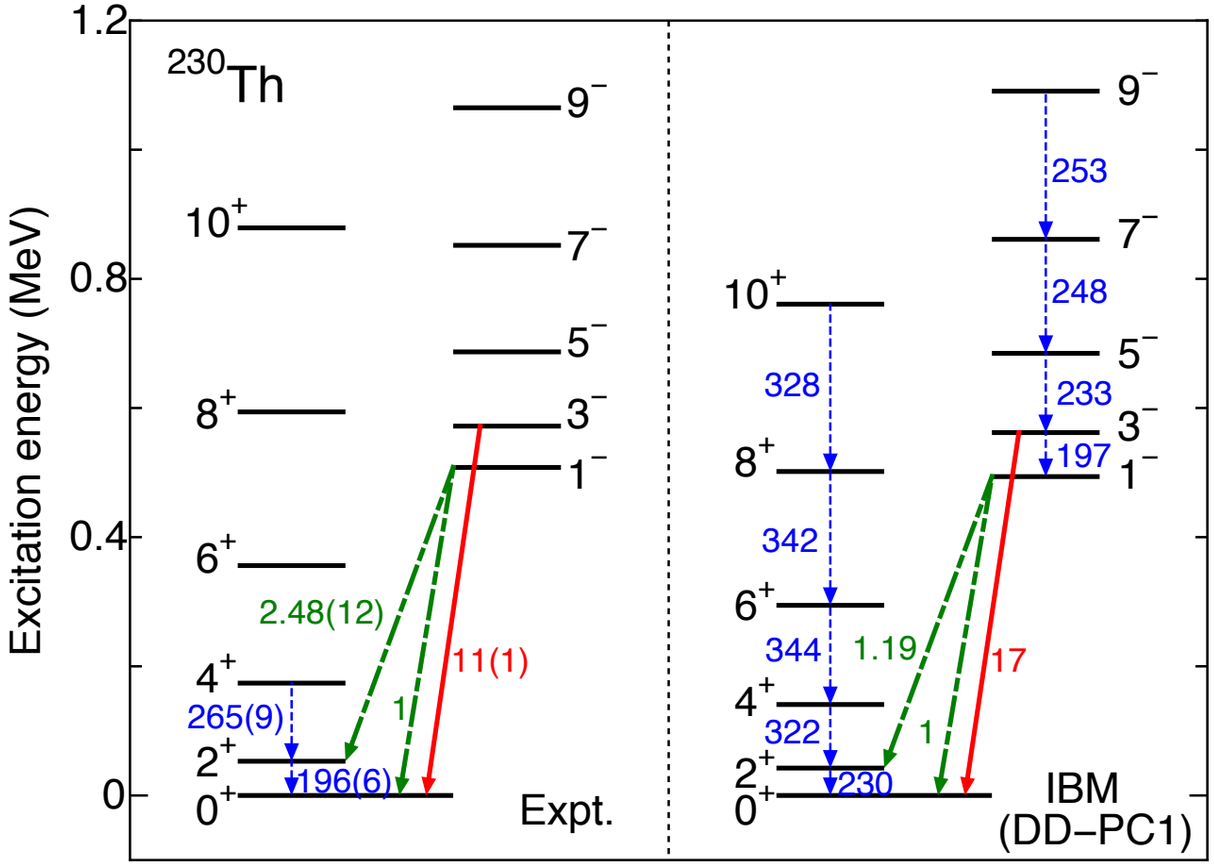


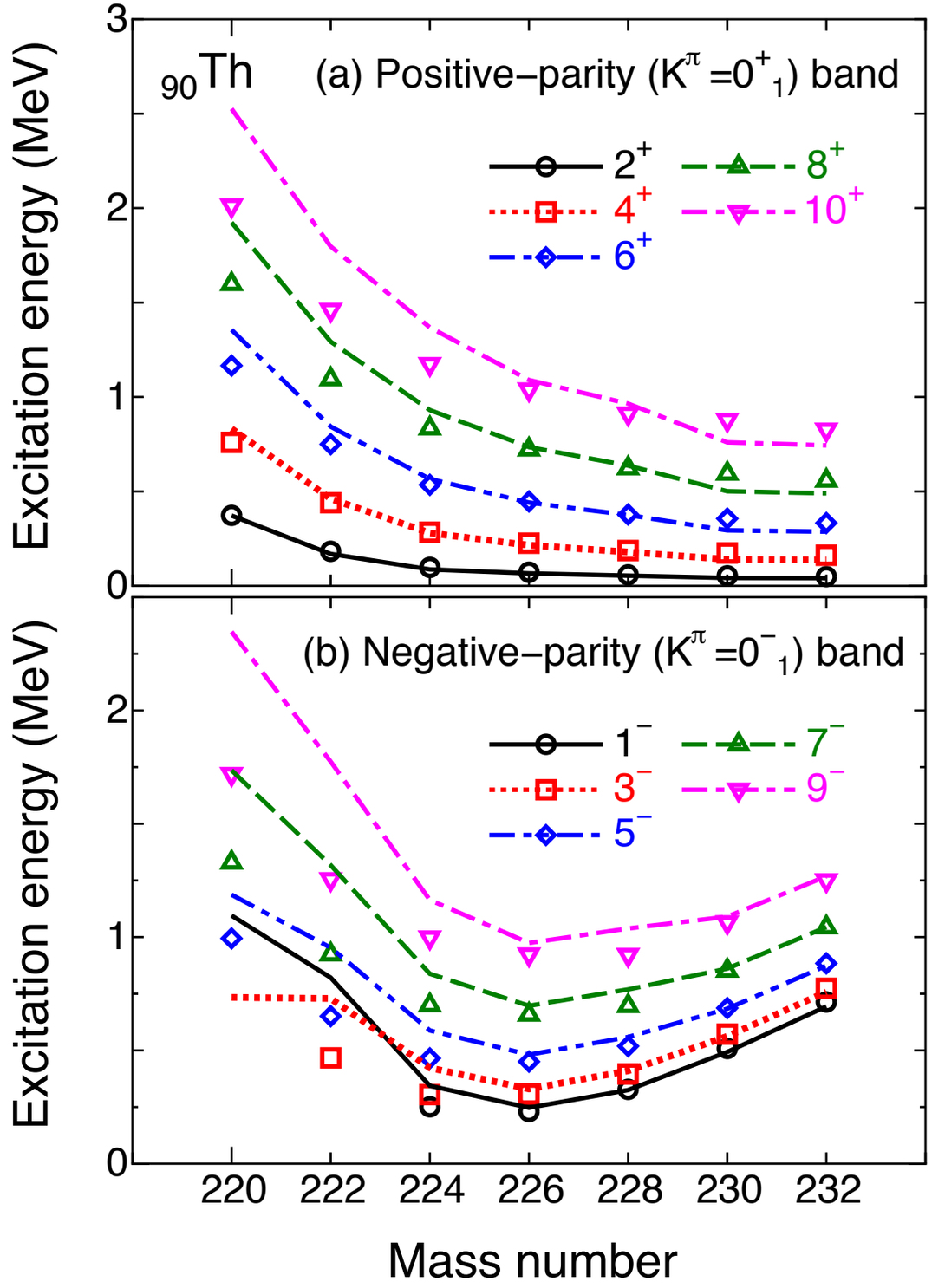


Mapping the microscopic PES on the expectation value of the IBM Hamiltonian in the *sdf*-boson condensate state:

$$\hat{H} = \epsilon_d \hat{n}_d + \epsilon_f \hat{n}_f + \kappa_2 \hat{Q} \cdot \hat{Q} + \alpha \hat{L}_d \cdot \hat{L}_d + \kappa_3 : \hat{V}_3^\dagger \cdot \hat{V}_3 :$$

$$|\phi\rangle = \frac{1}{\sqrt{N!}} (\lambda^\dagger)^N |-\rangle \qquad \lambda^\dagger = s^\dagger + \beta_2 d_0^\dagger + \beta_3 f_0^\dagger$$


230Th
Excitation energy (MeV)
1.2
0.8
0.4
0
10+
8+
6+
4+
2+
0+
9−
7−
5−
3−
1−
2.48(12)
265(9)
196(6)
1
11(1)
Expt.
328
342
344
322
230
1.19
17
253
248
233
197
IBM
(DD−PC1)


90Th
(a) Positive−parity (K^π =0+1) band
2+
4+
6+
8+
10+
(b) Negative−parity (K^π =0−1) band
1−
3−
5−
7−
9−
Excitation energy (MeV)
Mass number
220
222
224
226
228
230
232

Nuclear Energy Density Functional Framework

✔ unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.

✔ when extended to take into account collective correlations, EDFs describe deformations, shape-coexistence and shape-phase transition phenomena associated with shell evolution.

✔ Time-dependent NDFT → fully self-consistent (Q)RPA analysis of giant resonances, low-energy multipole response in weakly-bound nuclei, astro-physical applications.