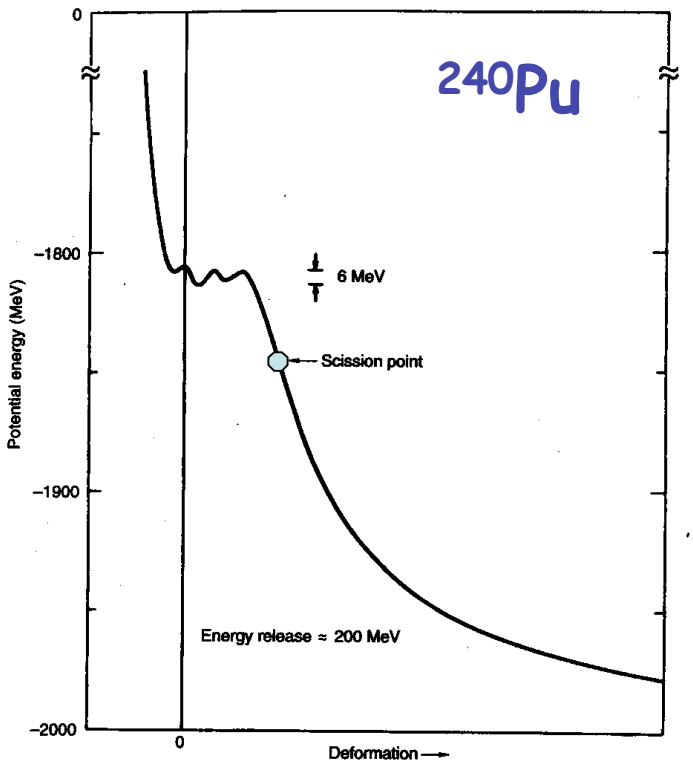
# Selfconsistent Barrier Calculations

## Theoretical Description of the Fission Process

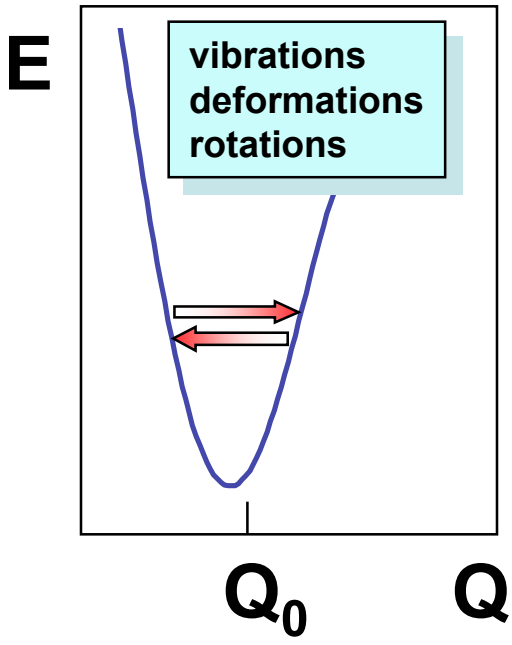
(DE-FG03-03NA00083)

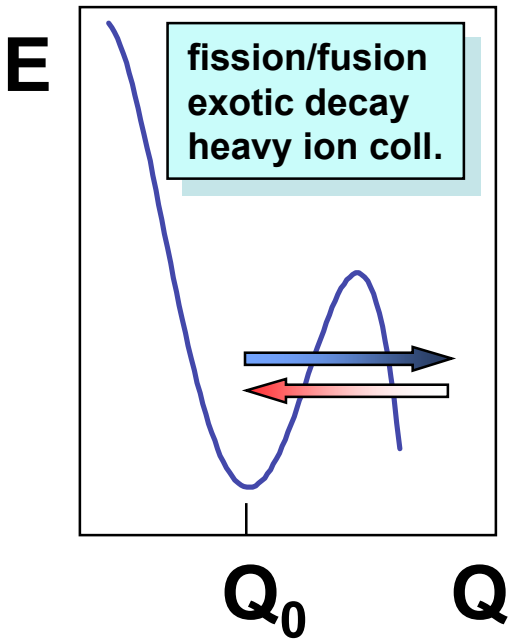
P. Borycki (UT, graduate student)
J. Dobaczewski (UT/Warsaw)
W. Nazarewicz (UT/ORNL, Principal Investigator)
A. Staszczak (UT/Lublin)
M. Stoitsov (UT/Sofia)

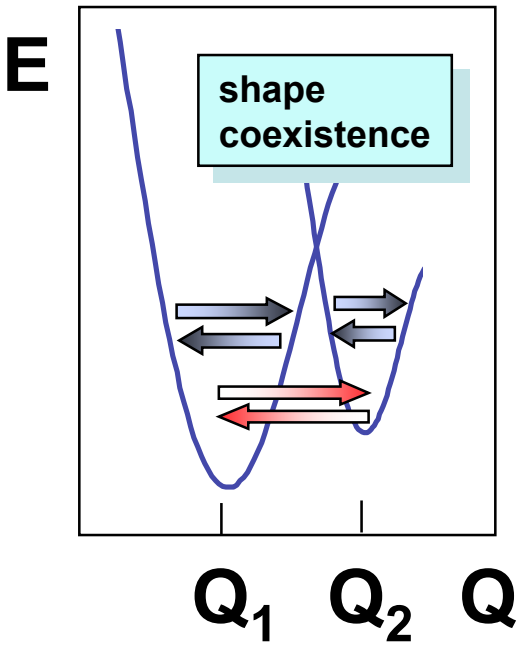



1938 - Hahn & Strassmann
1939 - Meitner & Frisch
1939 - Bohr & Wheeler
1940 - Petrzhak & Flerov

# Mean-field dynamics
## small/large amplitude collective motion




- Level crossing dynamics,
- Dynamics of symmetry breaking,
- Existence and disappearance of qantum numbers,
- Adiabaticity of LACM,
- Dissipation,
- Chaos.

# The Aim of the Project is…

…to attack the problem of spontaneous fission using modern theoretical methods and computational tools.

A. We intend to develop effective energy functionals that are appropriate for the description of heavy nuclei. Our goal is to improve the existing energy density (Skyrme) functionals to develop a force that will be used in calculations of fission dynamics. To this end, we will use recently written Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes.

B. Perform systematic self-consistent calculations of binding energies and fission barriers of actinide and trans-actinide nuclei using modern density functionals. This will be followed by calculations of spontaneous fission lifetimes and mass and charge divisions using dynamic adiabatic approaches based on the WKB approximation.

C. Investigate novel microscopic (non-adiabatic) methods to study the fission process. In particular, we are going to assess whether the imaginary time (instanton) method, the generator coordinate method, and the Walet-Klein approach to collective coordinates can be used in practical self-consistent calculations.

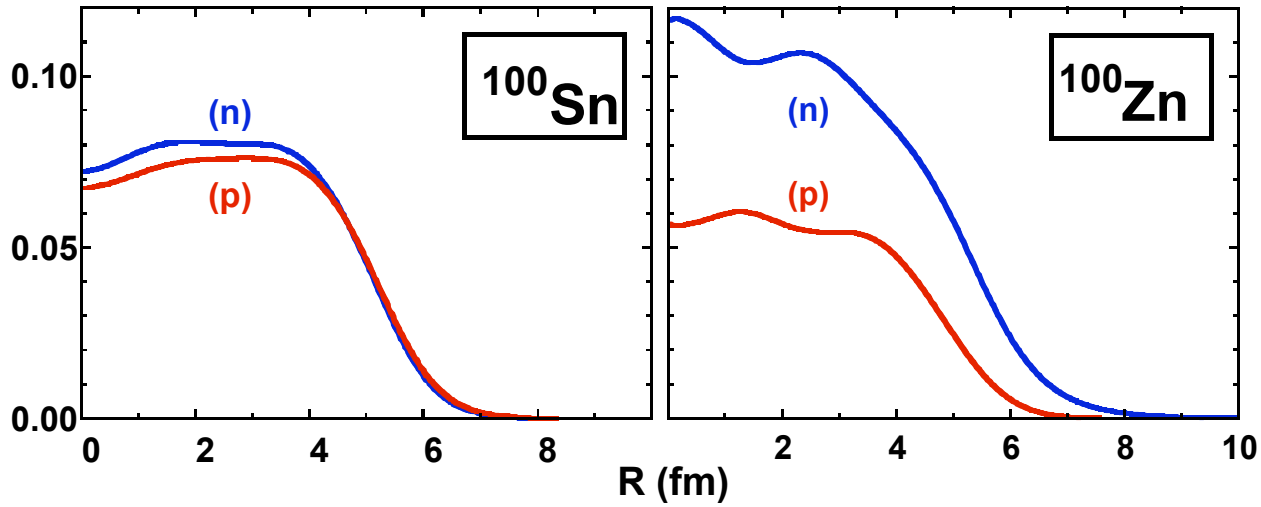
Our Recent relevant work:
Europhys. News 33, 1 (2002)
Nucl. Phys. A 701, 165c (2002).
Phys. Rev. C 68, 054312 (2003)
Phys. Rev. C 69, 014316 (2004)

# The Method

- The Skyrme SLy4 energydensity functional
- Pairing force (seniority pairing, delta pairing). The pairing strengths have been adjusted to reproduce the proton and neutron experimental pairing gaps in $^{252}$Fm.
- HF+BCS and HFB
- Cartesian (3D) harmonic oscillator finite basis code HFODD v.2.08i (Comput. Phys. Comm. 158, 158 (2004). This code makes it possible to break all self-consistent symmetries of the nuclear mean field, including axial symmetry, reflection symmetry, and time reversal.
- Calculations performed for transfermium and superheavy nuclei

# MEAN-FIELD APPROACH

## Towards Nuclear Energy Density Functional




Modern Mean-Field Theory ≡ Energy Density Functional

□ □ □ □ □

□, □, J, j, T, s, F,

+ pairing densities!

mean field □ one-body densities

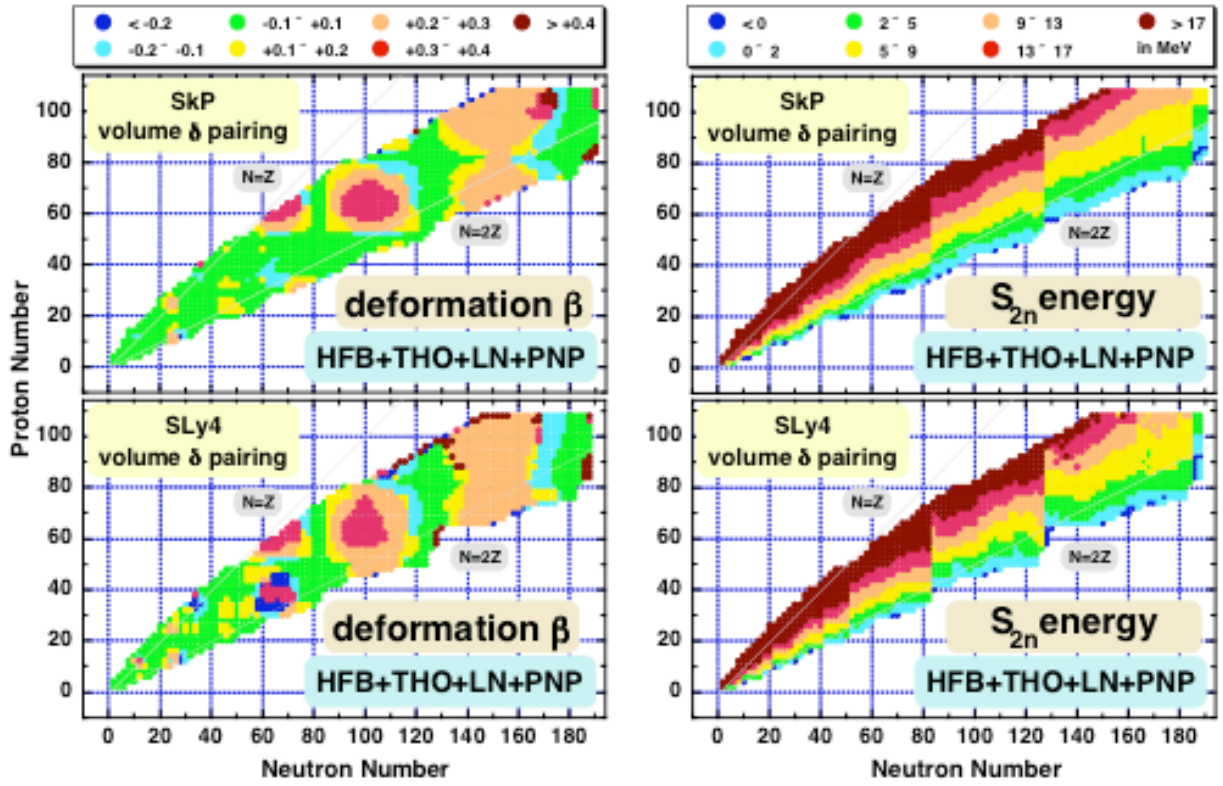
zero range □ local densities

finite range □ non-local densities

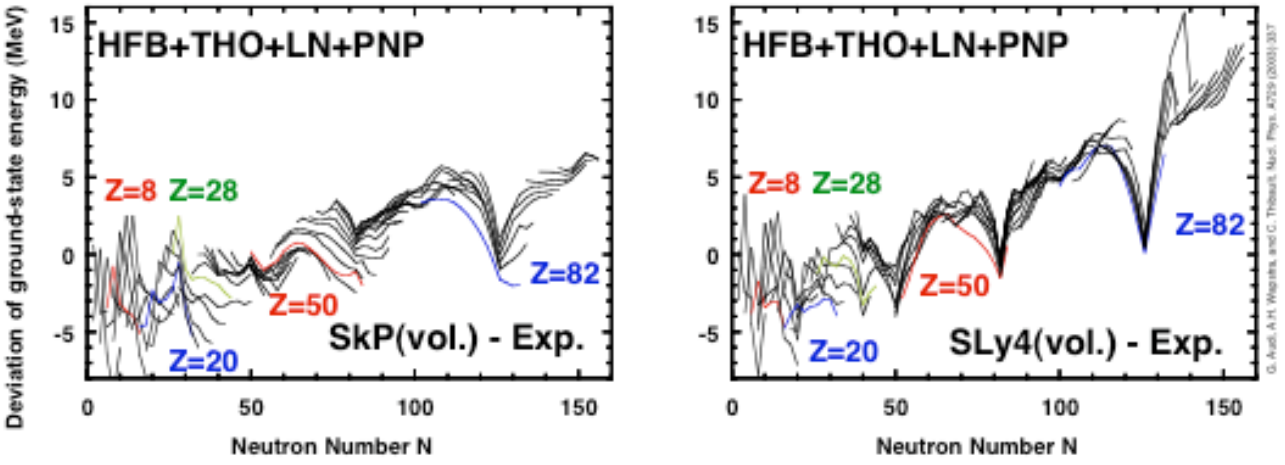
- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

# Microscopic Mass Table

M.V. Stoitsov et al., nucl-th/0406075
J. Dobaczewski et al., nucl-th/040407

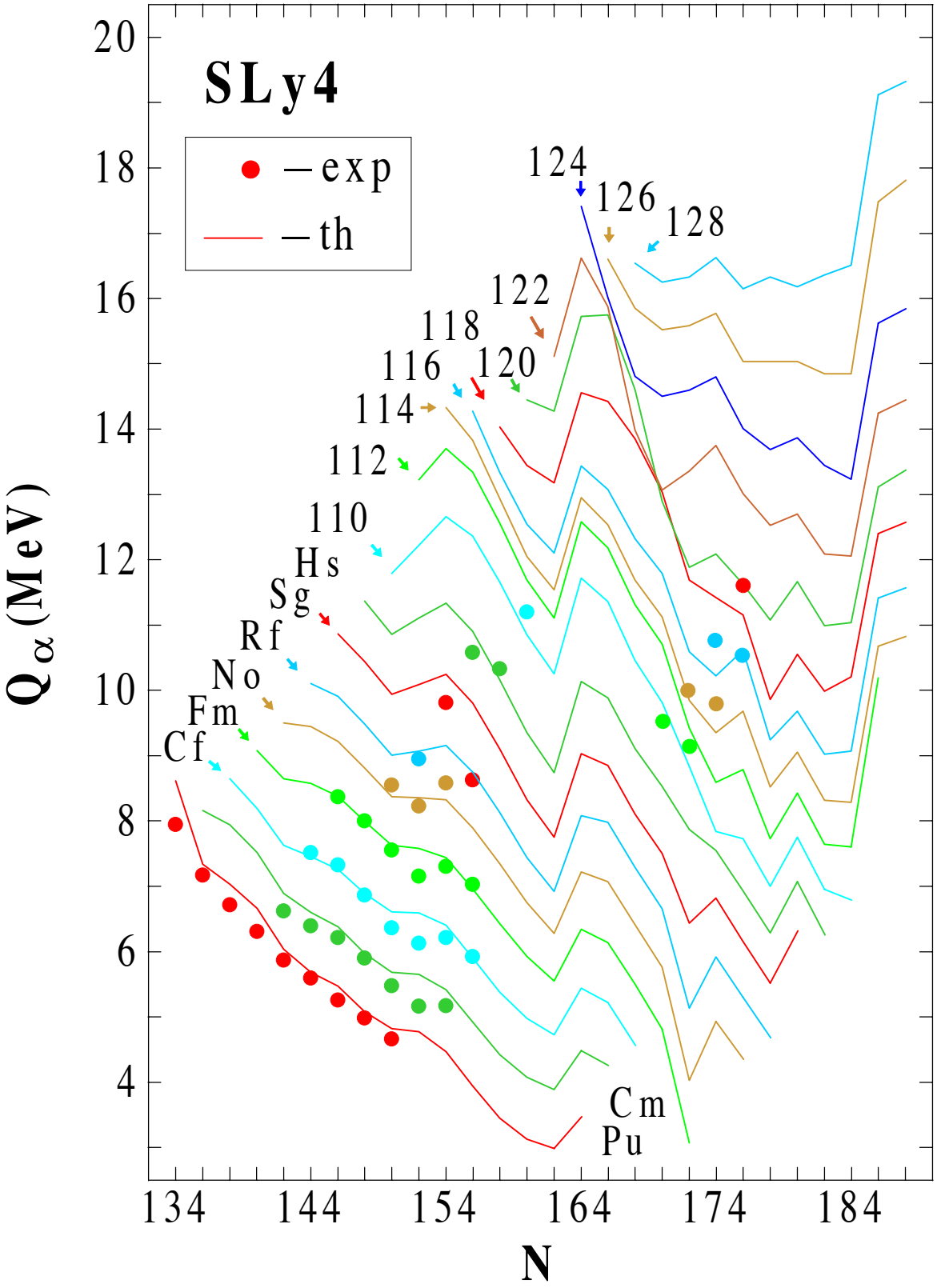



# Deviation from experiment




"Systematic study of deformed nuclei at the drip lines and beyond", M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, S. Pittel, and D.J. Dean, Phys. Rev. C **68**, 054312 (2003)

S. Cwiok, P.H. Heenen, W. Nazarewicz



# □ decay of $^{277}112_{165}$

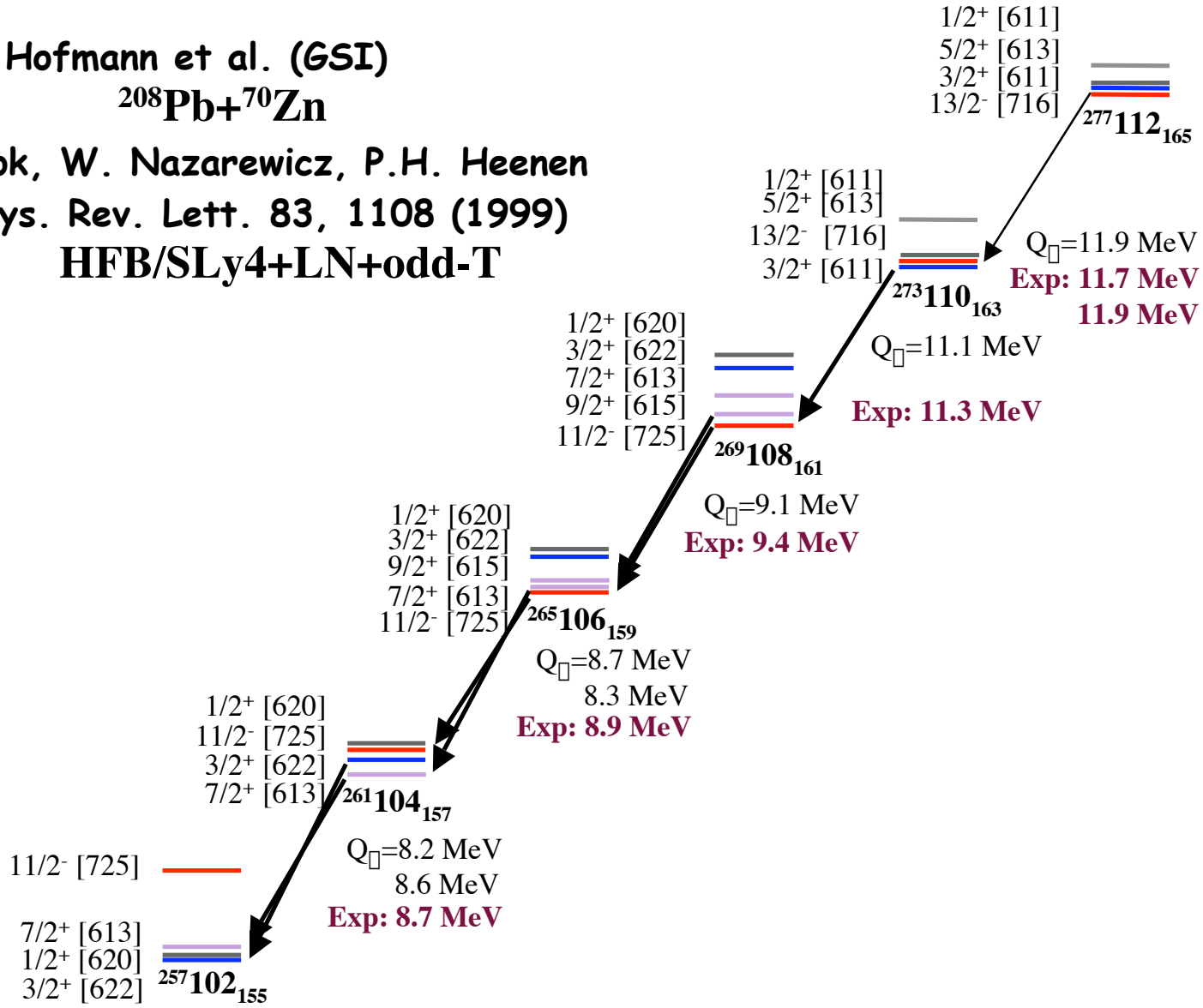
Experiment: S. Hofmann et al. (GSI)

$^{208}Pb+^{70}Zn$

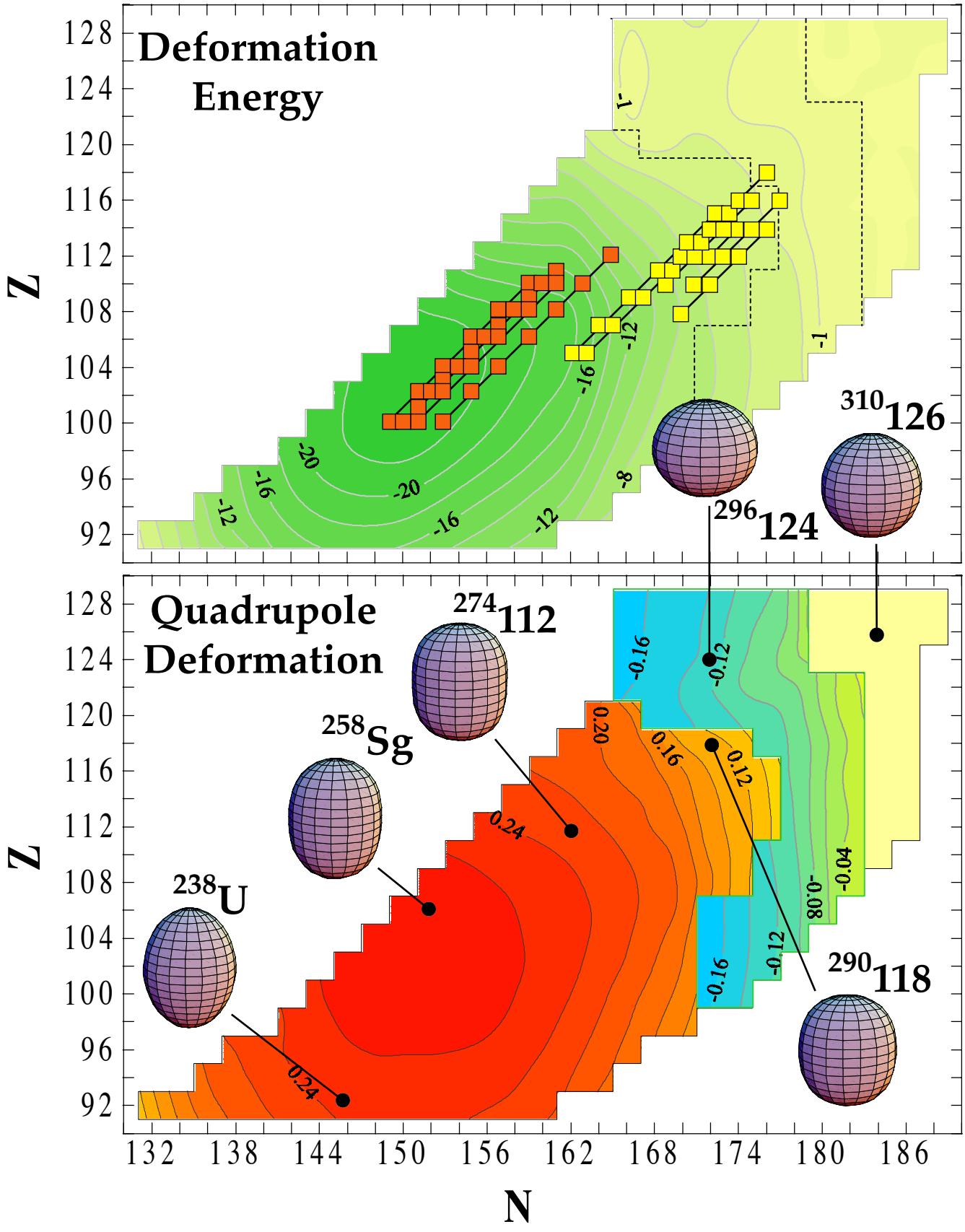
Theory: S. Cwiok, W. Nazarewicz, P.H. Heenen

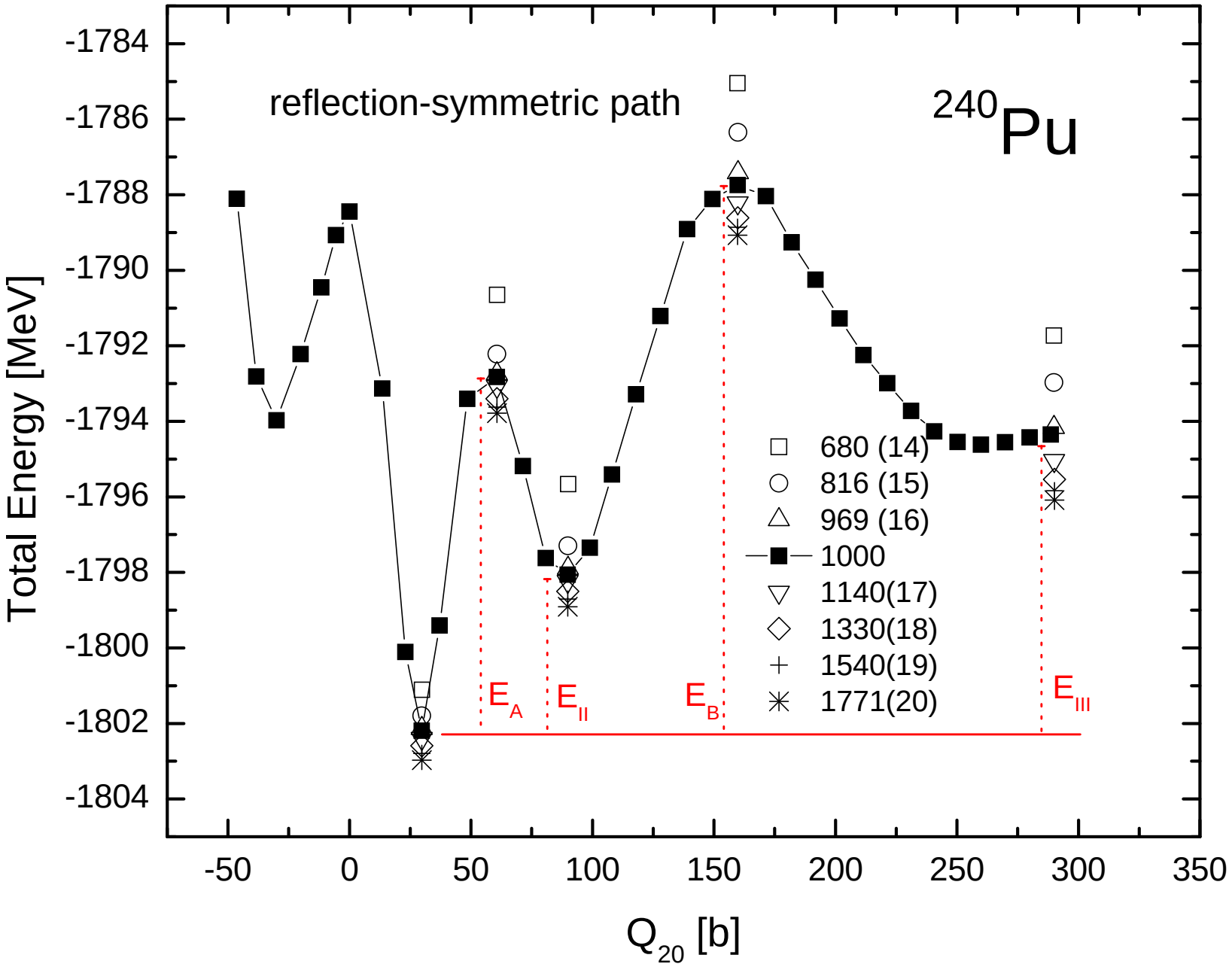
Phys. Rev. Lett. 83, 1108 (1999)

**HFB/SLy4+LN+odd-T**

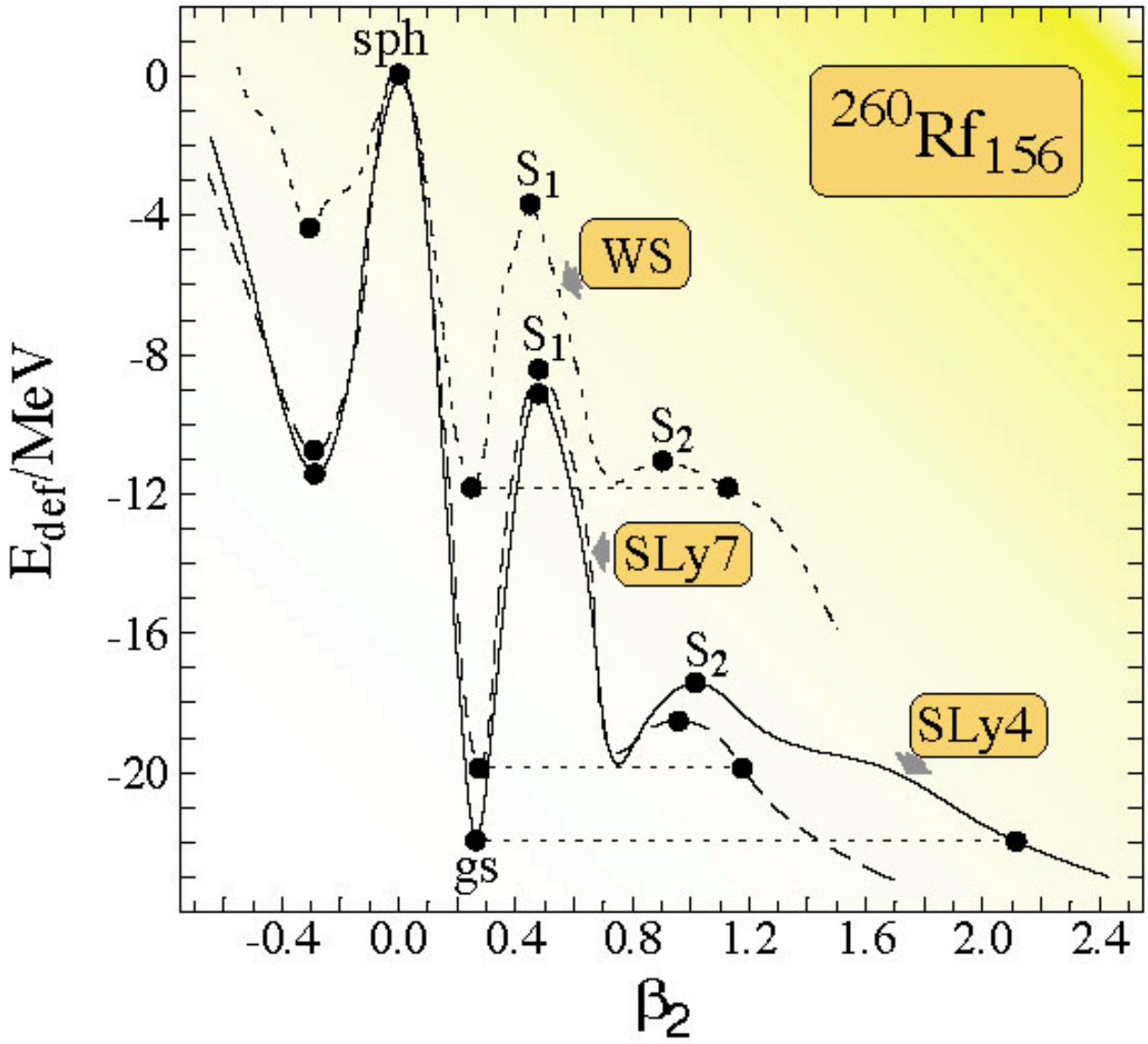


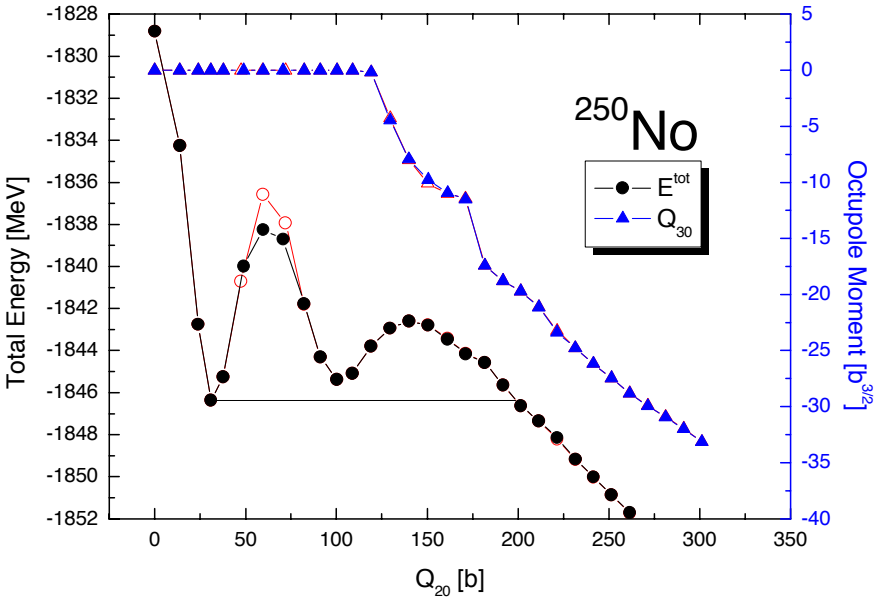
S. Cwiok, P.H. Heenen, W. Nazarewicz
Nature, 433, 705 (2005)

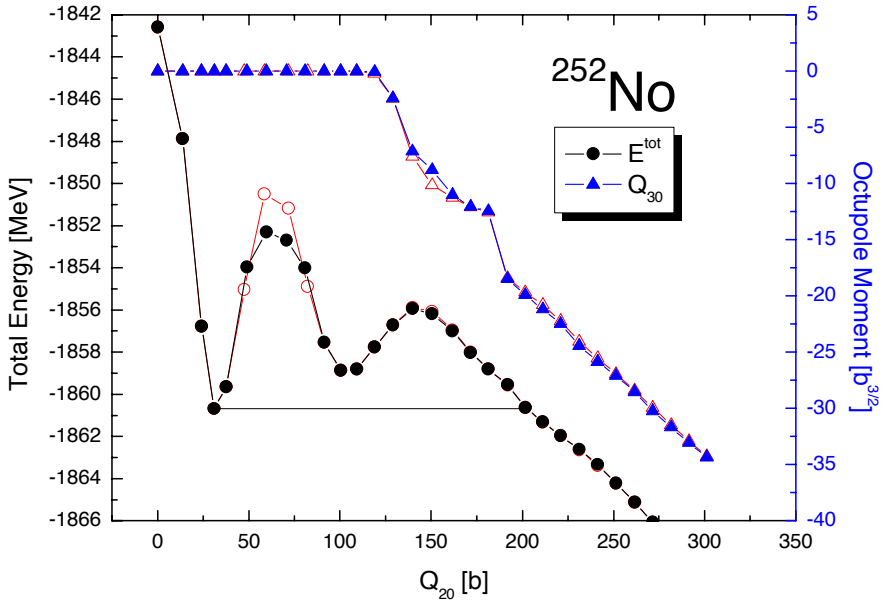



reflection-symmetric path
240Pu
Total Energy [MeV]
Q20 [b]
-1784
-1786
-1788
-1790
-1792
-1794
-1796
-1798
-1800
-1802
-1804
-50
0
50
100
150
200
250
300
350
680 (14)
816 (15)
969 (16)
1000
1140(17)
1330(18)
1540(19)
1771(20)
EA
EII
EB
EIII

# But… problems with self-consistent barriers and shape isomers




$^{250}$No
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]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$Q_{30}$
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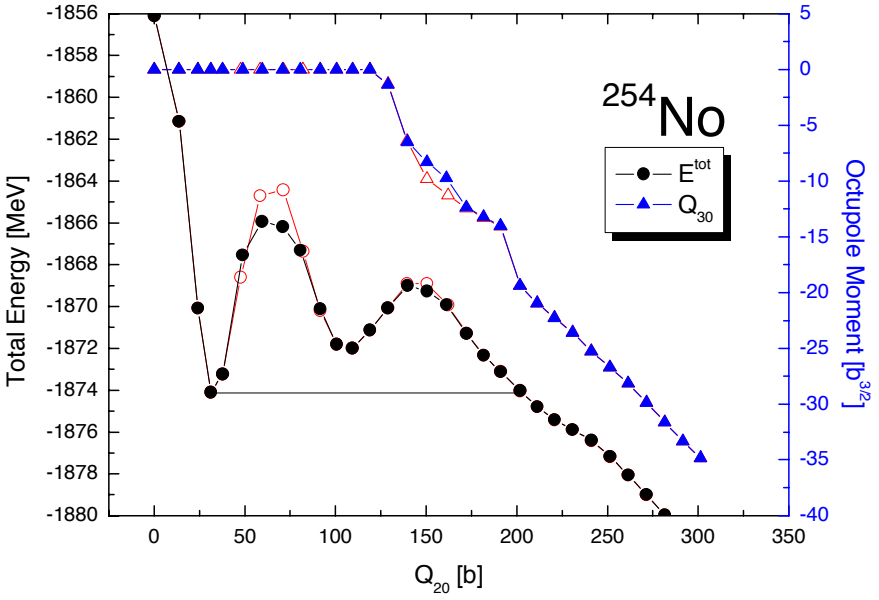
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]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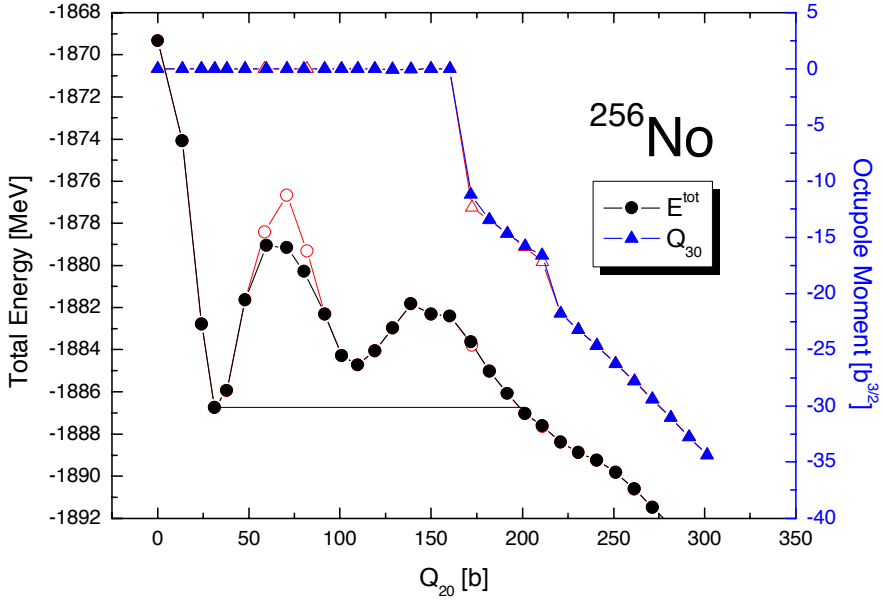
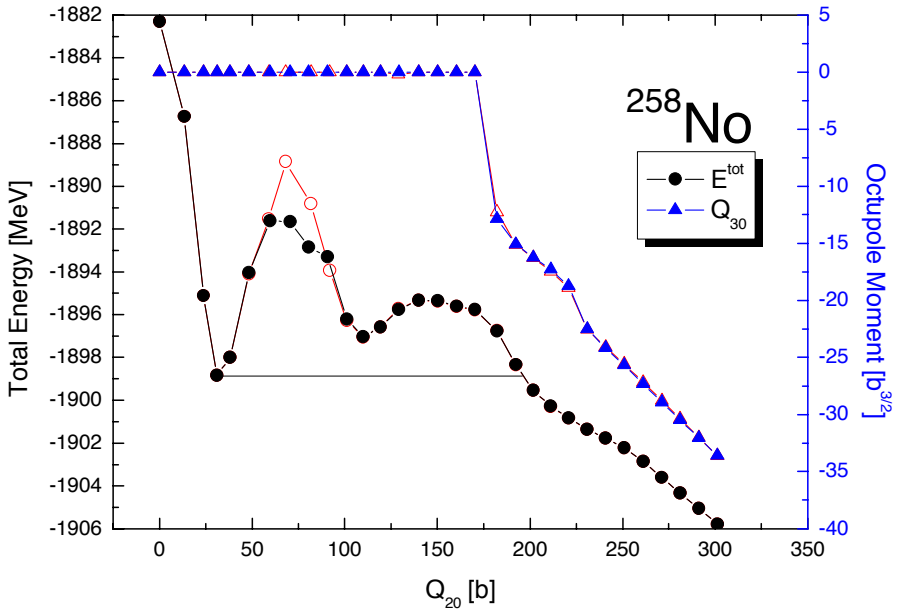
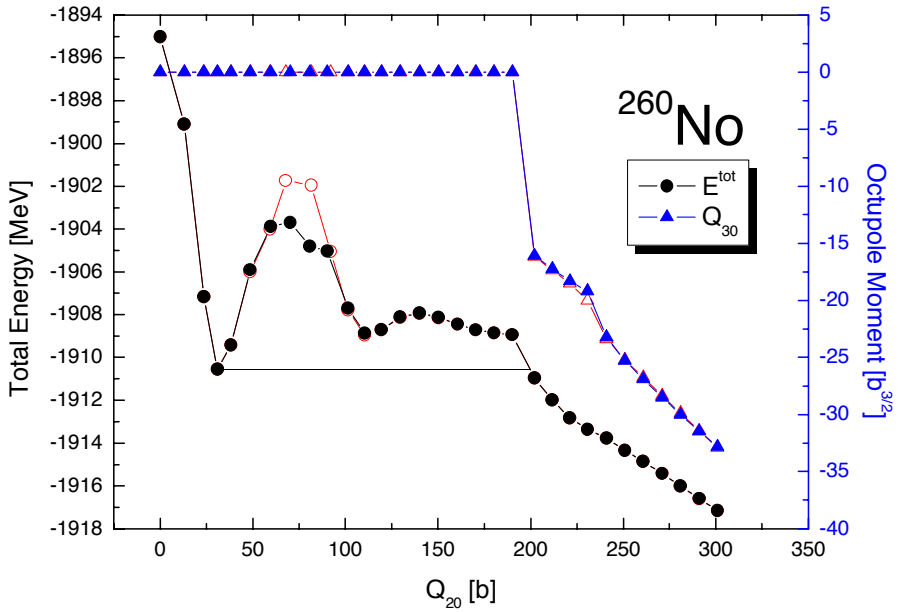
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{256}$No
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{258}$No
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]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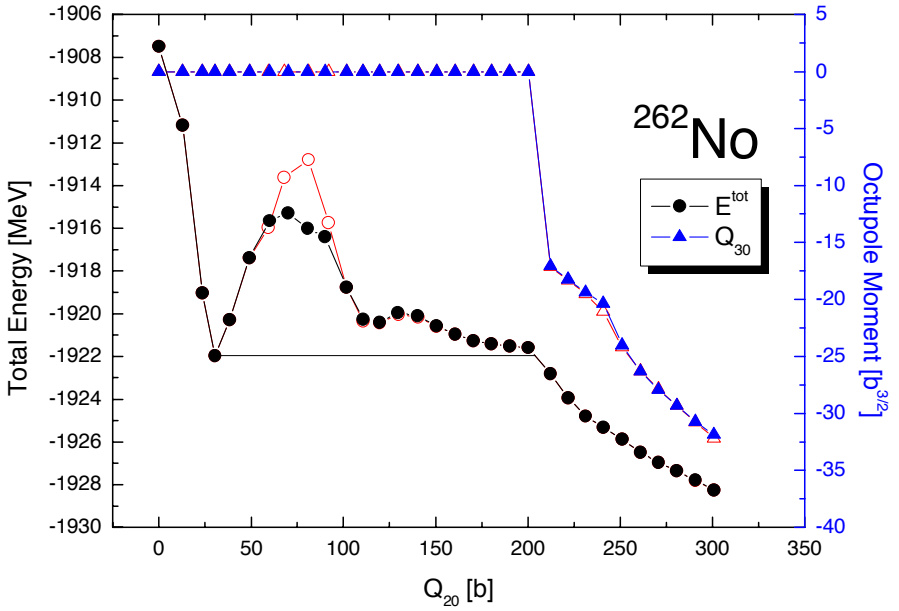
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]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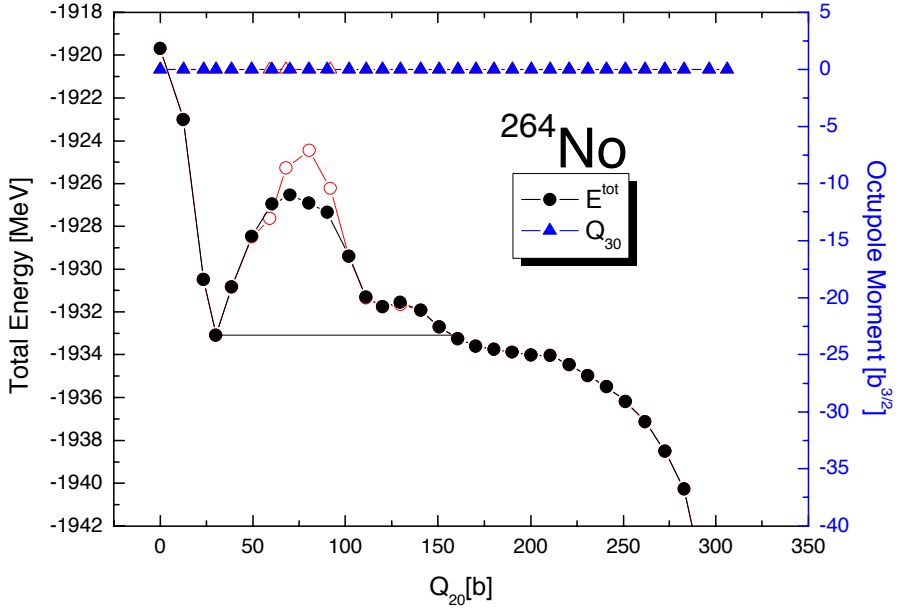
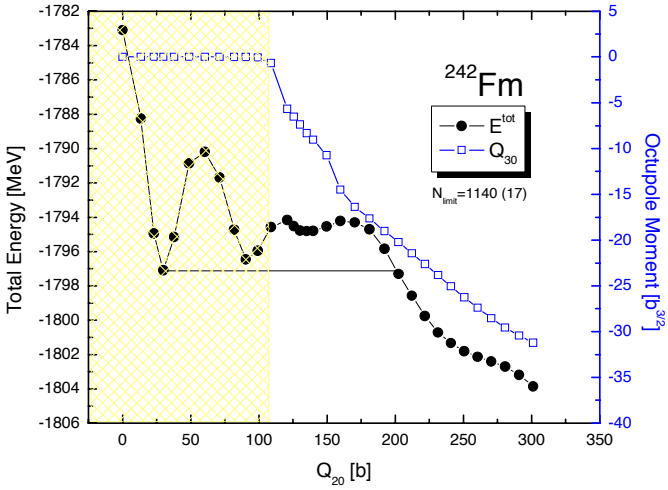
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{264}$No
$E^{tot}$
$Q_{30}$
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$[b]


$^{242}$Fm
$E^{tot}$
$Q_{30}$
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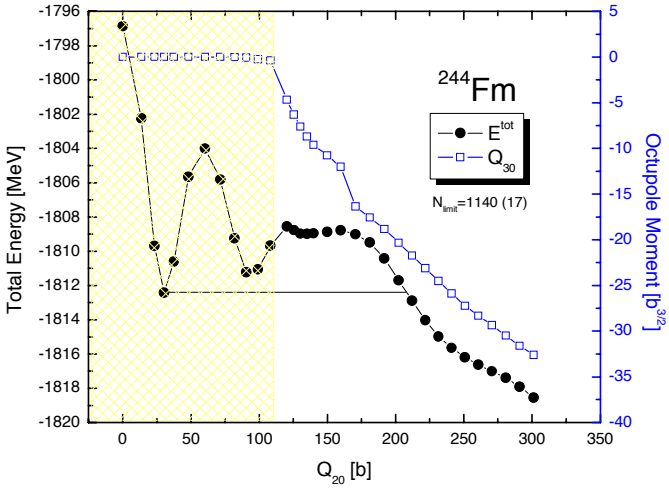
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{244}$Fm
$E^{tot}$
$Q_{30}$
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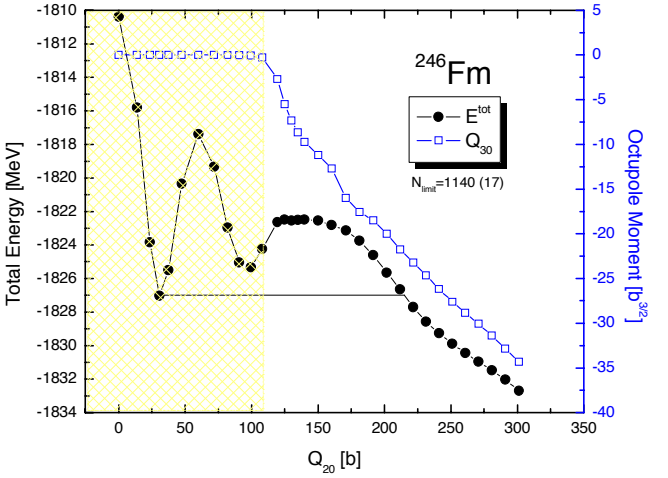
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{246}$Fm
$E^{tot}$
$Q_{30}$
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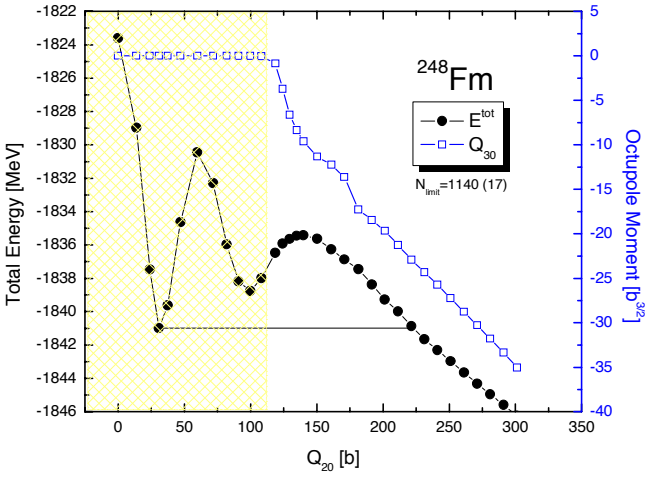
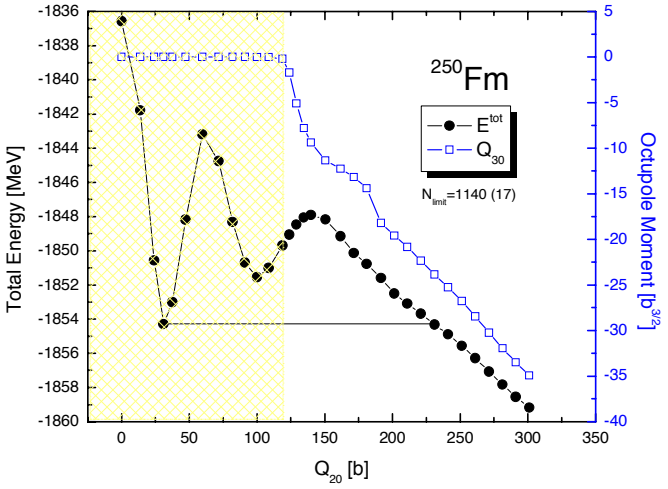
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{248}$Fm
$E^{tot}$
$Q_{30}$
$N_{limit}$=1140 (17)
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{250}$Fm
$E^{tot}$
$Q_{30}$
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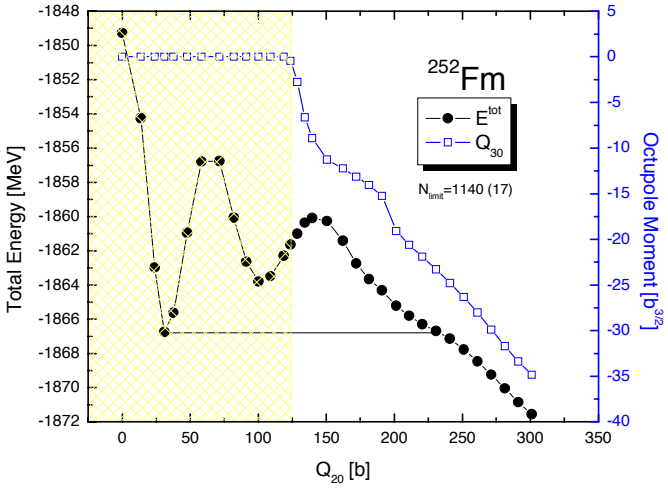
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{252}$Fm
$E^{tot}$
$Q_{30}$
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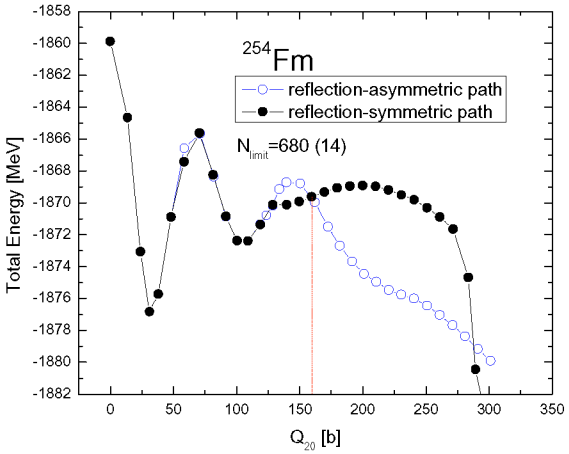
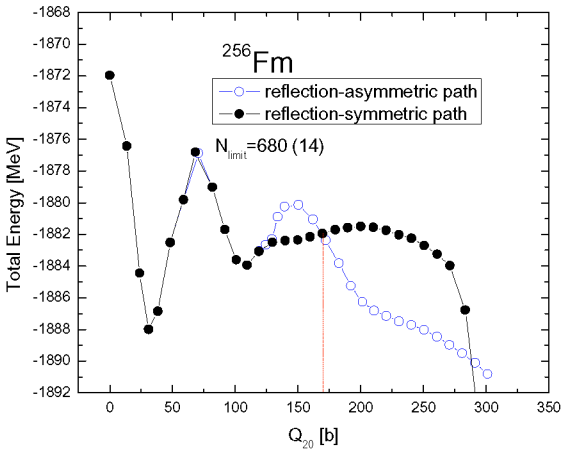
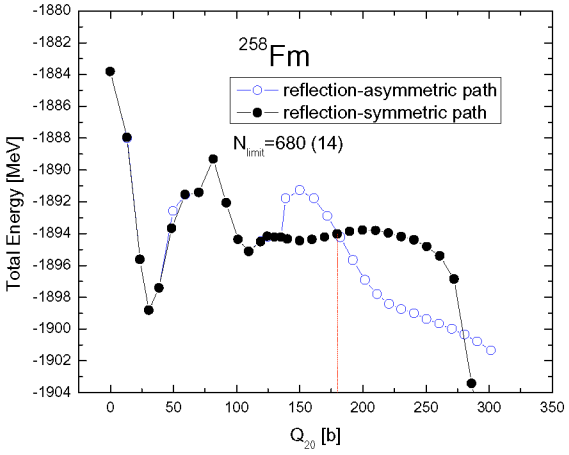
Total Energy [MeV]
Octupole Moment [b$^{3/2}$]
$Q_{20}$ [b]


$^{254}$Fm
reflection-asymmetric path
reflection-symmetric path
$N_{limit}$=680 (14)
Total Energy [MeV]
$Q_{20}$ [b]


$^{256}$Fm
reflection-asymmetric path
reflection-symmetric path
$N_{limit}$=680 (14)
Total Energy [MeV]
$Q_{20}$ [b]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reflection-asymmetric path
reflection-symmetric path
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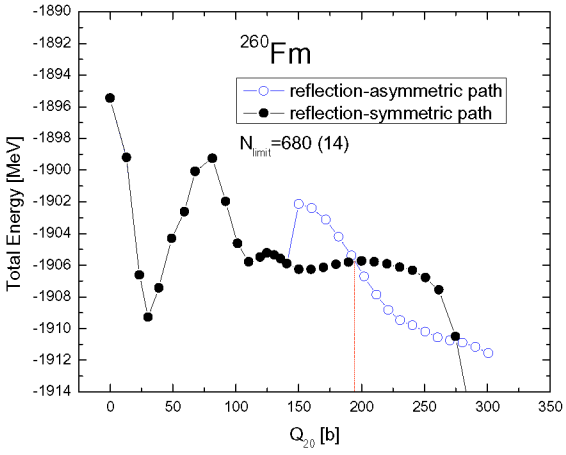
Total Energy [MeV]
$Q_{20}$ [b]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reflection-asymmetric path
reflection-symmetric path
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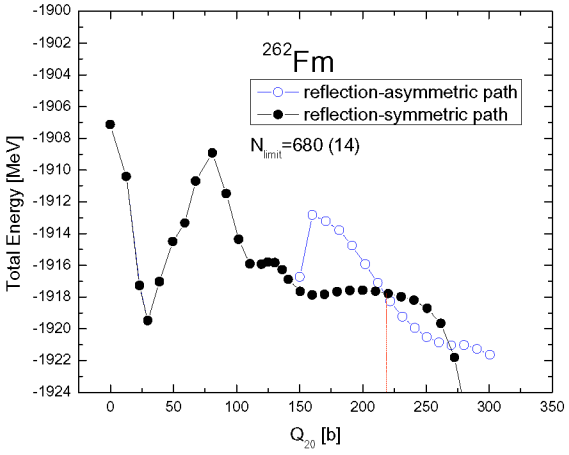
Total Energy [MeV]
$Q_{20}$ [b]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reflection-symmetric path
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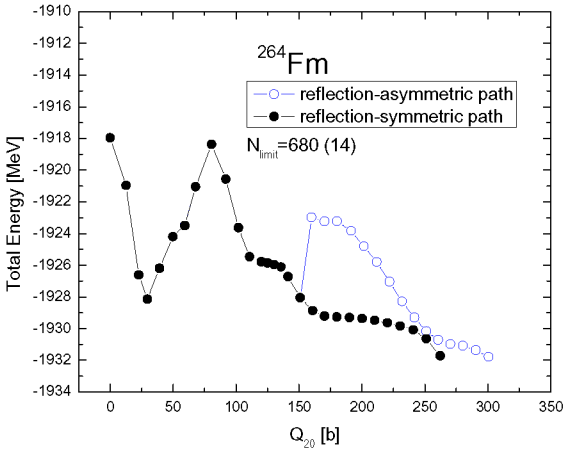
Total Energy [MeV]
$Q_{20}$ [b]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reflection-asymmetric path
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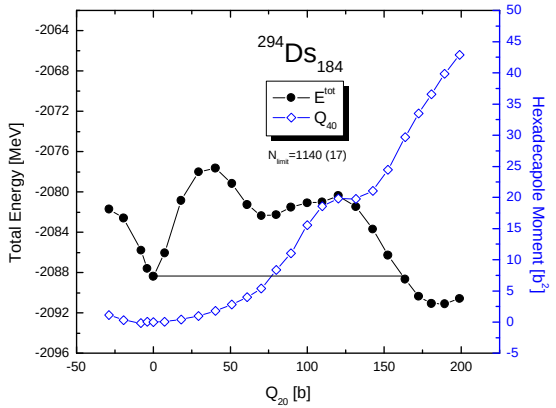
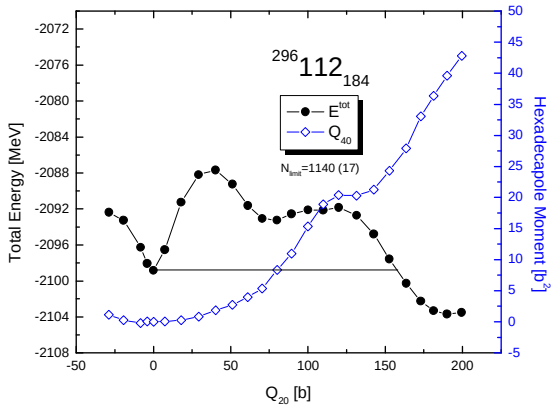
Total Energy [MeV]
$Q_{20}$ [b]


$^{294}Ds_{184}$
$E^{tot}$
$Q_{40}$
$N_{limit}$=1140 (17)
Total Energy [MeV]
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{296}112_{184}$
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Hexadecapole Moment [b$^2$]
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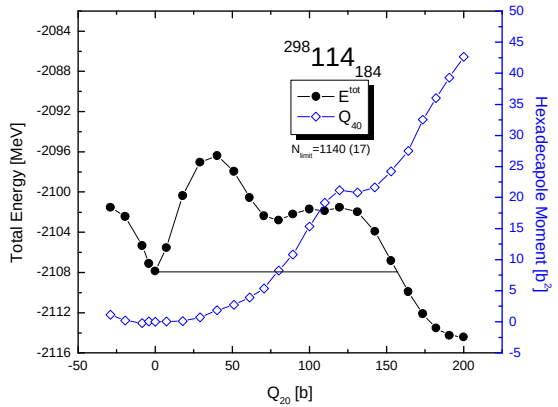
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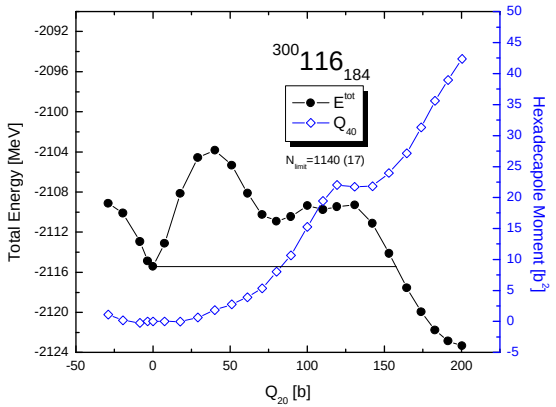
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{300}116_{184}$
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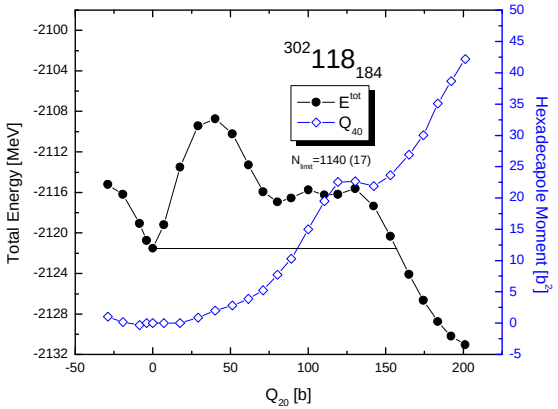
Total Energy [MeV]
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]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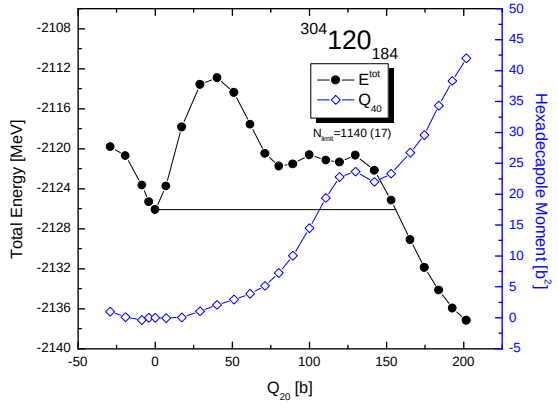
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{304}120_{184}$
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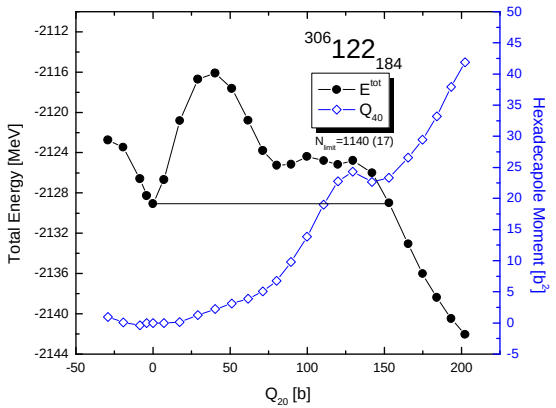
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{306}122_{184}$
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Hexadecapole Moment [b$^2$]
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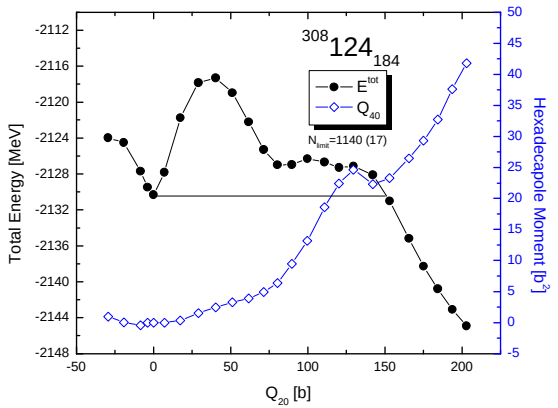
$^{308}124_{184}$
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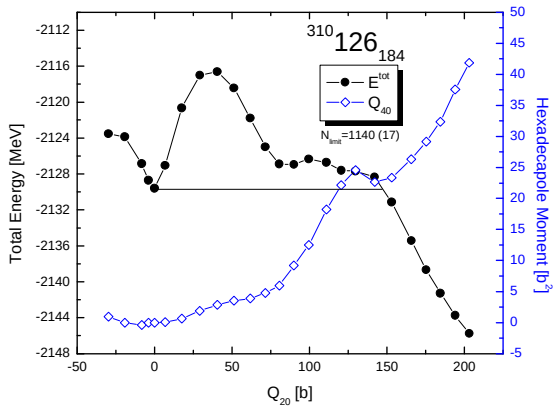
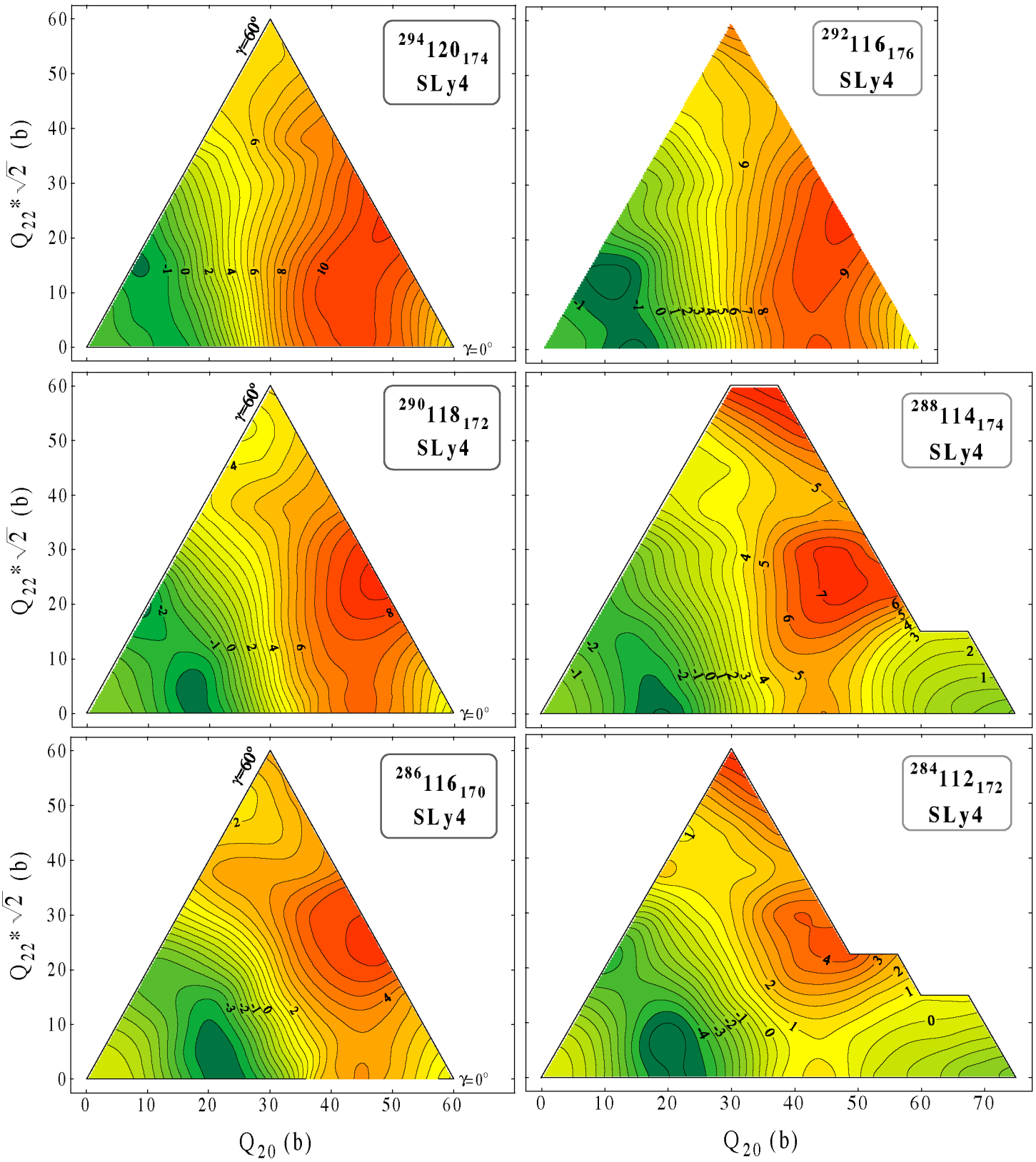
Total Energy [MeV]
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{310}126_{184}$
$E^{tot}$
$Q_{40}$
$N_{limit}$=1140 (17)
Total Energy [MeV]
Hexadecapole Moment [b$^2$]
$Q_{20}$ [b]


$^{294}120_{174}$ SLy4
$^{292}116_{176}$ SLy4
$^{290}118_{172}$ SLy4
$^{288}114_{174}$ SLy4
$^{286}116_{170}$ SLy4
$^{284}112_{172}$ SLy4
γ=60°
γ=0°
$Q_{22}*\sqrt{2}$ (b)
$Q_{20}$ (b)

S. Cwiok, P.H. Heenen, W. Nazarewicz