北京大學
PEKING UNIVERSITY

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Emergence of high-order deformation in atomic nuclei

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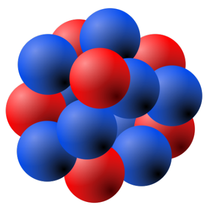
Outline

- High-order deformation parameters
- Non-axial octupole deformation
- High-order deformation in superheavy nuclei
- Summary

Nuclear deformation



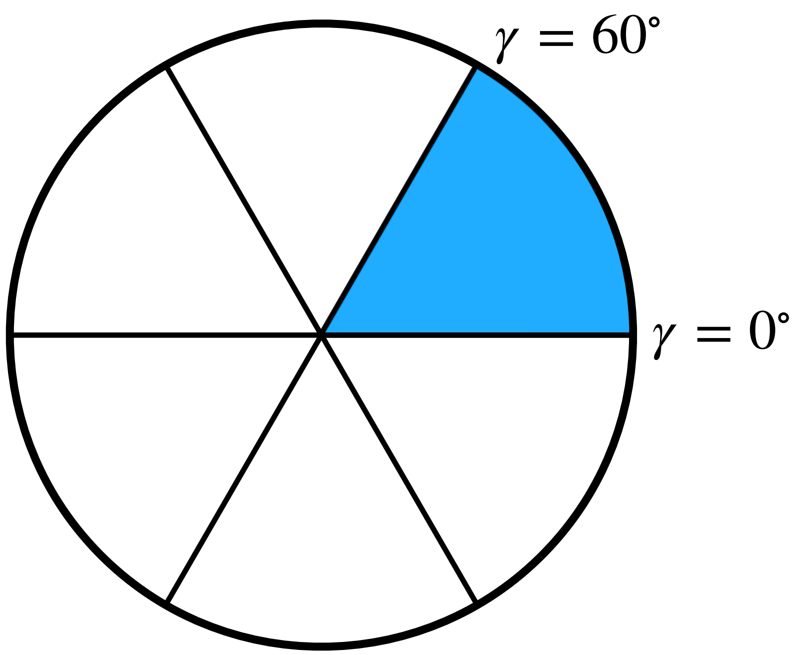
Nuclear shape: $R(\theta,\varphi) = R_0\left[1 + \sum_{\lambda=1}^{\infty}\sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu} Y^*_{\lambda\mu}(\theta,\varphi)\right]$

Quadrupole deformation

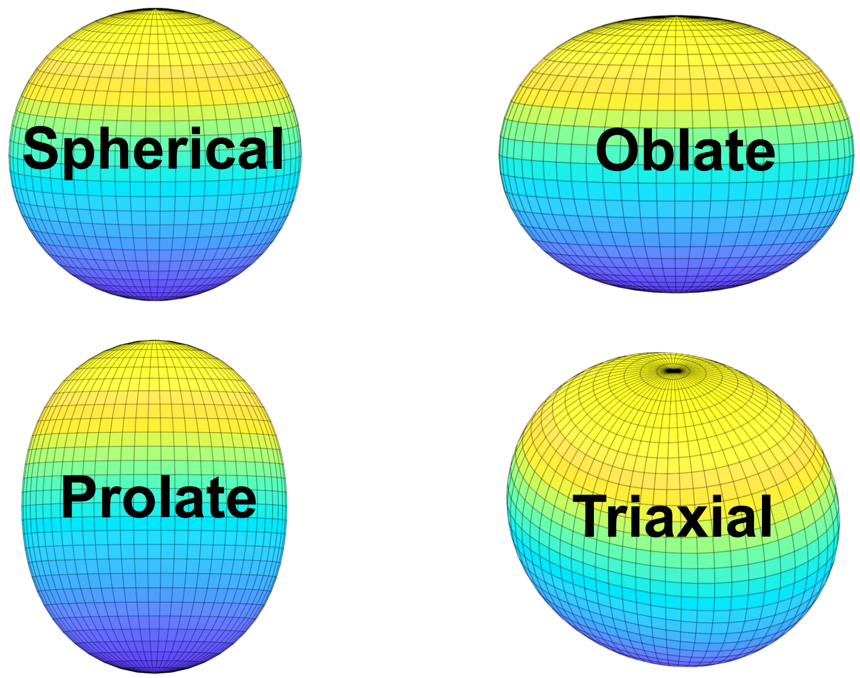
$$R(\theta,\varphi) = R_0\left[1 + \sum_{\mu=-2}^{2} \alpha_{2\mu} Y^*_{2\mu}(\theta,\varphi)\right]$$

5 - 3 = 2

Deformation parameters β and γ, defined in the **intrinsic frame**, which diagonalizes the inertia tensor.



uniquely covers all possible quadrupole shapes



Nuclear octupole deformation

Octupole deformation

$$R(\theta,\varphi) = R_0 \left[1 + \sum_{\mu=-3}^{3} \alpha_{3\mu} Y^*_{3\mu}(\theta,\varphi) \right]$$

7 - 3 = 4

Deformation parameters,
defined in the **intrinsic frame**,
which cannot be uniquely determined.

- Parametrized with the irreducible representations of the O_h group

$$R = R_0 \left[1 + \varepsilon_0 A_2 + \sum_{i=1}^{3} \varepsilon_1(i) F_1(i) + \sum_{i=1}^{3} \varepsilon_2(i) F_2(i) \right]$$

Hamamoto, Zhang, Xie, PLB 257, 1 (1991).

- The intrinsic frame can be defined by fixing $\varepsilon_2(i) = 0, \quad i = 1, 2, 3$

A certain Euler rotation between the intrinsic and laboratory frame is defined.

- The remain **4** parameters $\varepsilon_0,\ \varepsilon_1(i)$ are used to describe the octupole shapes.

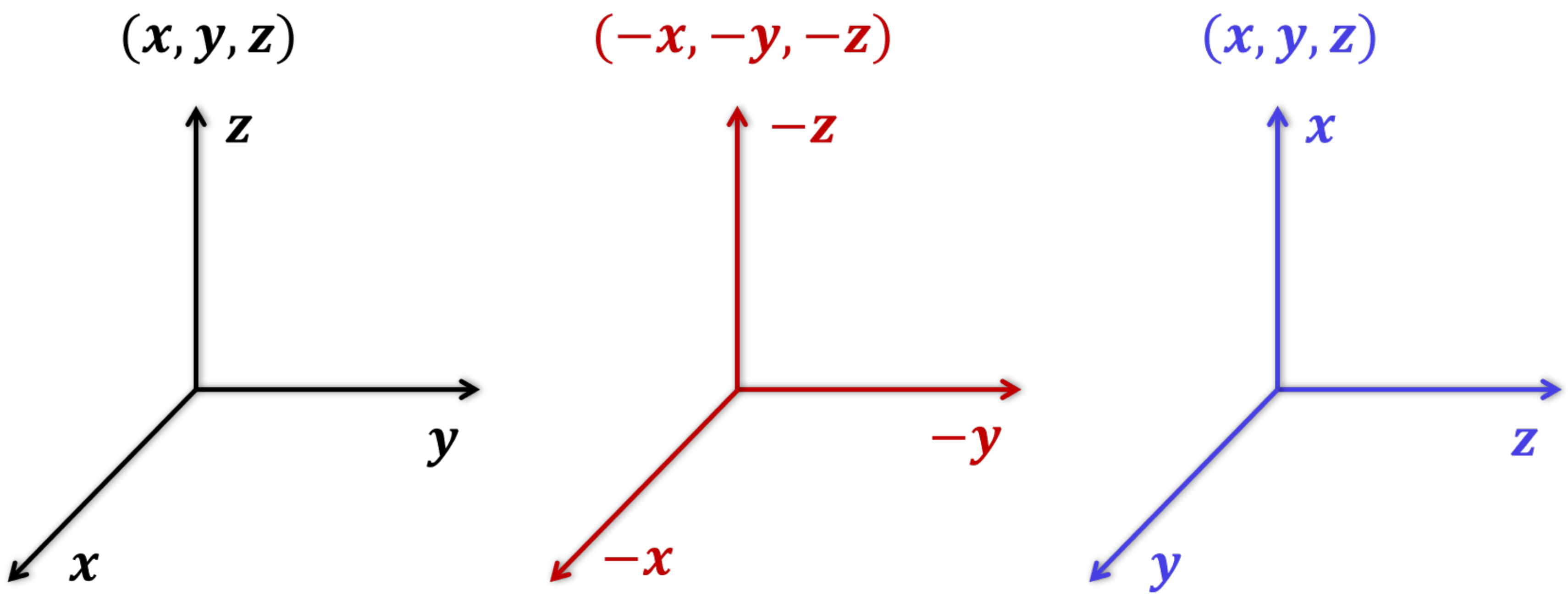
How about the range of these parameters ?

The range of octupole deformation parameters

- Restrict the range to uniquely cover all possible shapes without repeat.
- An intrinsic shape should be unchanged under the 48 transformations of coordinate system, i.e., the 48 elements of the O_h $[D_{2h} \otimes S_3]$ group.

D_{2h}: Change the signs of the x, y, and z axes → **8**

S_3: Change the names of the x, y, and z axes → **6**



Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024).

The range of the four parameters: $\varepsilon_0 \geq 0, \quad \varepsilon_1(1) \geq \varepsilon_1(2) \geq \varepsilon_1(3) \geq 0$

Definition of octupole deformation parameters

- Four octupole deformation parameters can be obtained by

$$a_{32} = \epsilon_0 = \frac{4\pi}{3AR^3} \int \mathrm{d}^3 r \rho_v(\boldsymbol{r}) r^3 A_2,$$

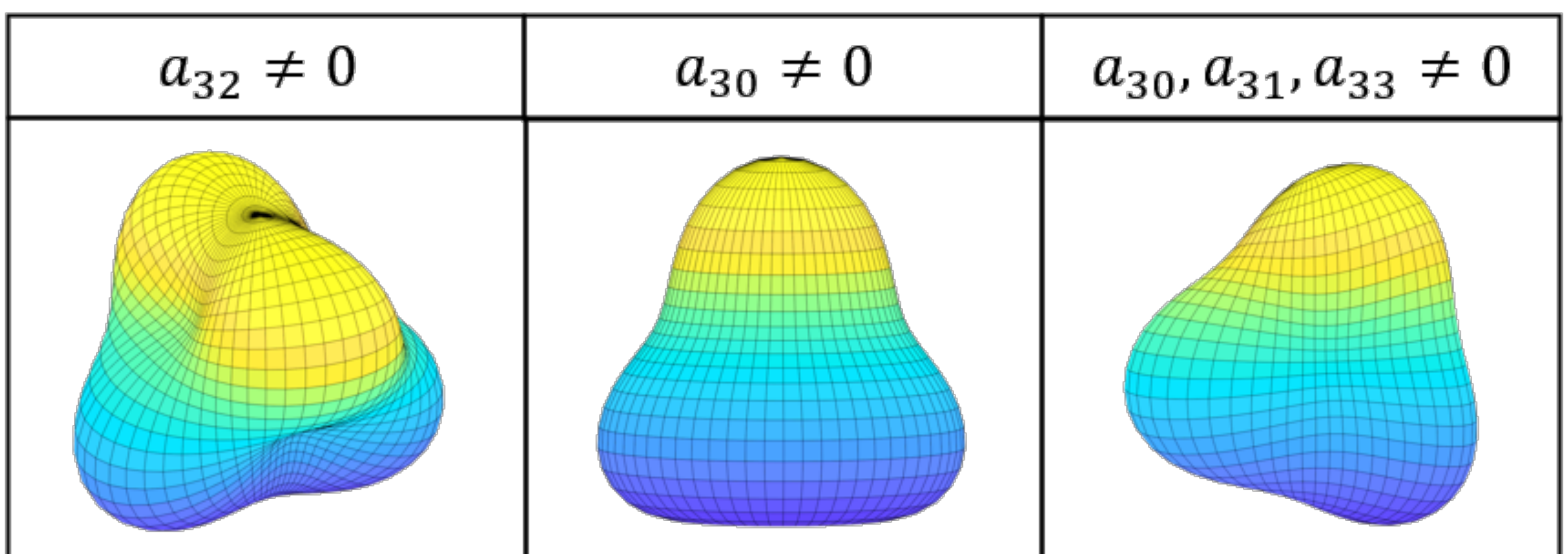
$$a_{30} = \epsilon_1(1) = \frac{4\pi}{3AR^3} \int \mathrm{d}^3 r \rho_v(\boldsymbol{r}) r^3 F_1(1),$$

$$a_{31} = \epsilon_1(2) = \frac{4\pi}{3AR^3} \int \mathrm{d}^3 r \rho_v(\boldsymbol{r}) r^3 F_1(2),$$

$$a_{33} = \epsilon_1(3) = \frac{4\pi}{3AR^3} \int \mathrm{d}^3 r \rho_v(\boldsymbol{r}) r^3 F_1(3).$$

$a_{32} \geq 0,\ a_{30} \geq a_{31} \geq a_{33} \geq 0.$

Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024).



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- High-order deformation in superheavy nuclei
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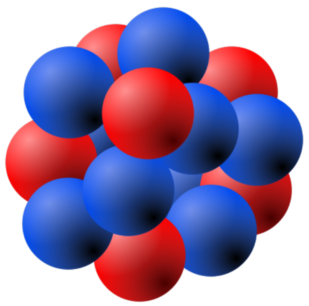
Relativistic nuclear many-body problem



Schrödinger Equation

$$H|\psi\rangle = (T+V)|\psi\rangle$$

Relativistic QFT

$$L = L_N + L_\sigma + L_\omega + L_{\text{int}}$$

Walecka, Ann. Phys., 83, 491 (1974)

Mean-field approximation

A Theory of Highly Condensed Matter*

J. D. WALECKA

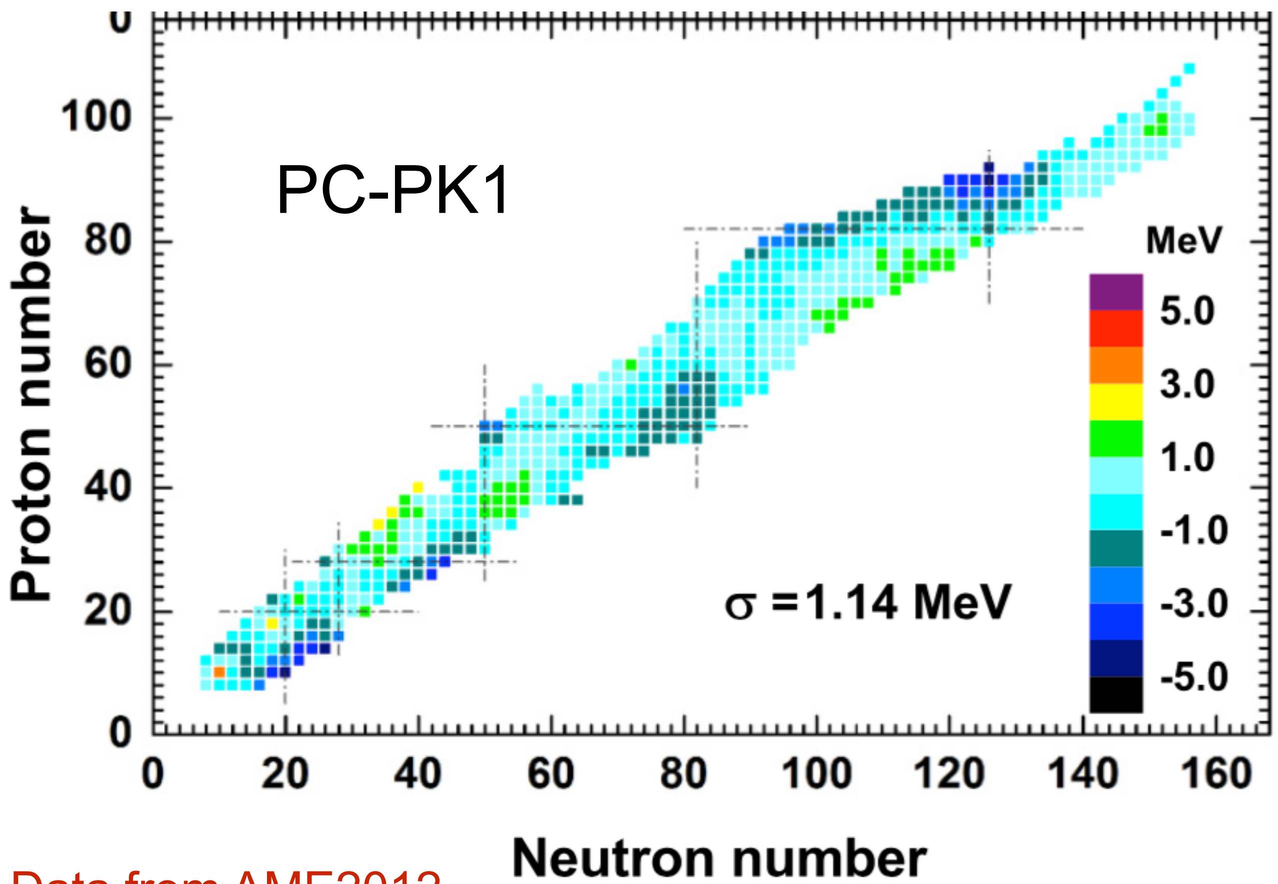
Institute of Theoretical Physics, Department of Physics, Stanford University, Stanford, California 94305

1. Mean-field approximation works surprisingly good !
2. Large mean fields *S ≈ -400 MeV, V ≈ 350 MeV*
3. Large spin-orbit splitting *predicts nuclear shell model, no adjustments to spin-orbit force*
4. Relativistic Saturation *non-relativistic calculations lead to a collapse*

A covariant formulation provides an efficient and comprehensive explanation of observed bulk and single-particle systematics.

Covariant density functional：PC-PK1

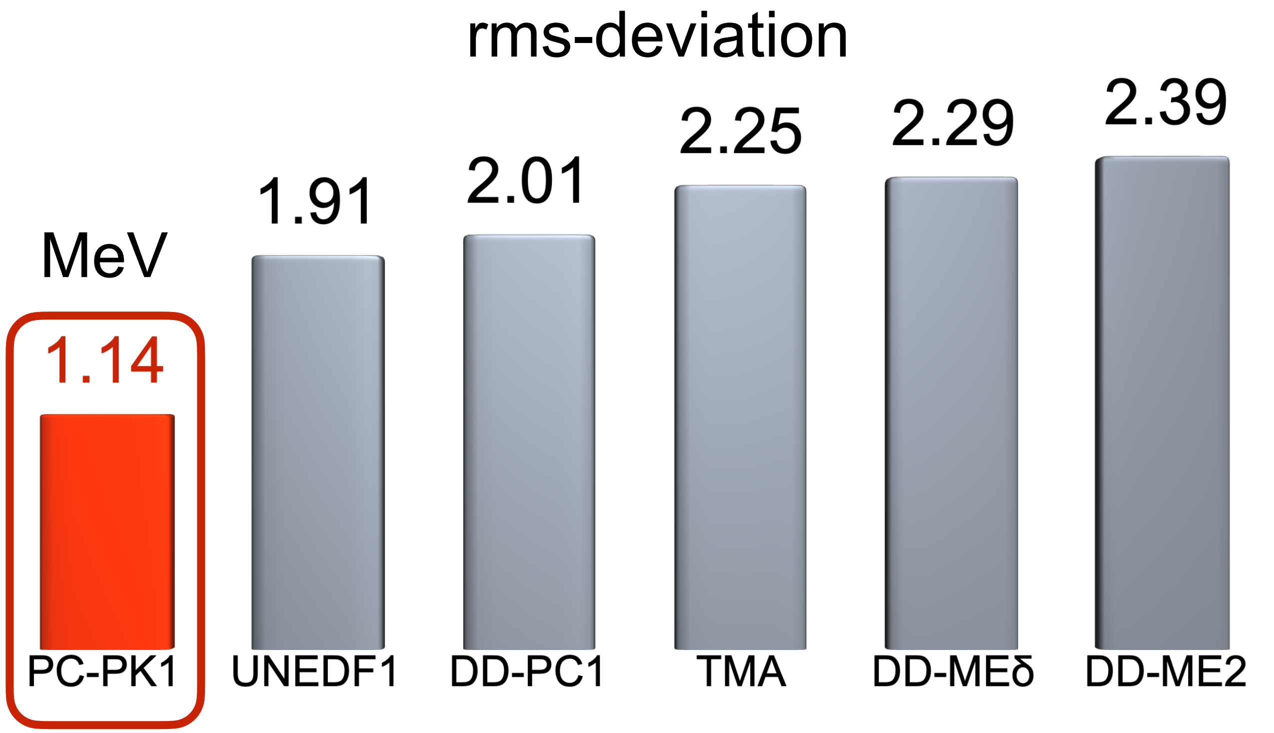
Mass Differences: M_{cal} - M_{exp}



Data from AME2012

PWZ, Li, Yao, Meng, PRC 82, 054319 (2010)

Lu, Li, Li, Yao, Meng, PRC 91, 027304 (2015)



http://nuclearmap.jcnp.org

Yang, Wang, PWZ, Li, PRC 104, 054312 (2021)

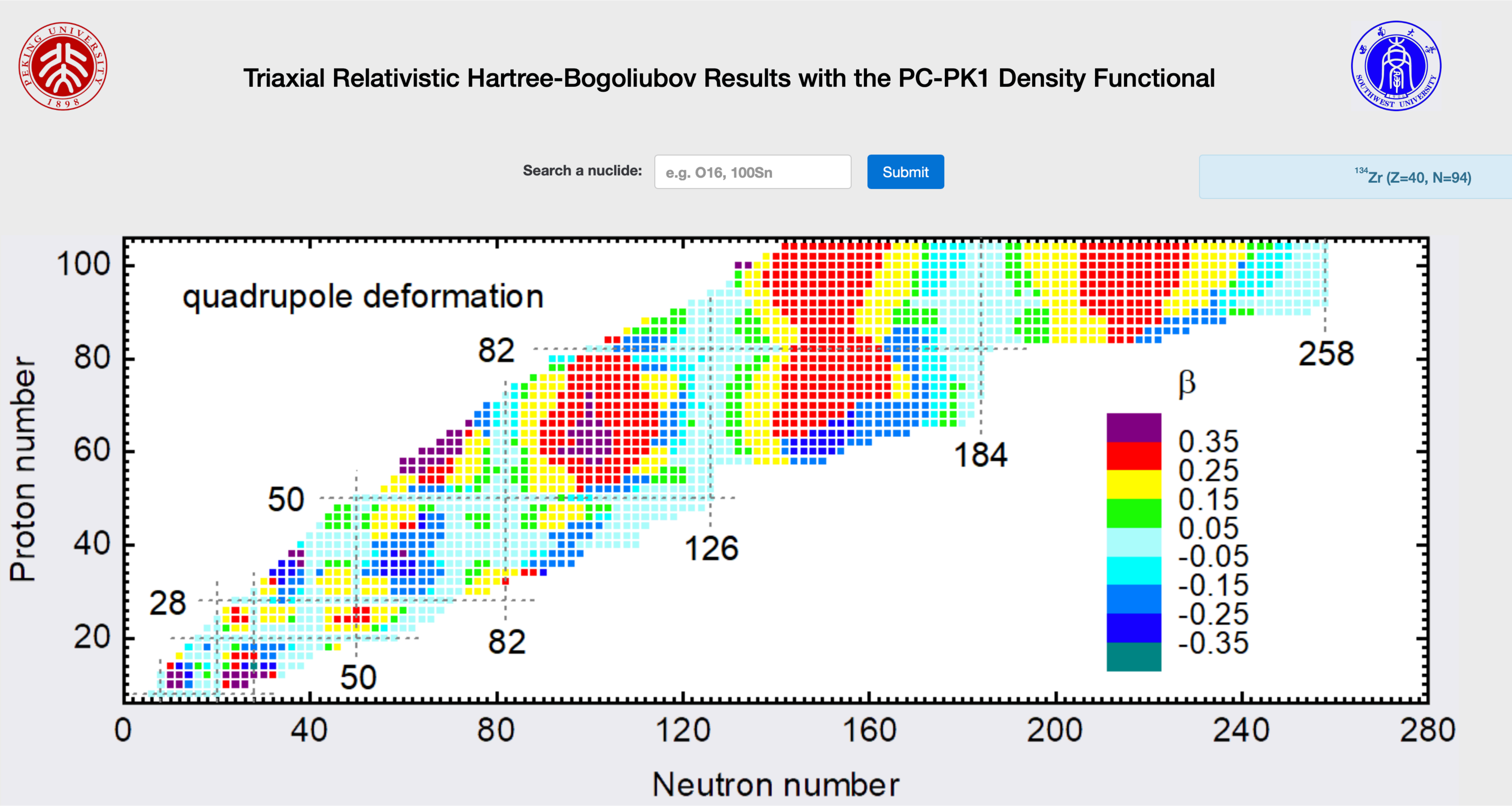
Yang, PWZ, Li, PRC 107, 024308 (2023)

Among the best density-functional description for nuclear masses!

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH



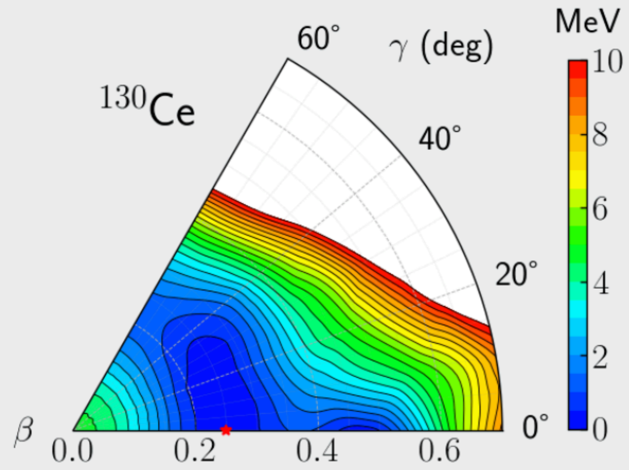
Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH

Results for Cerium 130 (Z=58, N=72)



Potential energy surface calculated by RHB theory with PC-PK1 density functional. All energies are normalized with respect to the binding energy of the absolute minimum. The contours join points on the surface with the same energy, and the energy difference between adjacent contours is 0.5 MeV.

Ground-state properties

Spectroscopy (coming soon)

E_{RHB} = -1079.46 MeV

E_{5DCH} = -1083.50 MeV

E_{exp} = -1083.32 MeV

β = 0.25

γ = 0°

To know the meaning of a quantity, please hold the mouse still on it.

Select a nuclide

Proton number

0

Neutron number

0

Submit

^{132}Nd

^{128}Ce ← → ^{132}Ce

^{128}Ba

Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

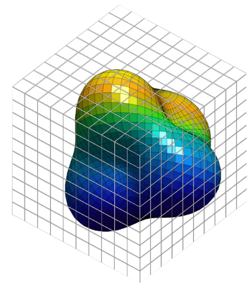
Lattice CDFT

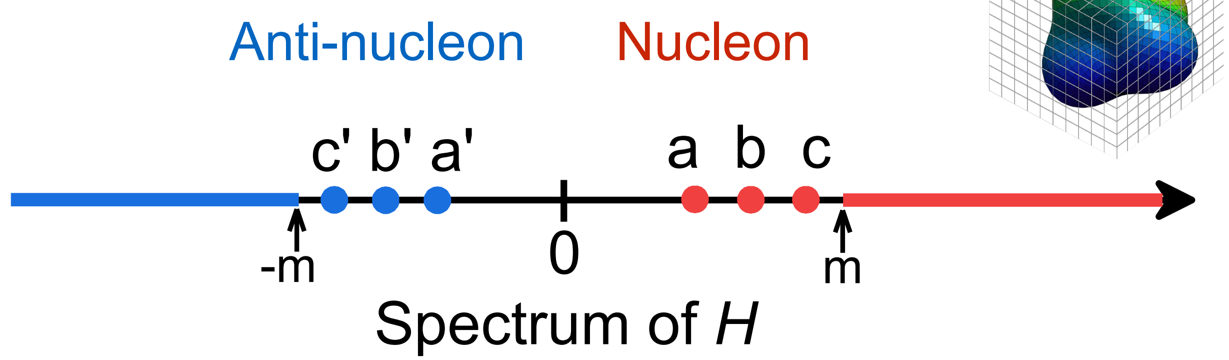
✓ No spatial symmetry restriction

✓ A long-term challenge due to

a) variational collapse problem

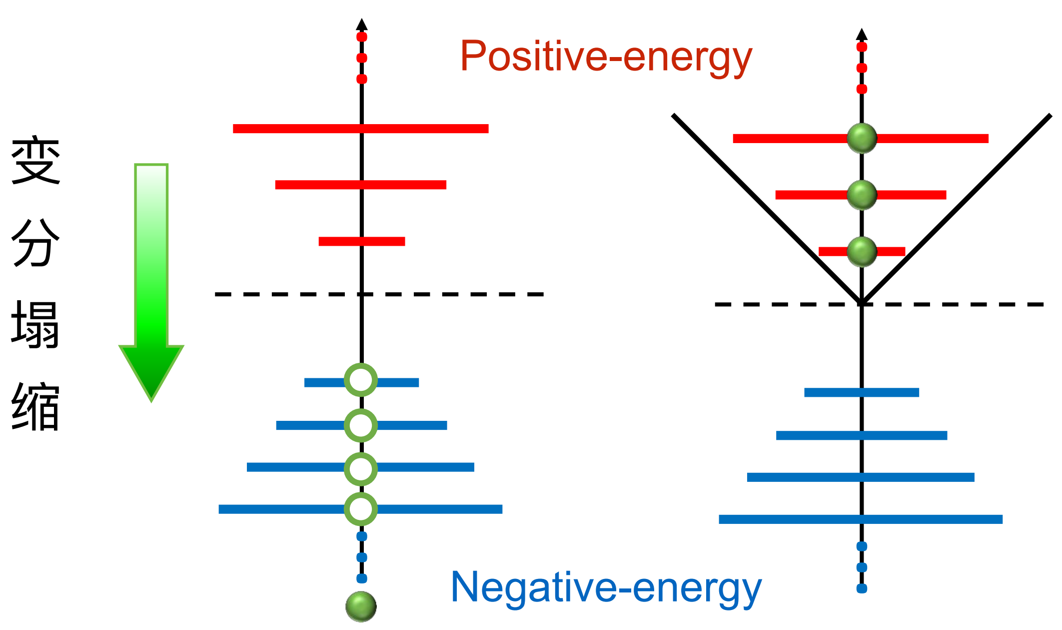
b) fermion doubling problem





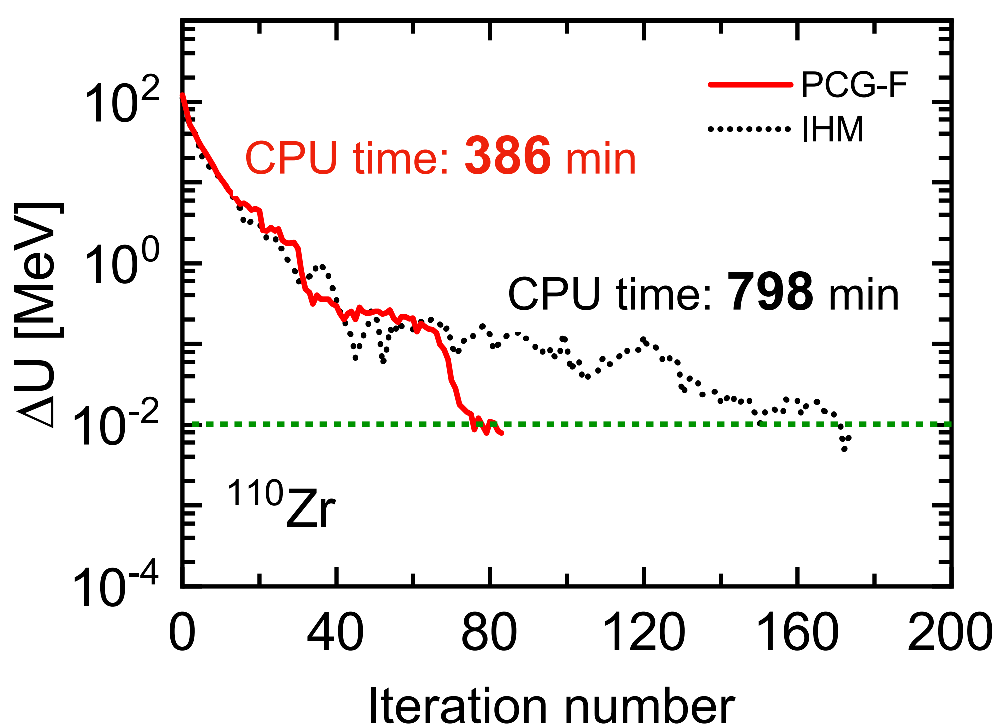
Hagino and Tanimura, PRC 82, 057301 (2010)

PCG-F Method



Li, Ren, PWZ, PRC 102, 044307 (2020)

PCG-F saves **~52%** of the CPU time



Xu, Li, Ren, PWZ, PRC 109, 014311 (2024)

Tetrahedral shape

The tetrahedral shape with a pure Y_{32}-type deformation is of particular interest and has been investigated extensively.

- Macroscopic-microscopic (MM) model

  Li and Dudek, PRC 49, 1250(R) (1994)
  Dudek, et al., PRL 88, 252502 (2002)
  Dudek, et al., PRL 97, 072501 (2006)

- Algebraic cluster model

  Bijker and Iachello, PRL 112, 152501 (2014)

- Lattice EFT

  Epelbaum, Krebs, Lähde, Lee, Meißner, Rupak, PRL 112, 102501 (2014)

- Non-relativistic density functional theories (DFTs)

  Schunck, Dudek, Góźdź, Regan, PRC 69, 061305(R) (2004)
  Zberecki, Magierski, Heenen, Schunck, PRC 74, 051302(R) (2006)
  Tagami, Shimizu, Dudek, PRC 87, 054306 (2013)
  Miyahara, Nakada, PRC 98, 064318 (2018)

- Covariant density functional theories (CDFTs)

  Zhao, Lu, Zhao, Zhou, PRC 95, 014320 (2017)
  Rong, Wu, Lu, Yao, PLB 840, 137896 (2023)

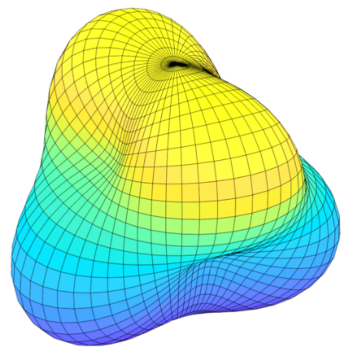
V_4 symmetry/partial shape space assumed in DFT calculations …

Potential energy surface (PES)

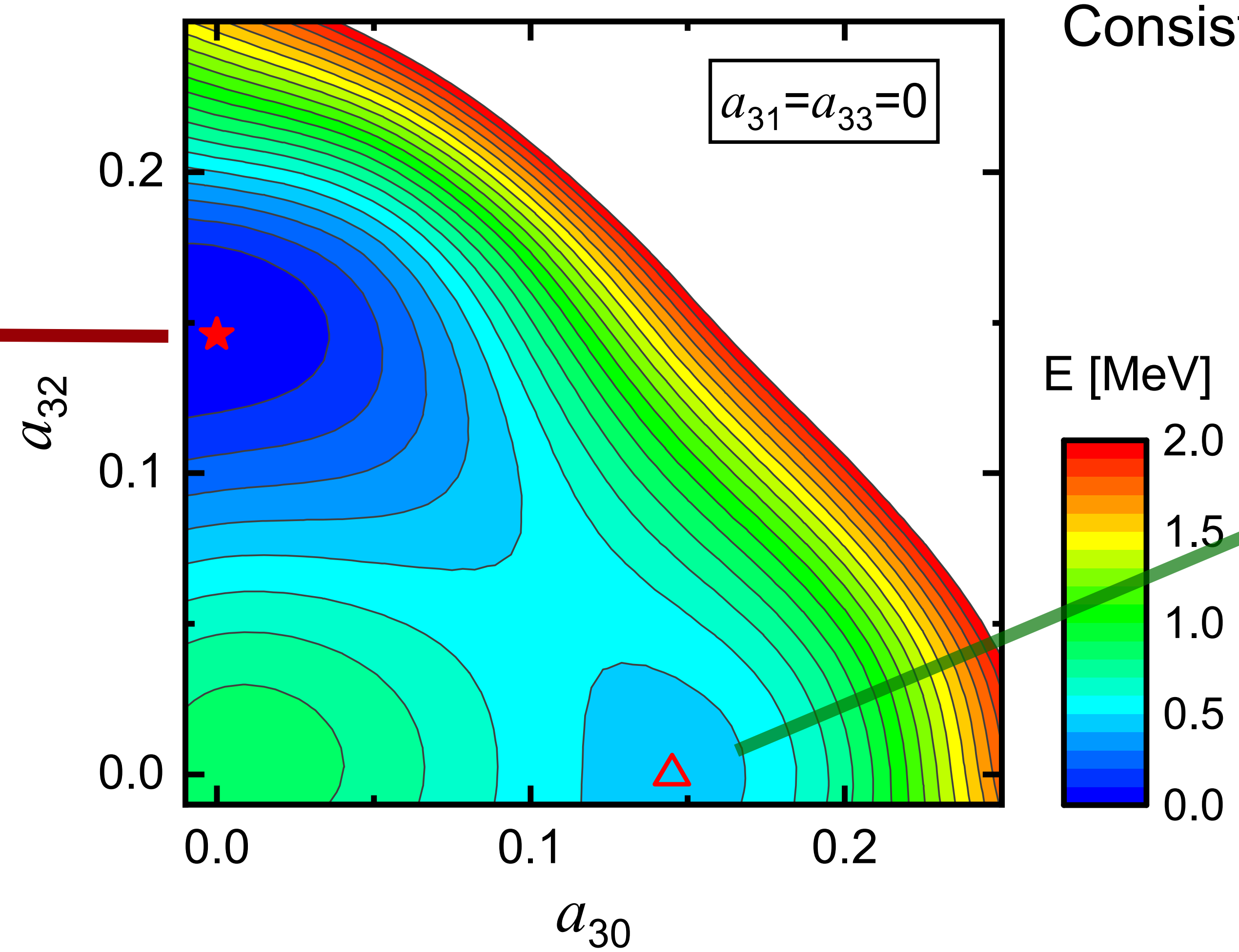
^{110}Zr

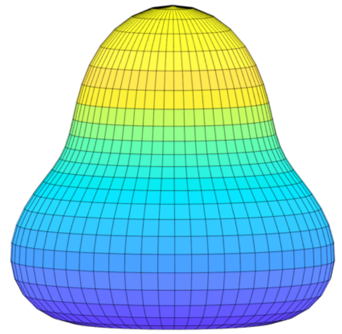
Lattice CDFT calculations with V_4 symmetry

Consistent with the MDC-RHB results
PRC 95, 014320 (2017)



Tetrahedral ground state



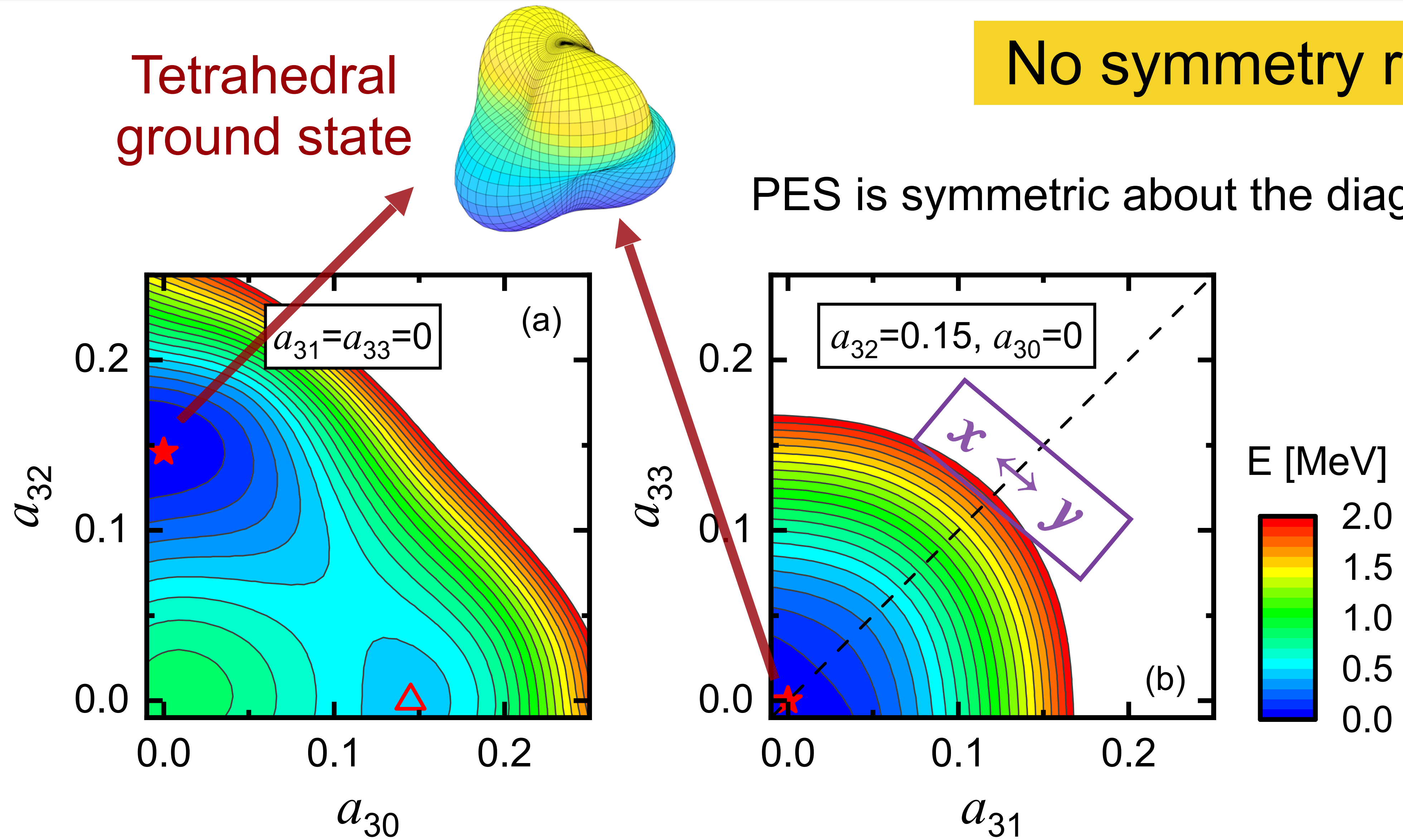


Pear-like isomeric state

Energy minimum	a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
Ground state	0.00	0.00	0.15	0.00	-902.49
Isomeric state	0.15	0.00	0.00	0.00	-902.02

Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024)

The tetrahedral ground state

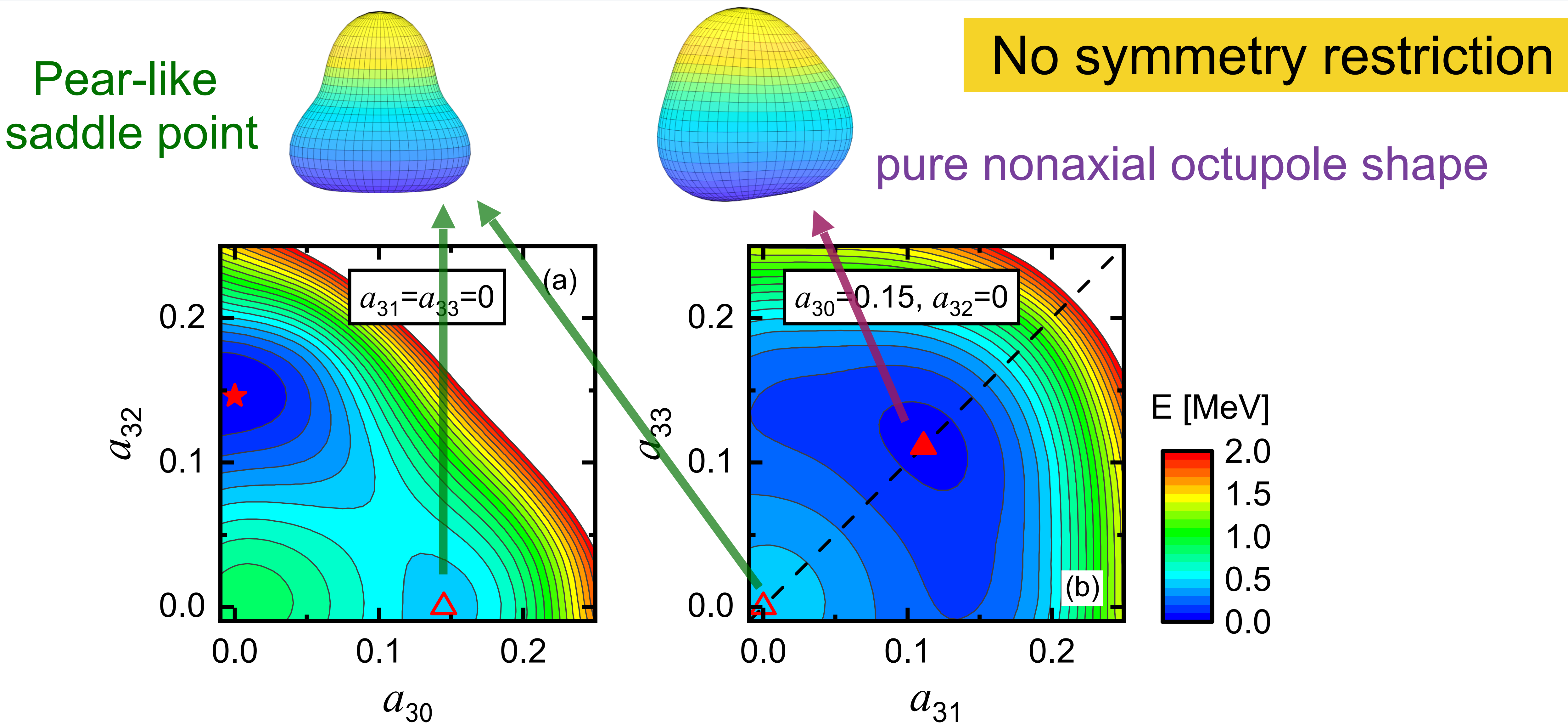


Energy minimum	a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
Ground state	0.00	0.00	0.15	0.00	-902.49

Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024)

The ground state of ^{110}Zr has a tetrahedral shape.

Nonaxial octupole isometric state



Energy minimum	a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
Ground state	0.00	0.00	0.15	0.00	-902.49
Isomeric state	0.15	0.11	0.00	0.11	-902.42

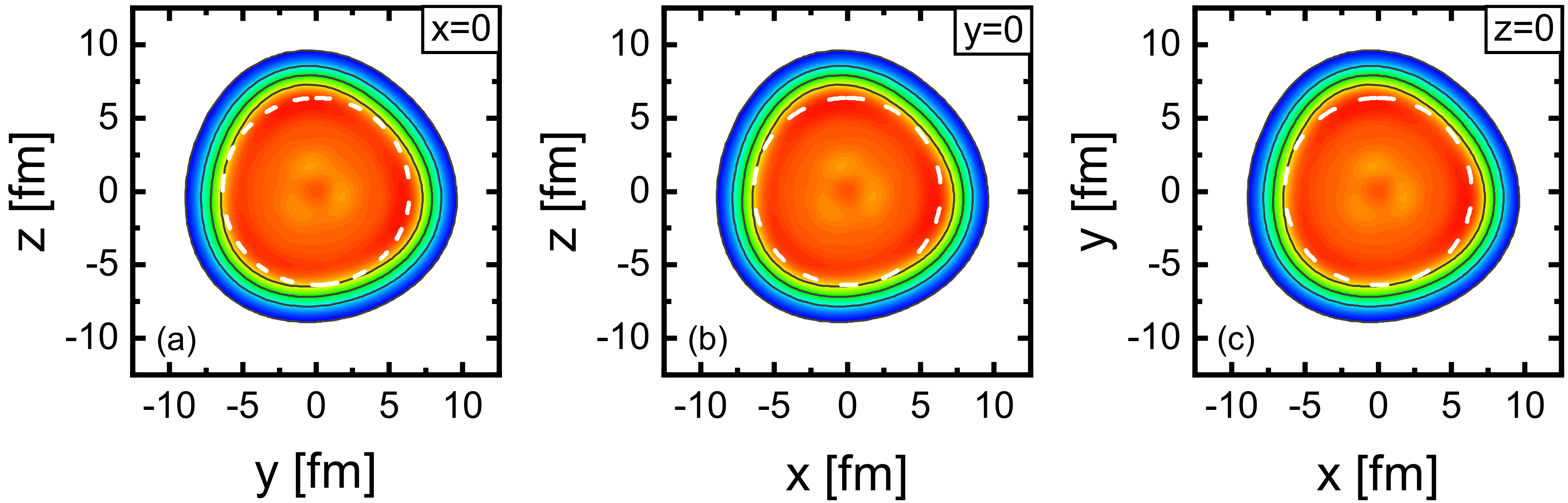
Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024)

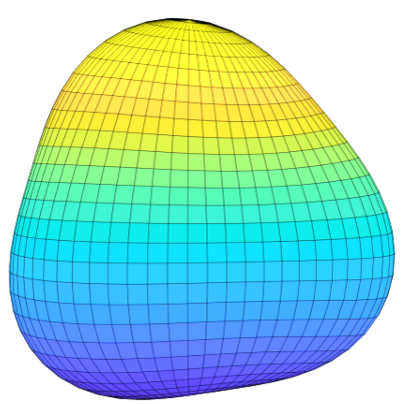
The isomeric state of ^{110}Zr has a pure non-axial octupole shape.

Y_{31} and Y_{33} deformations

^{286}No Ground-state density profiles

No symmetry restriction





a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
0.07	0.07	0.01	0.07	-2046.65

Xu, Li, Ring, **PWZ**, In preparation

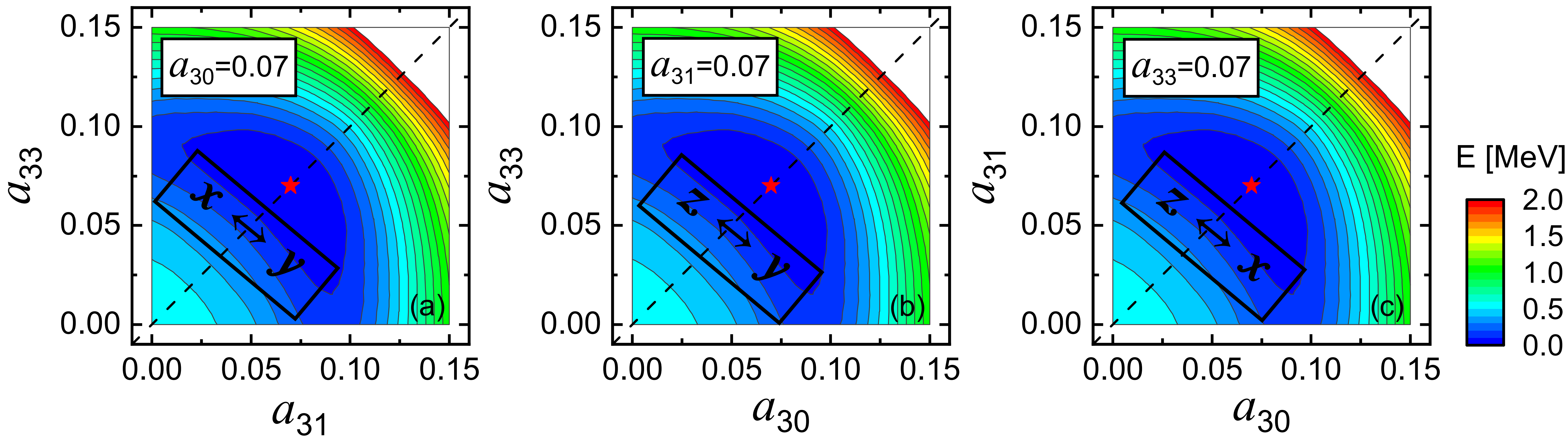
The ground state of ^{286}No has a pure non-axial octupole shape.

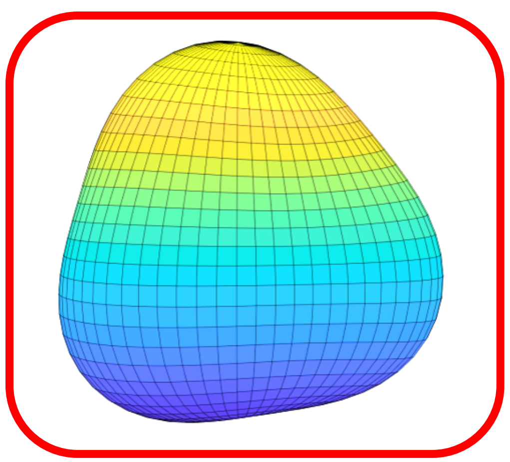
Softness of the ground state

^{286}No

No symmetry restriction

PES is symmetric about the diagonal.





a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
0.07	0.07	0.01	0.07	-2046.65

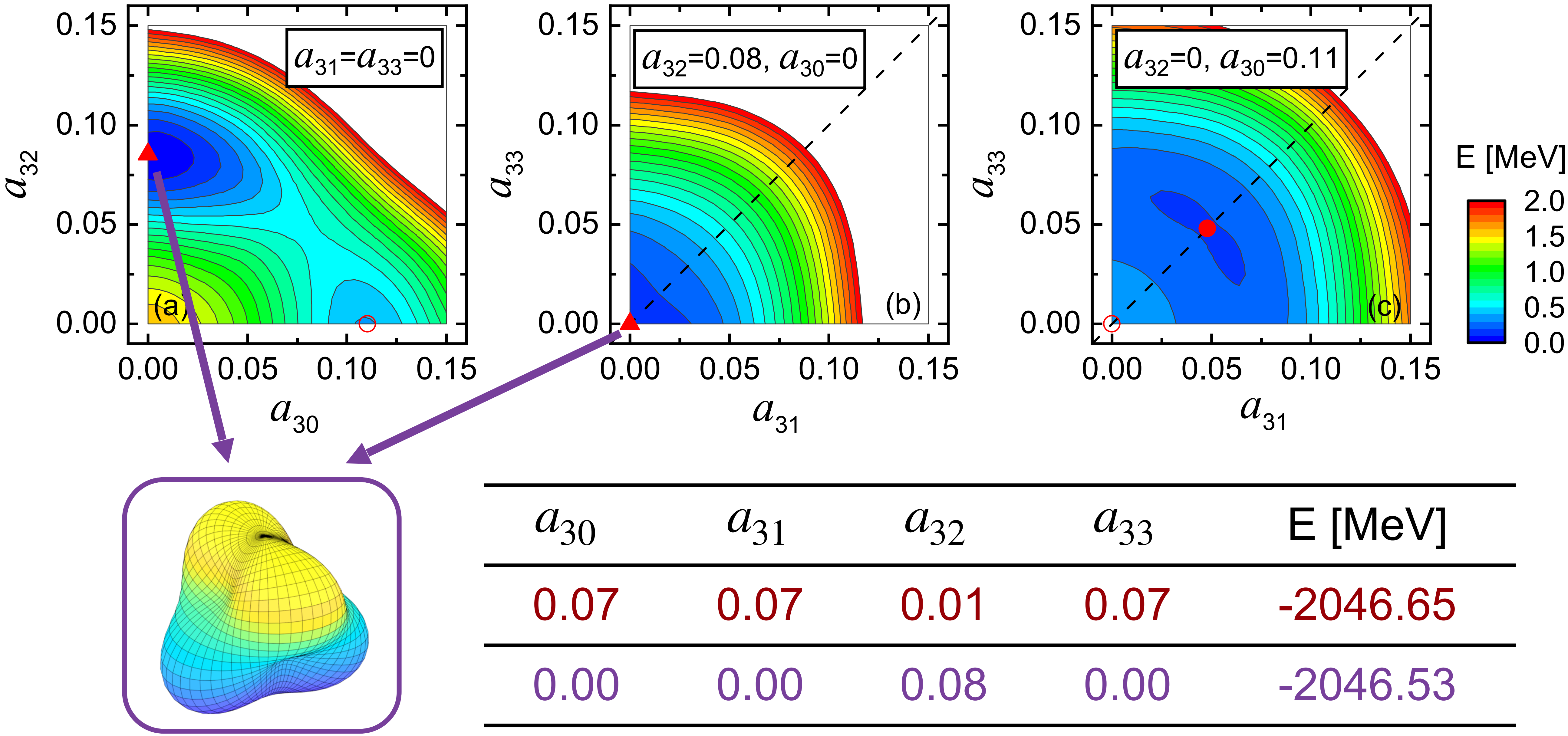
Xu, Li, Ring, **PWZ**, In preparation.

The ground state of ^{286}No is soft in the octupole directions.

Potential energy surface for ^{286}No

^{286}No

Lattice-CDFT results



a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
0.07	0.07	0.01	0.07	-2046.65
0.00	0.00	0.08	0.00	-2046.53

Xu, Li, Ring, **PWZ**, In preparation.

The isomeric state of ^{286}No has a tetrahedral shape.

Outline

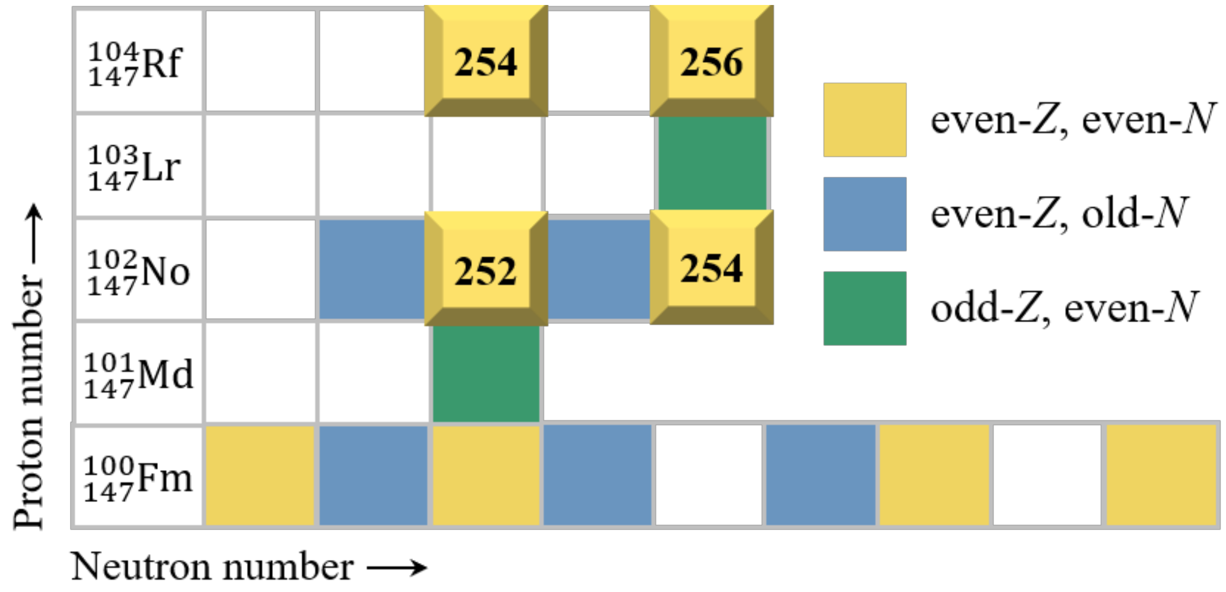
- High-order deformation parameters
- Non-axial octupole deformation
- High-order deformation in superheavy nuclei
- Summary

Rotating transfermium nuclei

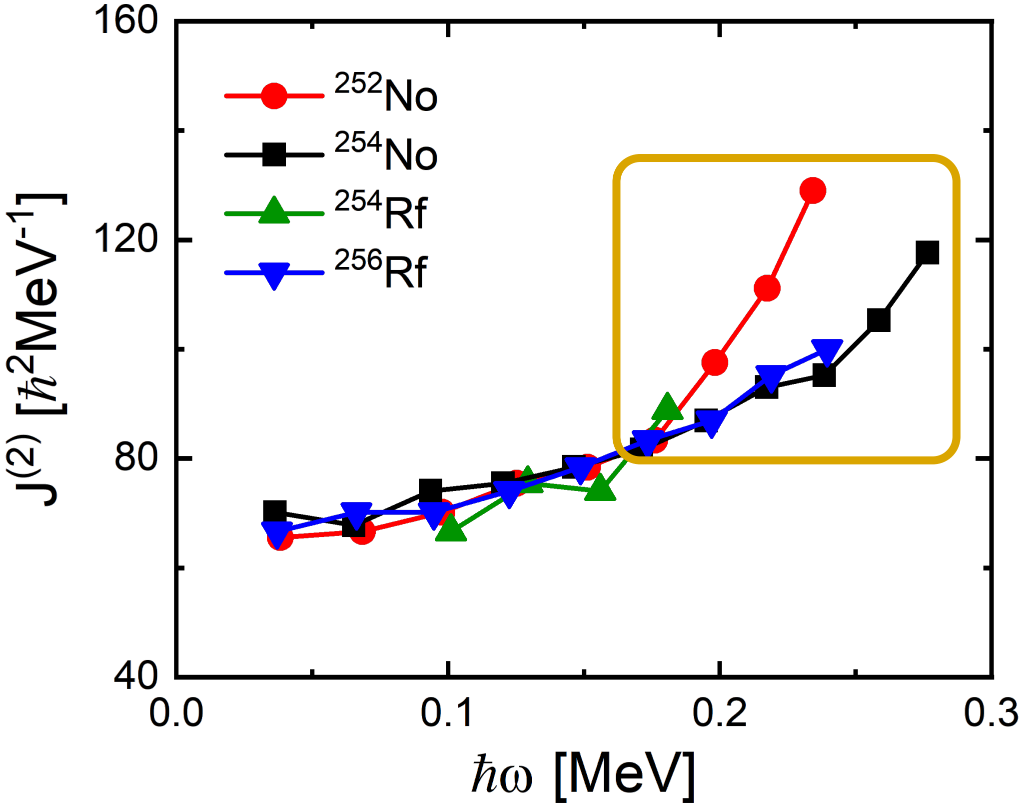
- Transfermium nuclei are the heaviest ones, whose rotational spectra have been measured experimentally.
- They are important for determining the location of the "island of stability".

Herzberg, Greenlees, Prog. Part. Nucl. Phys. 61, 674 (2008).
Ackermann, Theisen, Phys. Scr. 92, 083002 (2017).

ANL、FLNR、GANIL、GSI、JAEA、JYFL …



PRL 82, 509 (1999). PRL 85, 1198 (2000). PRL 89, 202501 (2002).
PRL 95, 102502 (2005). PRL 95, 032501 (2005).
PRL 97, 082502 (2006). PRL 98, 132503 (2007).
PRL 102, 212501 (2009). PRL 109, 102501 (2012).
…



PRL 82, 509 (1999). PRL 109, 102501 (2012).
PRC 65, 014303 (2001). PRC 107, L061302 (2023).

The physical mechanism of the rotational behavior in ^{252}No and ^{254}No?

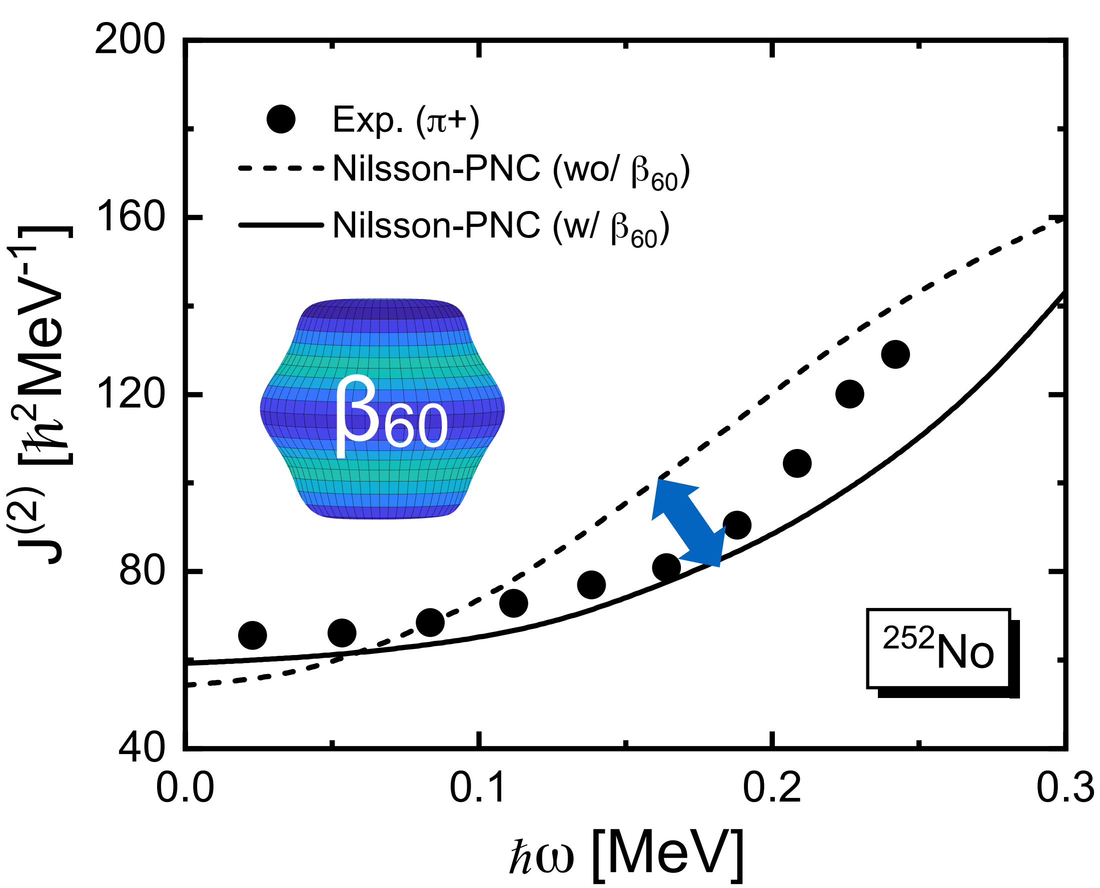
Theoretical investigations

- Theoretical studies on the rotational properties of ^{252}No and ^{254}No include:

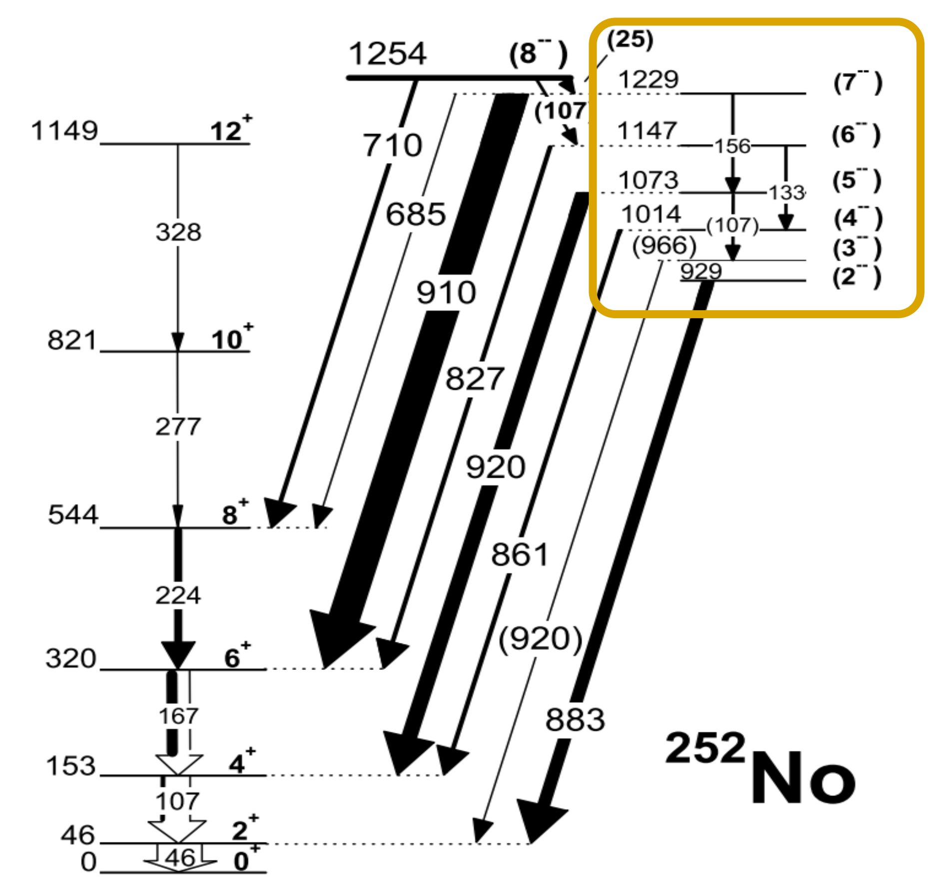
✓ Density functional theories
✓ Projected shell model
✓ Reflection asymmetric shell model
✓ Total Routhian surface (TRS) method
✓ PNC cranked shell model (PNC-CSM)
✓ …

Duguet NPA (2001); Sun PRC (2008); Chen PRC (2008); Liu PRC (2012); Zhang PRC (2013) …

- β_{60} deformation is considered to be reason for the upbending of the moments of inertia in ^{252}No, but the octupole deformation is ignored.



Zhang, Meng, Zhao, Zhou, Phys. Rev. C 87, 054308 (2013).



Sulignano, et al., Eur. Phys. J. A 33, 327 (2007).

Dynamic moments of inertia

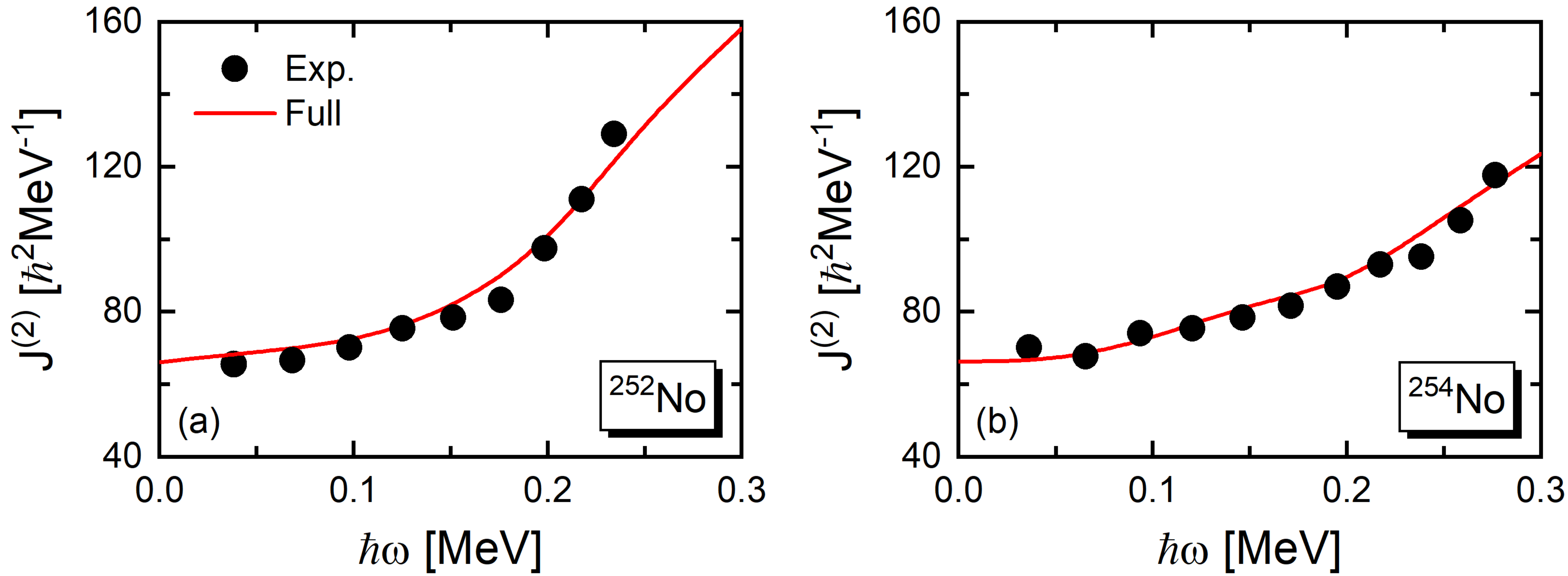
Cranking CDFT in 3D lattice with a shell-model-like approach (SLAP):

✓ self-consistent and microscopic description

✓ no adjustable parameter beyond a well-determined functional

✓ no spatial symmetry restriction

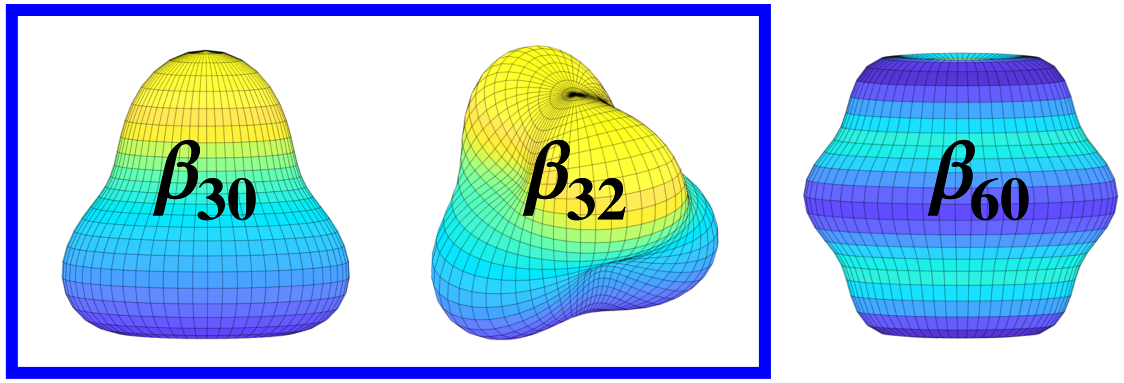
✓ pairing correlations is treated with particle number conservation

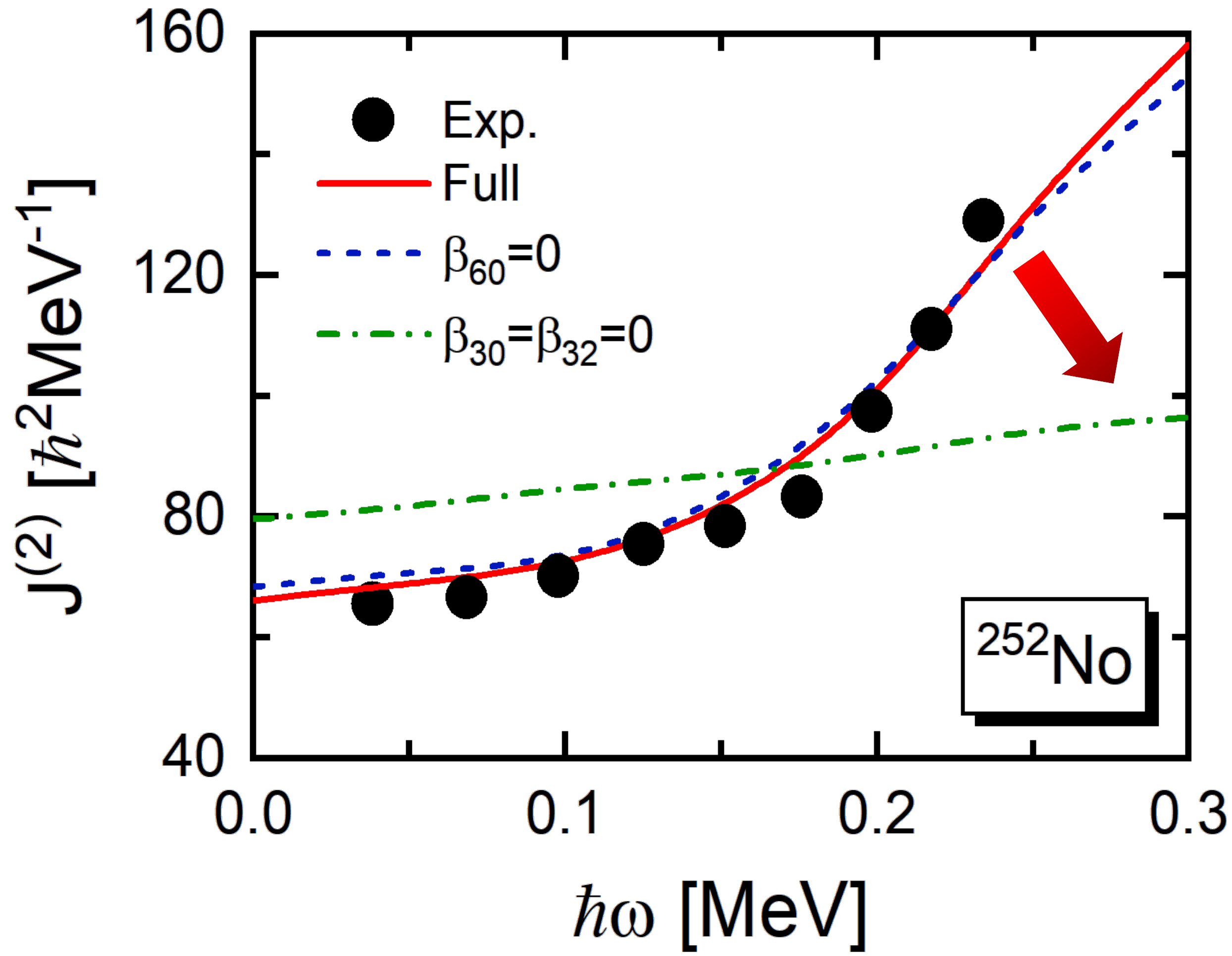


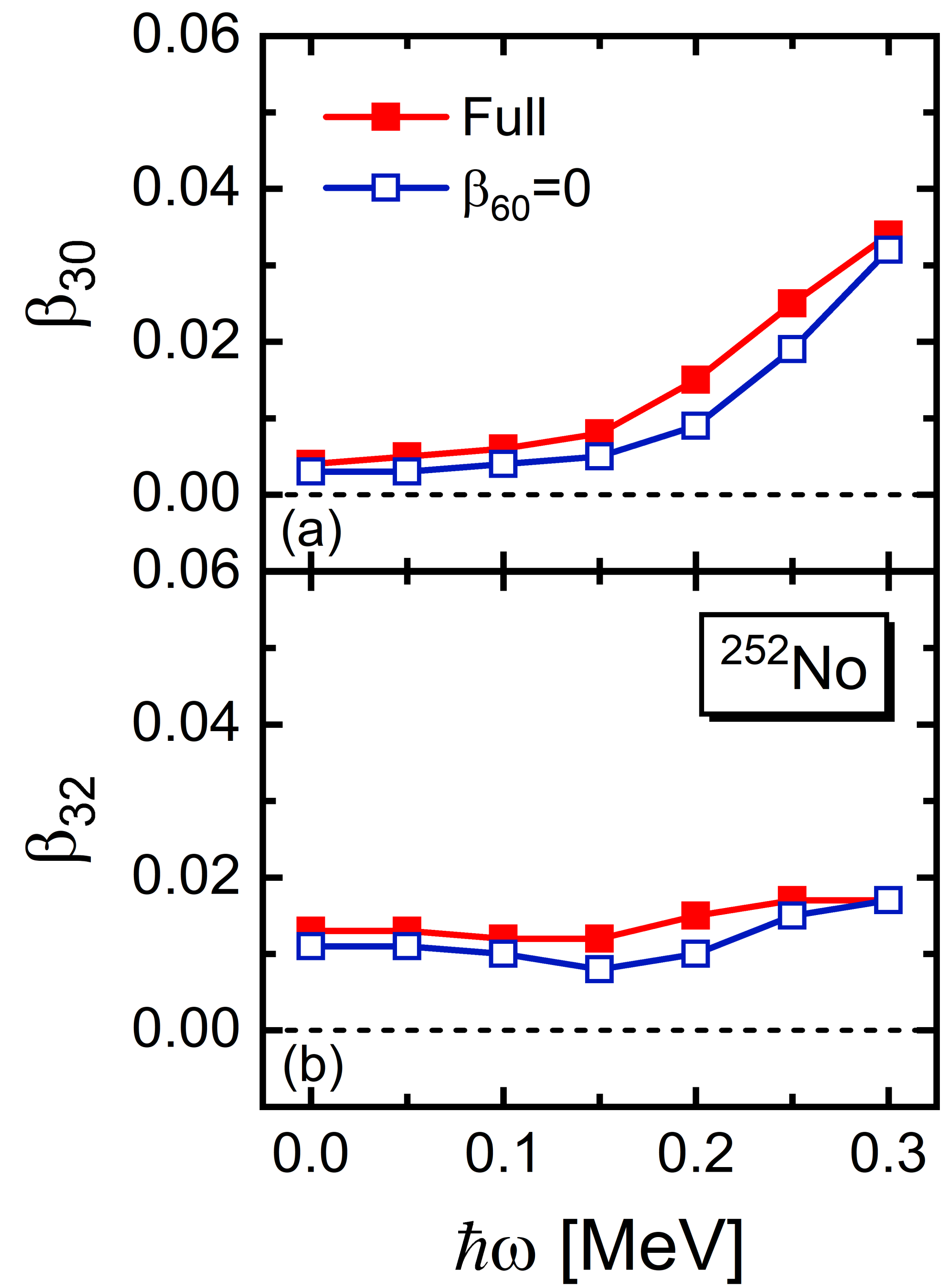
Xu, Wang, Wang, Ring, **PWZ**, Under review.

The experimental moments of inertia are well reproduced.

High-order deformation in ^{252}No



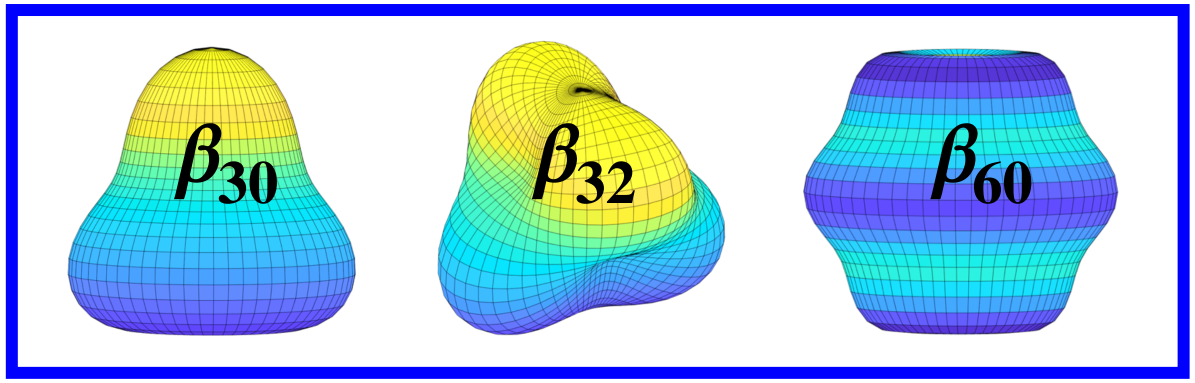


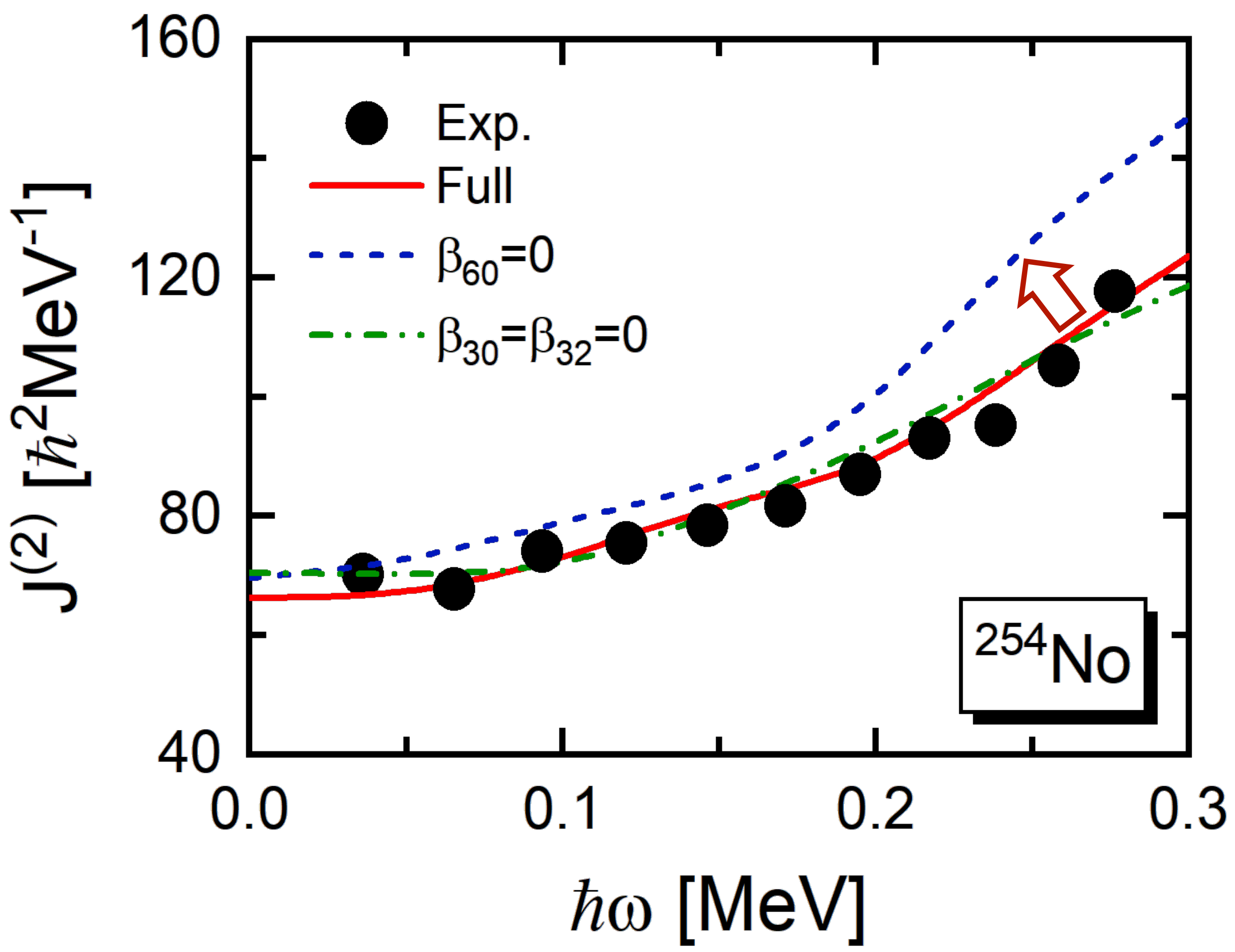


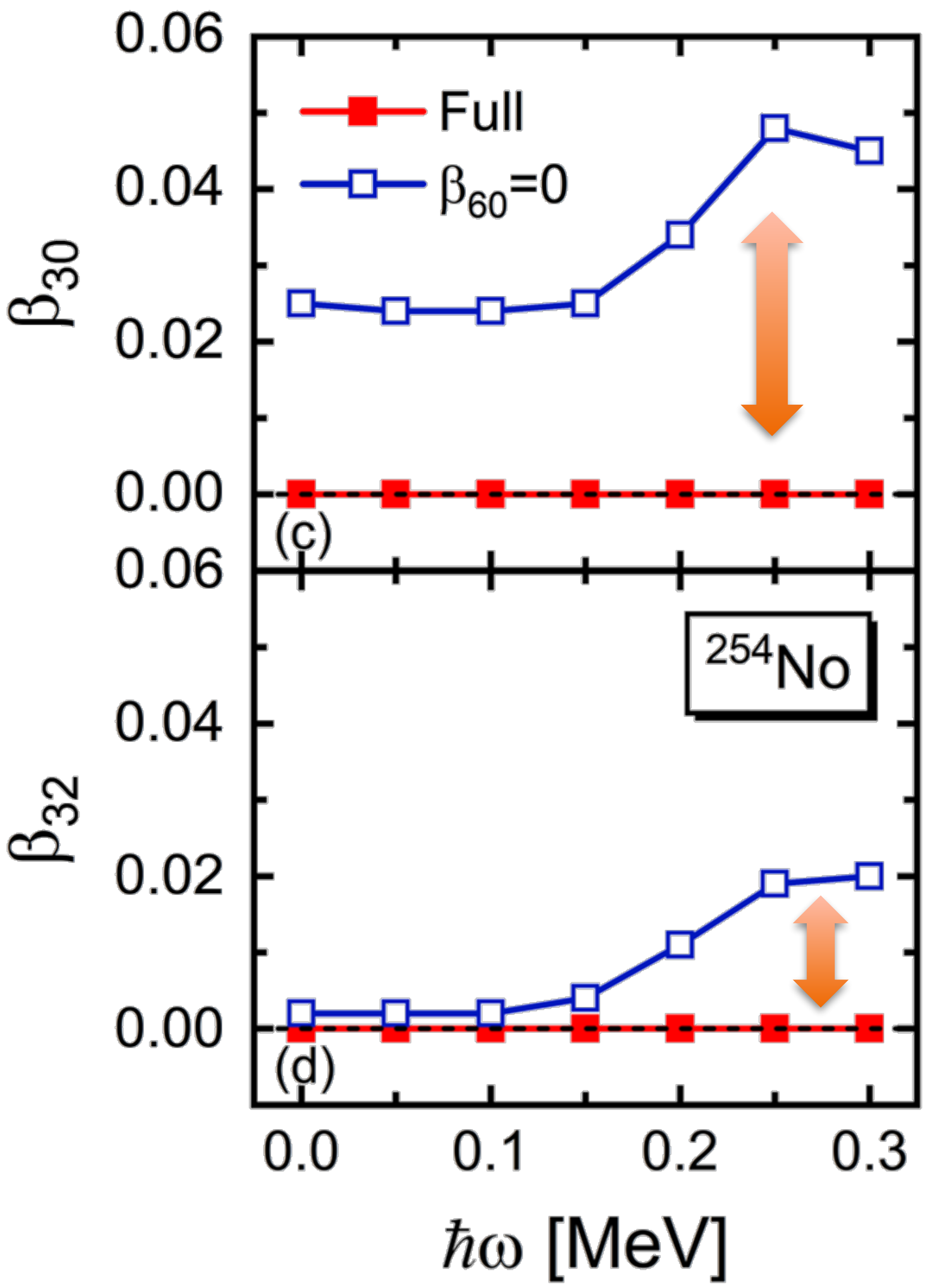
Xu, Wang, Wang, Ring, **PWZ**, Under review.

Octupole deformation is responsible for the upbending in ^{252}No.

High-order deformation in ^{254}No







Xu, Wang, Wang, Ring, **PWZ**, Under review.

Octupole and β_{60} deformations are coupled with each other in ^{254}No.

Summary

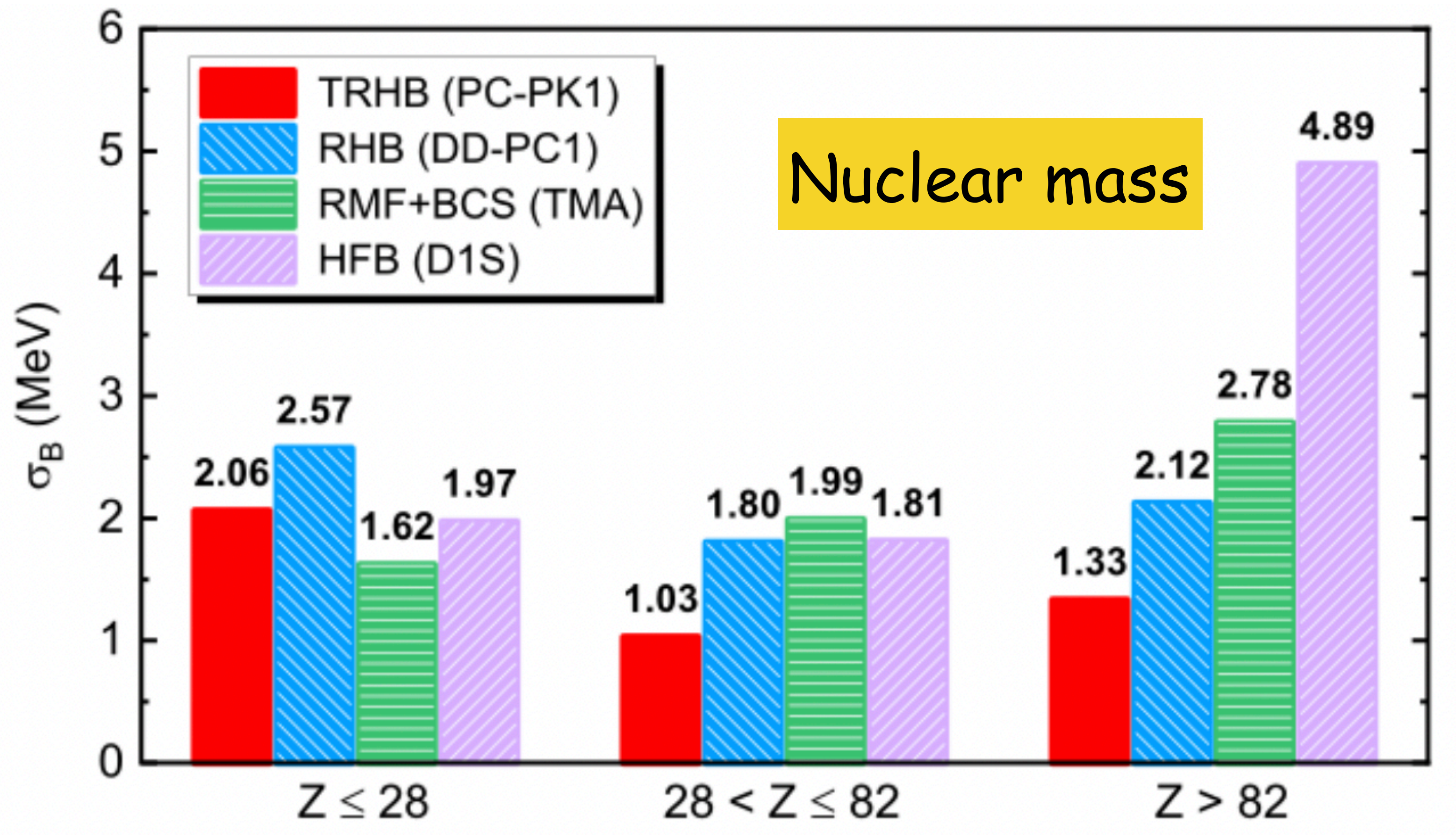
Covariant density functional theory has been solved in 3D lattice and used to study high-order deformations in nuclei.

- CDFT has been solved in 3D lattice by PCG-F
  more efficient in computation
- Tetrahedral, Y_{31}, and Y_{33} deformations in ^{110}Zr and ^{286}No
  a tetrahedral state and a pure non-axial octupole state
  shape softness / coexistence
- Cranking CDFT+SLAP has been developed in 3D lattice
  no spatial symmetry restriction
  particle number conservation
- High-order deformation in superheavy nuclei
  octupole deformation effects
  coupling between the octupole and β_{60} deformation


Thank you.

Relativistic density functional theory

The relativistic density functional theory is very successful in the description of many nuclear phenomena



Total rms deviation

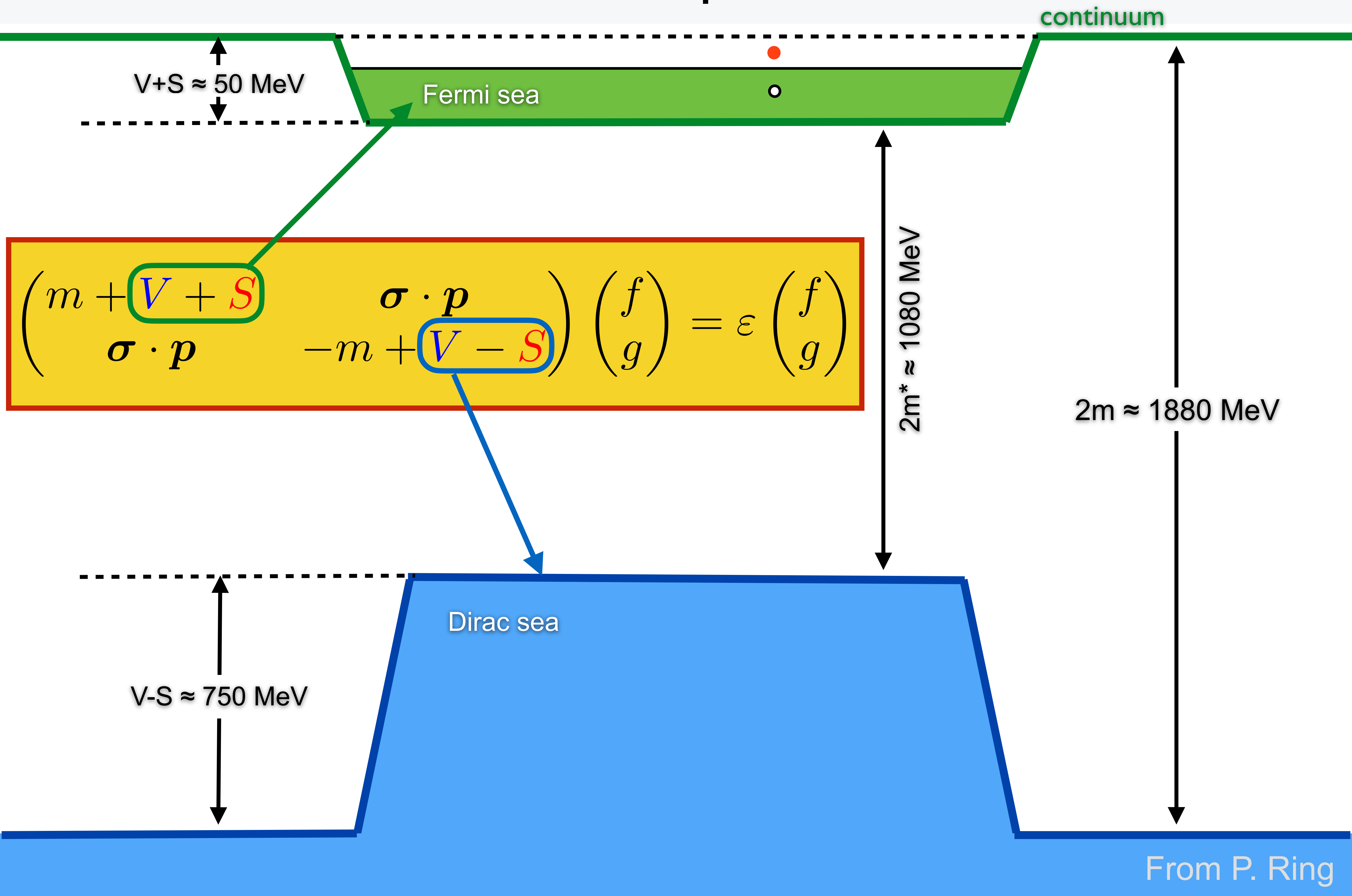
RHB (PC-PK1): 1.31 MeV

HFB (UNEDF1): 1.91 MeV

PC-PK1: PWZ, Li, Yao, and Meng, PRC 82, 054319 (2010)
Ground states: Yang, Wang, PWZ, and Li, PRC 104, 054312 (2021)
Low-lying spectra: Yang, PWZ, and Li, PRC 107, 024308 (2023)

Triaxial RHB mass table
http://nuclearmap.jcnp.org

Relativistic potentials



$$\begin{pmatrix} m + V + S & \boldsymbol{\sigma}\cdot\boldsymbol{p} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} & -m + V - S \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \varepsilon \begin{pmatrix} f \\ g \end{pmatrix}$$