Emergence of high-order deformation in atomic nuclei

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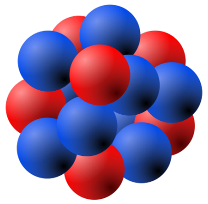
Outline

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

Nuclear deformation



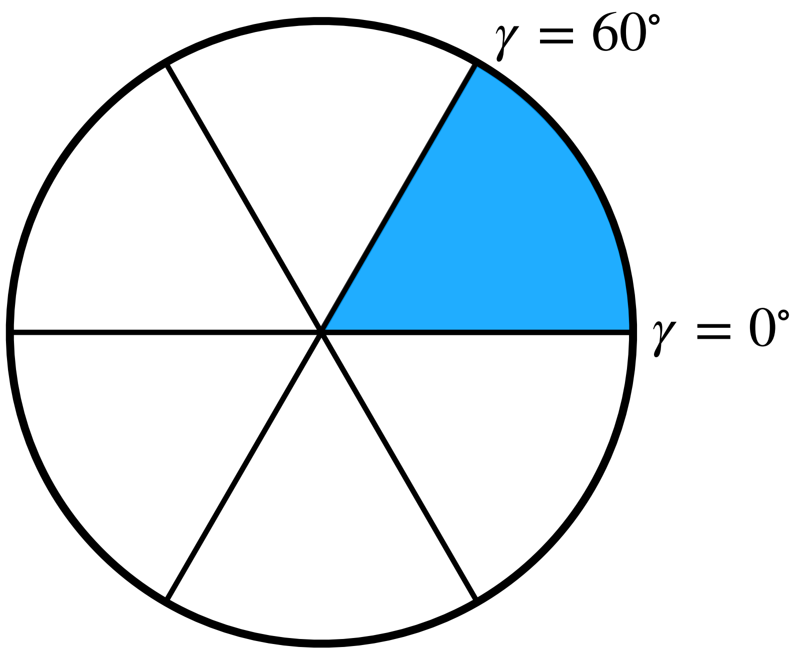
Nuclear shape: $R(\theta,\varphi) = R_0\left[1 + \sum_{\lambda=1}^{\infty}\sum_{\mu=-\lambda}^{\lambda}\alpha_{\lambda\mu}Y^*_{\lambda\mu}(\theta,\varphi)\right]$

Quadrupole deformation

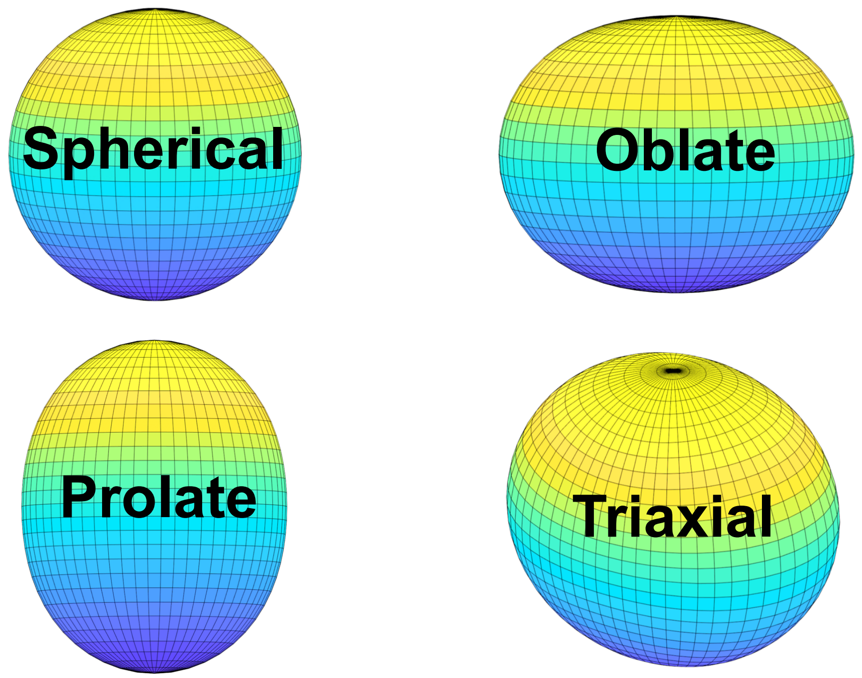
$$R(\theta,\varphi) = R_0\left[1 + \sum_{\mu=-2}^{2}\alpha_{2\mu}Y^*_{2\mu}(\theta,\varphi)\right]$$

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.

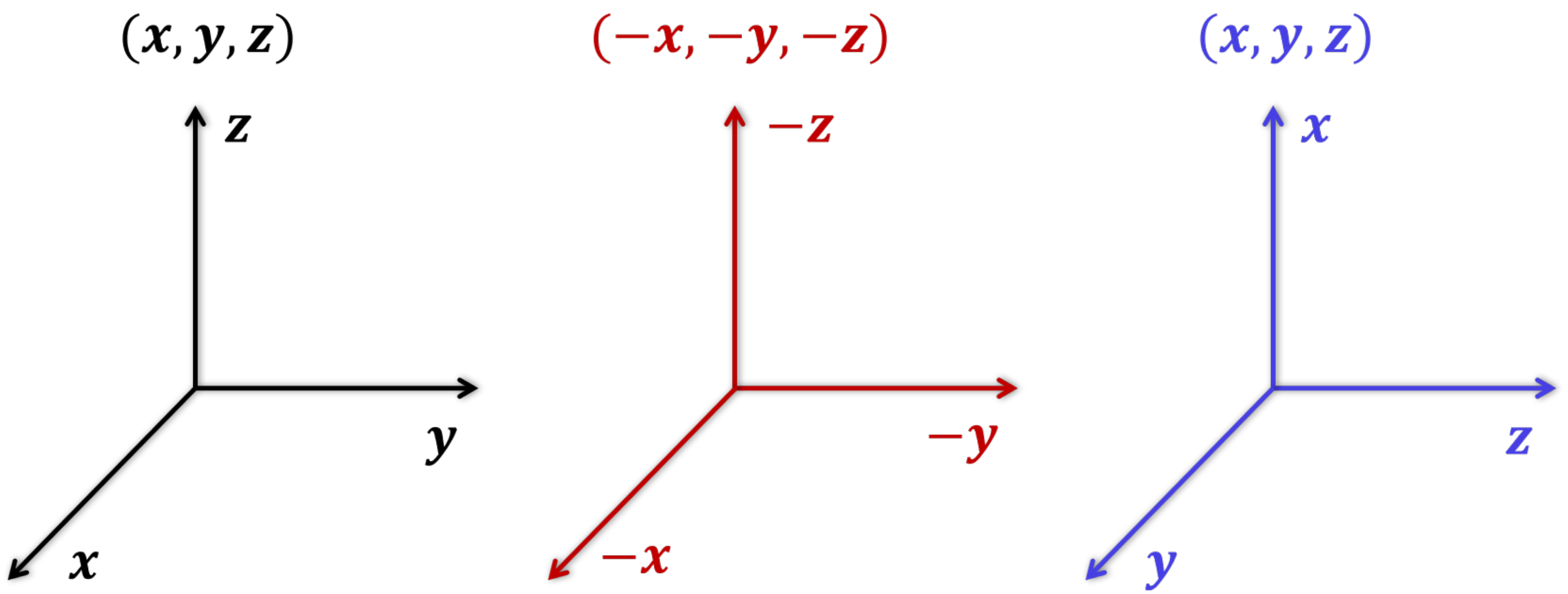
How about the range of these parameters ?

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

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

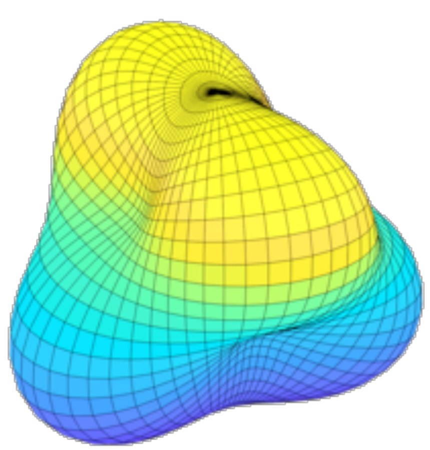
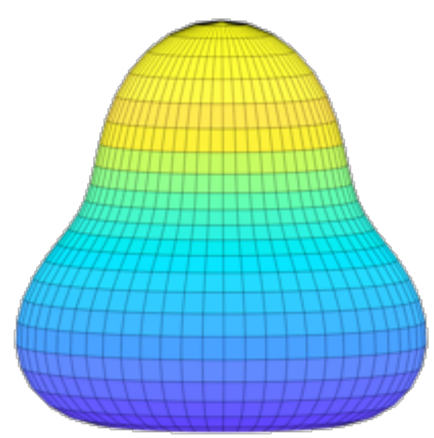
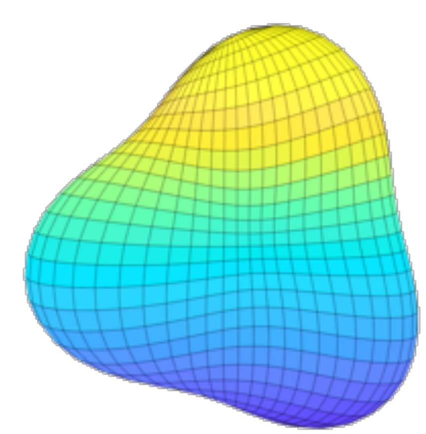
$$a_{30} = \epsilon_1(1) = \frac{4\pi}{3AR^3} \int \mathrm{d}^3 r \rho_v(\boldsymbol{r}) r^3 F_1(1),$$

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

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

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

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

$a_{32} \neq 0$	$a_{30} \neq 0$	$a_{30}, a_{31}, a_{33} \neq 0$
		

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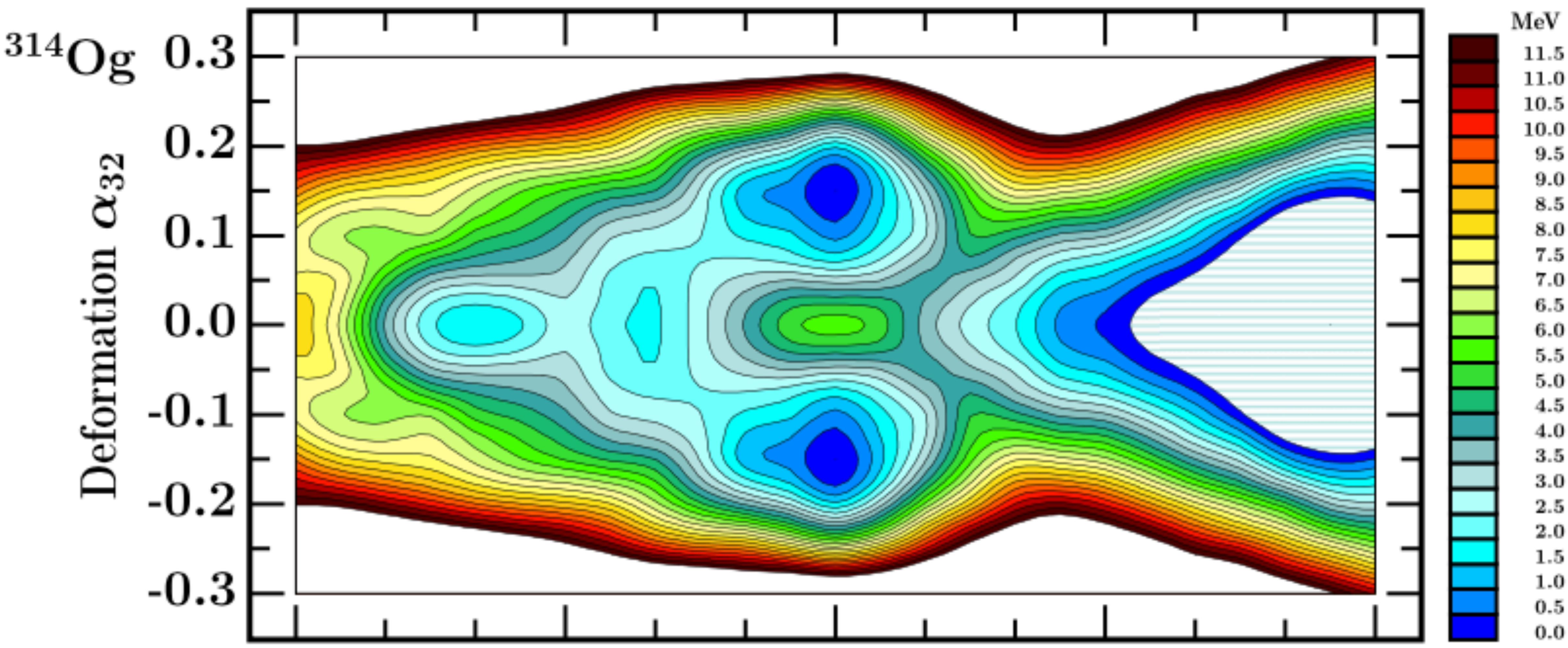
Prediction of octupole shapes within the Mac-mic method

Strong shell closures are predicted in the actinide (N=136) and superheavy regions (N=196) with **nonvanishing all four octupole deformations**.

Yang, Dudek, Dedes, et al., PRC 105, 034348 (2022); 106, 054314 (2022); 107, 054304 (2023)

Mac-mic method with Woods-Saxon potential **See talks by Dedes and Yang**



Deformation α_{20}

Density functional theory

The many-body problem is mapped onto a one-body problem

Hohenberg-Kohn Theorem

The exact ground-state energy of a quantum mechanical many-body system is a universal functional of the local density.

$$E[\rho] = T[\rho] + U[\rho] + \int V(\mathbf{r})\rho(\mathbf{r})\, d^3\mathbf{r}$$

Kohn-Sham DFT

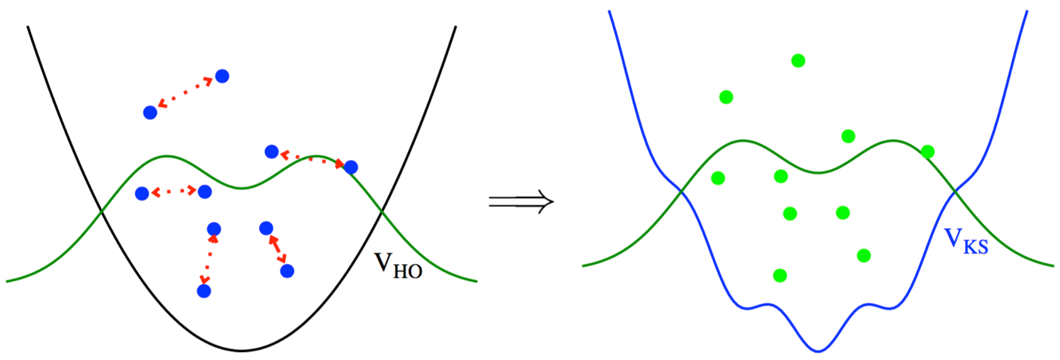


Figure from Drut PPNP 2010

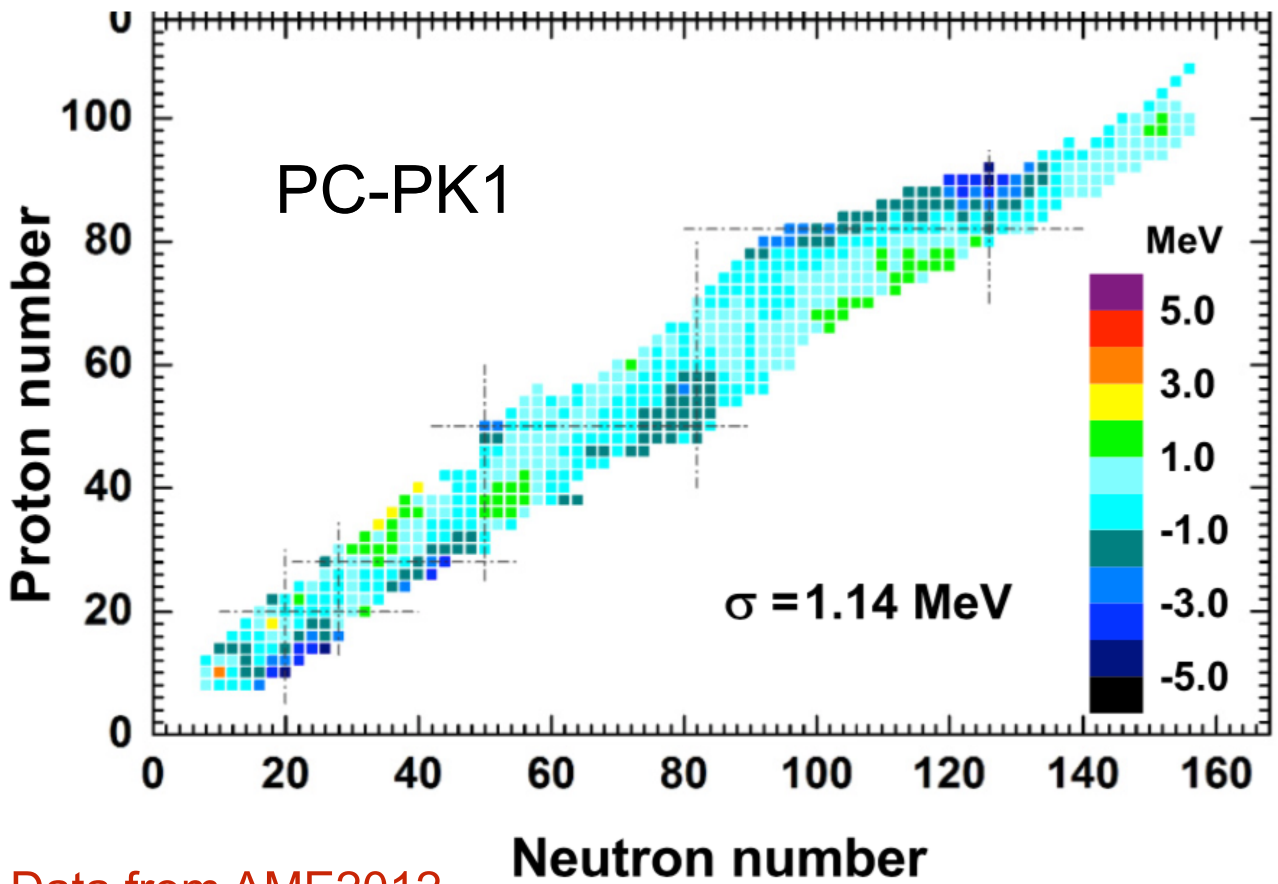
$$T[\rho] \doteq \sum_{i=1}^{N} \left\langle \varphi_i \left| -\frac{\hbar^2}{2m}\nabla^2 \right| \varphi_i \right\rangle$$

$$E[\rho] \Rightarrow \boxed{\hat{h} = \frac{\delta E}{\delta \rho}} \Rightarrow \boxed{\hat{h}\varphi_i = \varepsilon_i \varphi_i} \Rightarrow \boxed{\rho = \sum_{i=1}^{A} |\varphi_i|^2}$$

The practical usefulness of the Kohn-Sham theory depends entirely on whether an **Accurate Energy Density Functional** can be found!

Covariant density functional： PC-PK1

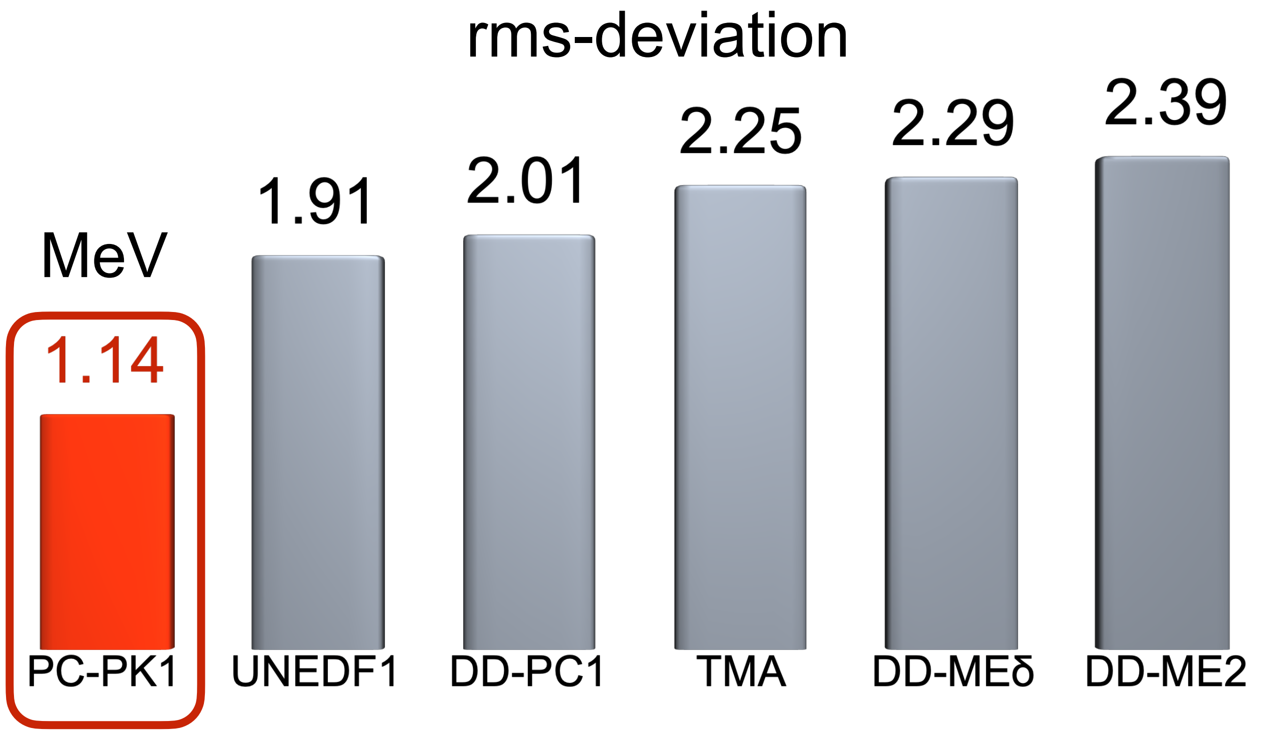
Mass Differences: M_{cal} - M_{exp}



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!

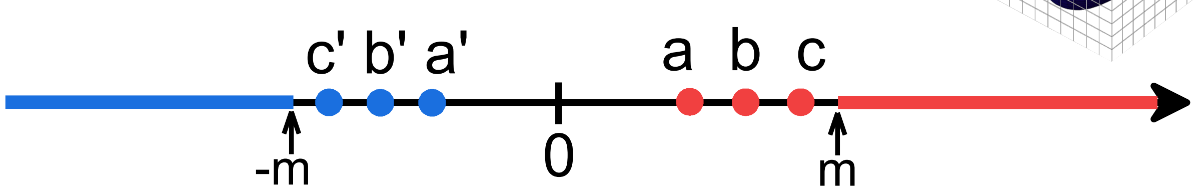
Lattice CDFT

✓ No spatial symmetry restriction

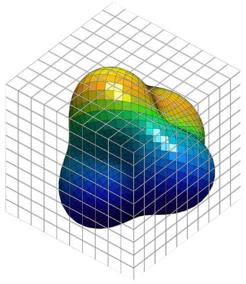
✓ A long-term challenge due to

a) variational collapse problem

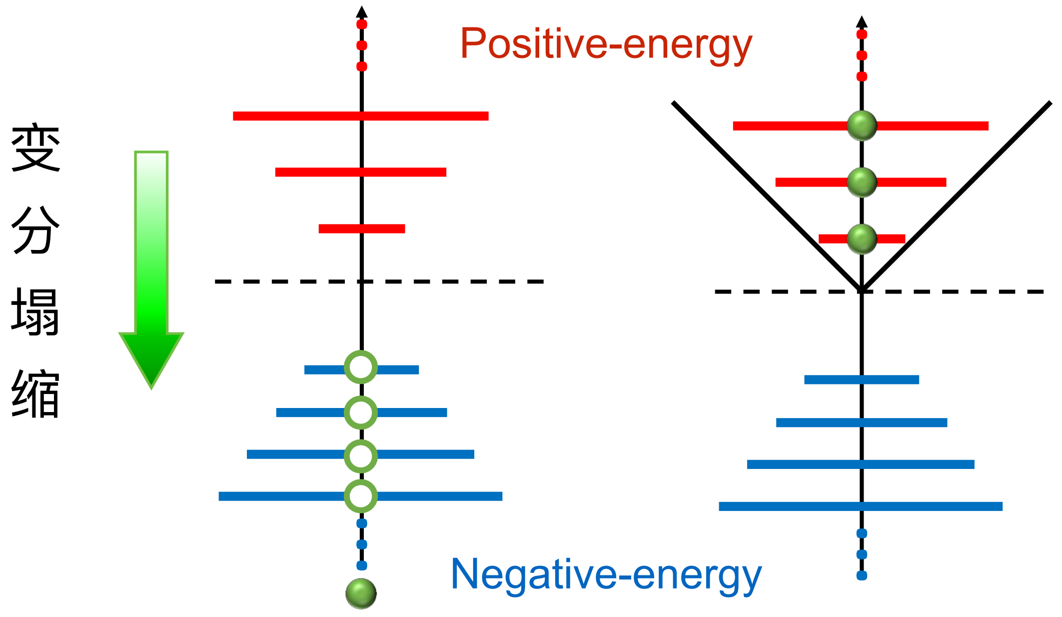
b) fermion doubling problem



Hagino and Tanimura, PRC 82, 057301 (2010)

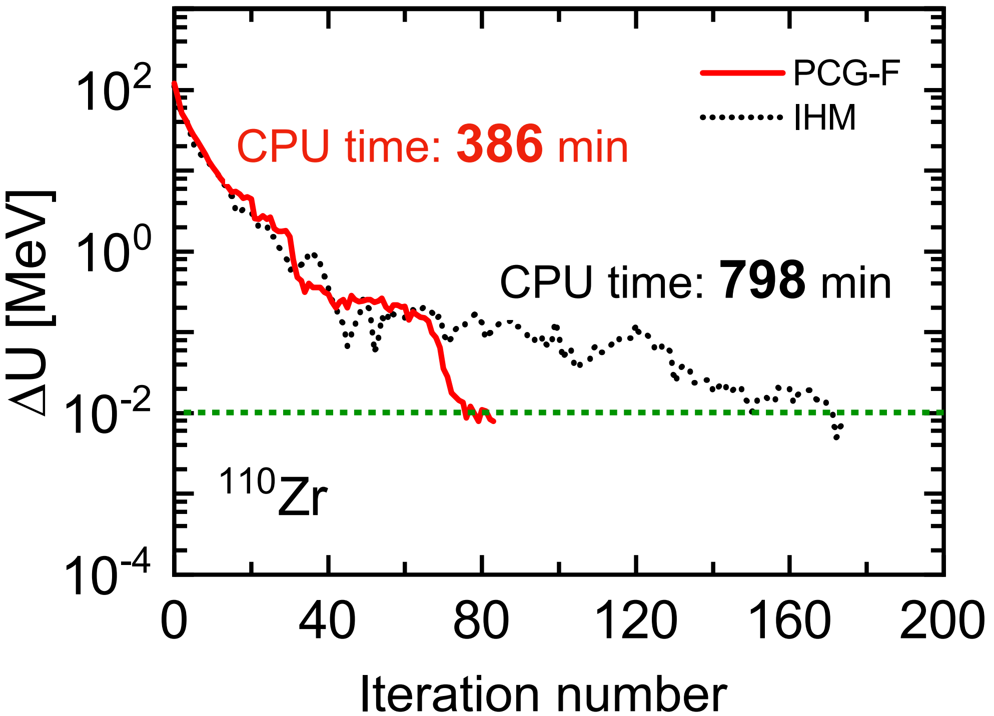


PCG-F Method



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

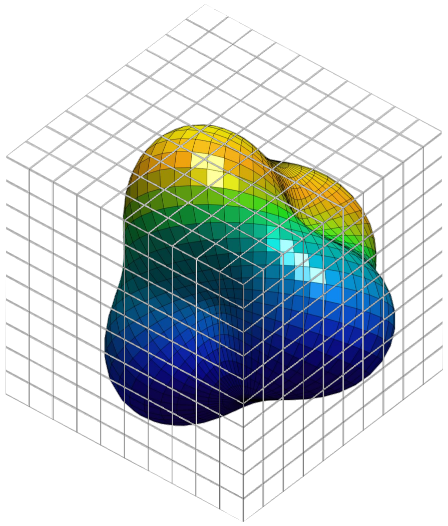
PCG-F saves **~52%** of the CPU time



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

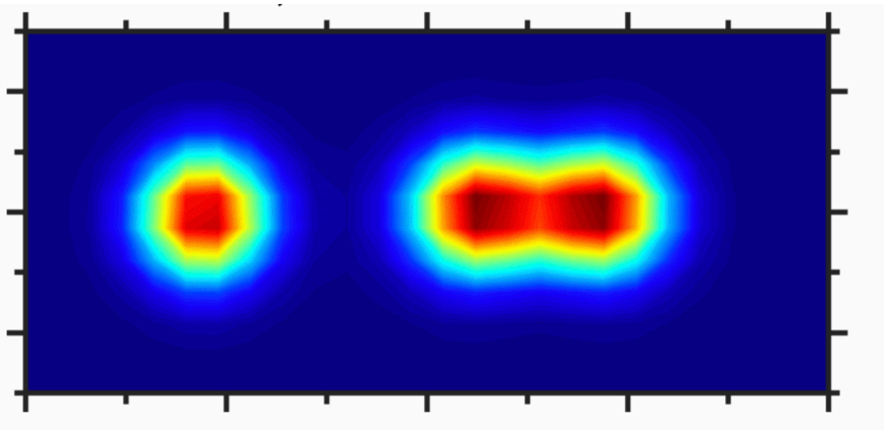
Applications of the TD-CDFT

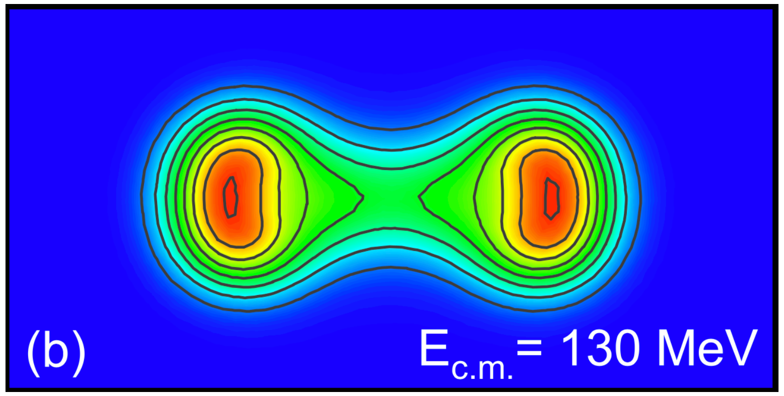
3D Lattice: no spatial symmetry restriction

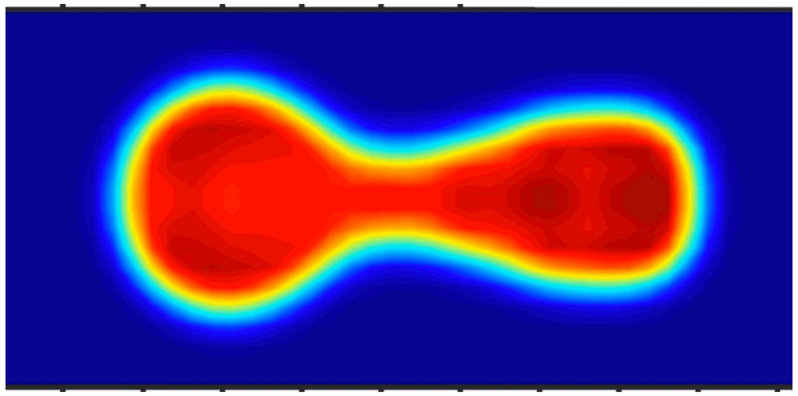


✓ Applications include:

- Linear alpha-chain — PRL 115, 022501 (2015) PLB 801,135194 (2020)
- Nuclear fission — PRL 128, 172501 (2022) PRC 105, 044313 (2022) PRC 107, 014303 (2023)
- Chiral dynamics — PRC 105, L011301 (2022) PLB 856, 138877 (2024)
- Nuclear reaction — PRC 102, 044603 (2020) PRC 109, 024614 (2024) PRC 109, 024316 (2024) Editors' Suggestion
- …







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, Goźdź, 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)

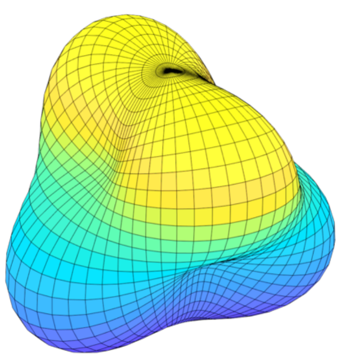
  Zhao, Lu, Zhao, Zhou, PRC 95, 014320 (2017)
  Rong, Wu, Lu, Yao, PLB 840, 137896 (2023)

V_4 symmetry/partial shape space assumed in CDFT calculations …

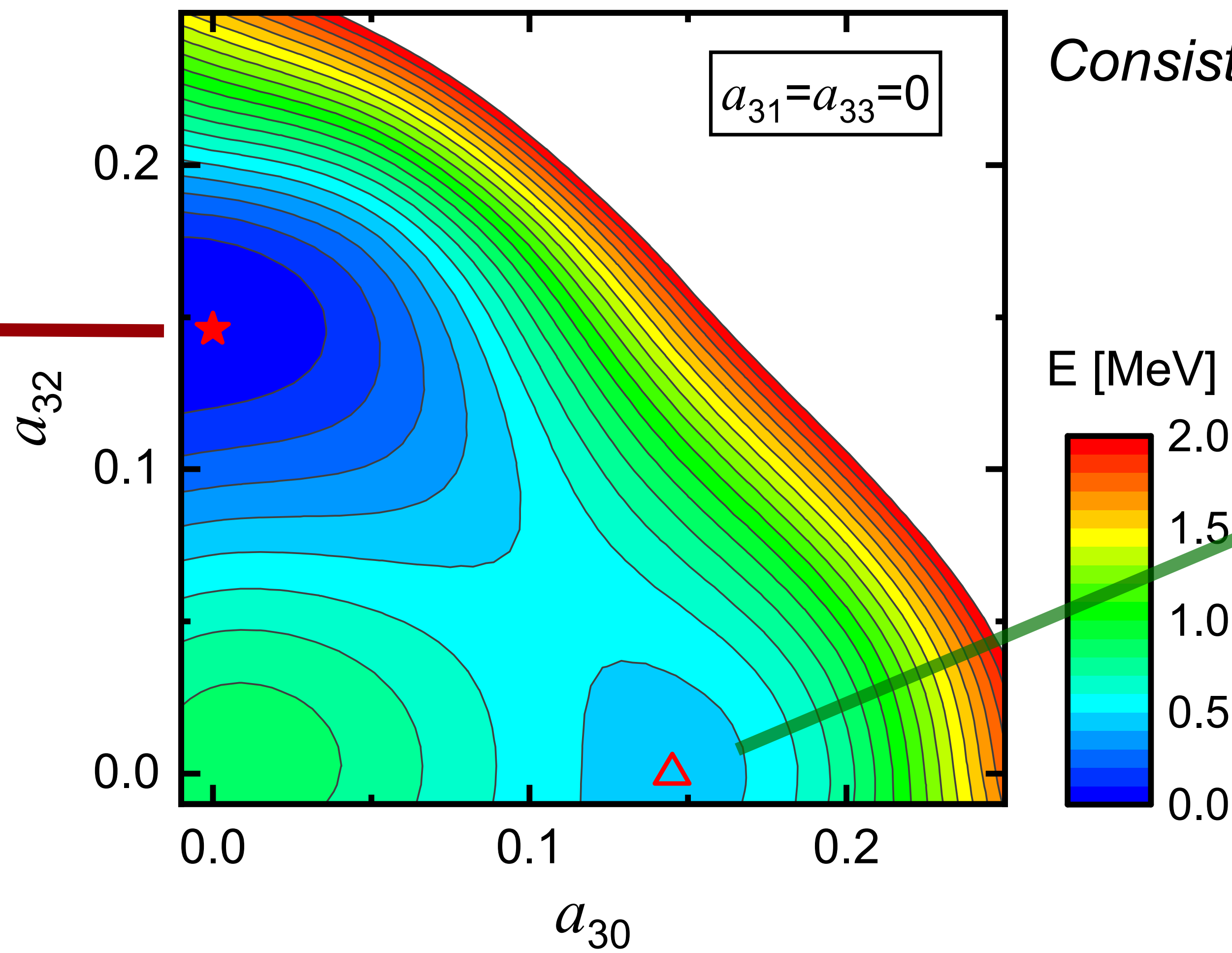
Potential energy surface (PES)

^{110}Zr

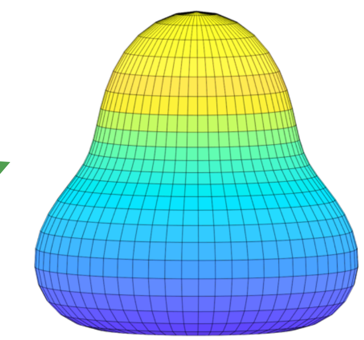
Lattice CDFT calculations with V_4 symmetry



Tetrahedral ground state



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

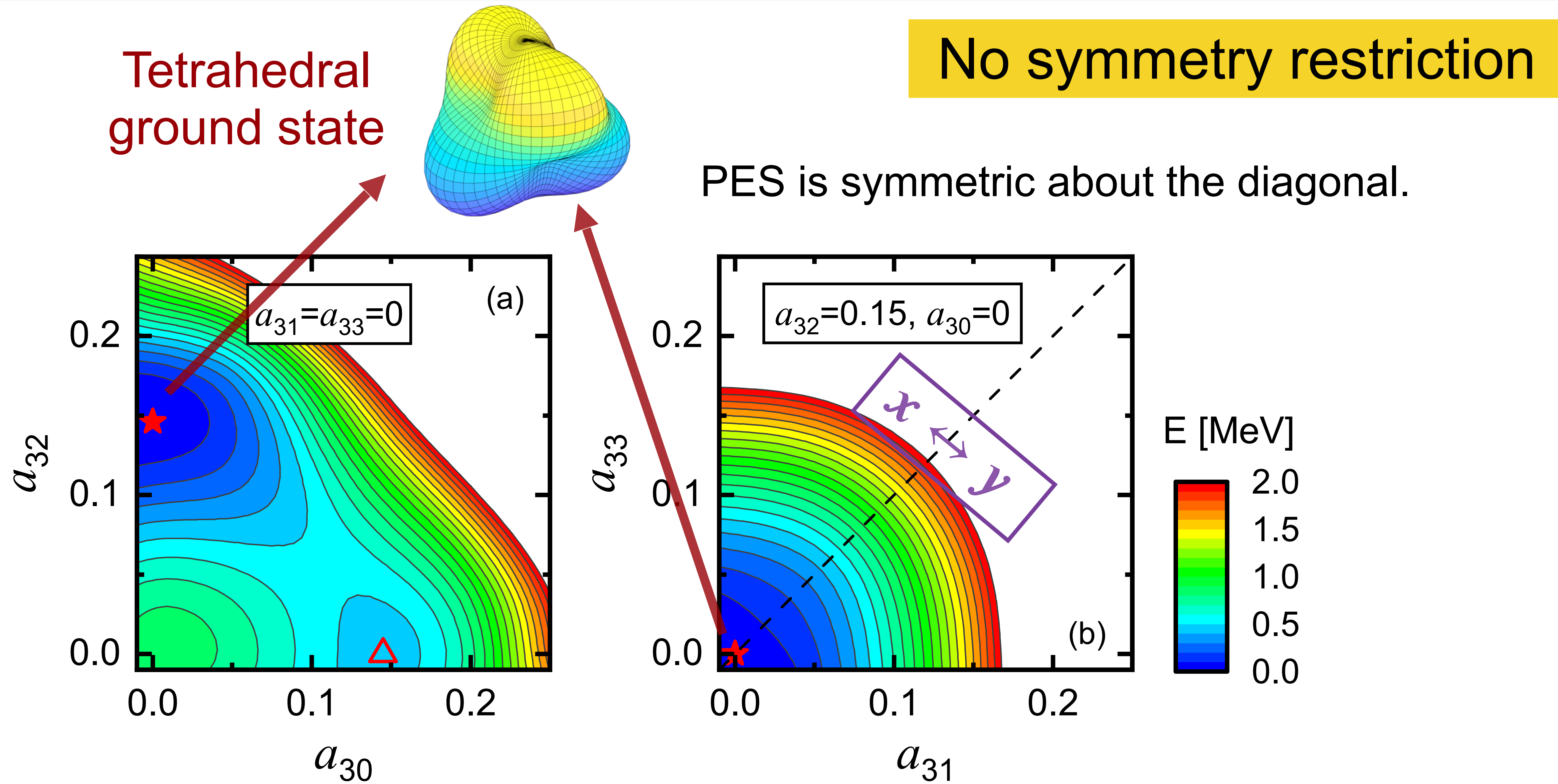


Pear-like isomeric state

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

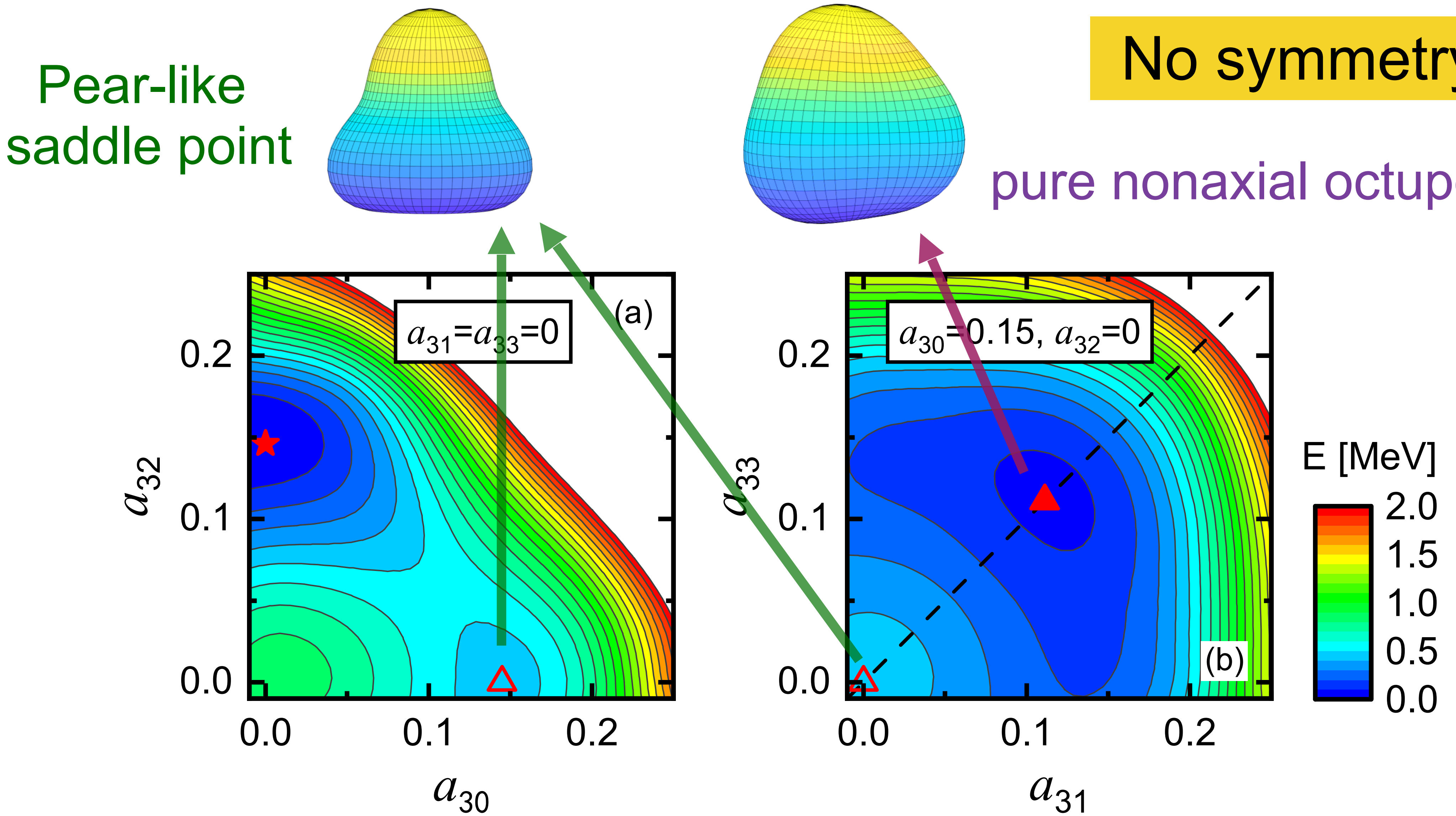


Energy minimum	a_{30}	a_{31}	a_{32}	a_{33}	E [MeV]
Ground state	0.00	0.00	0.15	0.00	-902.49

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

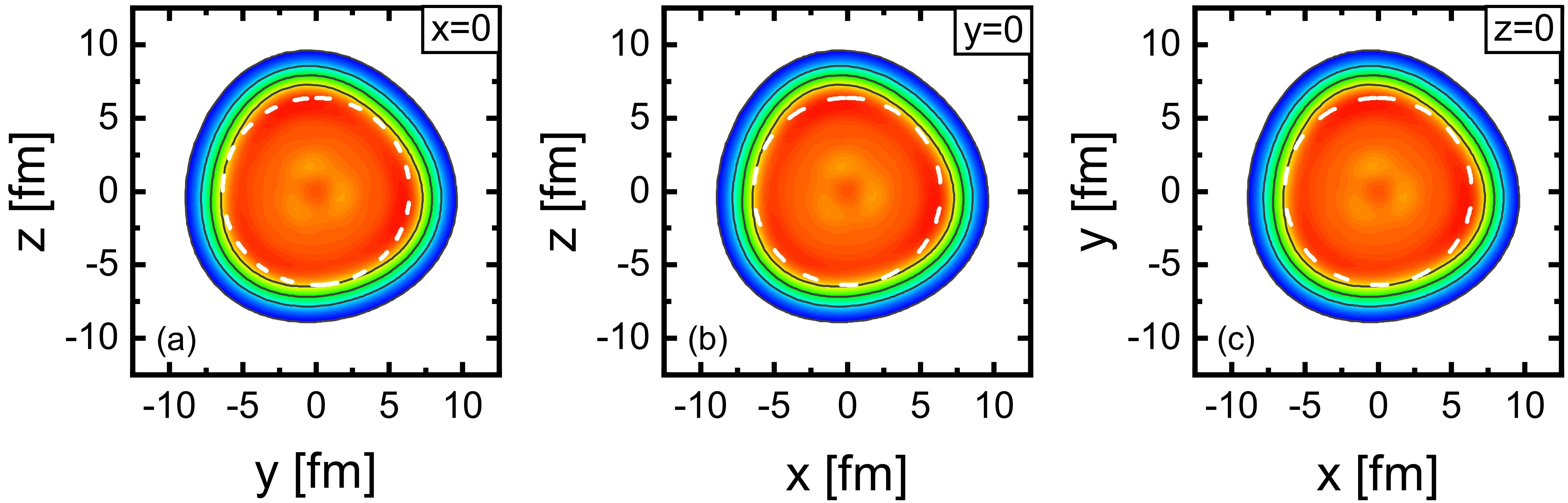
Xu, Li, Ren, **PWZ**, Phys. Rev. C 109, 014311 (2024)

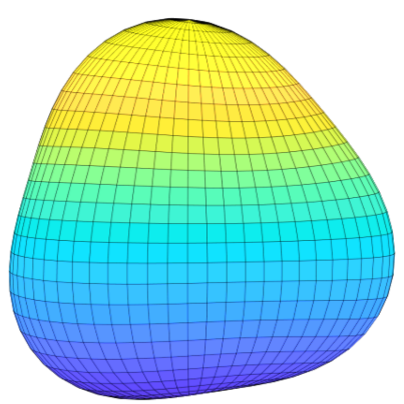
The isomeric state of ^{110}Zr has a pure non-axial octupole shape.

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**, PLB 856, 138893 (2024)

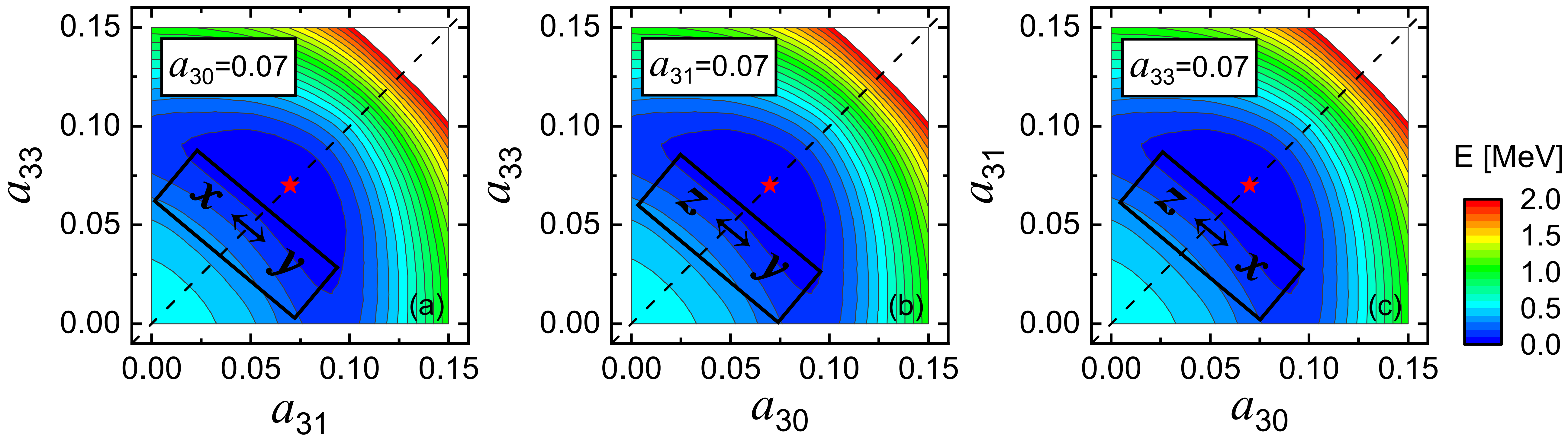
The ground state of ^{286}No has a pure non-axial octupole shape.

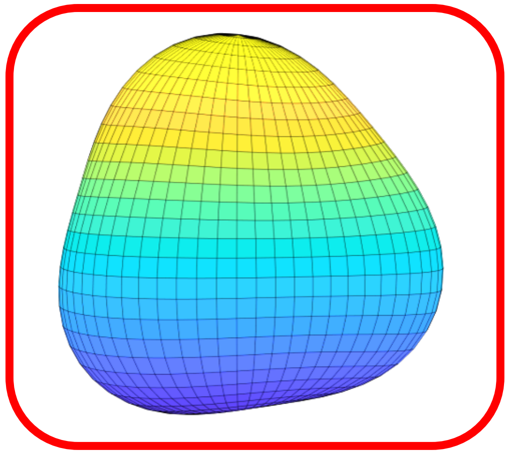
Softness of the ground state

^{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

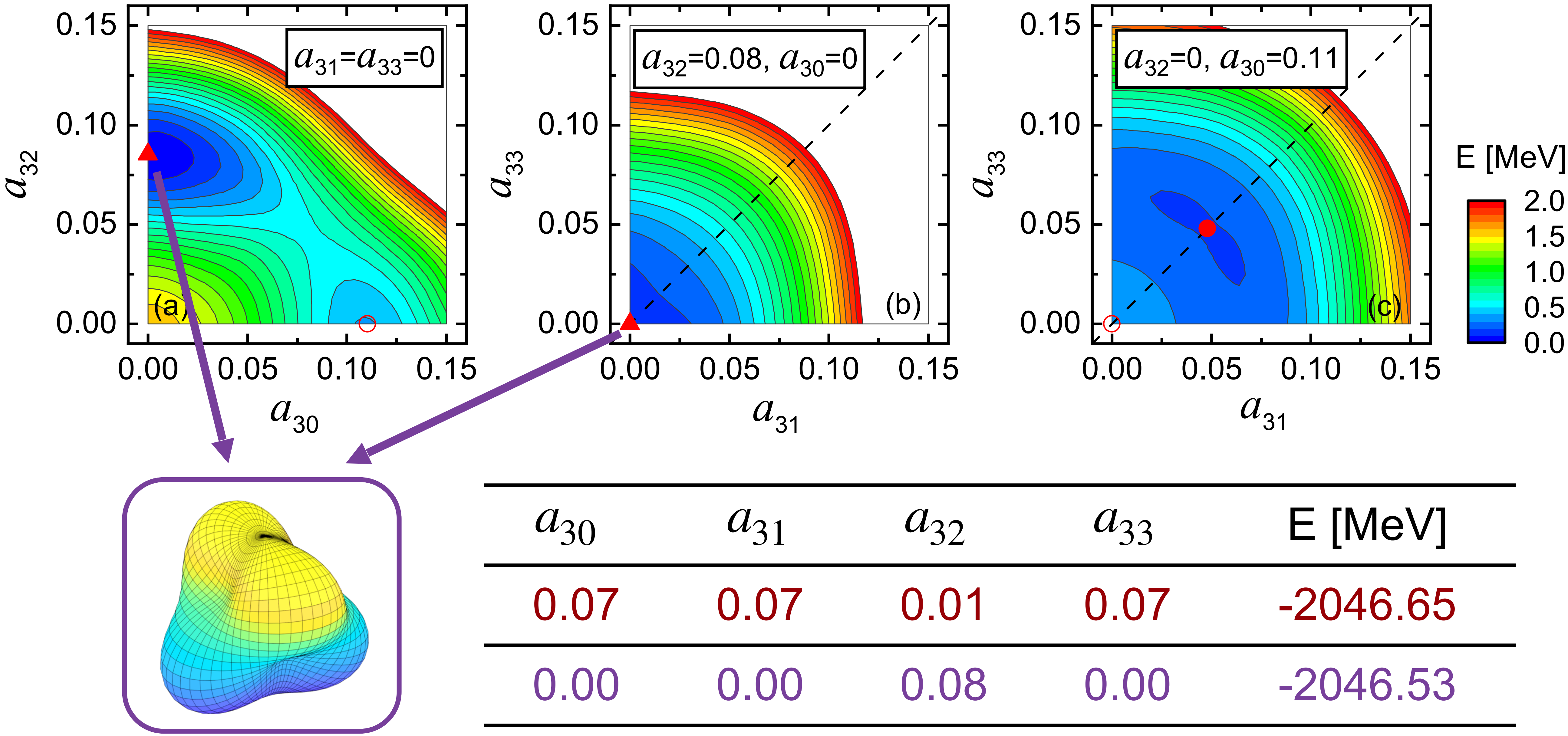
Xu, Li, Ring, **PWZ**, PLB 856, 138893 (2024)

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**, PLB 856, 138893 (2024)

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

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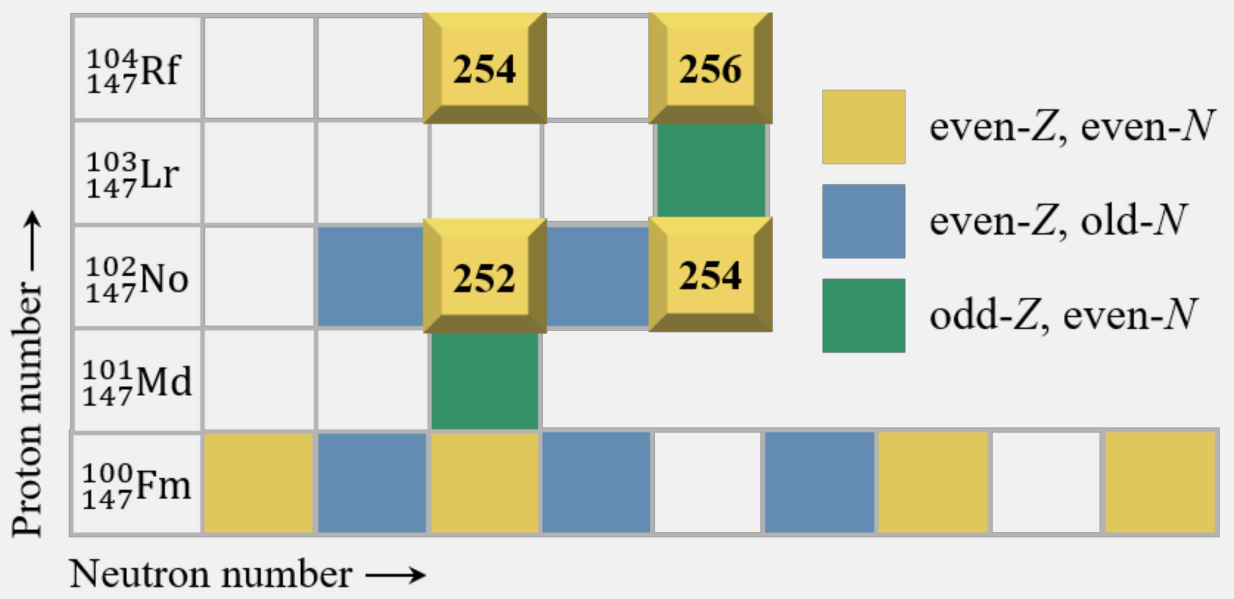
Rotating transfermium nuclei

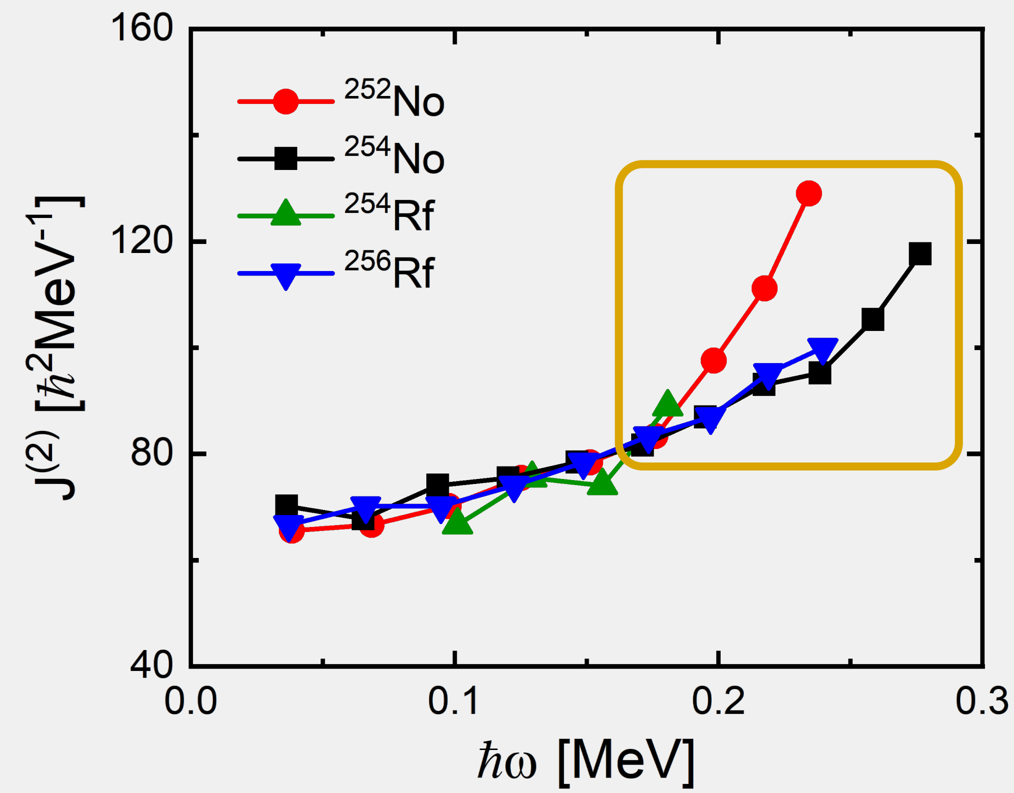
- **Transfermium nuclei** are the heaviest ones, whose rotational spectra have been measured experimentally; important for the location of the **"island of stability"**.

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

ANL、FLNR、GANIL、GSI、JAEA、JYFL ... **Dariusz's talk**



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 abnormal behavior in ^{252}No and ^{254}No?

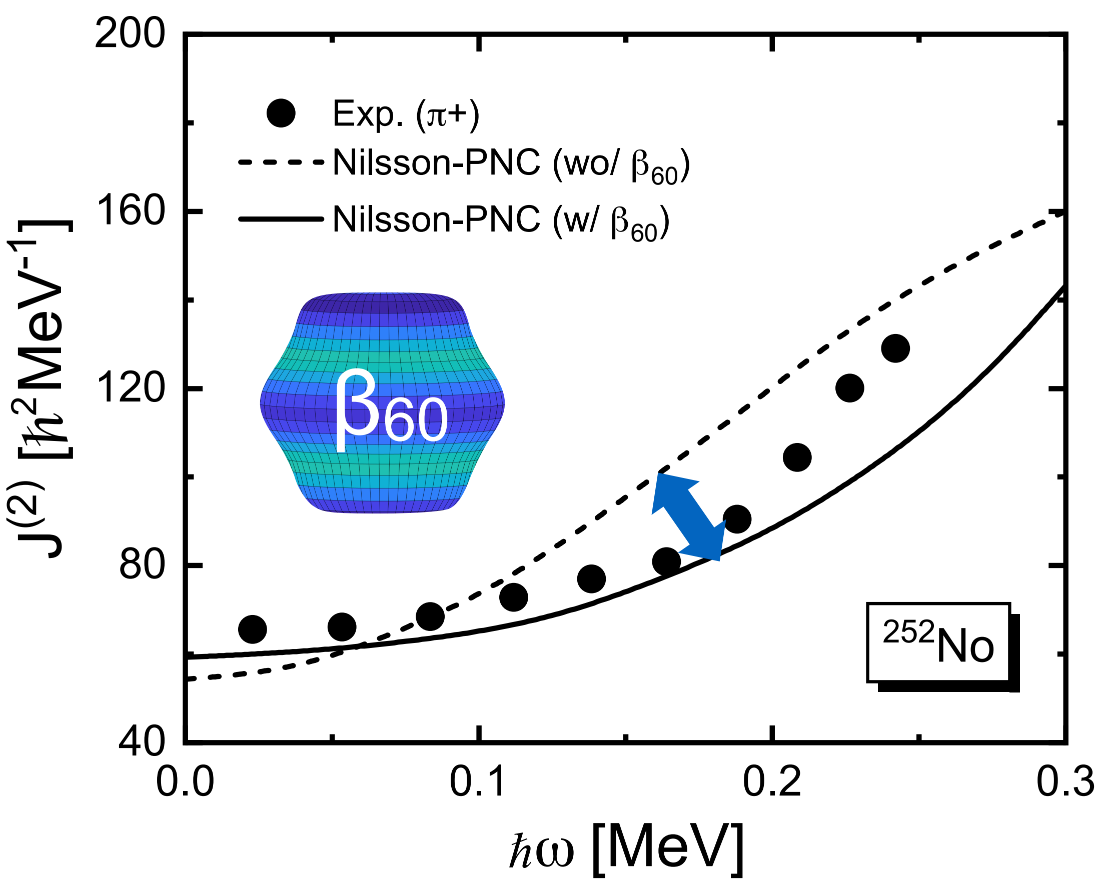
Theoretical investigations

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

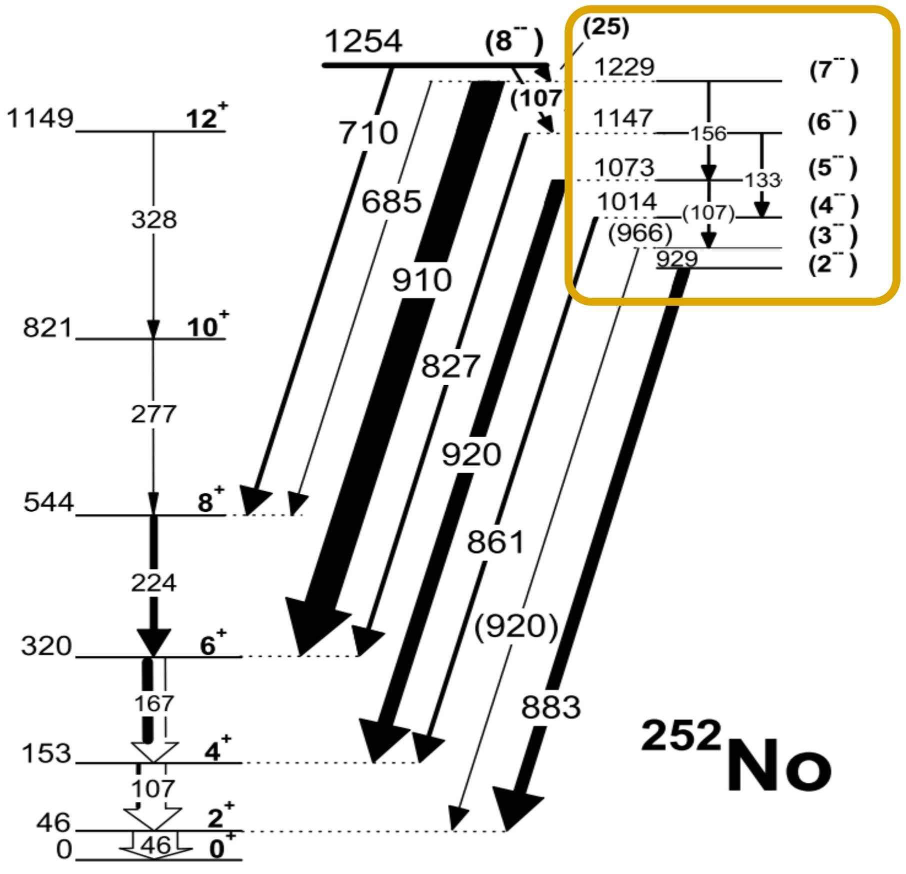
✓ Density functional theories	✓ Total Routhian surface (TRS) method
✓ Projected shell model	✓ PNC cranked shell model (PNC-CSM)
✓ Reflection asymmetric shell model	✓ …

Duguet NPA (2001); Afanasjev PRC (2003); 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

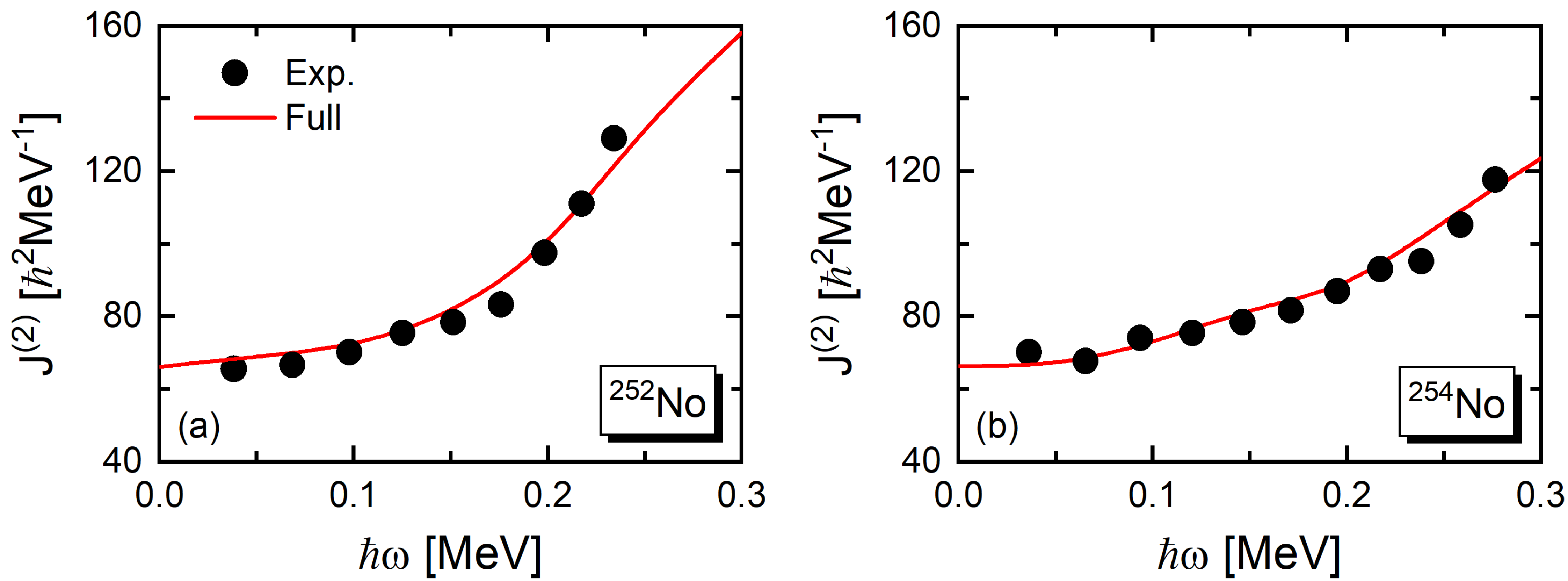
Cranking CDFT in 3D lattice with a shell-model-like approach (SLAP):

✓ self-consistent and microscopic description

✓ no adjustable parameter beyond a well-determined functional

✓ no spatial symmetry restriction

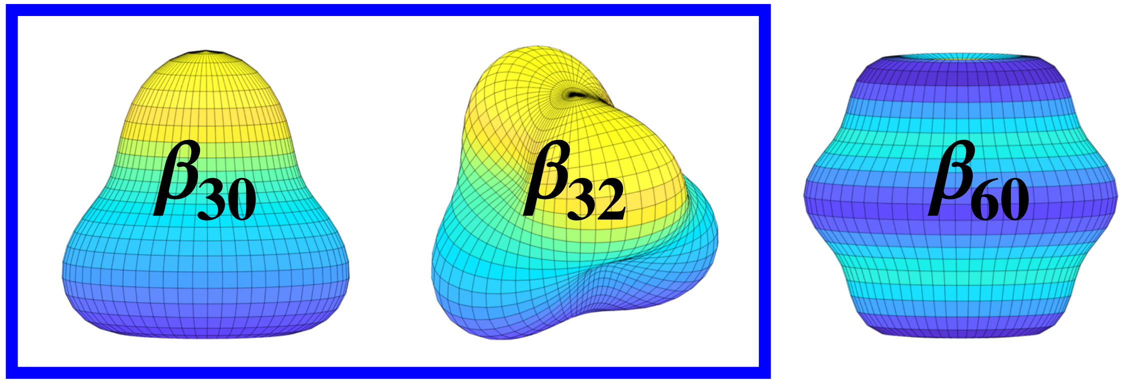
✓ pairing correlations is treated with particle number conservation

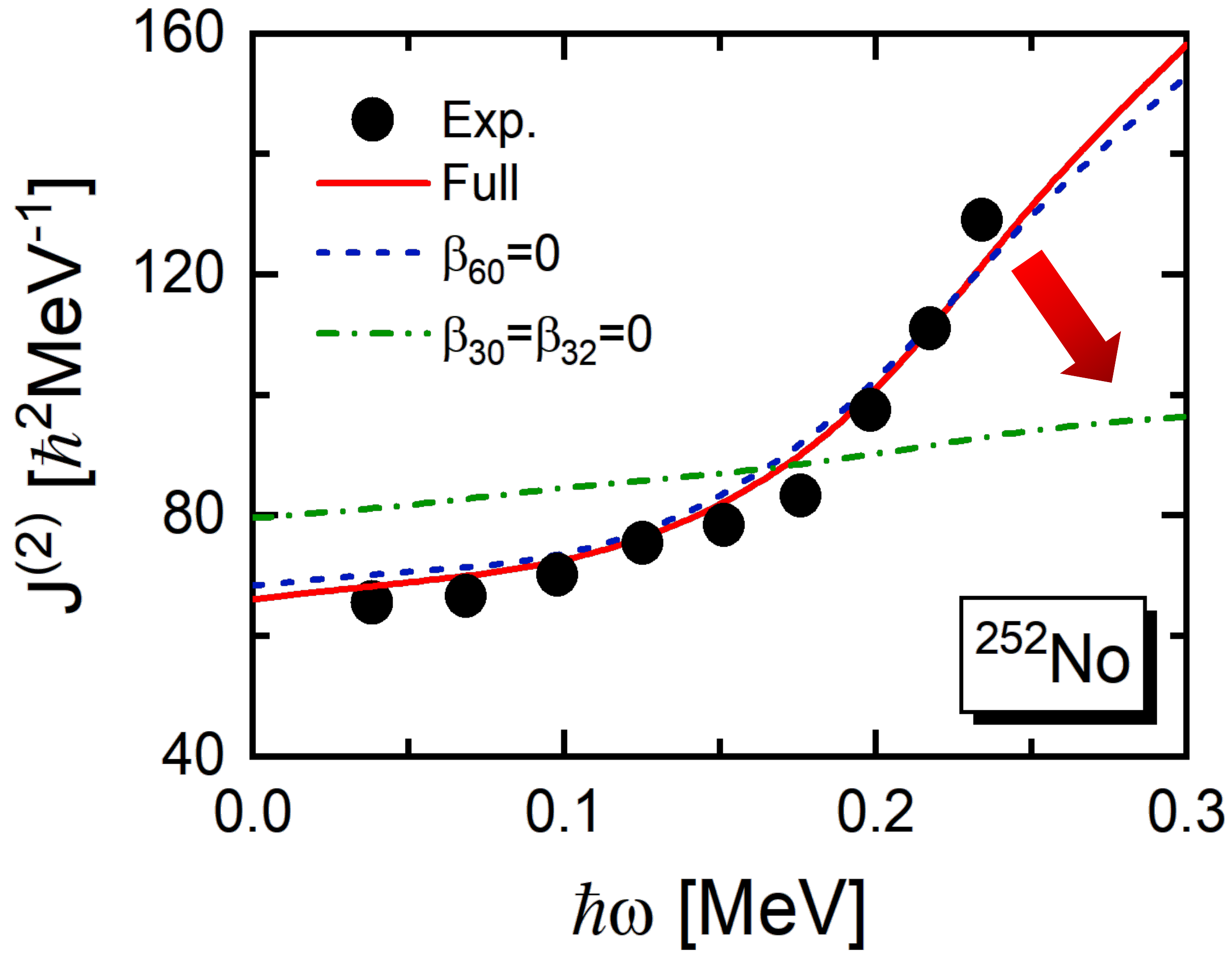


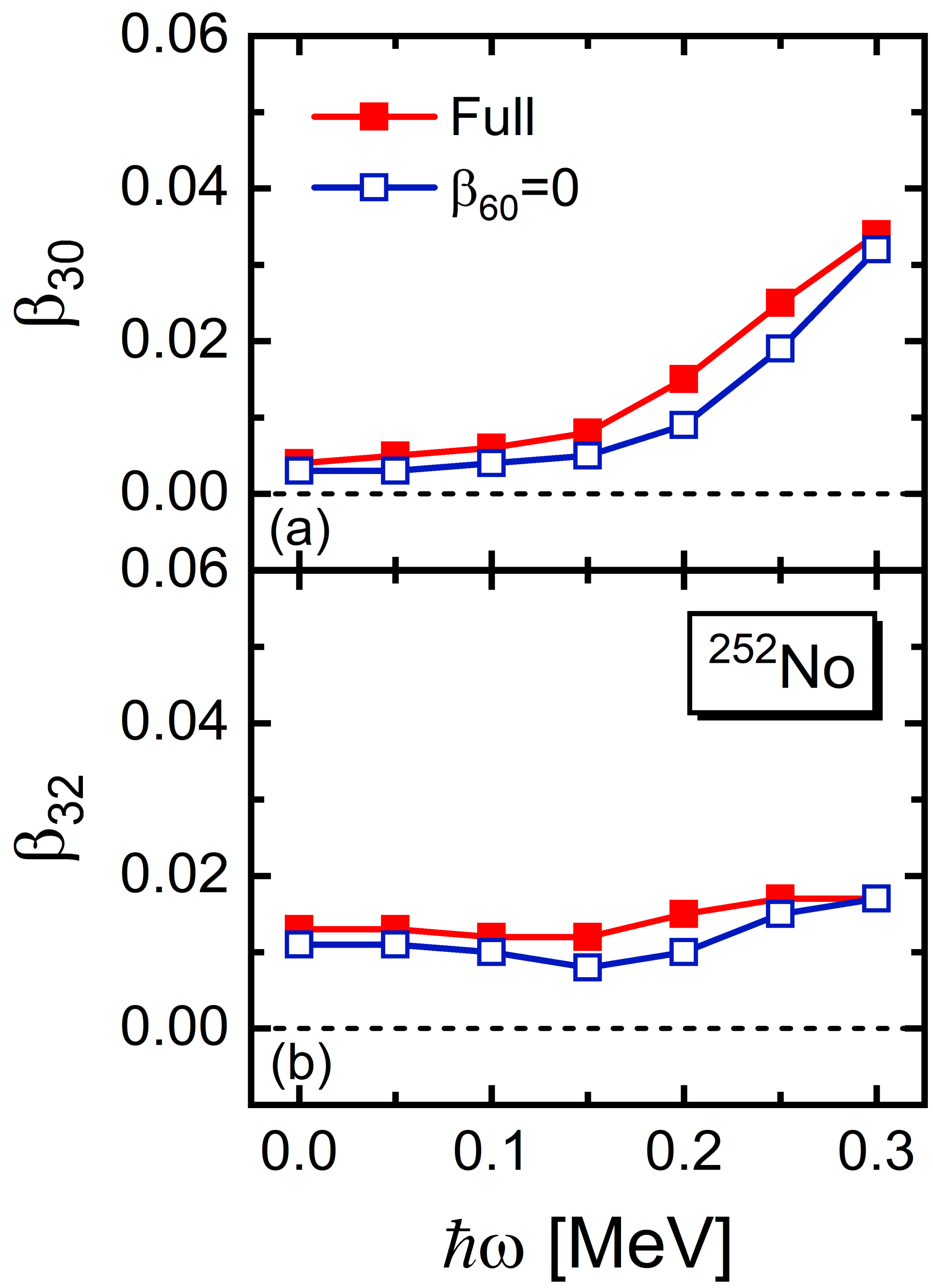
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

The experimental moments of inertia are well reproduced.

High-order deformation in ^{252}No



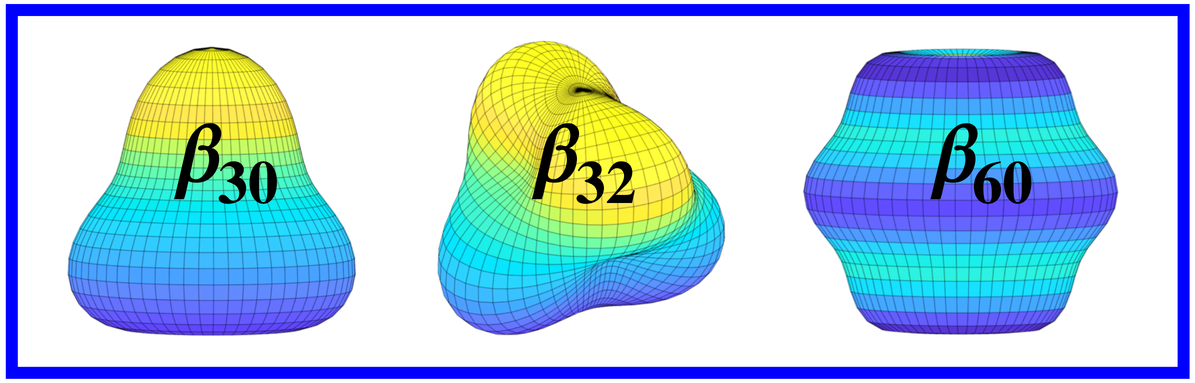


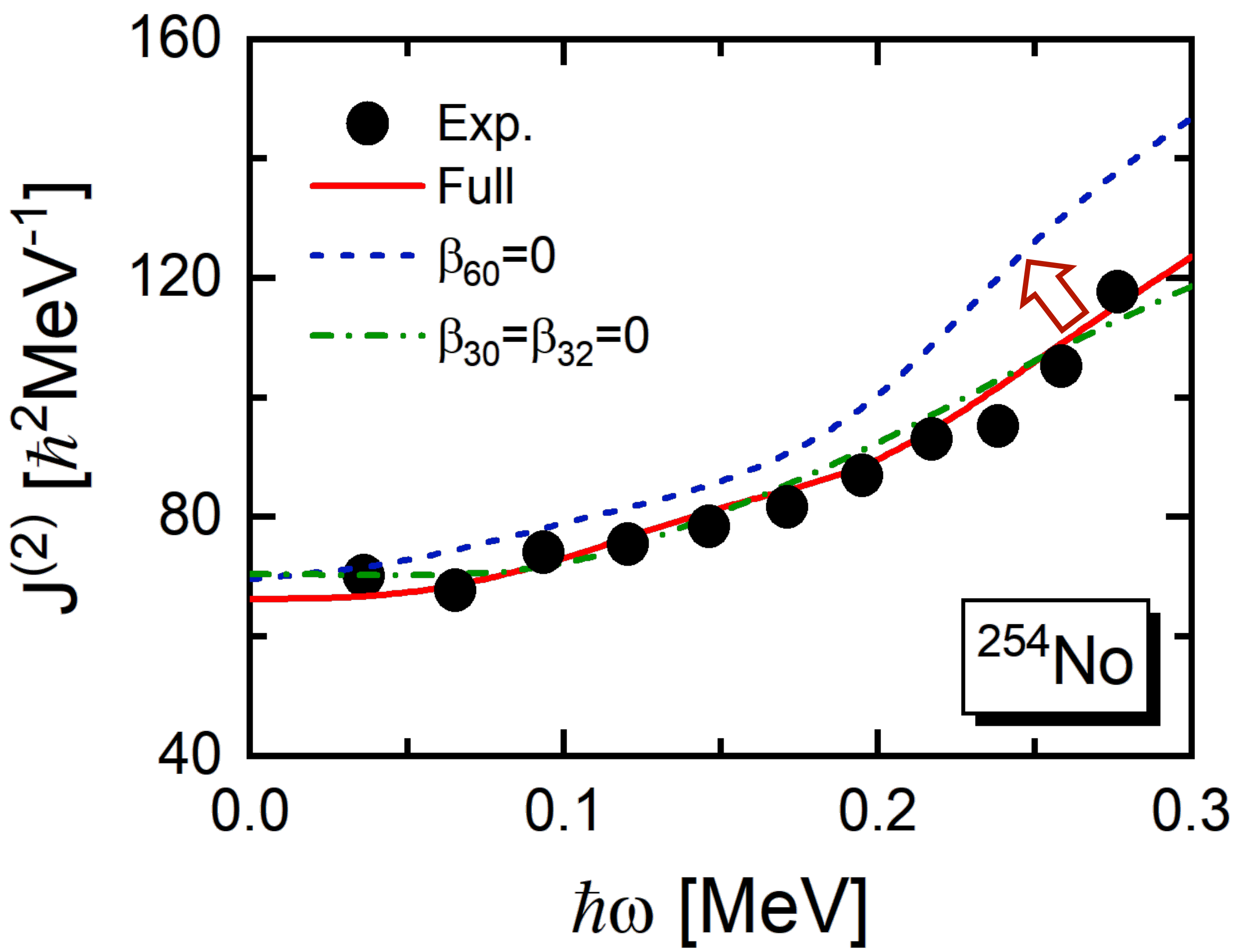


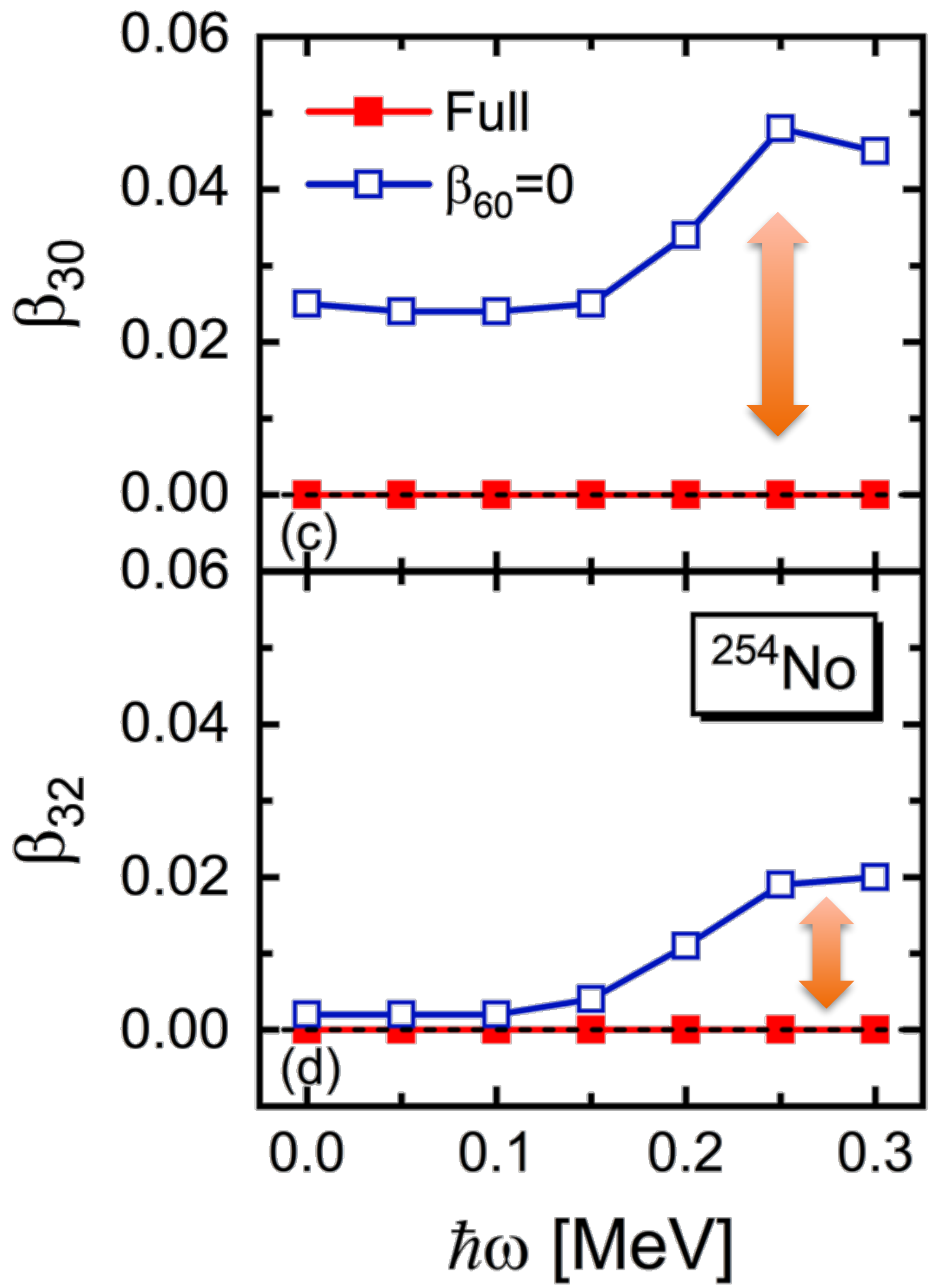
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

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

High-order deformation in ^{254}No







Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

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

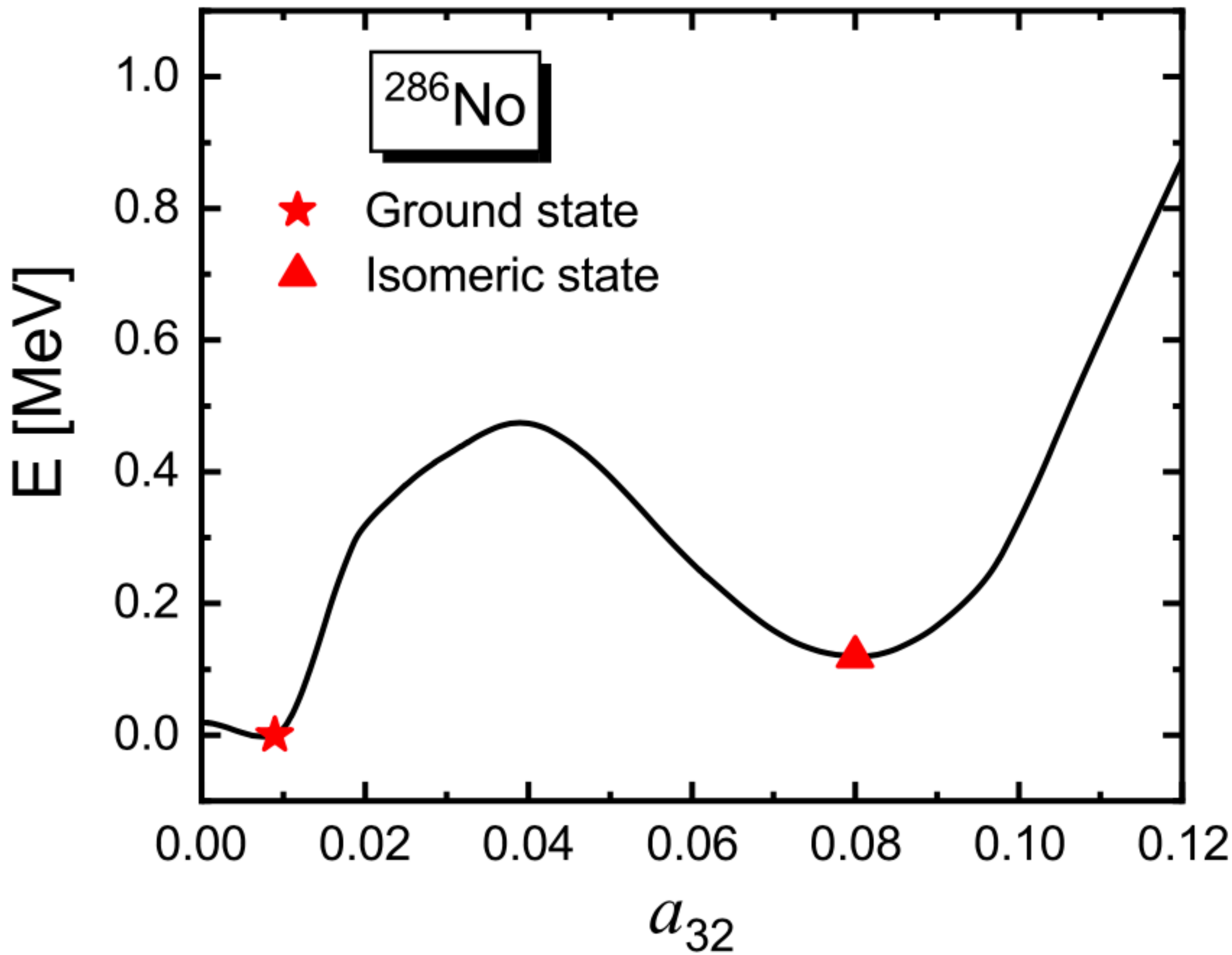
  particle number conservation

- High-order deformation in superheavy nuclei

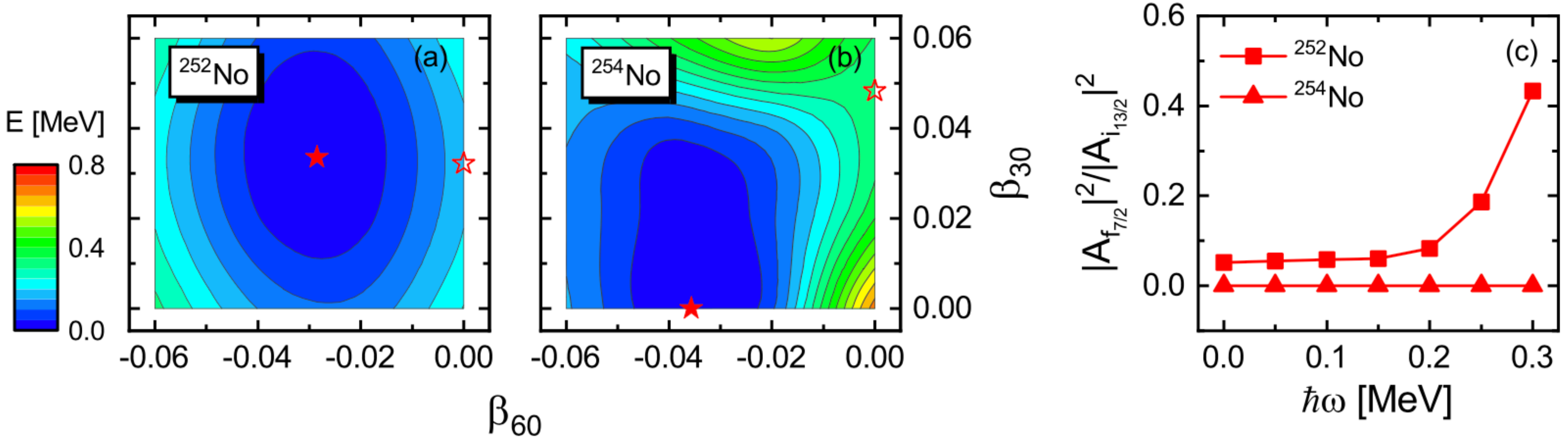
  octupole deformation effects

  coupling between the octupole and β_{60} deformation


Thank you.



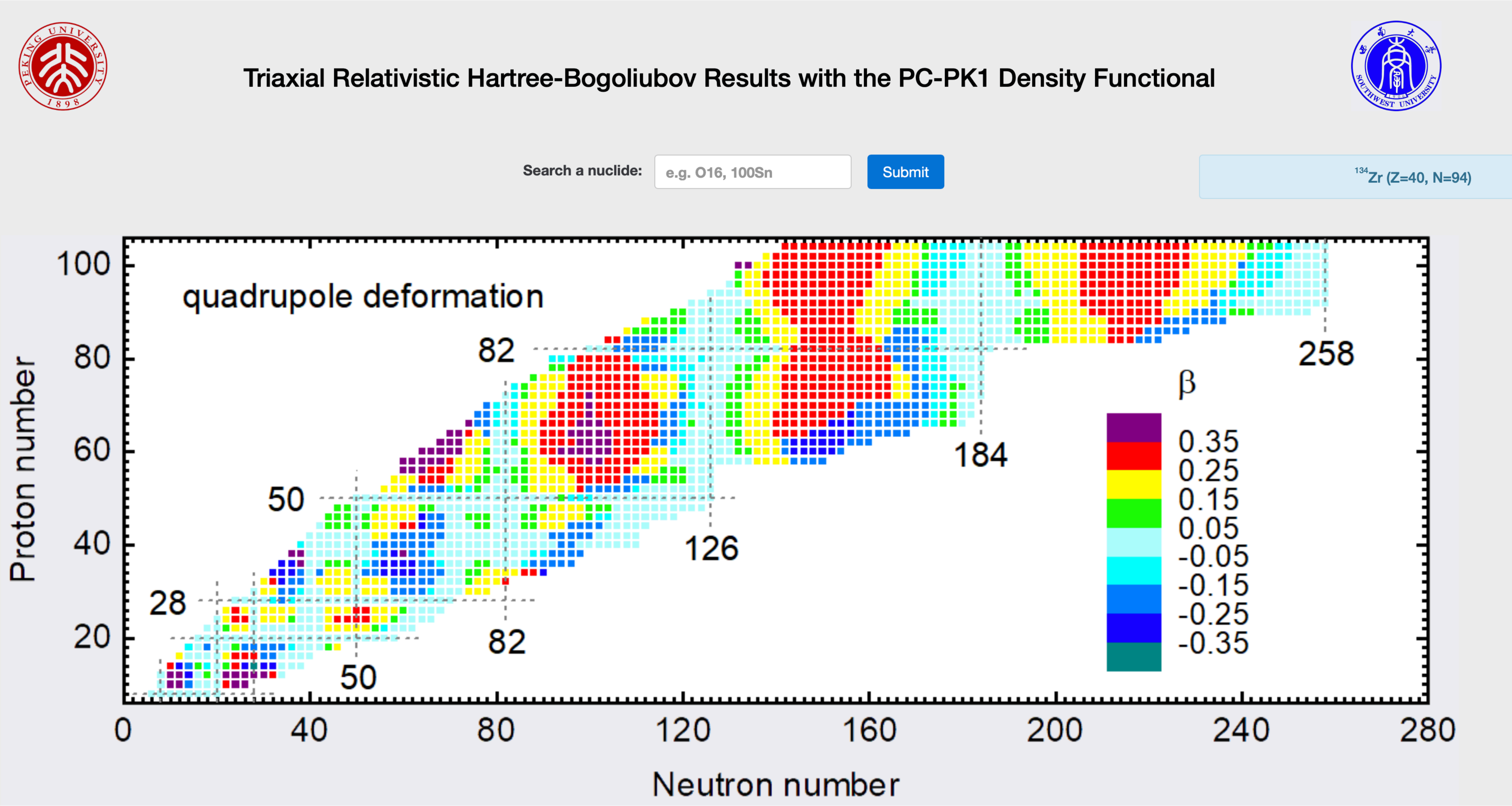
^{286}No
Ground state
Isomeric state
E [MeV]
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.02
0.04
0.06
0.08
0.10
0.12
a_{32}


E [MeV]
0.8
0.4
0.0
^{252}No
(a)
^{254}No
(b)
-0.06
-0.04
-0.02
0.00
0.06
0.04
0.02
0.00
β_{30}
β_{60}
0.6
0.4
0.2
0.0
$|A_{f_{7/2}}|^2/|A_{i_{13/2}}|^2$
^{252}No
^{254}No
(c)
0.0
0.1
0.2
0.3
$\hbar\omega$ [MeV]

How many nuclei are bound?

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

Triaxial RHB + 5DCH



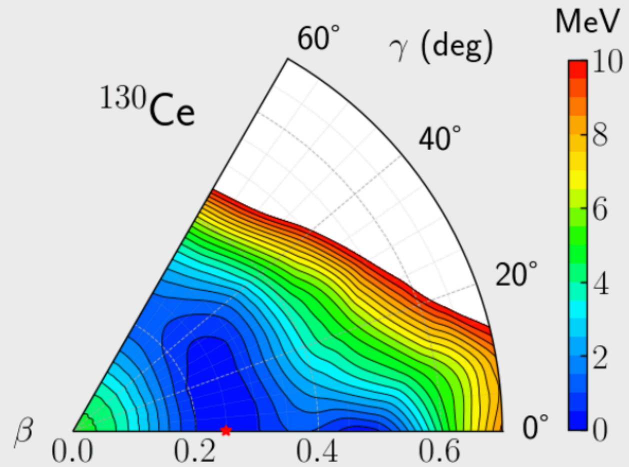
Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

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

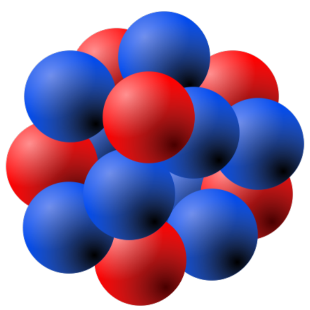
^{132}Nd

^{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)

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

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 Theory of Highly Condensed Matter*

J. D. Walecka

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

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