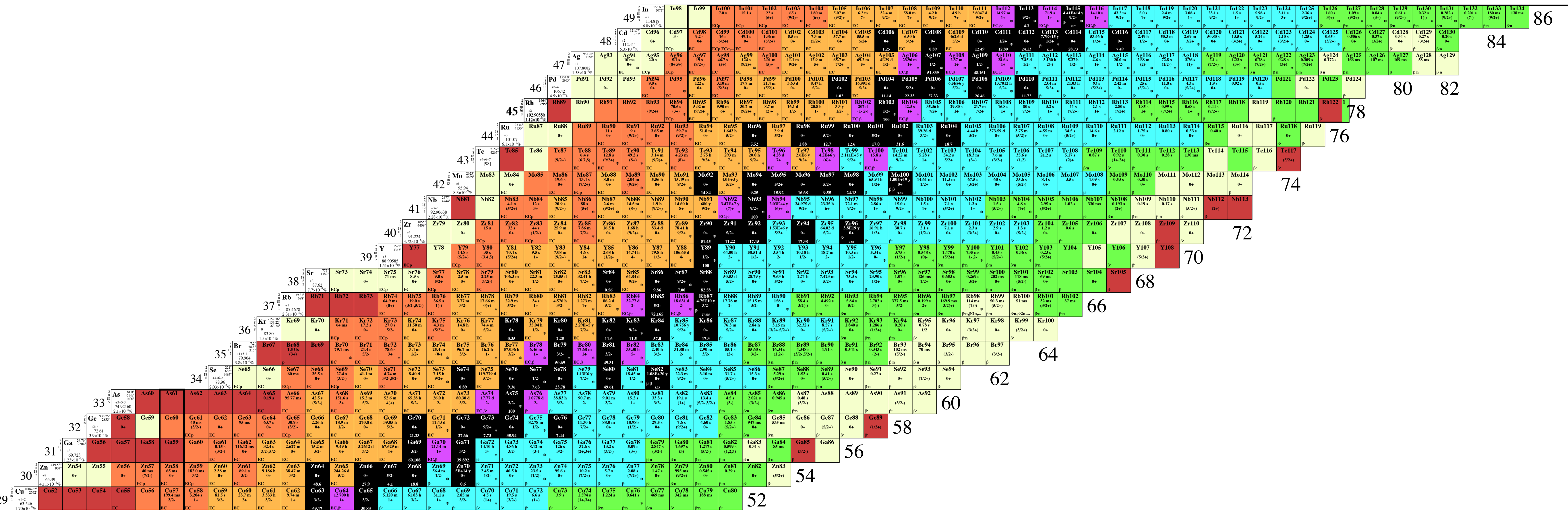
Shape evolution, mixing and coexistence around Z = 30-48 studied with beyond-mean-field methods



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CGS 17 Grenoble

July 17th, 2023

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gfn UCM Grupo de Física Nuclear

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J. L. Egido (UAM)

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Outline

1. Introduction. Theoretical framework

2. Multiple shapes in ^{84}Mo, ^{80}Zr and ^{110}Cd

3. Shape evolution and systematics

4. Summary and outlook

Outline

1. Introduction. Theoretical framework
2. Multiple shapes in ^{84}Mo, ^{80}Zr and ^{110}Cd
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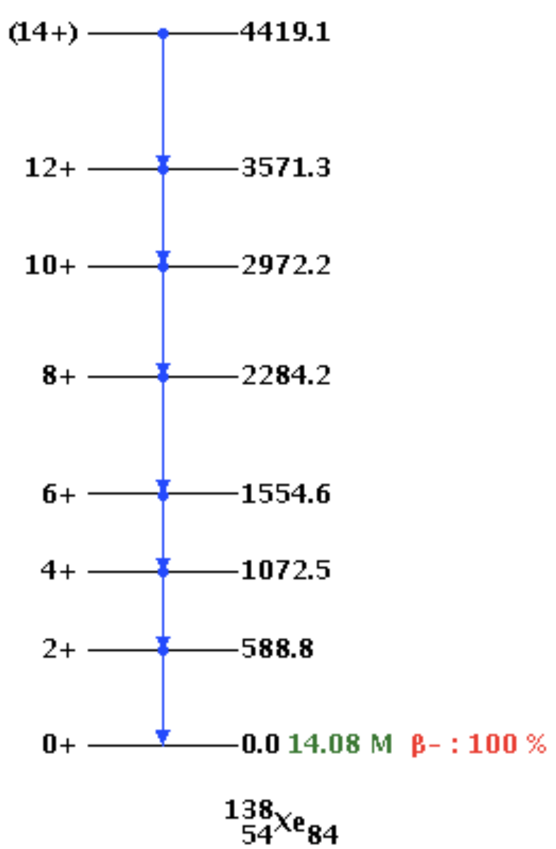
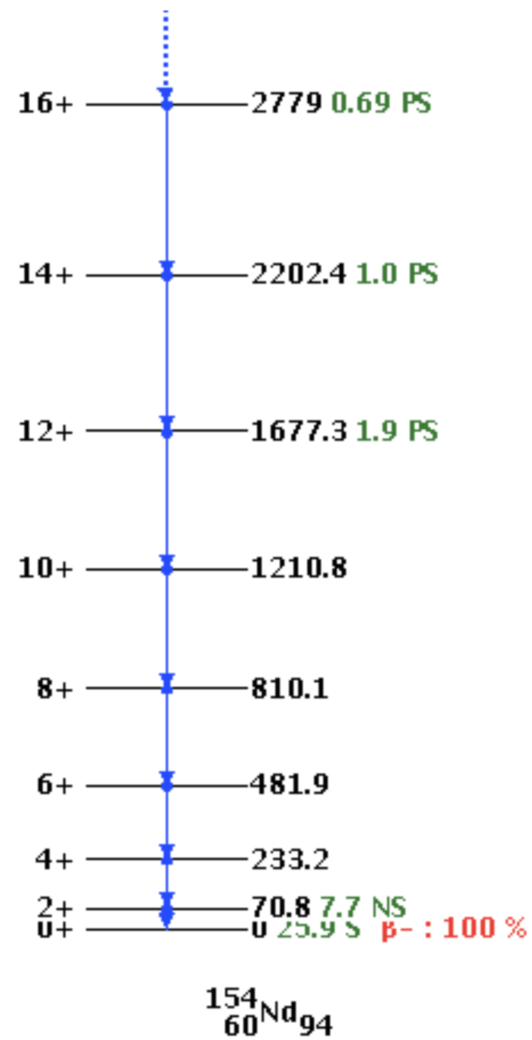
Introduction

- Intrinsic nuclear shapes can be inferred from the experimental data (energies and electromagnetic moments and transitions) by comparison with the predictions given by geometrical (simple) models.





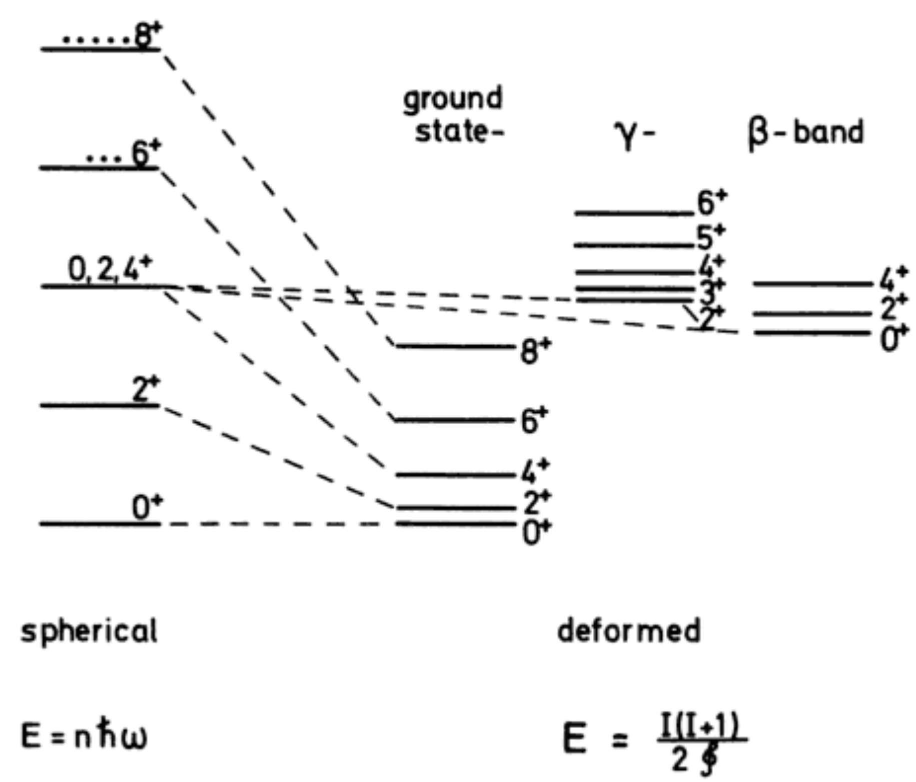


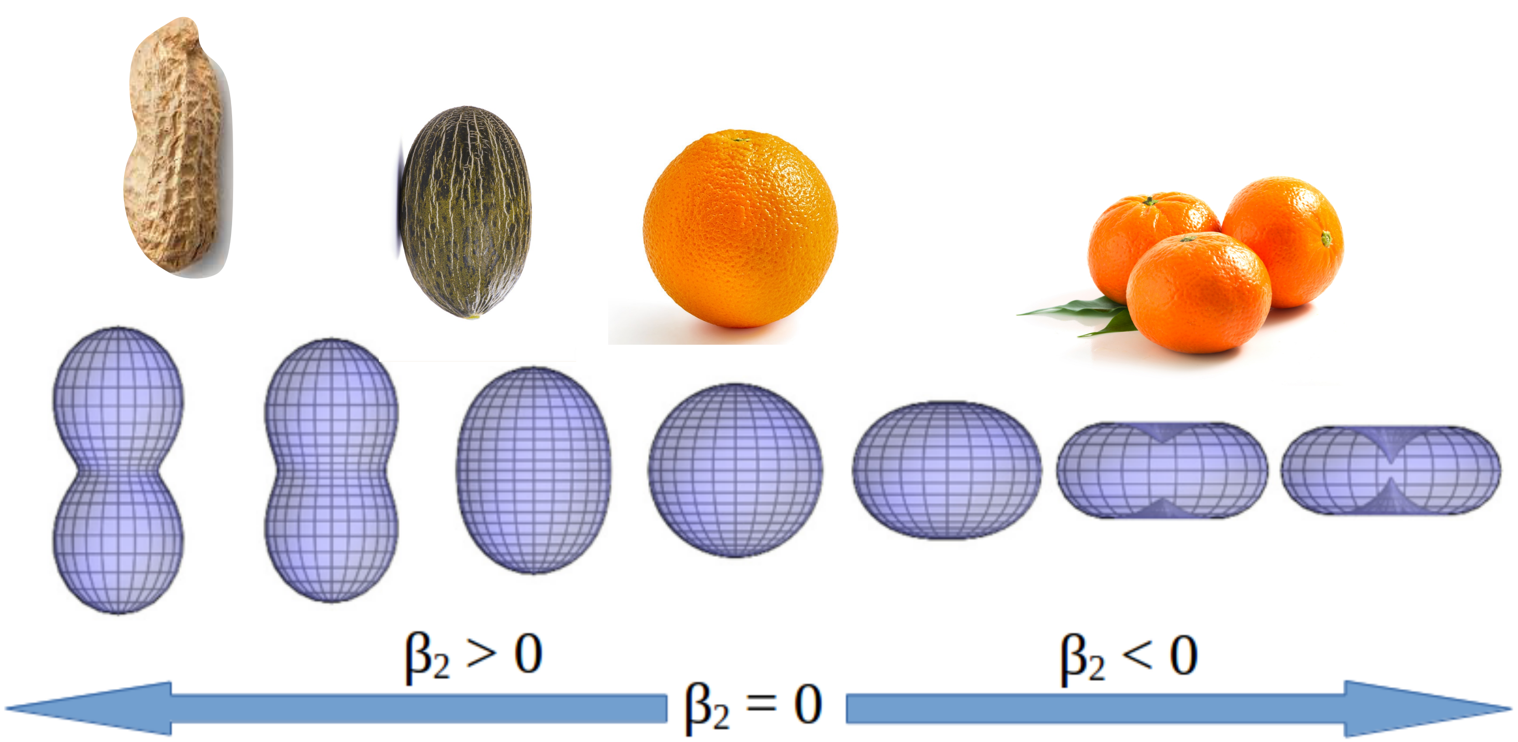
Figure 1.12. Schematic level schemes of spherical and deformed nuclei. (From [SDG 76].)

P. Ring and P. Schuck, *The Nuclear Many-Body Problem*

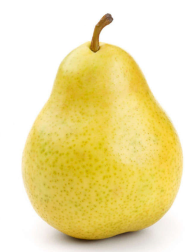
Introduction

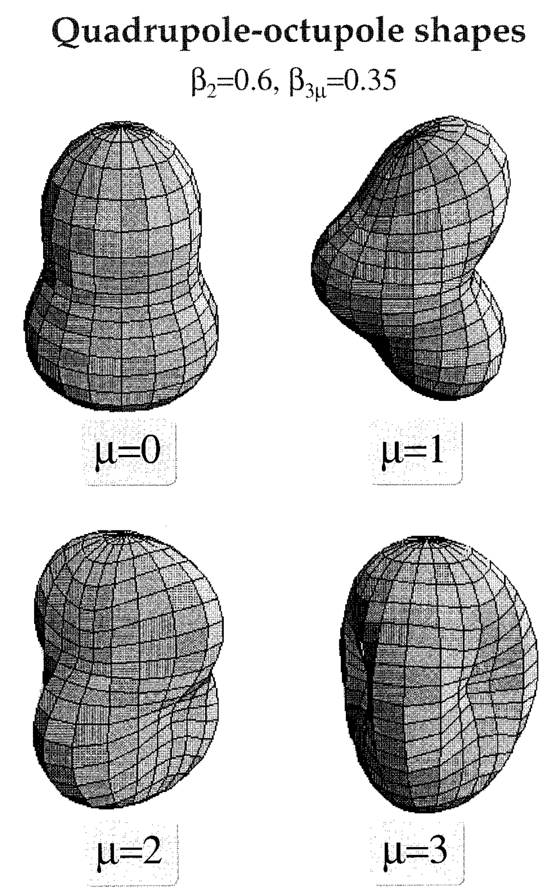
- **Collective models** are based on the parametrization of the nuclear radius with a multipole expansion

$$R(\Omega) = c(\alpha) R_0 \left[1 + \sum_{\lambda=2}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{+\lambda} \alpha_{\lambda\mu} Y^*_{\lambda\mu}(\Omega) \right]$$



axial quadrupole shapes

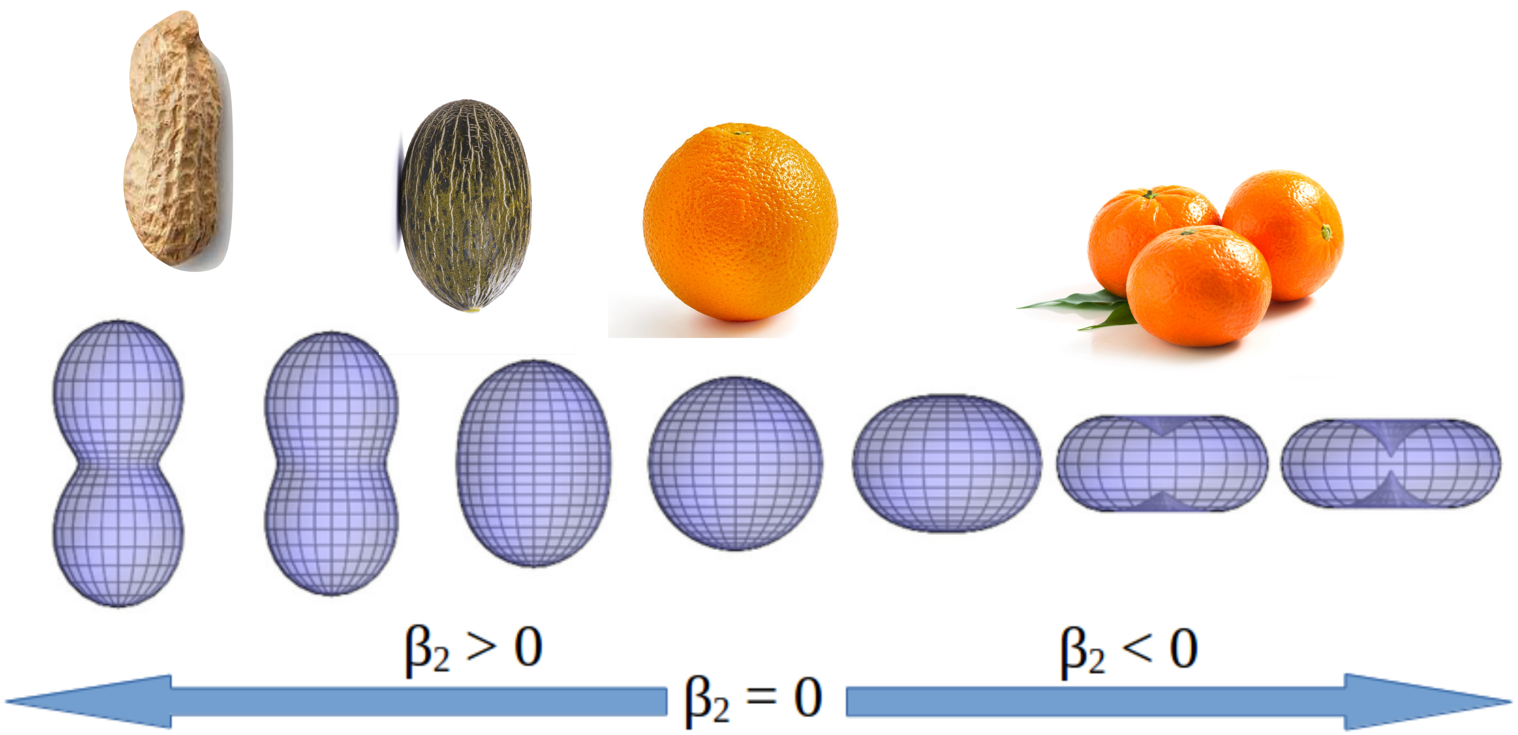




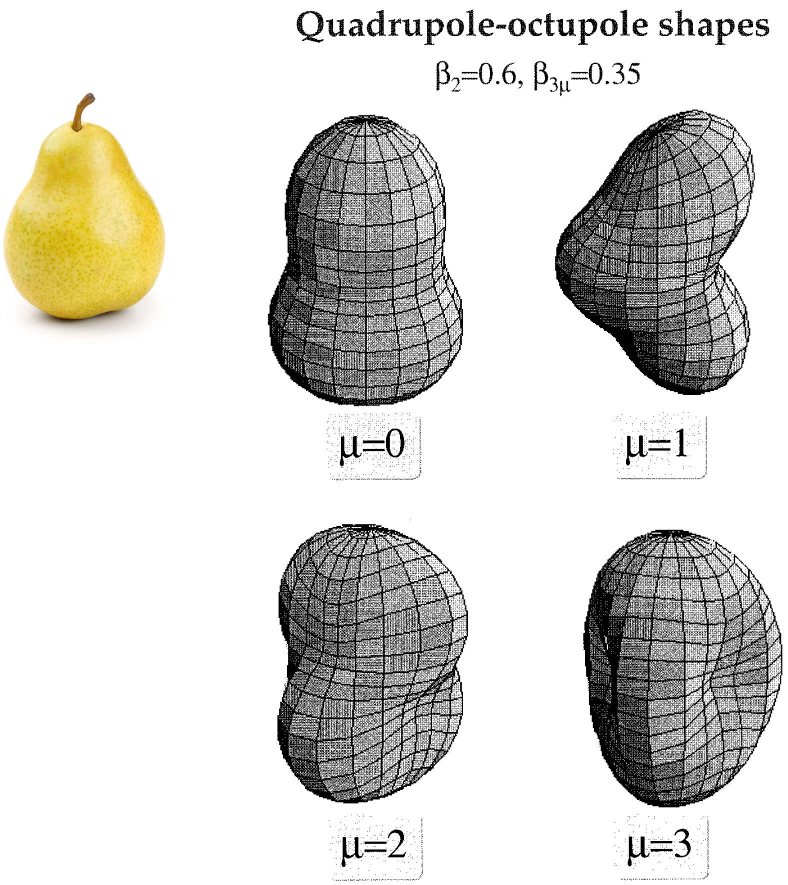
P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

Introduction

Can we provide a **microscopic** description of these collective phenomena?



axial quadrupole shapes



P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

Introduction

The nuclear many-body problem is solved using

Gogny energy density functional as the underlying nuclear interaction

Symmetry conserving configuration mixing (SCCM)

A.K.A.

Projected generator coordinate method (PGCM)

Multi-reference energy density functional (MR-EDF)

to solve the quantum *A*-body problem

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P^{J}_{MK} P^{N} P^{Z} P^{\pi} \boxed{|\Phi(q)\rangle}$$

$$\Gamma \equiv (JMNZ\pi)$$

"basis" states

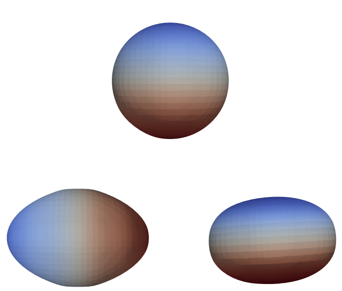
Intrinsic (HFB-like, Bogoliubov quasiparticle vacuum) state:

$$|\Phi(q)\rangle \rightarrow \beta_b(q)|\Phi(q)\rangle = 0 \quad \forall \quad b \qquad \beta_b^{\dagger}(q) = \sum_a U_{ab}(q)c_a^{\dagger} + V_{ab}(q)c_a$$

variational!

We minimize the particle number projected energy functional

even-even



$$E'_{\mathrm{PNVAP}}\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^{N}P^{Z}|\Phi(q)\rangle}{\langle\Phi(q)|P^{N}P^{Z}|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q\hat{Q}|\Phi(q)\rangle$$

M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A 696, 467 (2001).

Constraints $q \rightarrow$ quadrupole deformations; octupole deformations; pairing content; intrinsic rotations

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} \boxed{P_{MK}^{J} P^{N} P^{Z} P^{\pi}} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

“basis” states

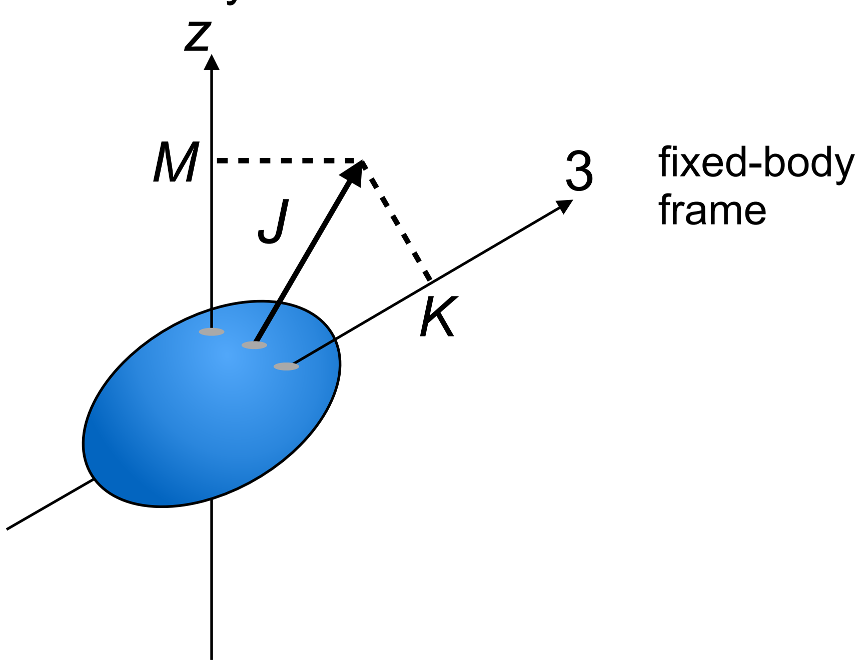
Symmetry restoration

$P_{MK}^{J} \longrightarrow$ angular momentum projector

$P^{N} \longrightarrow$ neutron number projector

$P^{Z} \longrightarrow$ proton number projector

$P^{\pi} \longrightarrow$ spatial parity projector



Theoretical framework

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} \boxed{f_{\sigma;qK}^{JMNZ\pi}} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

coefficients of the linear combination

The coefficients are obtained by minimizing the expectation value of the Hamiltonian (energy) with those coefficients as the variational parameters:

$$\sum_{q'K'} \left(\mathcal{H}_{qK,q'K'}^{\Gamma} - \boxed{E_{\sigma}^{\Gamma}} \mathcal{N}_{qK,q'K'}^{\Gamma}\right) \boxed{f_{\sigma;q'K'}^{\Gamma}} = 0$$

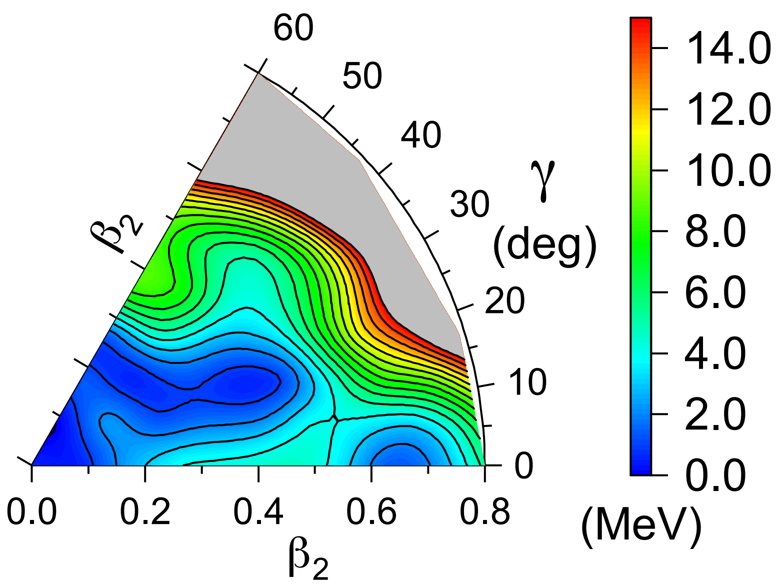
Hill-Wheeler-Griffin (HWG) equation

$$\mathcal{H}_{qK,q'K'}^{\Gamma} = \langle\Phi(q)|\hat{H} P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle,$$
$$\mathcal{N}_{qK;q'K'}^{\Gamma} = \langle\Phi(q)|P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle$$

Hamiltonian and norm kernels

(β_2, γ)-plane

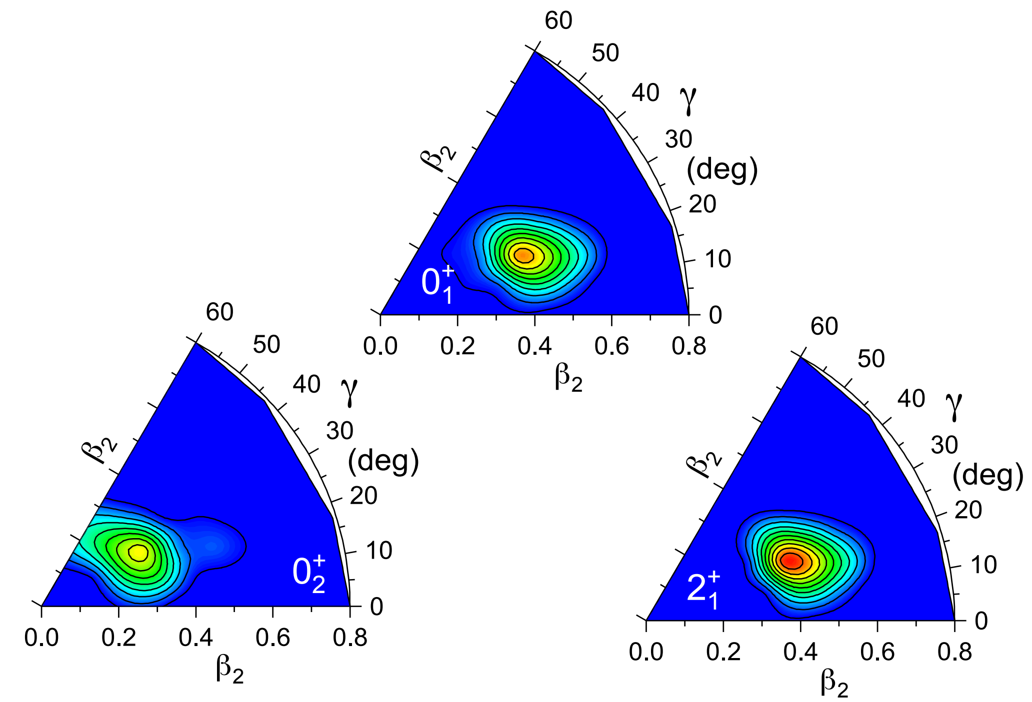
Total energy surface (TES)



PN-VAP **energy** in the triaxial plane:

- no angular momentum projection
- no shape mixing
- Wrongly named Potential energy surface (PES)

Collective wave functions

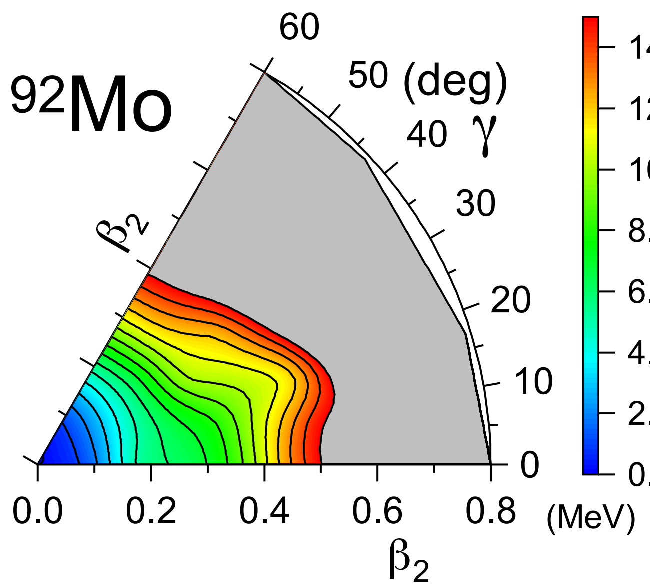


Most relevant shapes to build an individual SCCM state

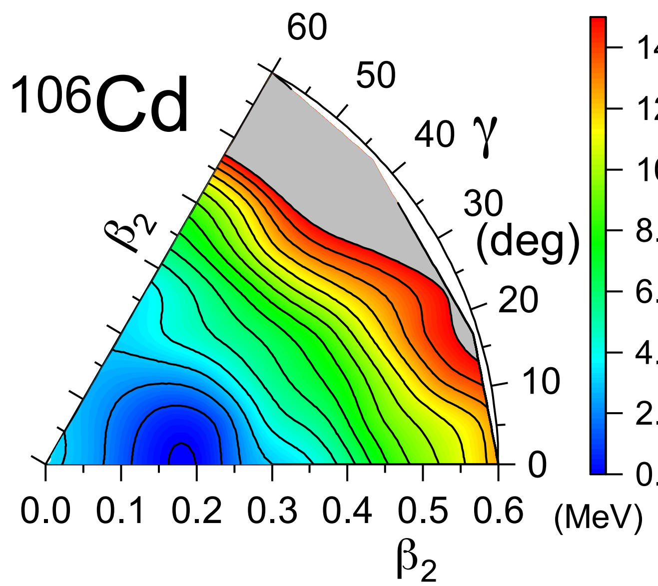
- **“probability"**
- after angular momentum projection and shape-mixing

Taxonomy of quadrupole shapes

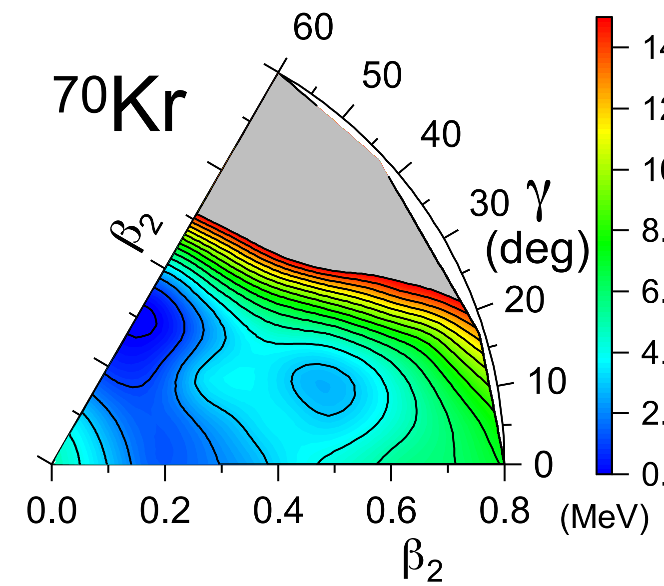
Spherical



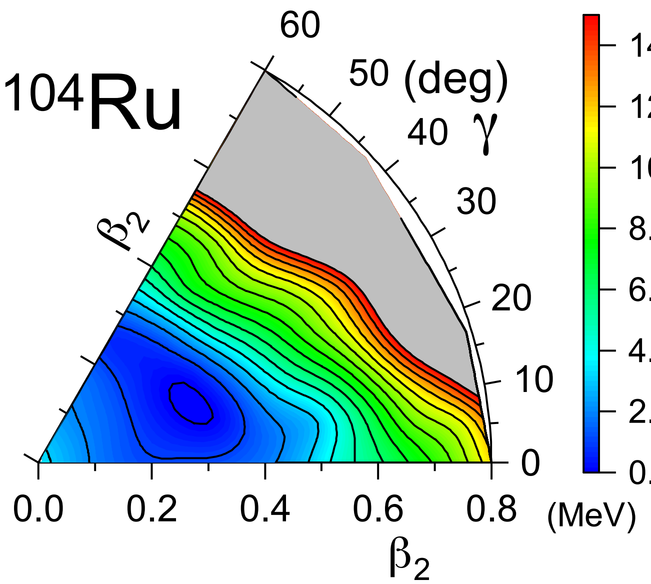
Axial prolate



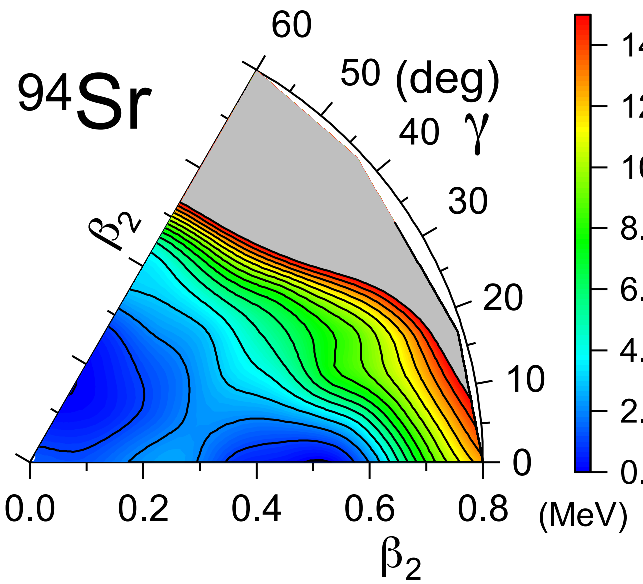
Axial oblate



Triaxial / γ-soft



Shape-coexistence



- First classification of the collective quadrupole behavior of the nucleus based on the **total energy surfaces** (**TESs**)

- Shape-coexistent TESs are rather common in the Ni-Sn region

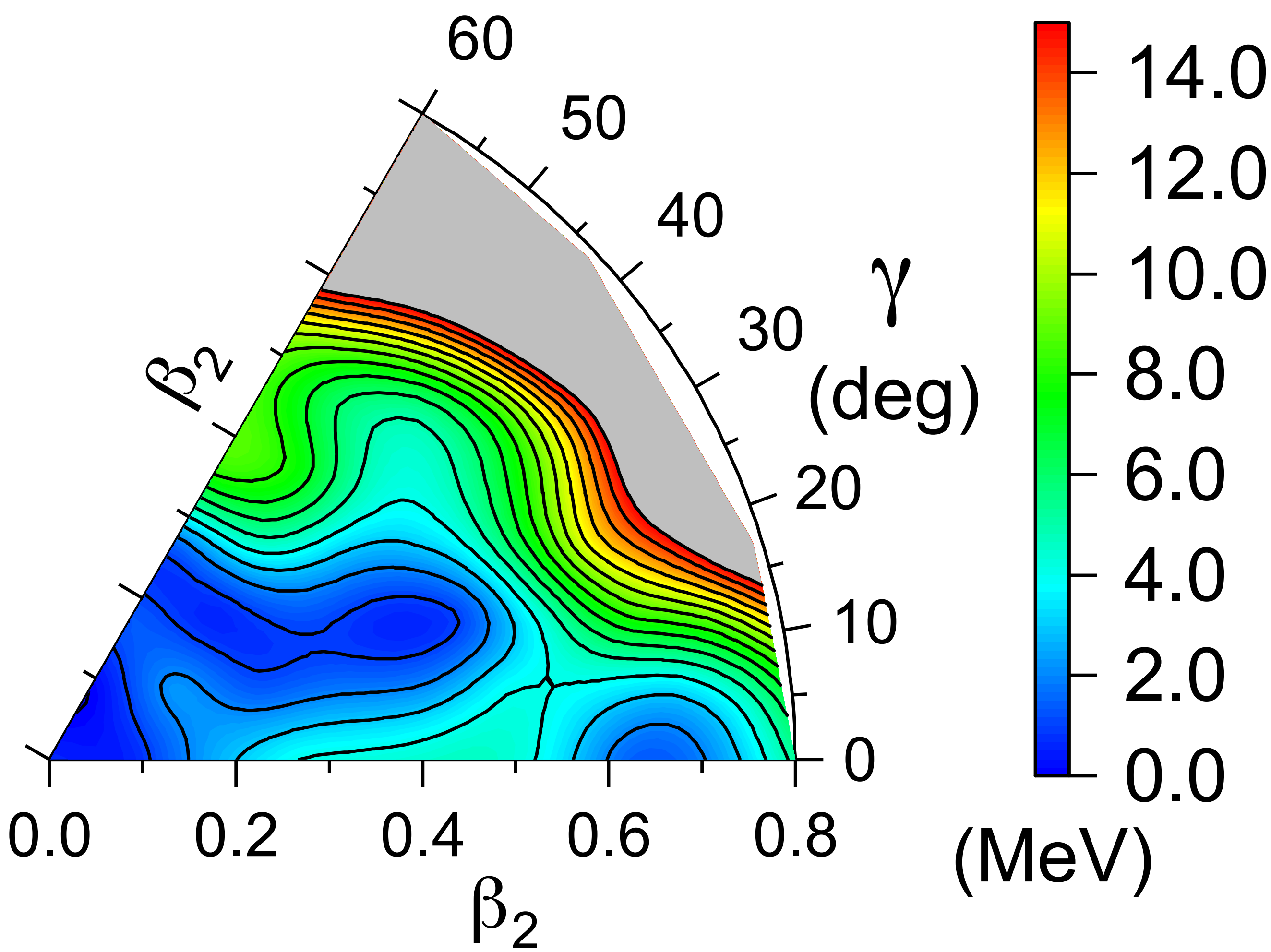
- Final theoretical interpretation of the spectrum is given by the analysis of the excitation energies, electromagnetic properties and the collective wave functions

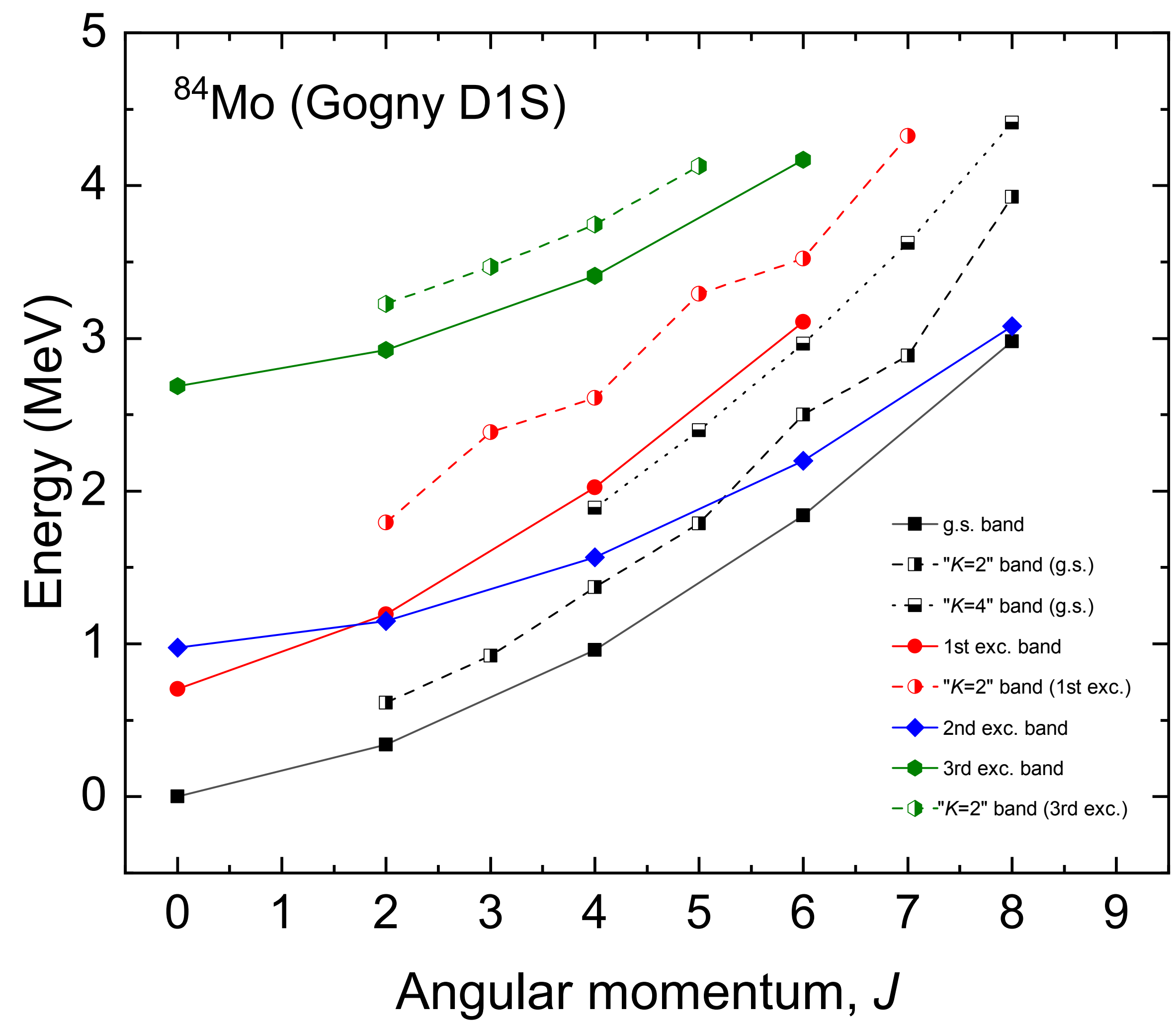
Outline

Multiple Shape Coexistence (A)

$^{84}Mo_{42}$

- Several minima in the total energy surfaces (TES)
- Different collective bands are built on top of those minima





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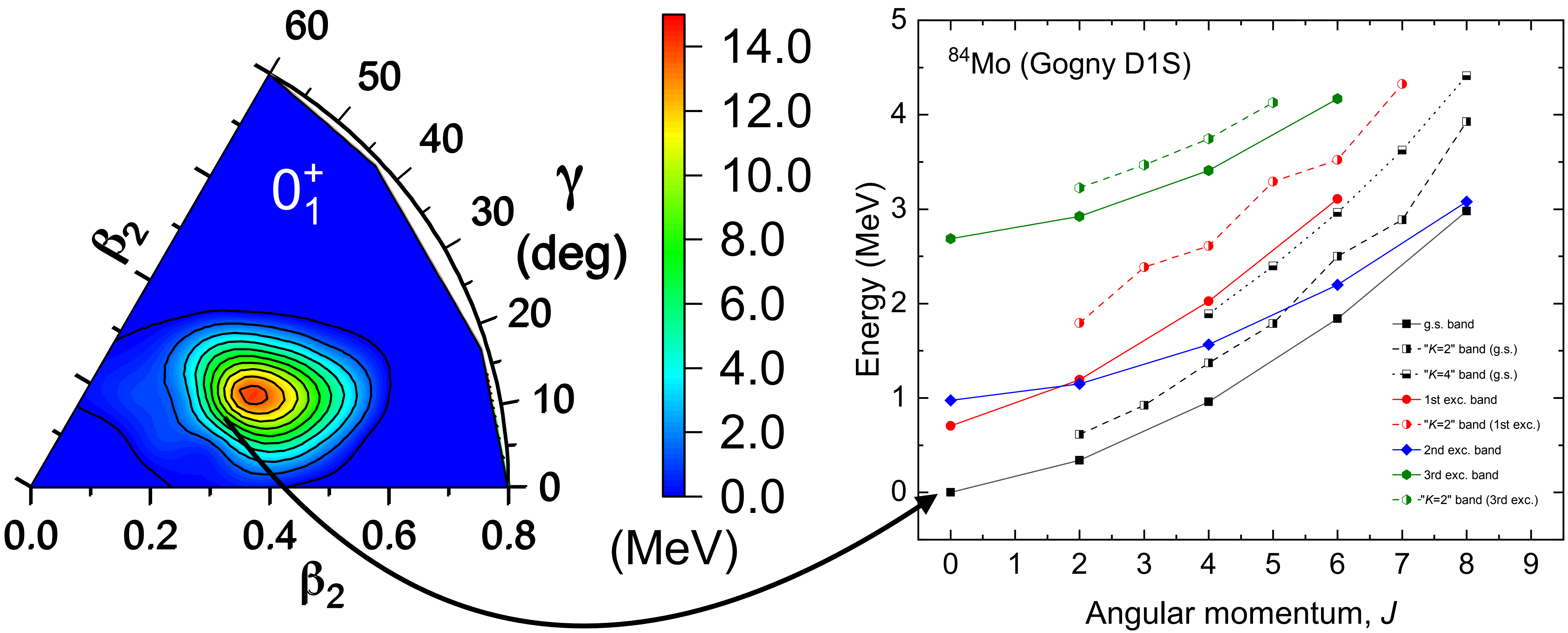

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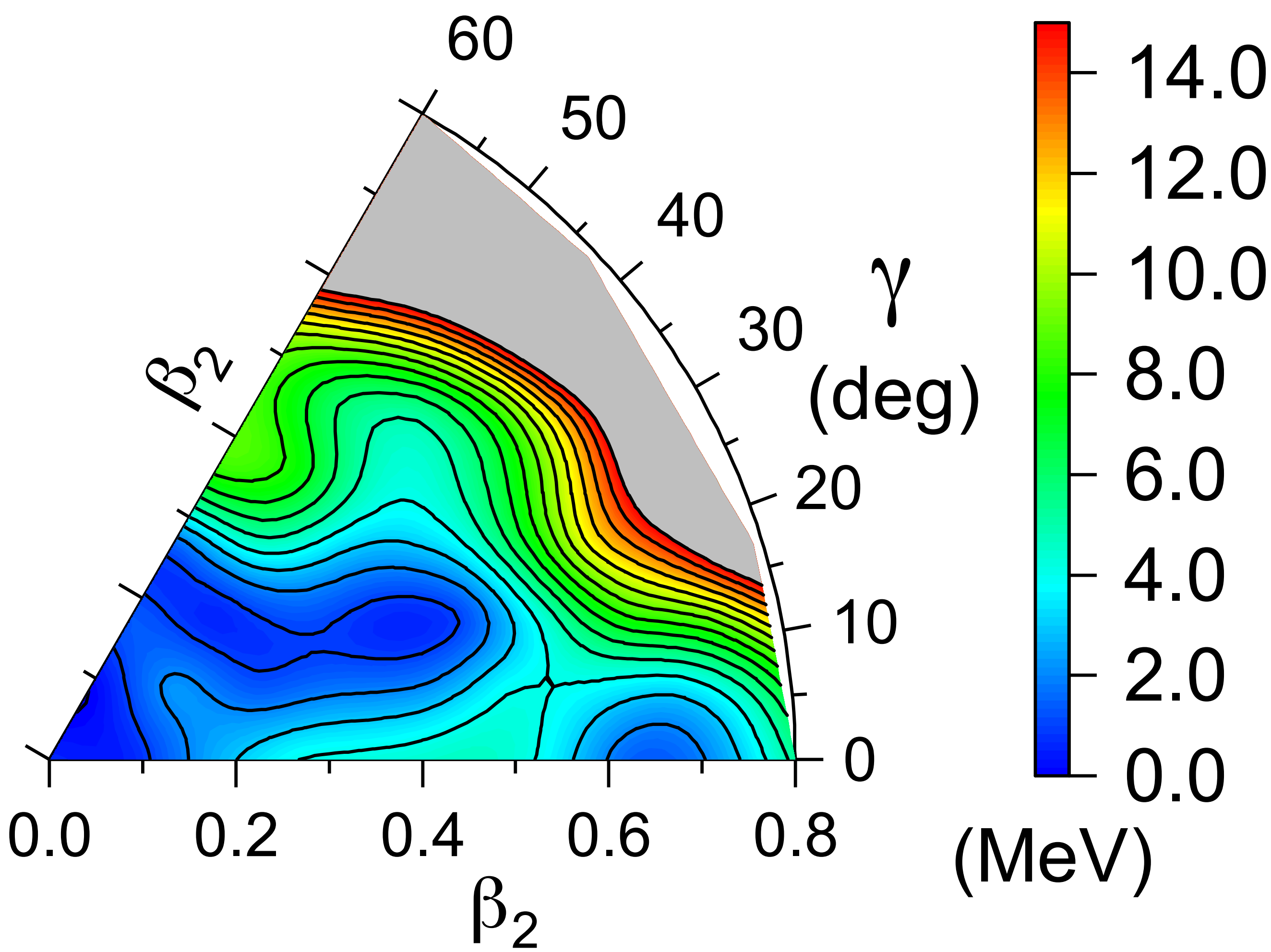

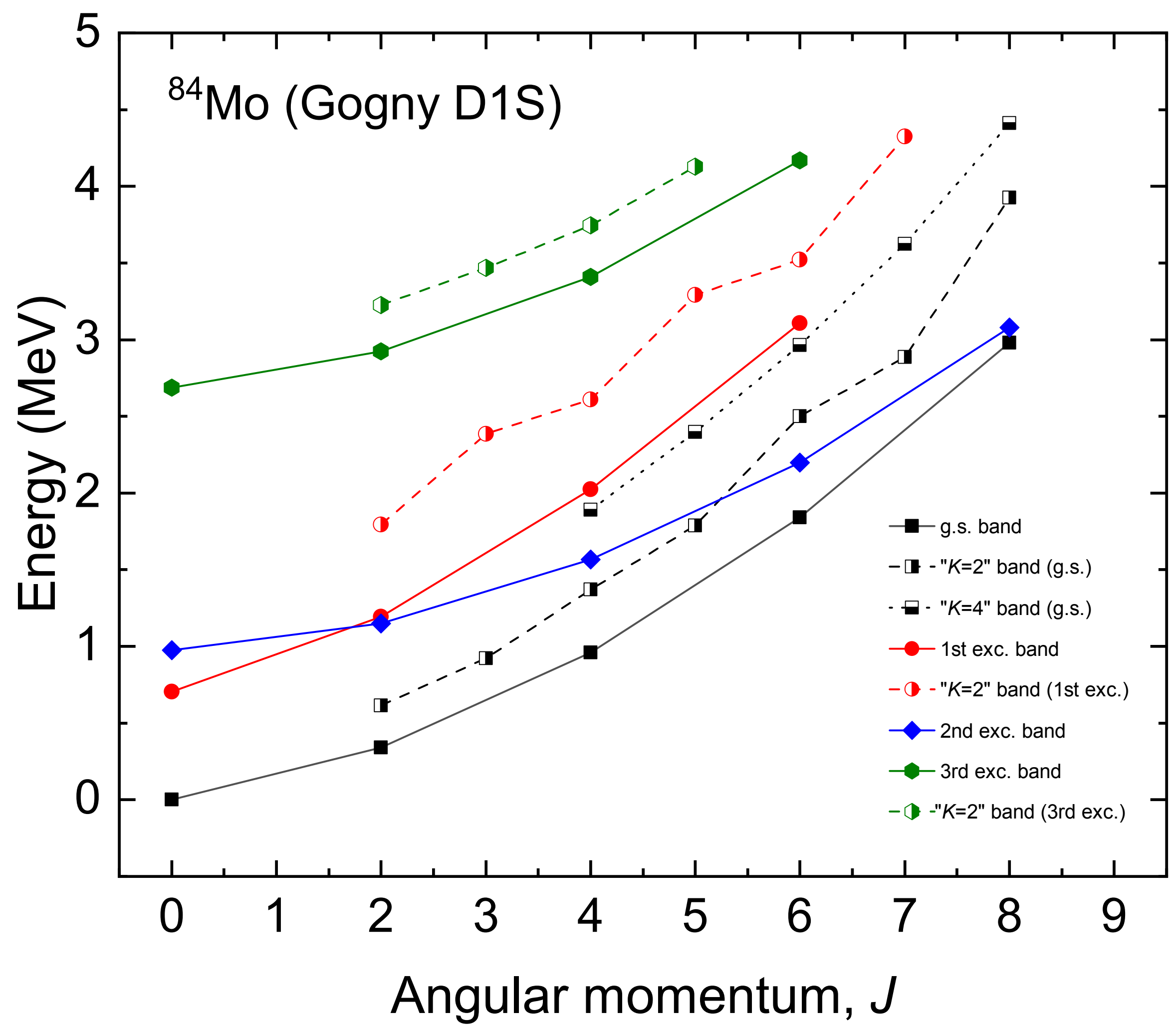

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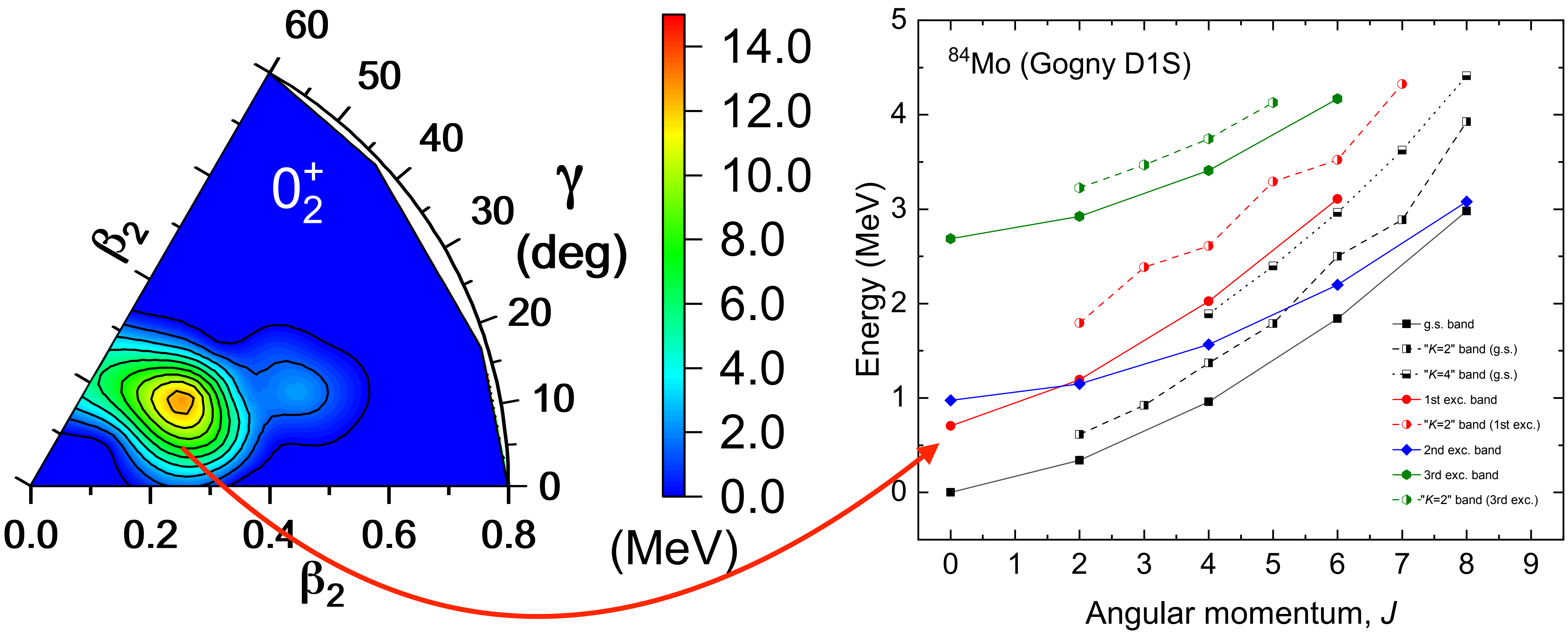

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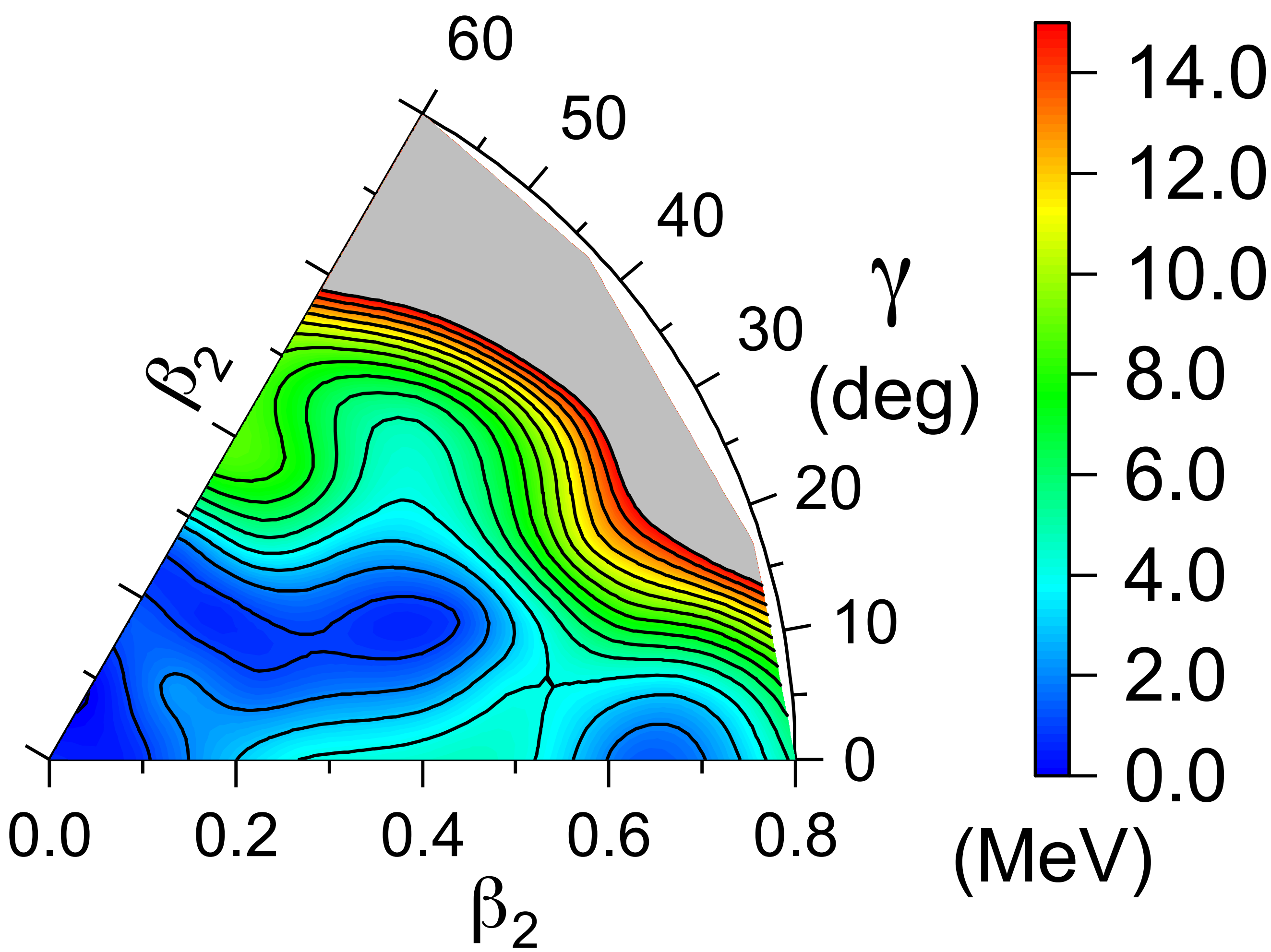

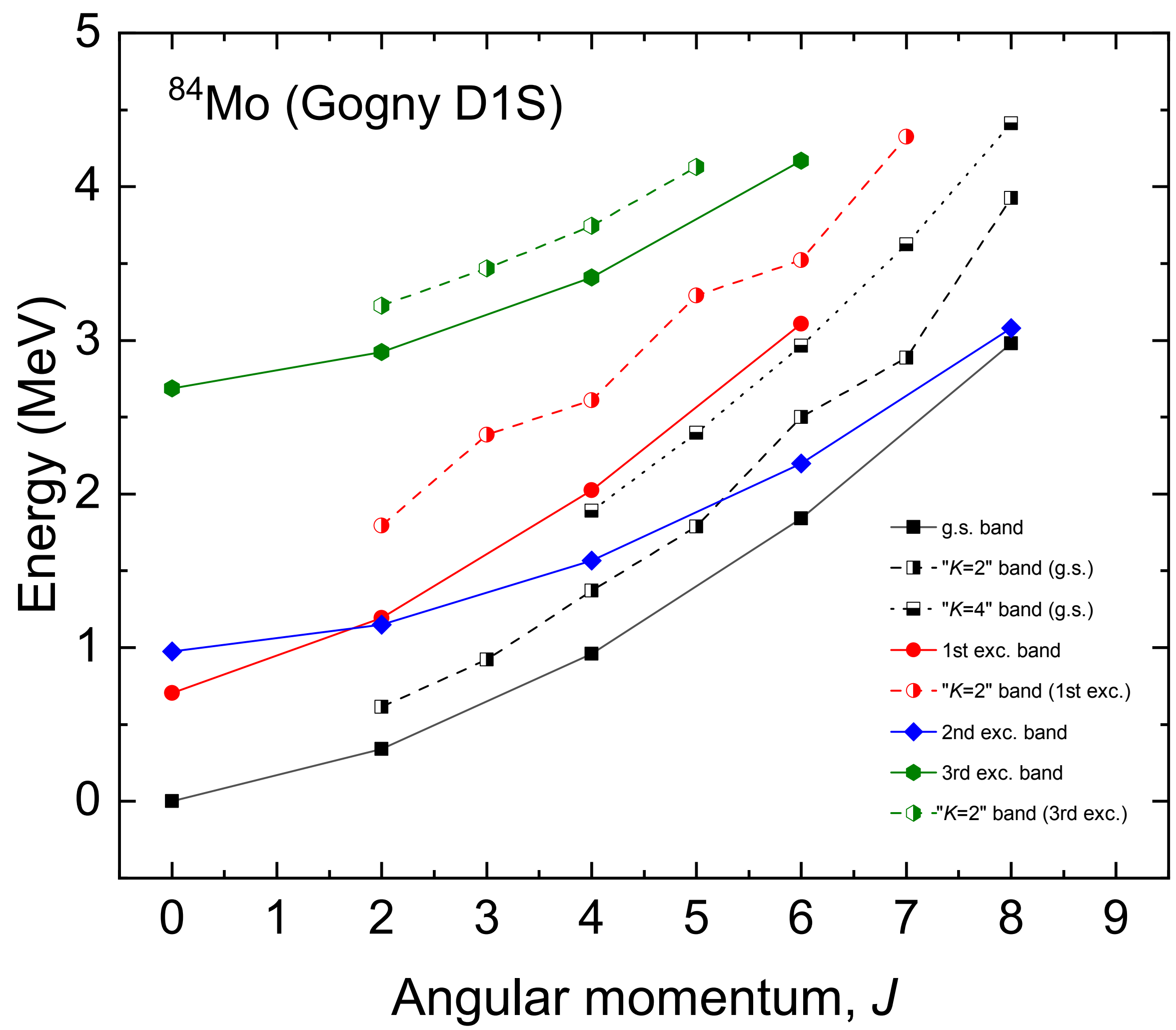

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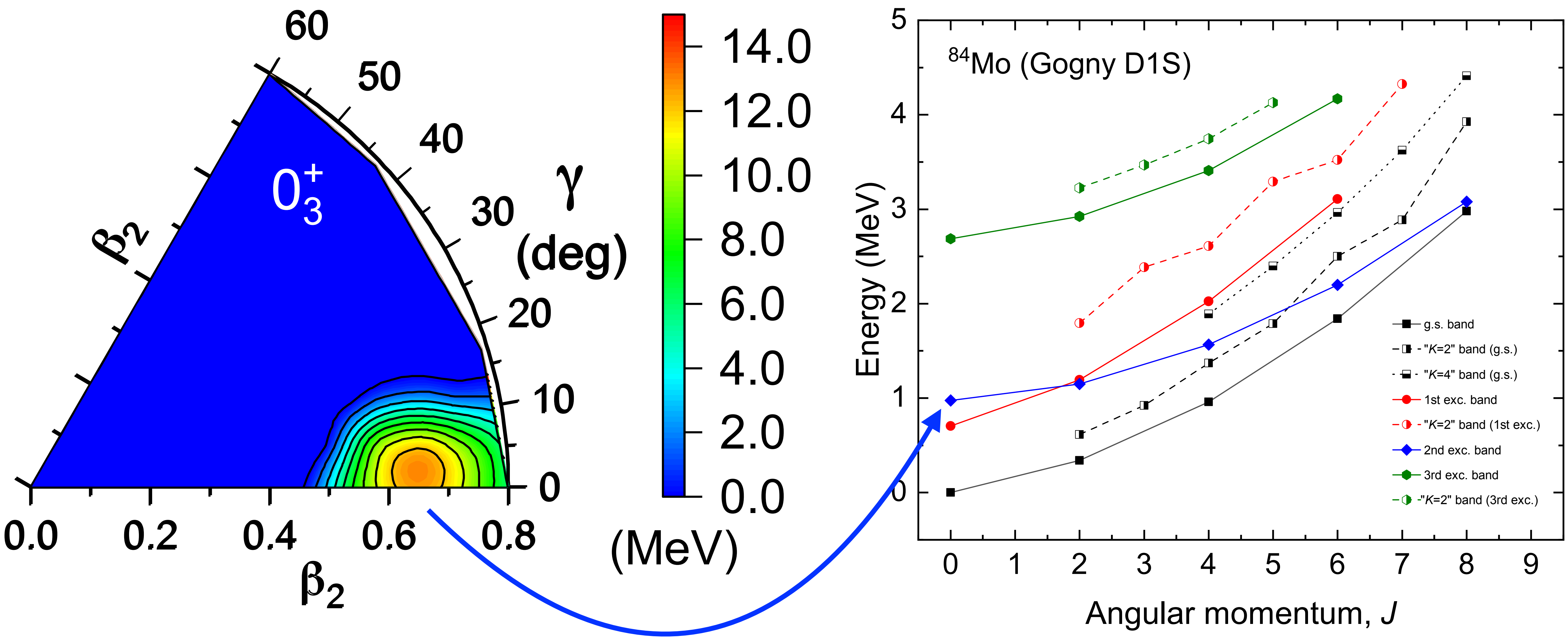

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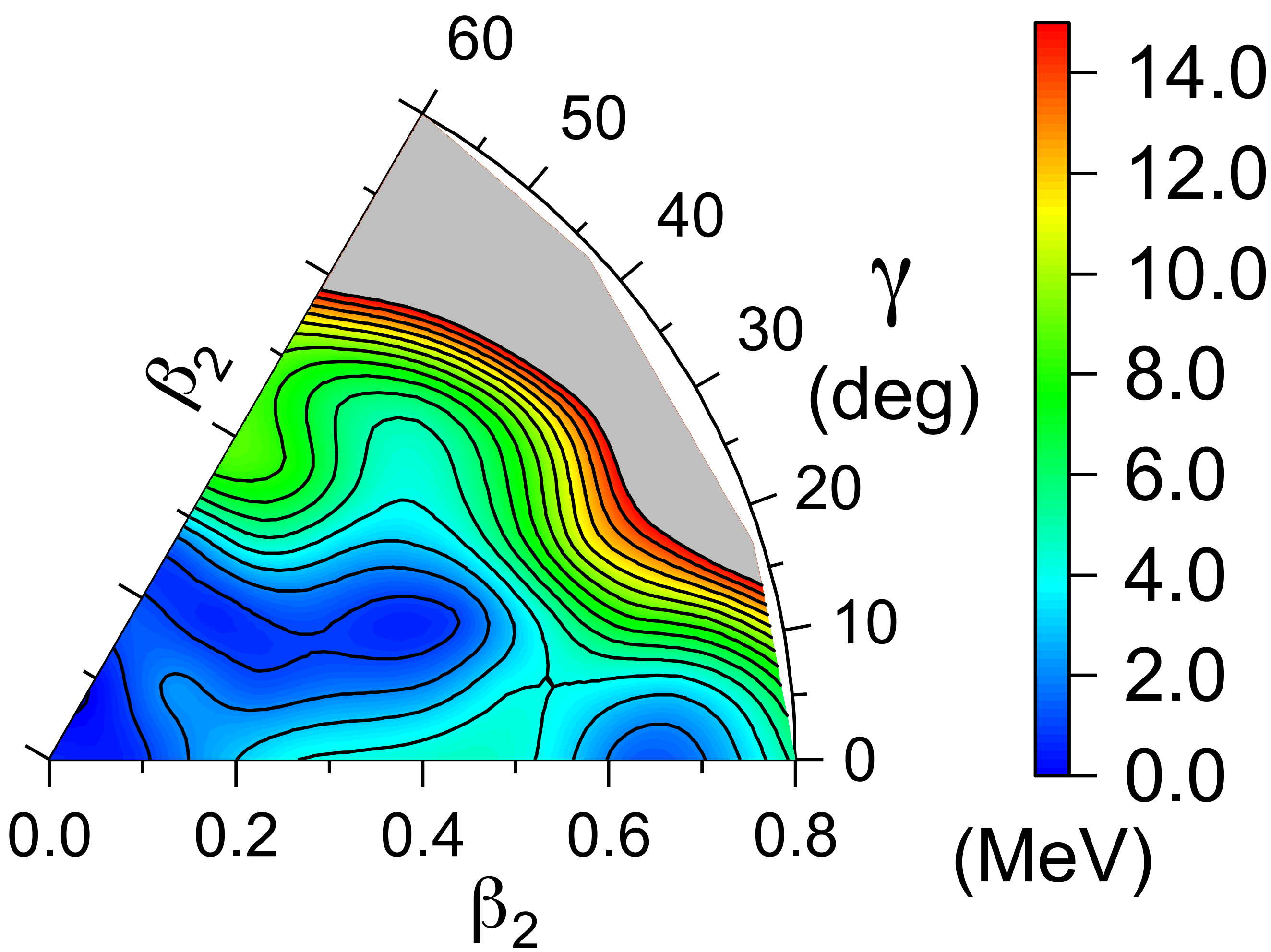

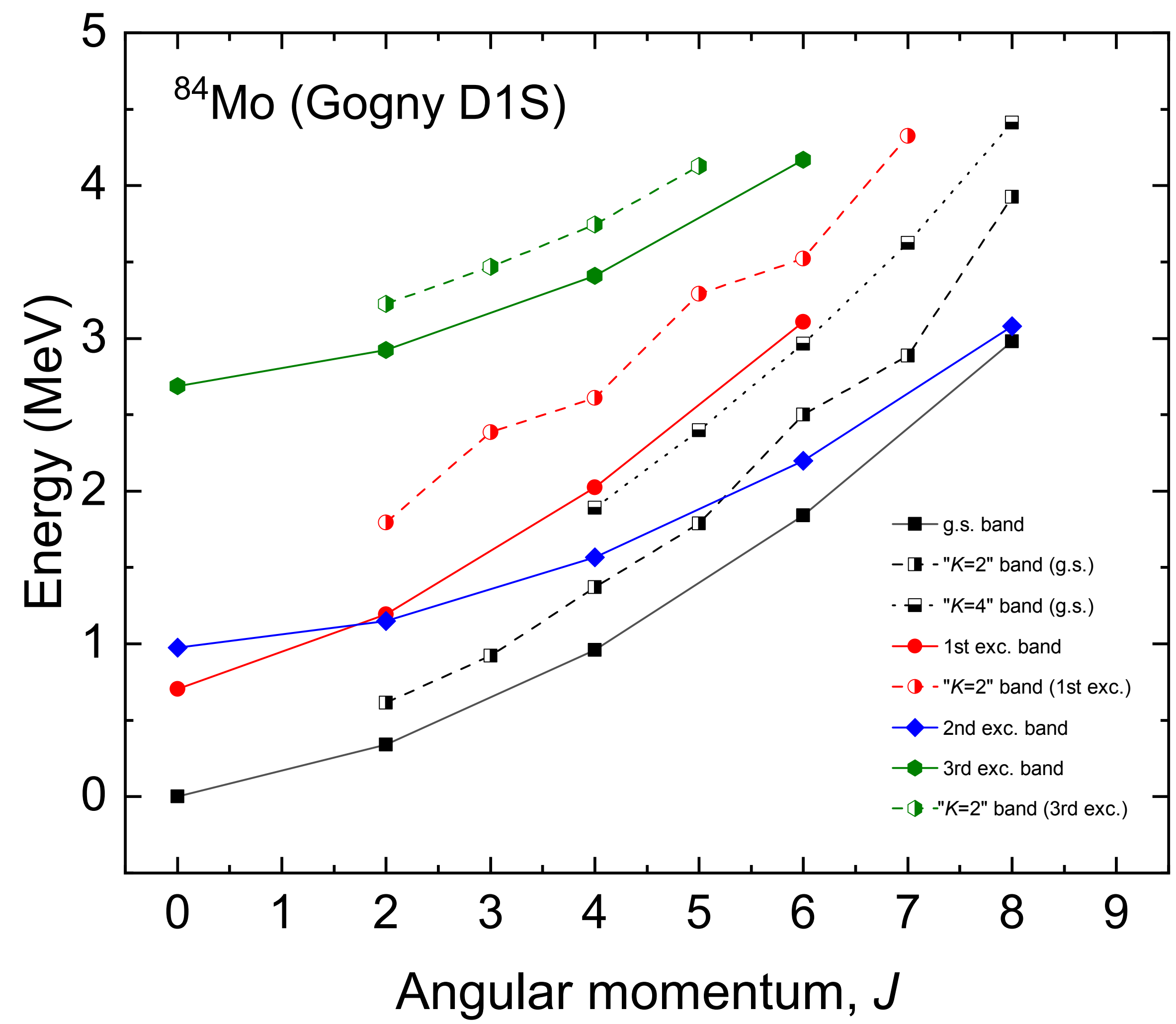

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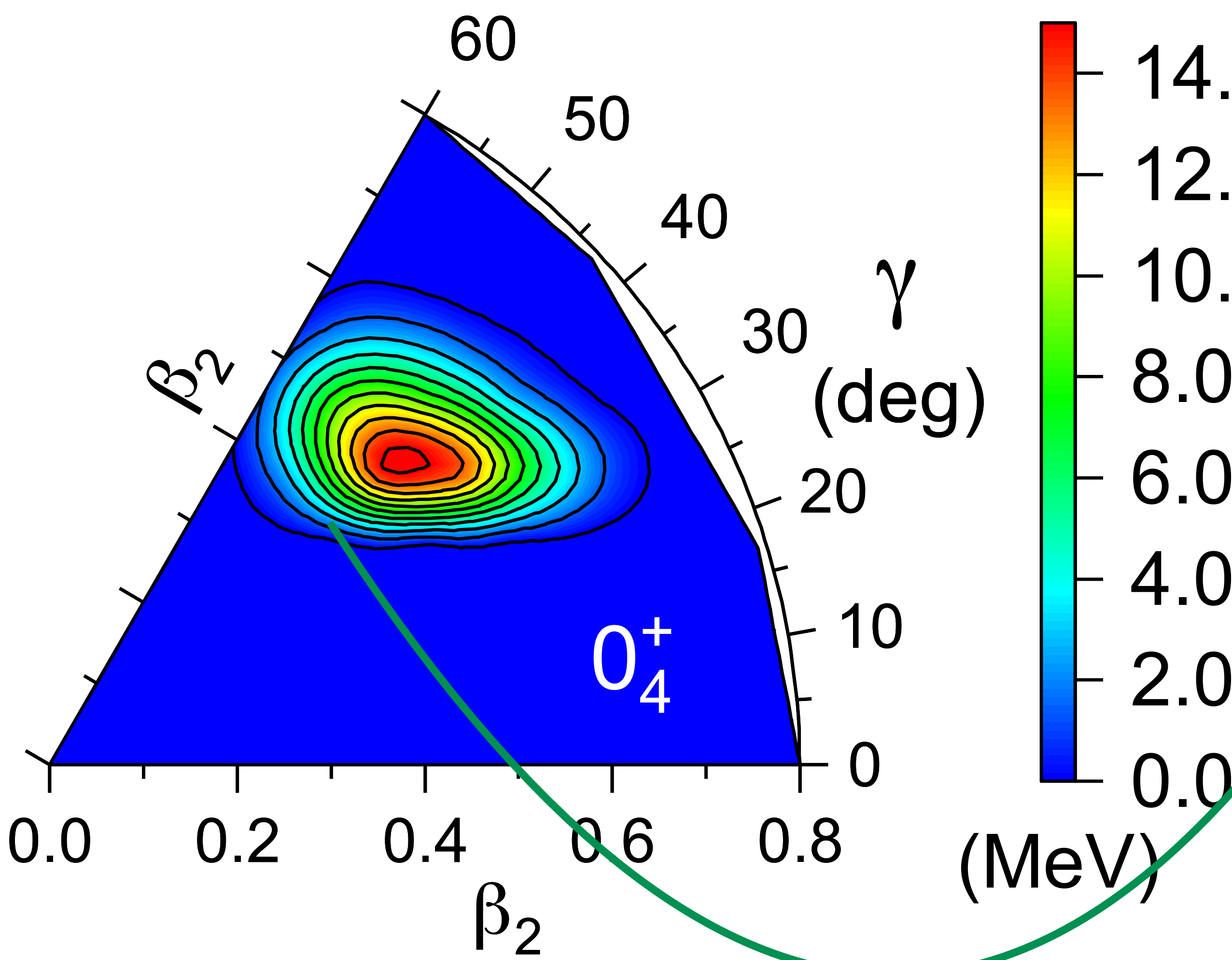

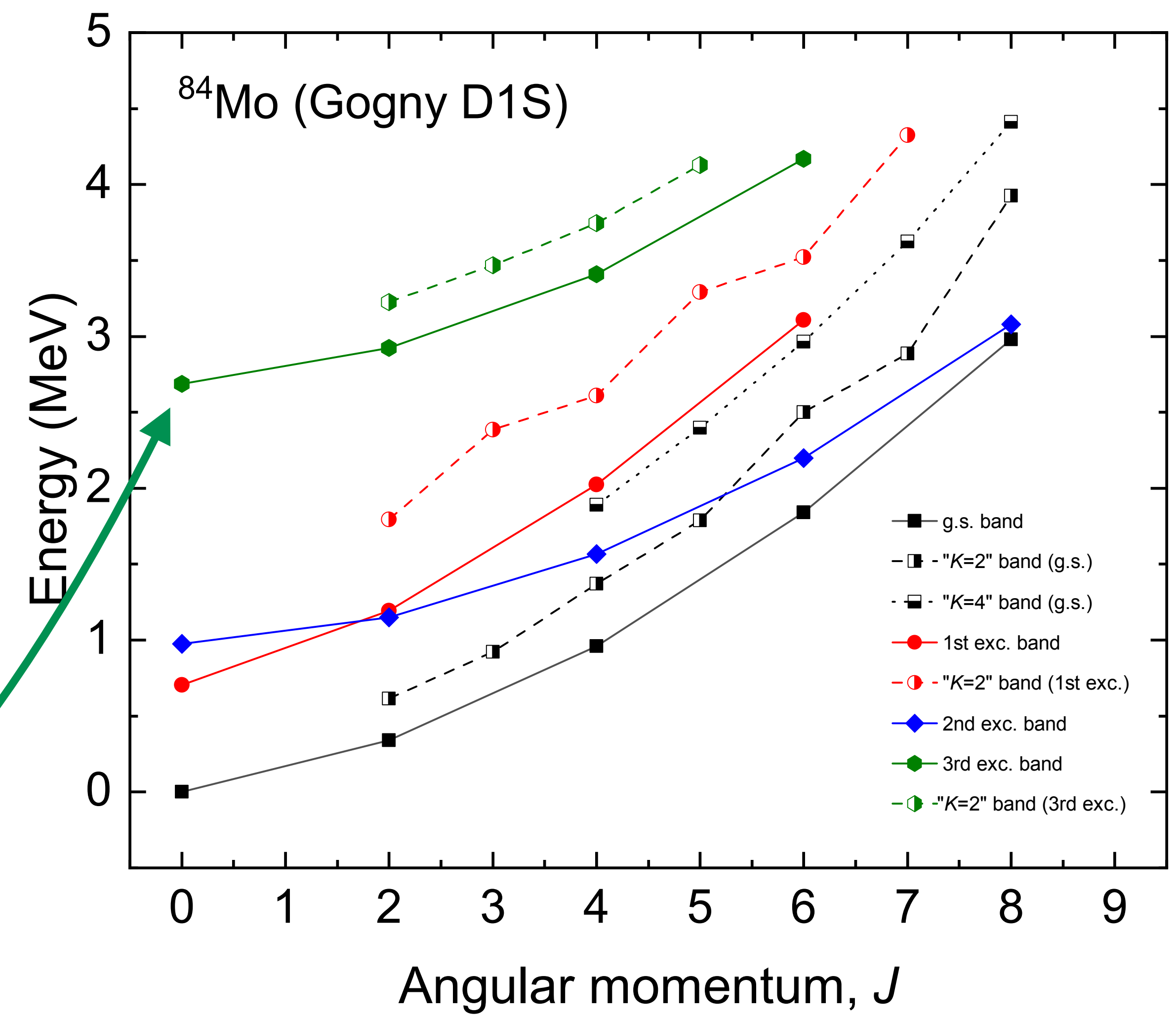

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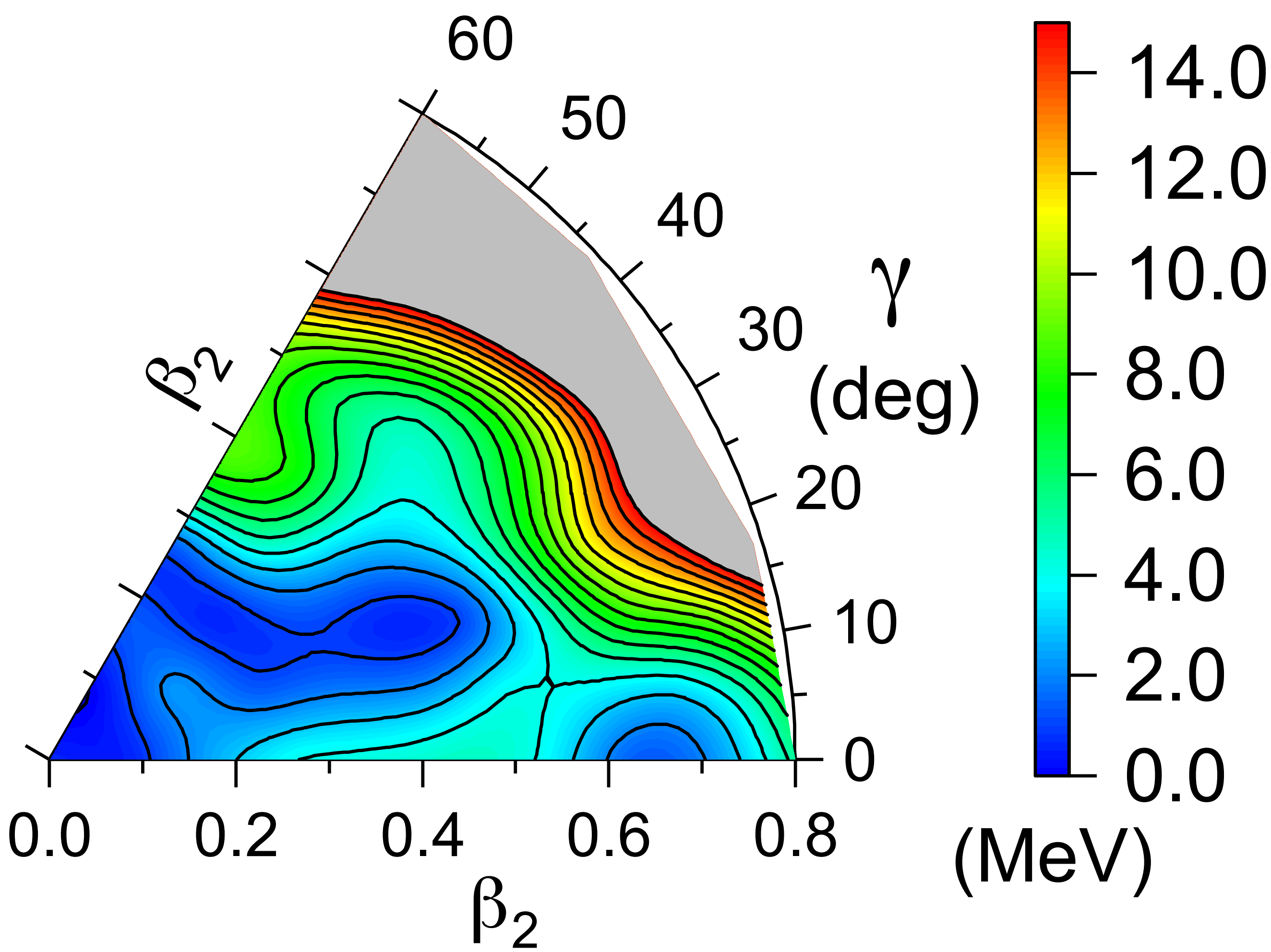

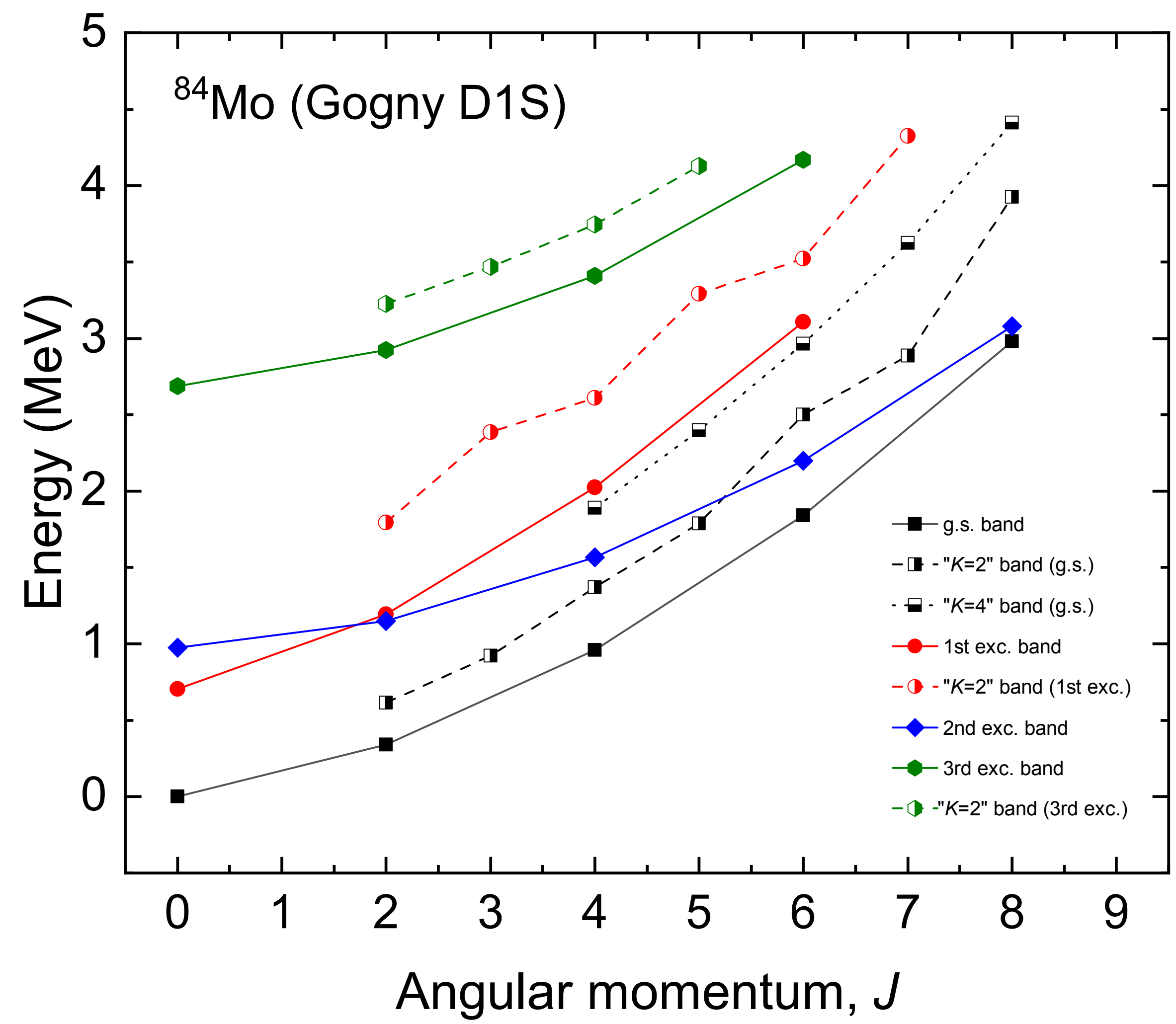

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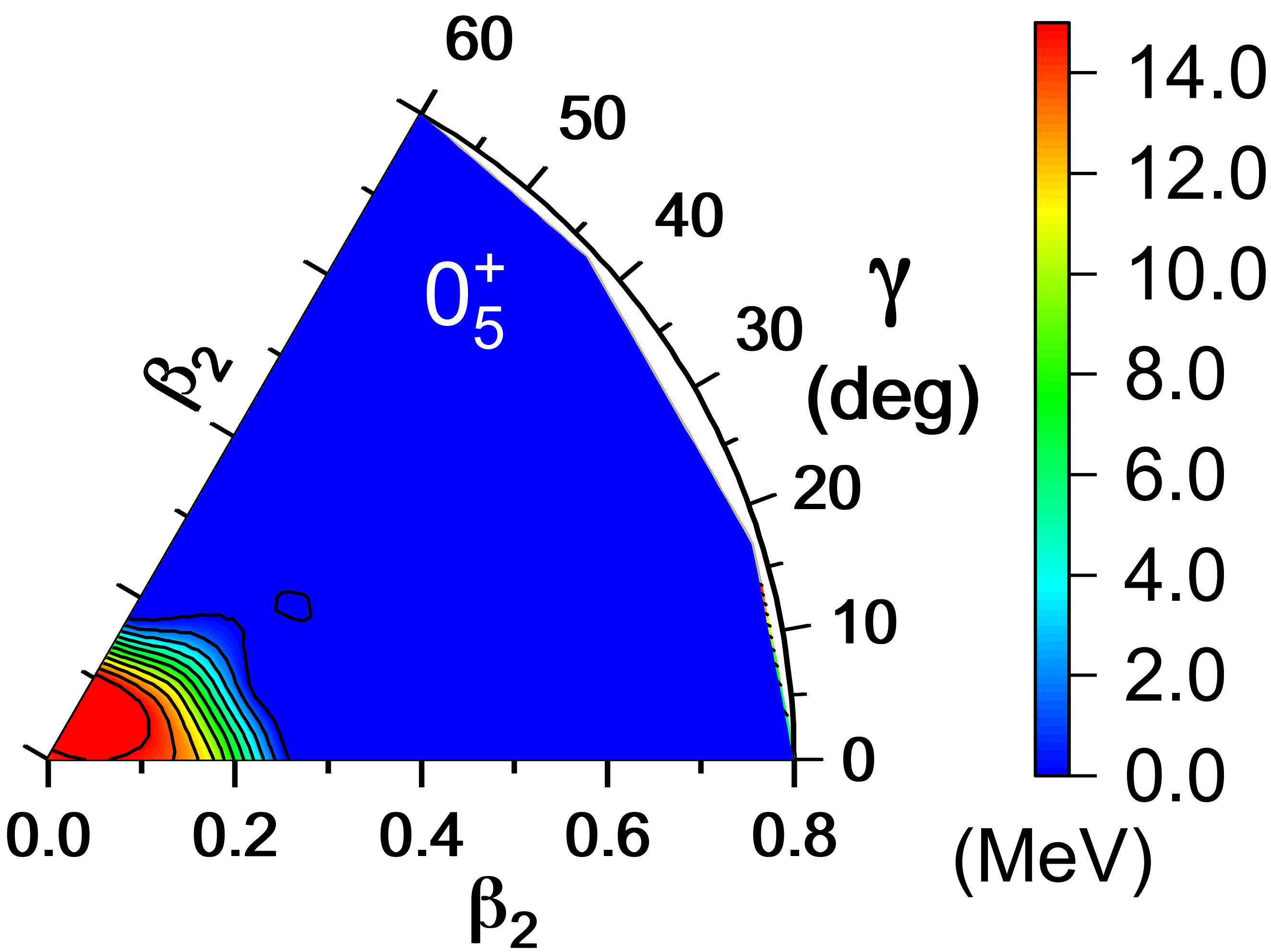

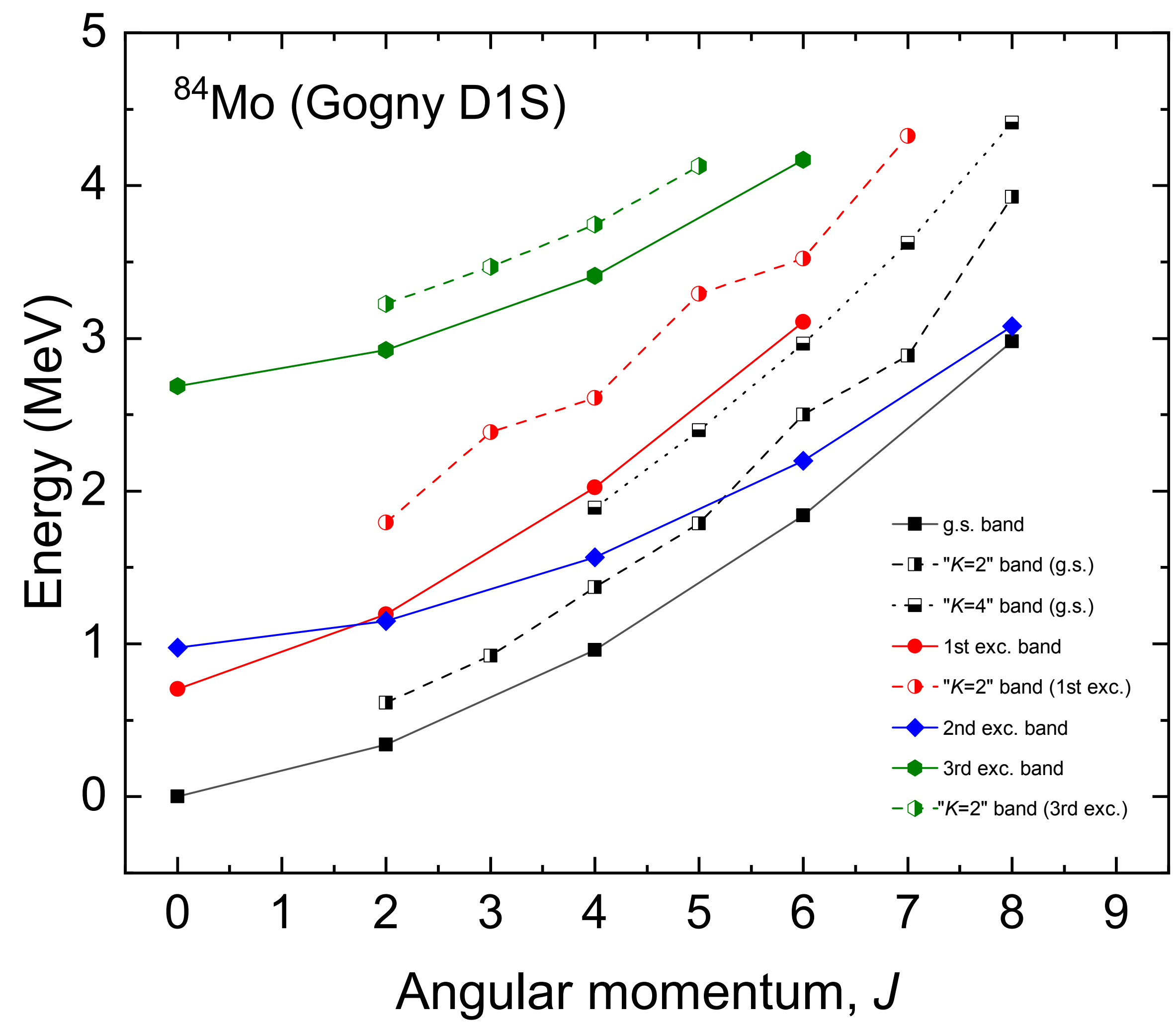

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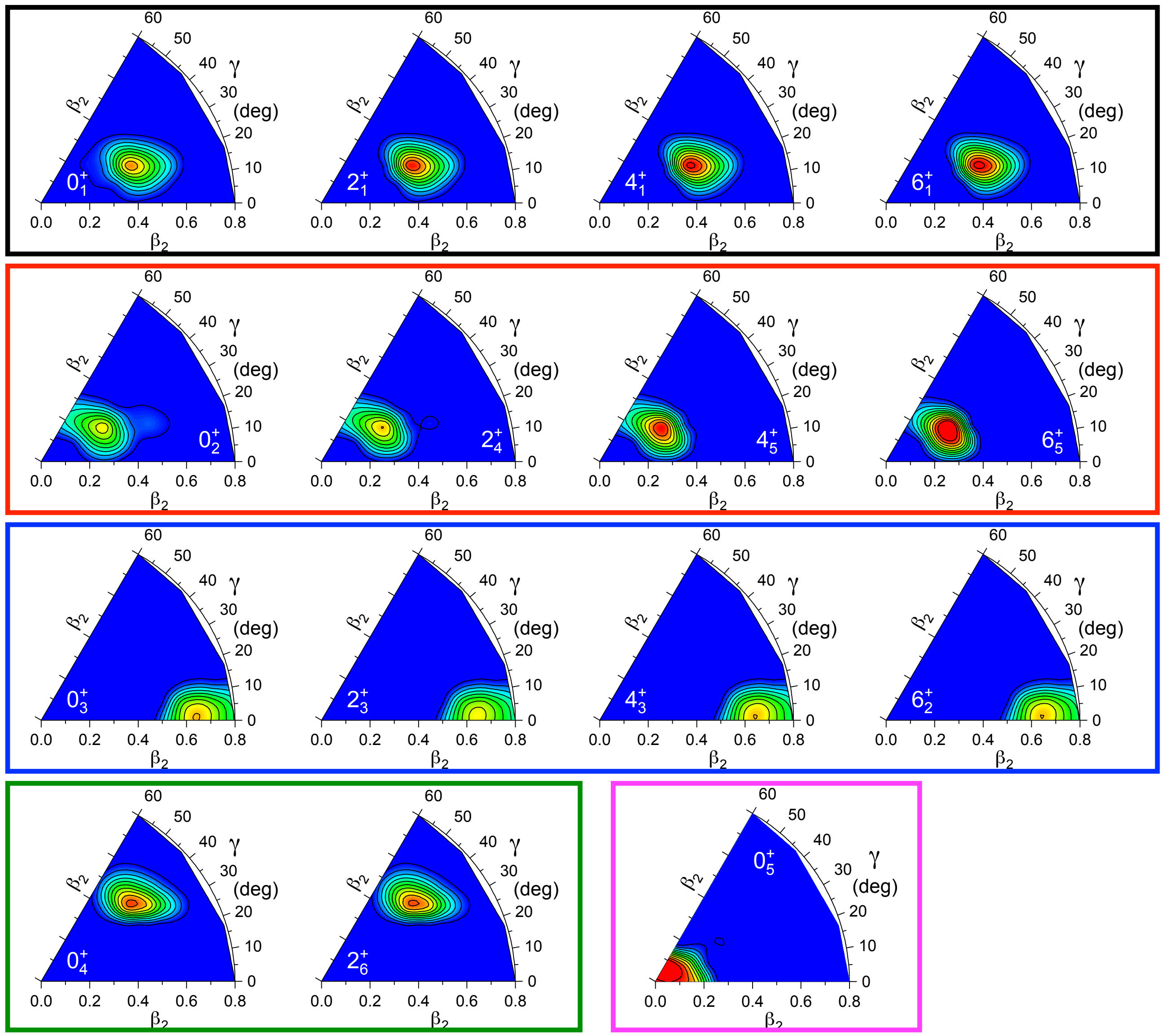
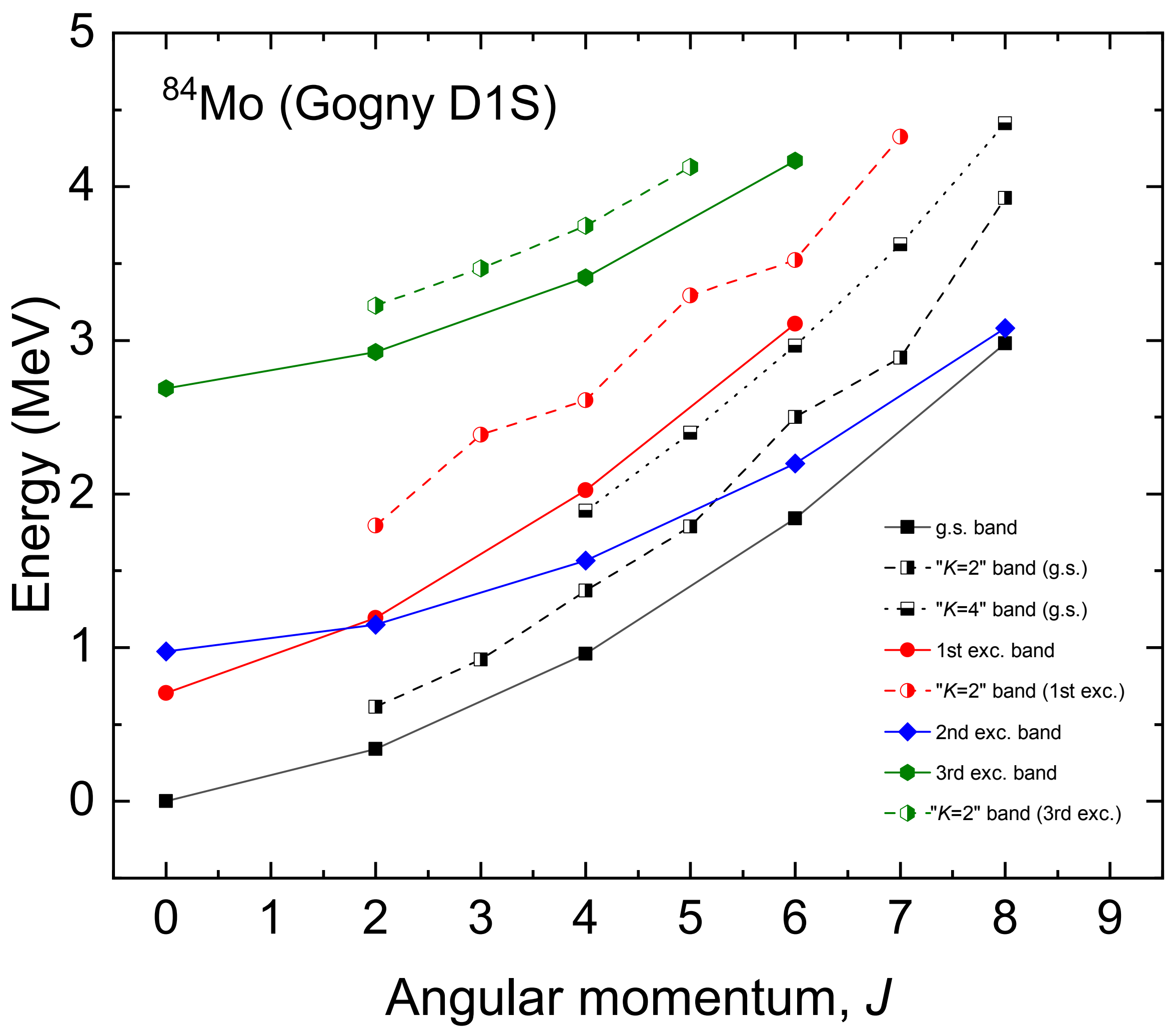
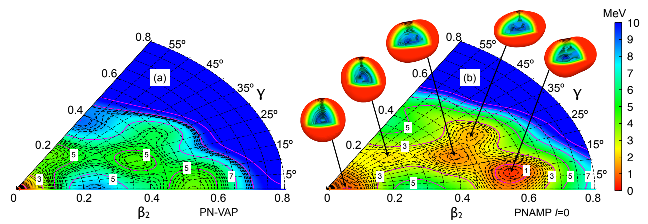
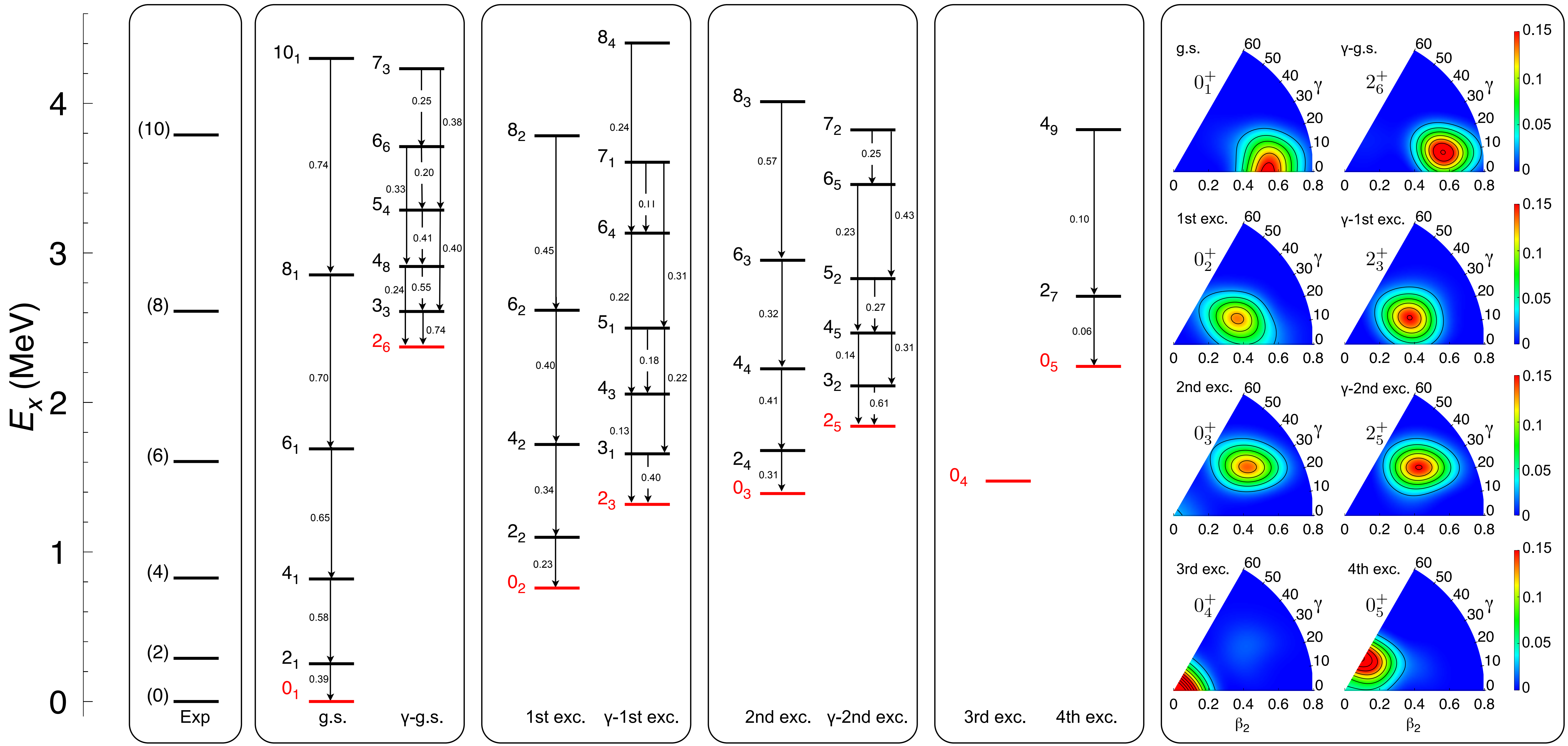




Multiple Shape Coexistence (A)

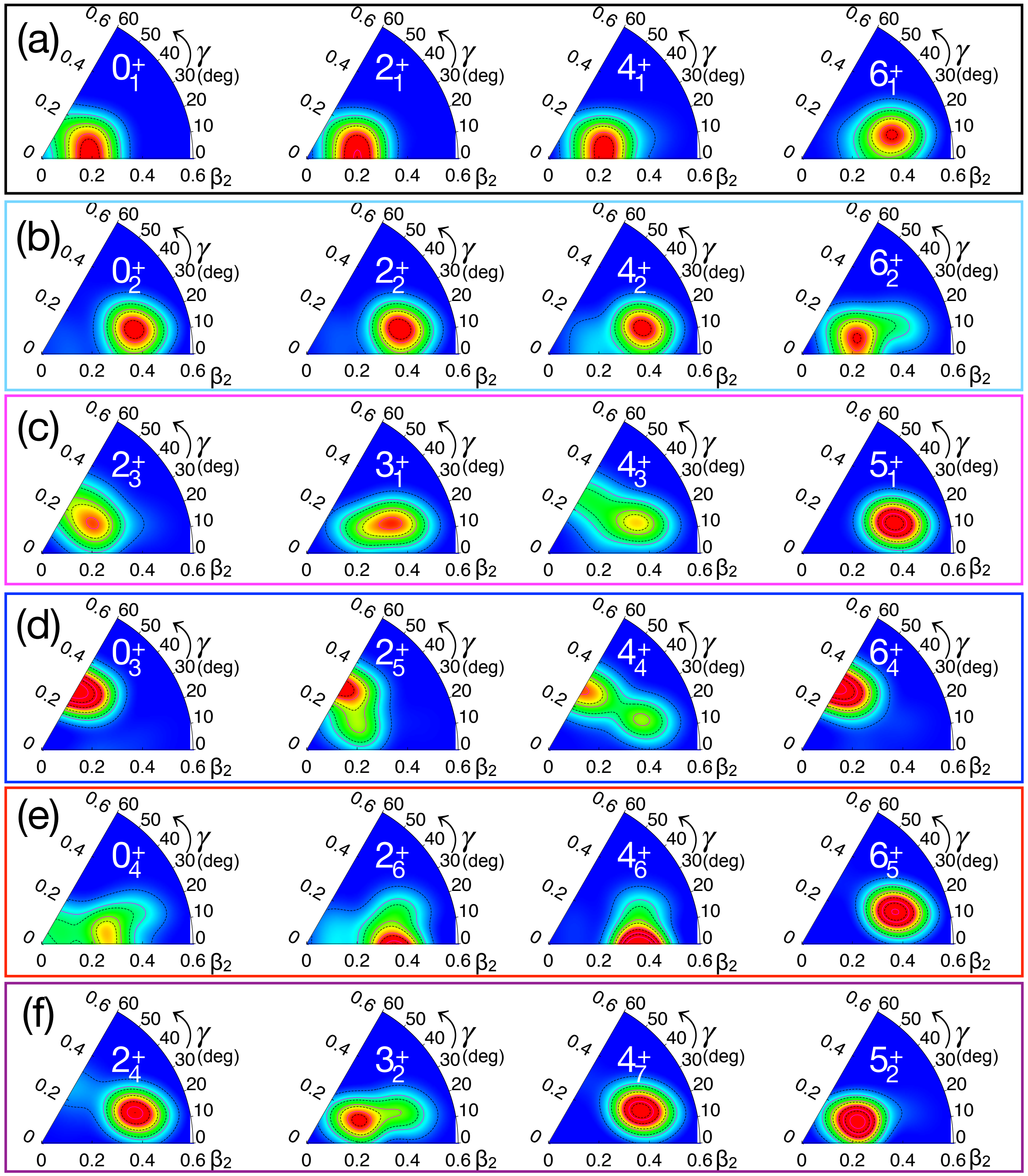


$^{80}Zr_{40}$

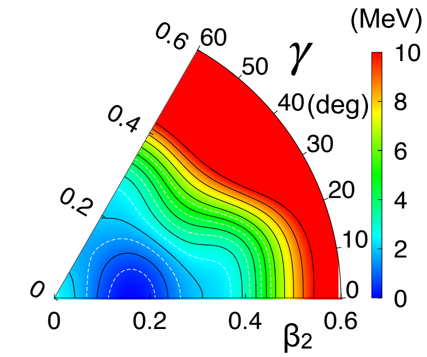


T. R. R., J. L. Egido, Phys. Lett. B 705, 255 (2011)

Multiple Shape Coexistence (B)



^{110}Cd



- Shape coexistence in stable cadmium isotopes

➡ Appearance of different bands with different collective structures without a clear connection with the underlying TES

➡ Prolate slightly deformed ground state band

➡ Triaxial-prolate deformed 2nd excited band

➡ Axial-oblate deformed 3rd excited bands

➡ Shape-mixing-prolate band

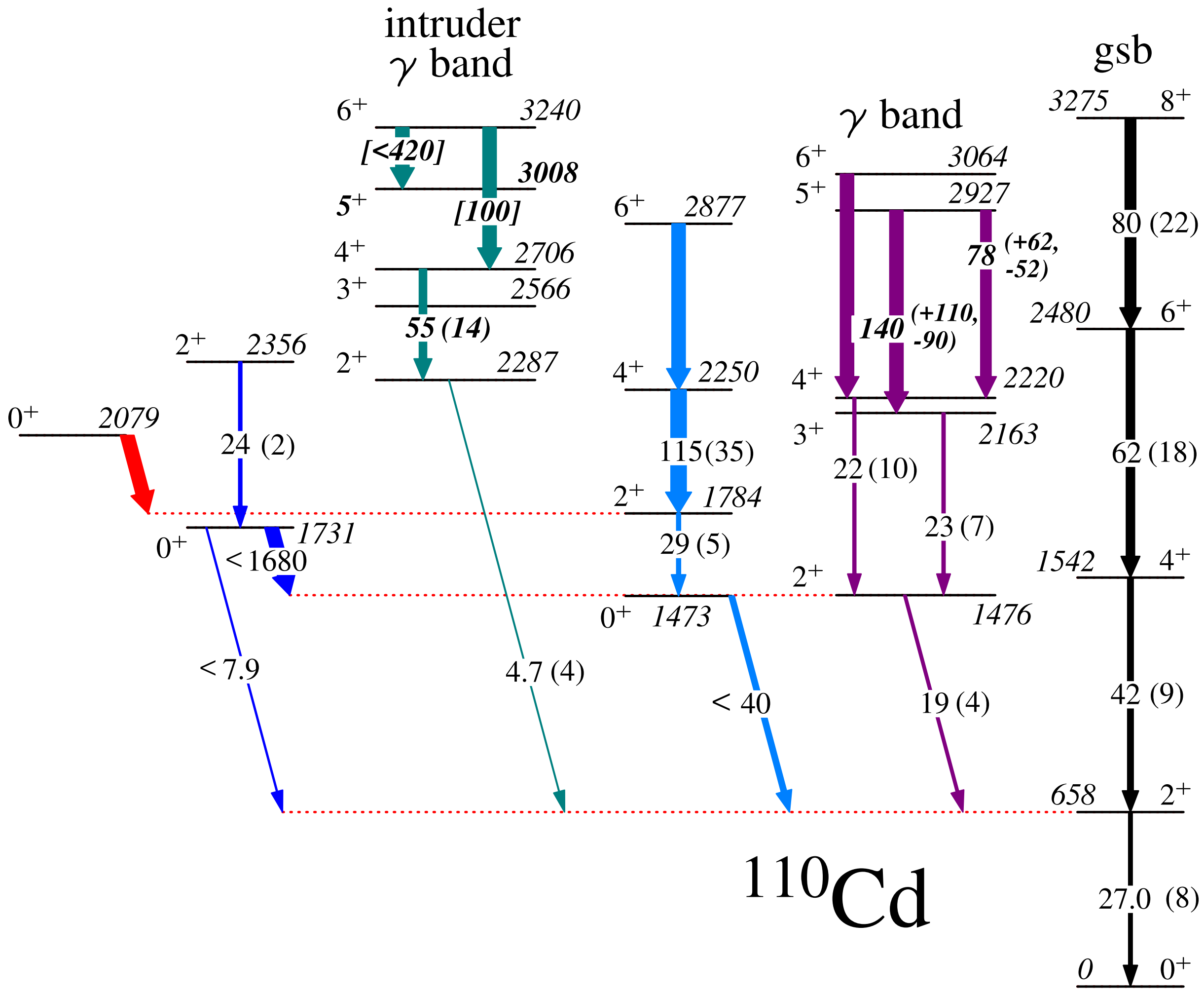
➡ Band-crossings are observed

➡ Pseudo-gamma-bands are observed

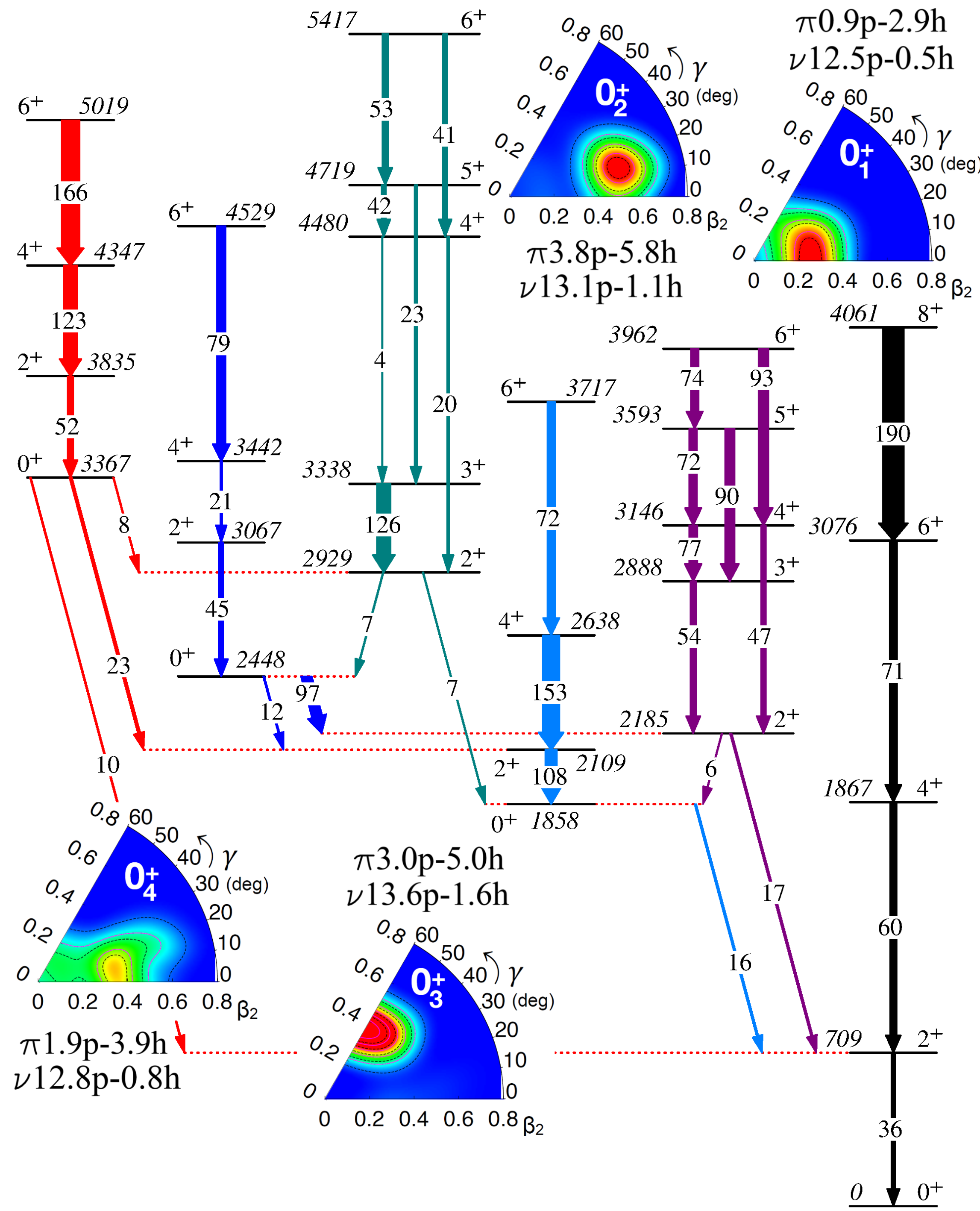
P. Garrett et al., Physical Review Letters 123, 142502 (2019)

Multiple Shape Coexistence (B)

Experiment



Theory



P. Garrett et al., Physical Review Letters 123, 142502 (2019)

Outline

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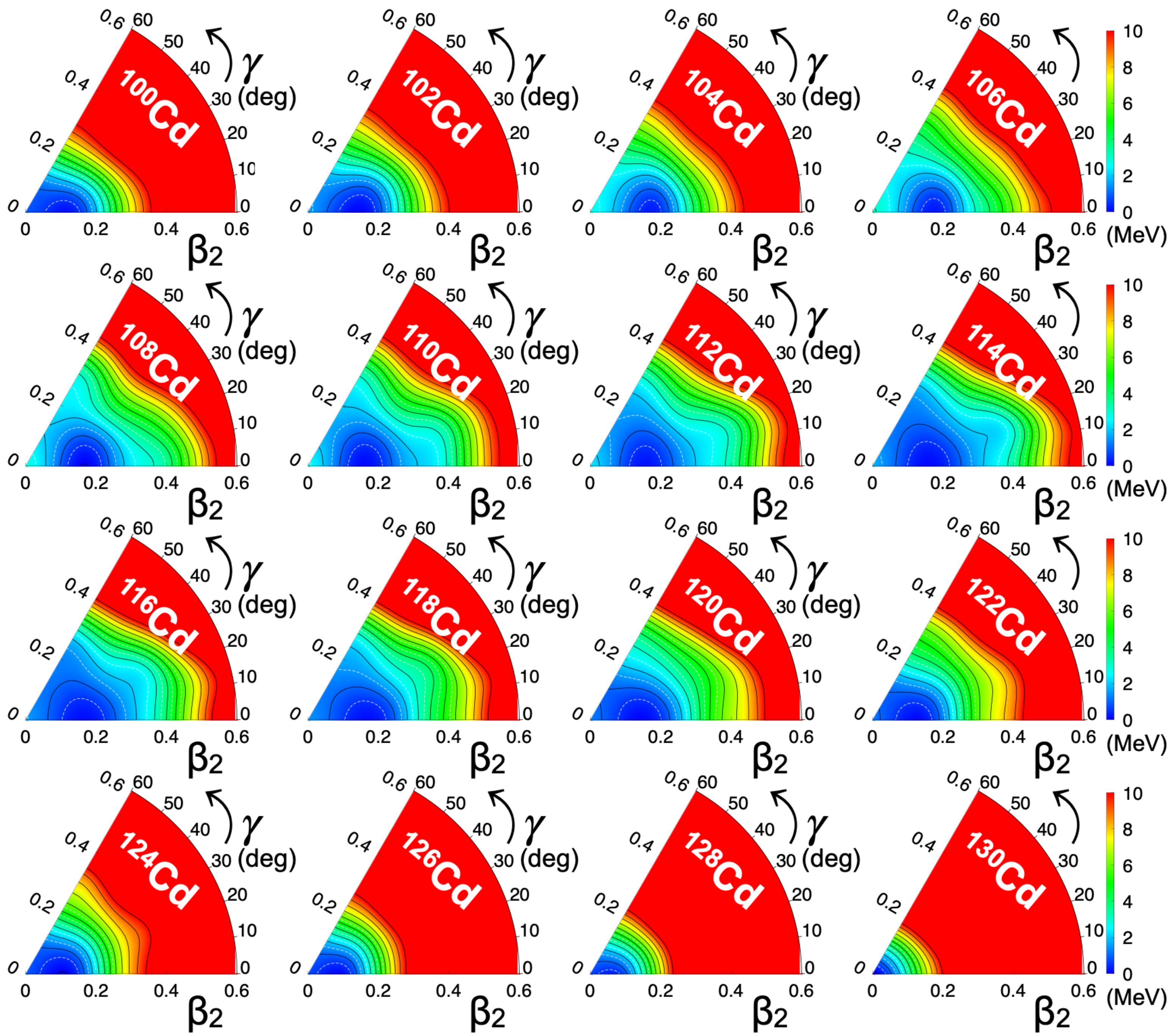
Shape evolution in Cd isotopes

▸ Shape evolution in cadmium isotopes



➡ Slightly prolate deformed minima are found along the whole isotopic chain.

➡ Deformation is larger (and almost constant) in the mid-shell and smaller when approaching to the magic neutron numbers (N = 50, 82).

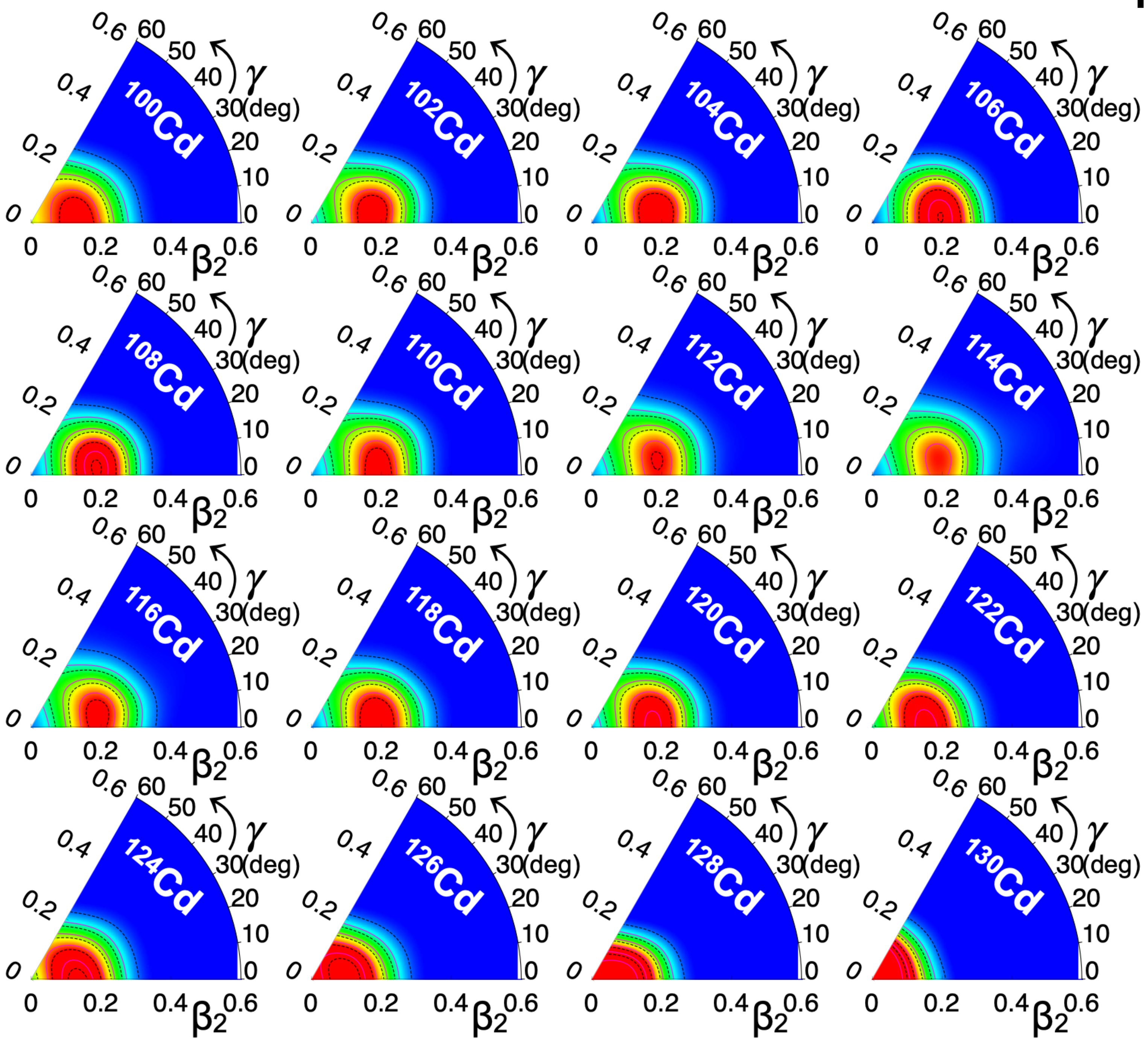
➡ A depression at β_2~0.35, γ~20 is found in $^{110-118}$Cd.

M. Siciliano et al., Physical Review C 104, 034320 (2021)

Shape evolution in Cd isotopes

Shape evolution in cadmium isotopes

0^+_1



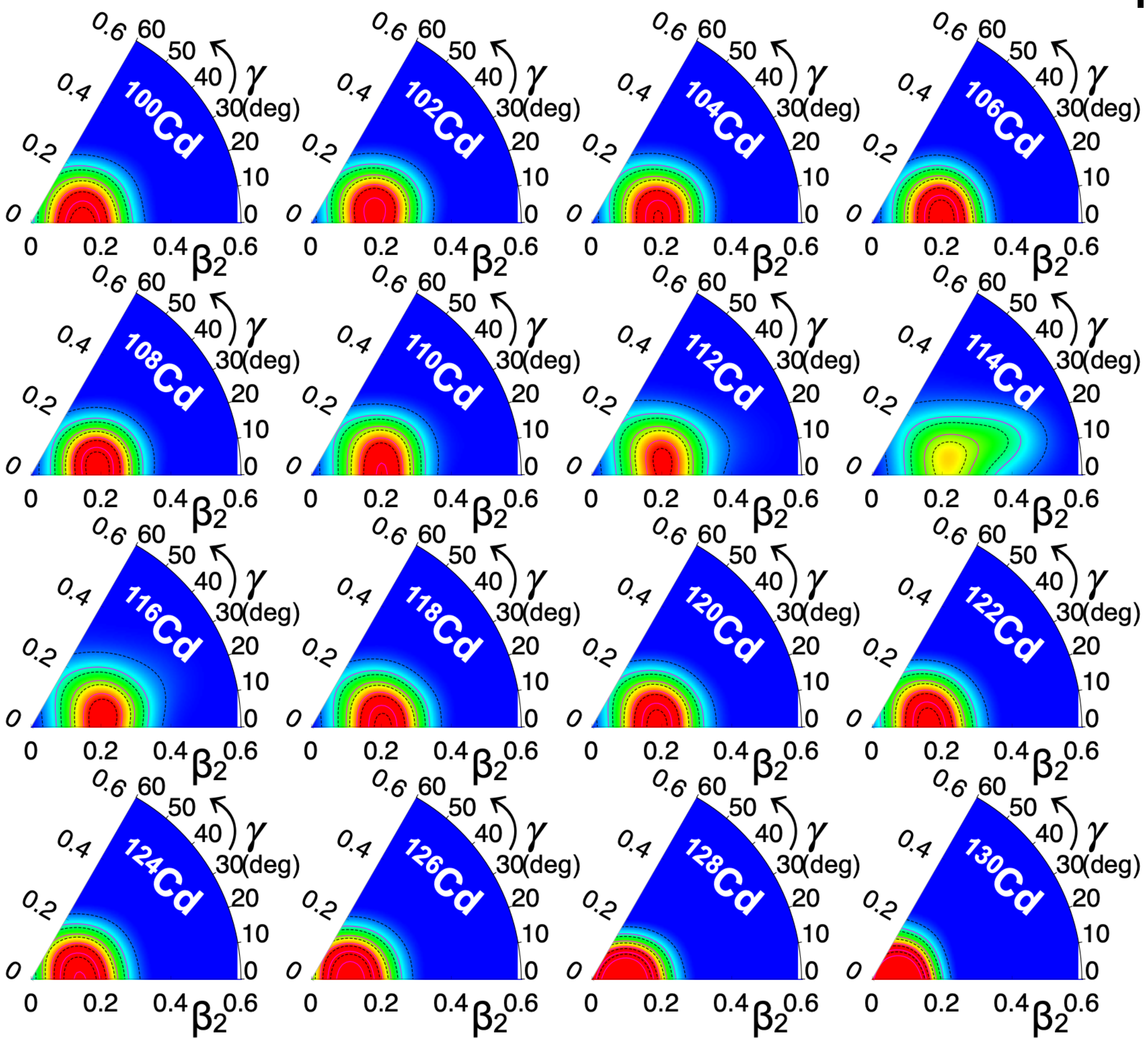
- ➡ Slightly prolate deformed ground state collective wave functions are found after performing PGCM.
- ➡ Deformation is larger (and almost constant) in the mid-shell and smaller when approaching to the magic neutron numbers (N = 50, 82).

M. Siciliano et al., Physical Review C 104, 034320 (2021)

Shape evolution in Cd isotopes

Shape evolution in cadmium isotopes

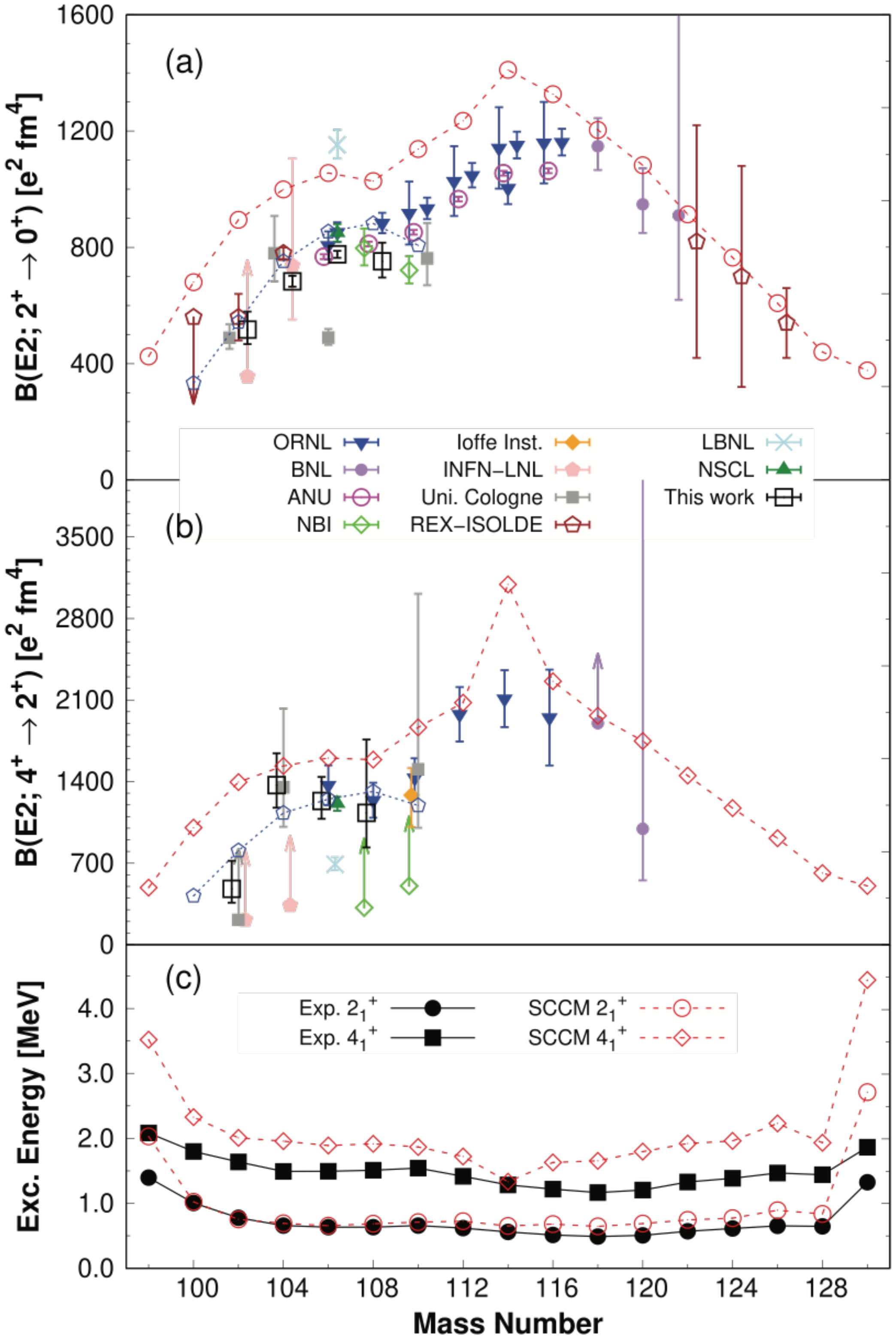
2_1^+



- ➡ Slightly prolate deformed 2_1^+ collective wave functions are found after performing PGCM.
- ➡ Similar to the 0_1^+ collective wave functions except for ^{114}Cd.

M. Siciliano et al., Physical Review C 104, 034320 (2021)

Shape evolution in Cd isotopes



Shape evolution in cadmium isotopes

➡ Qualitative good agreement between theory and experiment for excitation energies and transition probabilities in the whole isotopic chain.

➡ 2^+, 4^+ excitation energies are stretched (lack of cranking components) although some 2^+ energies are on top of the experimental data, meaning that the deformation could be overestimated.

➡ B(E2) are systematically larger than the experimental data (deformation overestimated).

➡ $^{126-128}$Cd lowering of the 2^+ is well-reproduced contrary to most of the shell model calculations that predict a parabolic trend.

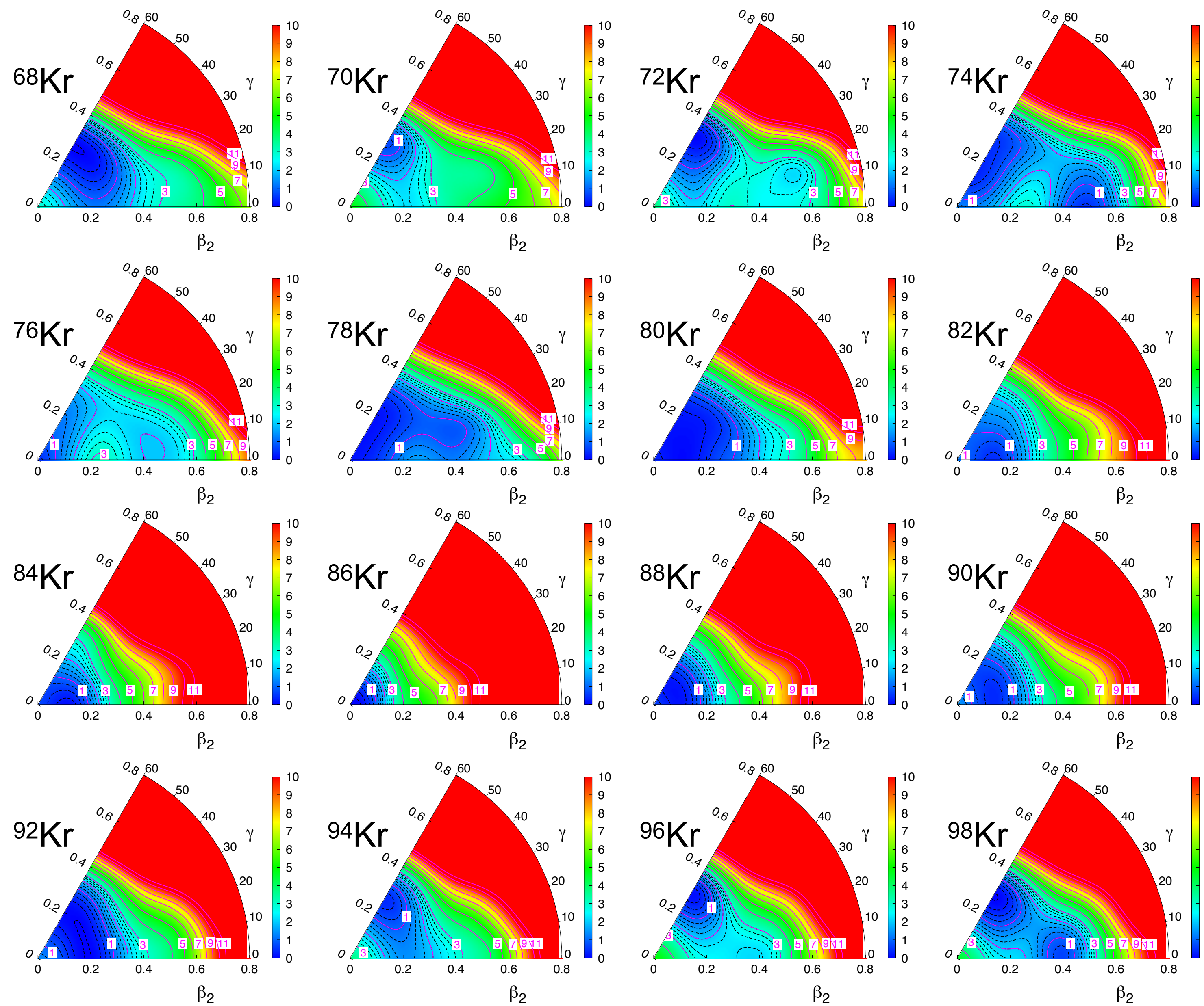
➡ Poor reproduction of excitation energies at the magic numbers (problems to describe pure spherical single-particle excitations)

M. Siciliano et al., Physical Review C 104, 034320 (2021)

TRR, J. L. Egido, A. Jungclaus, Phys. Lett. B 668, 410 (2008)

Krypton (Z=36)

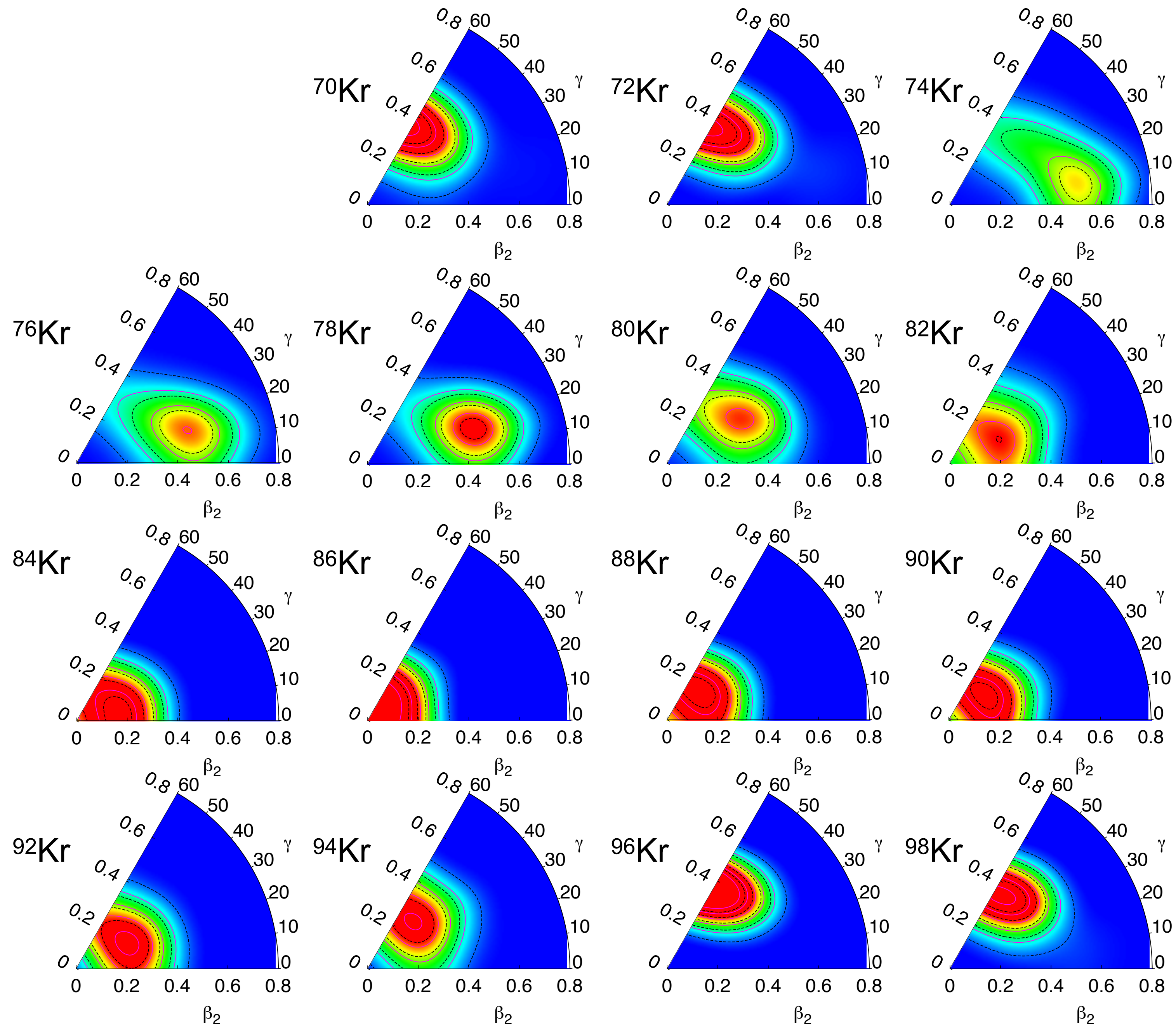
- ✓ Oblate shape in $^{68\text{-}70}$Kr
- ✓ Two minima in $^{72\text{-}76}$Kr
- ✓ γ-softness in $^{78\text{-}80}$Kr
- ✓ Slightly prolate deformation in $^{82\text{-}84}$Kr
- ✓ Spherical semi-magic ^{86}Kr
- ✓ γ-softness in $^{88\text{-}92}$Kr
- ✓ Oblate shape in ^{94}Kr
- ✓ Oblate/prolate minima in $^{96\text{-}98}$Kr



TRR, Physical Review C 90, 034306 (2014)

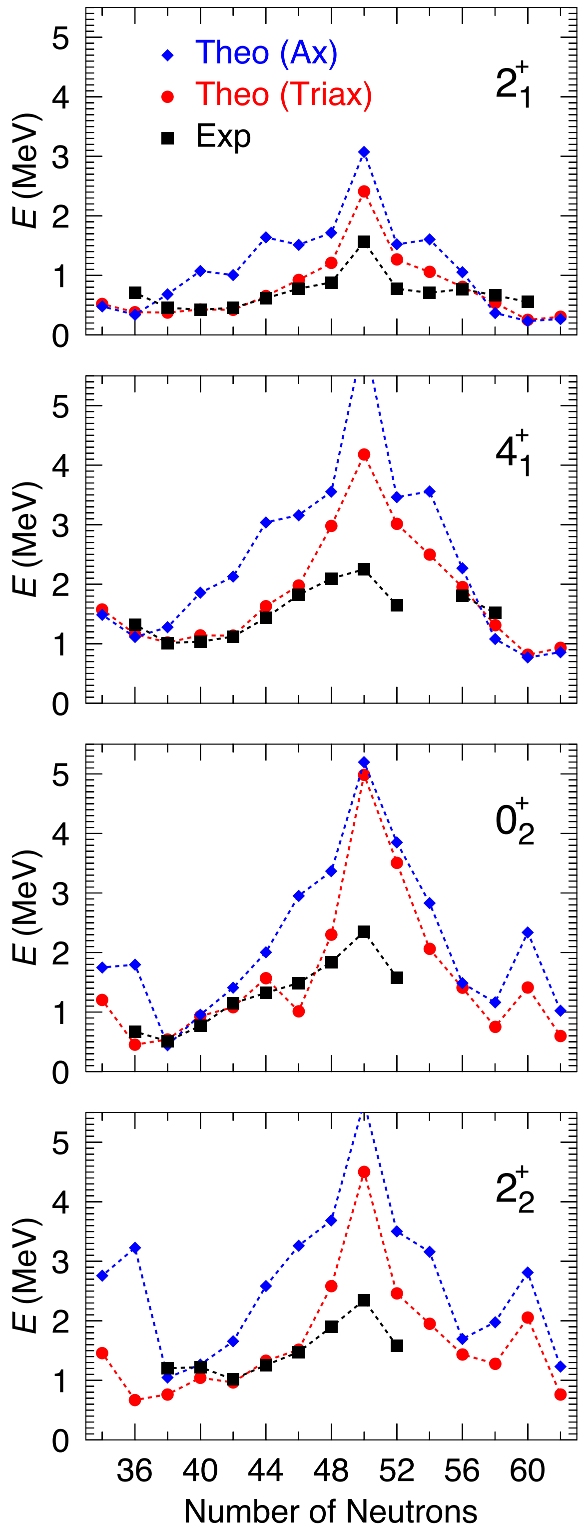
Krypton (Z=36)

- ✓ Oblate shape in $^{70-72}$Kr. Transition $^{72-74}$Kr
- ✓ Triaxial/prolate $^{74-78}$Kr
- ✓ Triaxial/oblate ^{80}Kr
- ✓ γ-softness in ^{82}Kr
- ✓ Slightly prolate deformation in ^{84}Kr
- ✓ Spherical semi-magic ^{86}Kr
- ✓ γ-softness/oblate in ^{88}Kr
- ✓ γ-softness/oblate in $^{90-92}$Kr
- ✓ Oblate shape in ^{94}Kr
- ✓ Oblate/prolate minima in $^{96-98}$Kr



TRR, Physical Review C 90, 034306 (2014)

Krypton (Z=36)



Krypton isotopes

✓ Good agreement with the experimental data in the triaxial case.

✓ Poor performance of the axial approximation.

✓ Main differences around the magic nucleus ^{86}Kr (quasiparticle excitations are not included explicitly)

✓ In neutron rich nuclei, a flatter behavior than the theoretical results is found experimentally in the 2_1^+ energies.

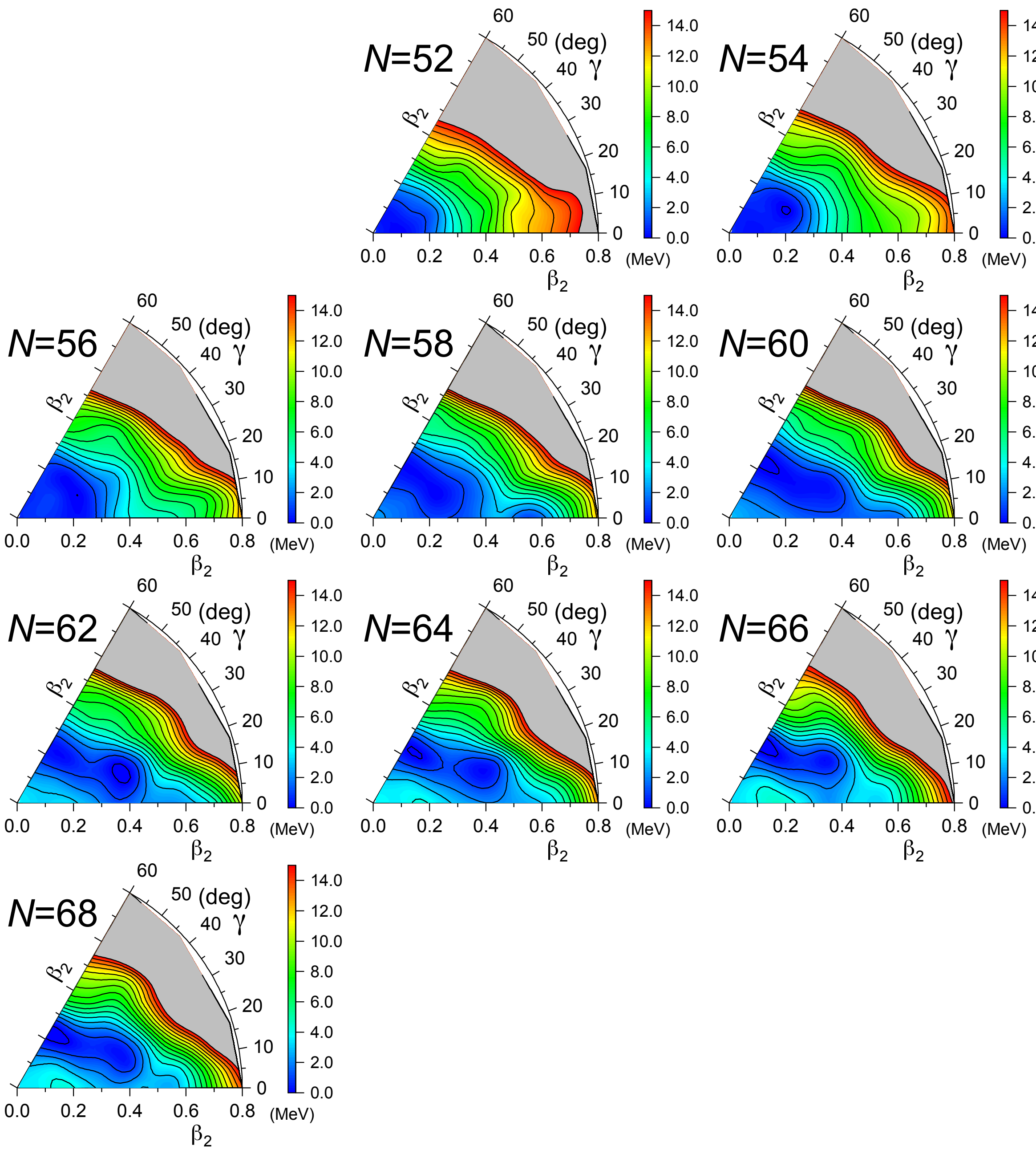
✓ There is not a sharp transition at N=60 (^{96}Kr).

✓ Several candidates for shape coexistence (low-lying 0_2^+).

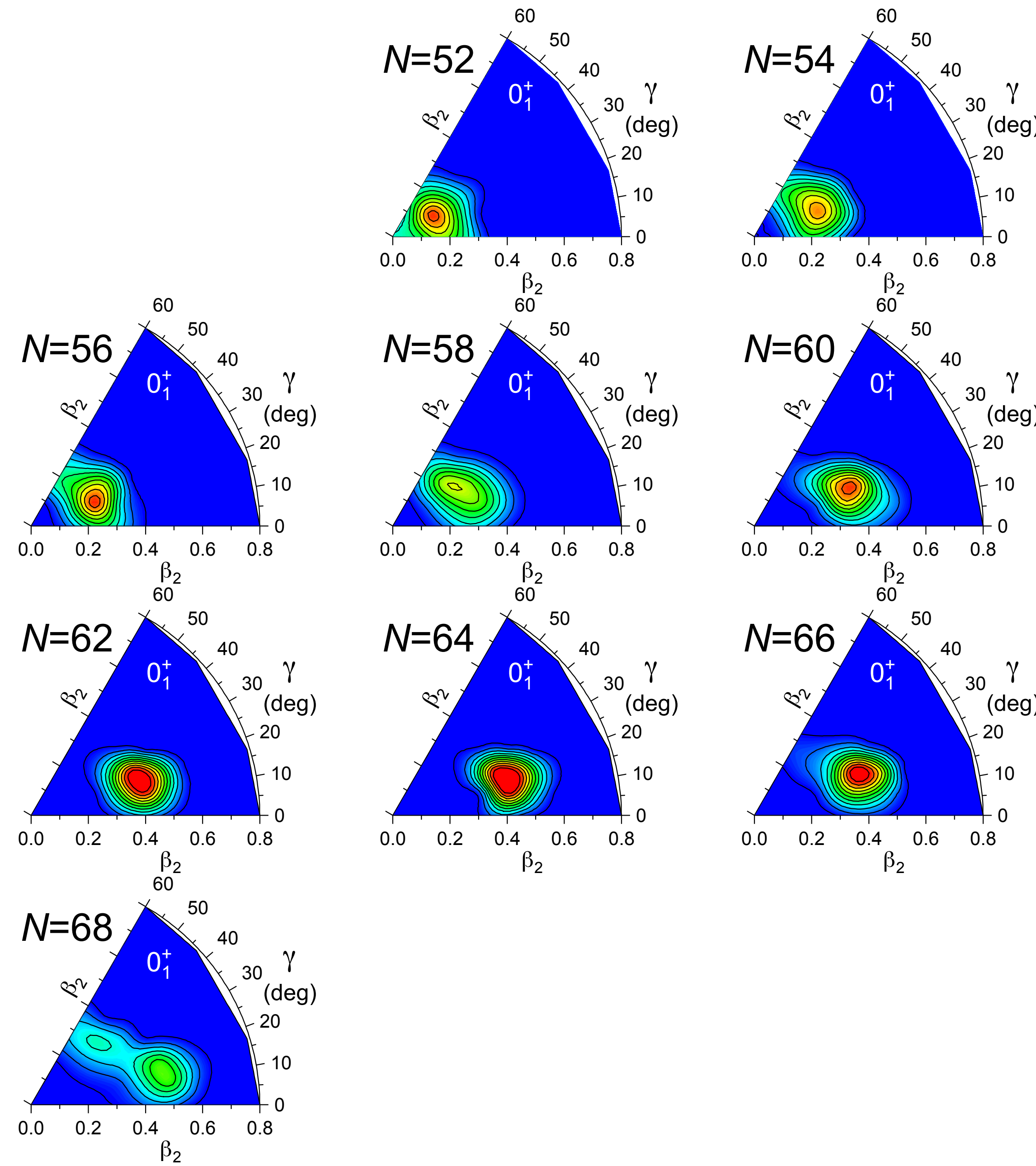
TRR, Physical Review C 90, 034306 (2014)

Molybdenum (Z=42)

Total PN-VAP Energy Surfaces

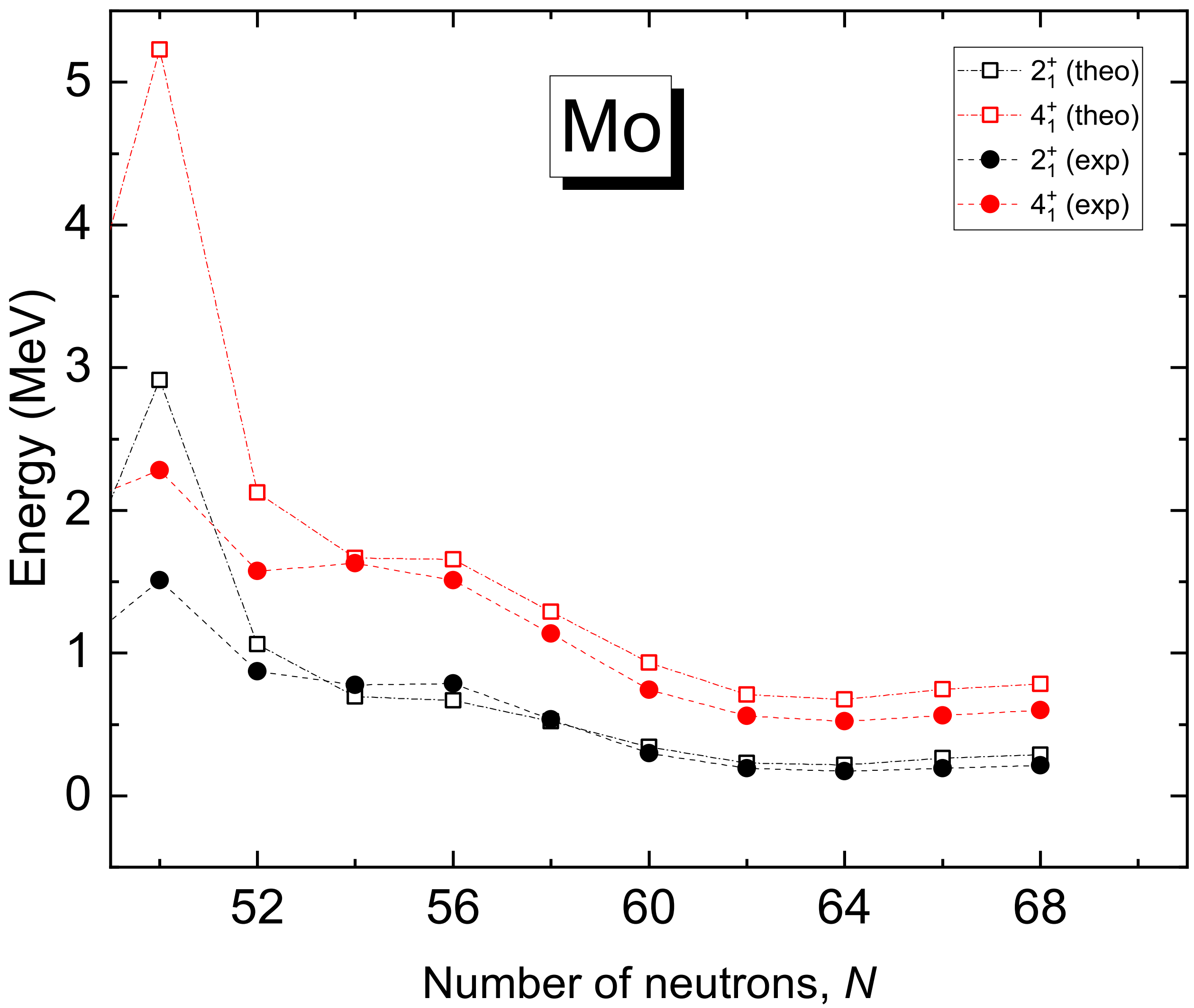


Ground state collective wave functions

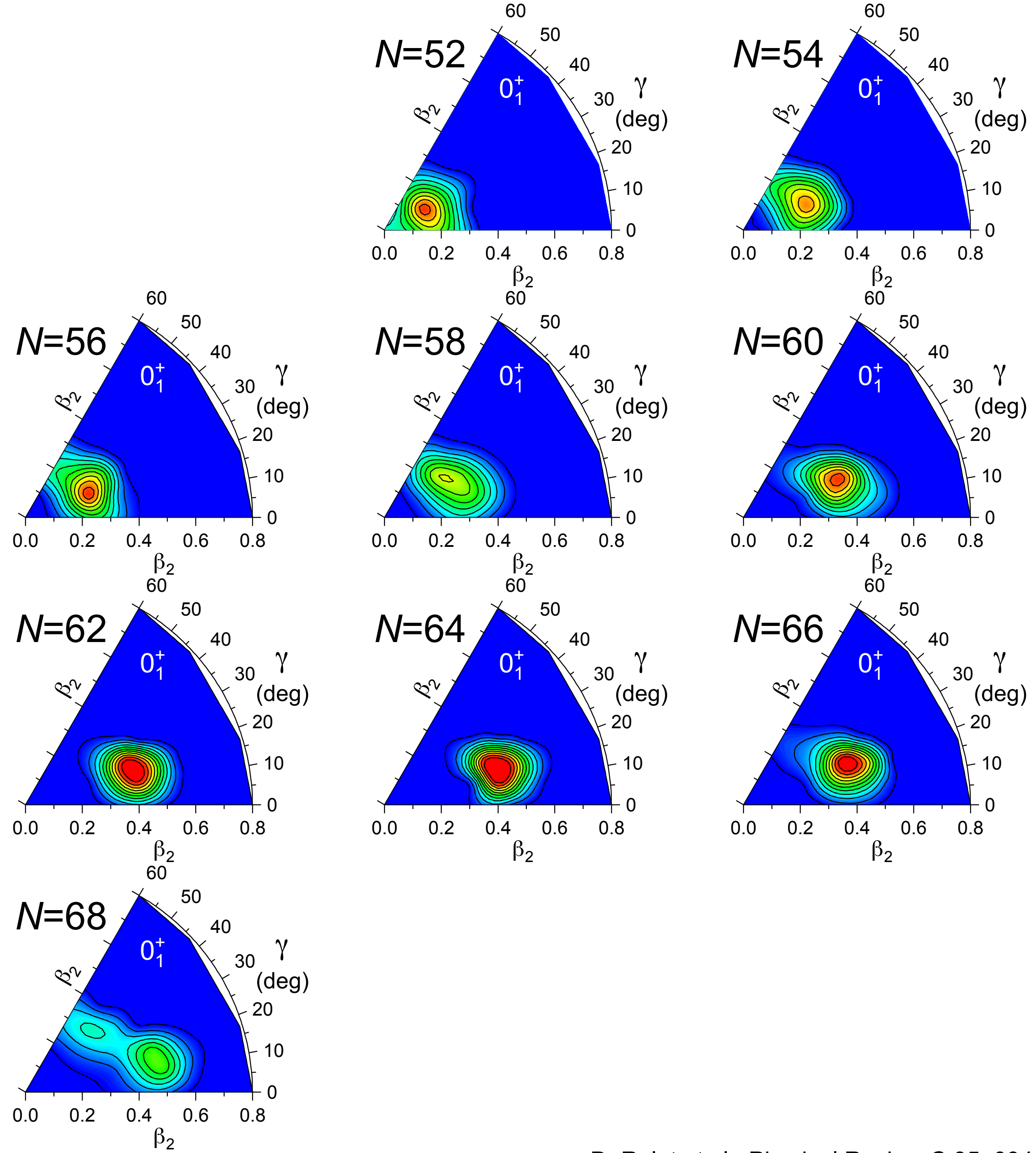


Molybdenum (*Z*=42)

Excitation energies



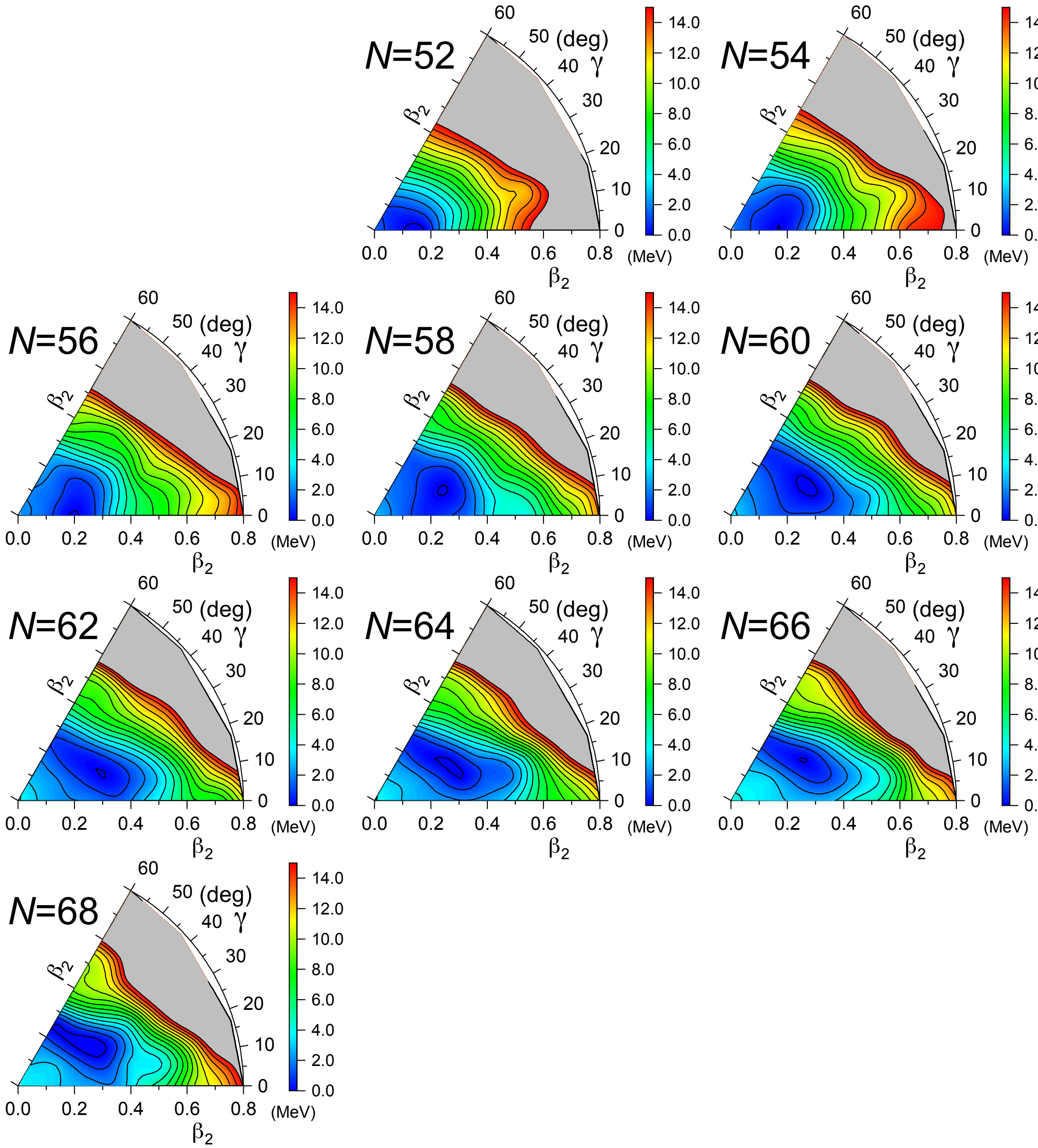
Ground state collective wave functions



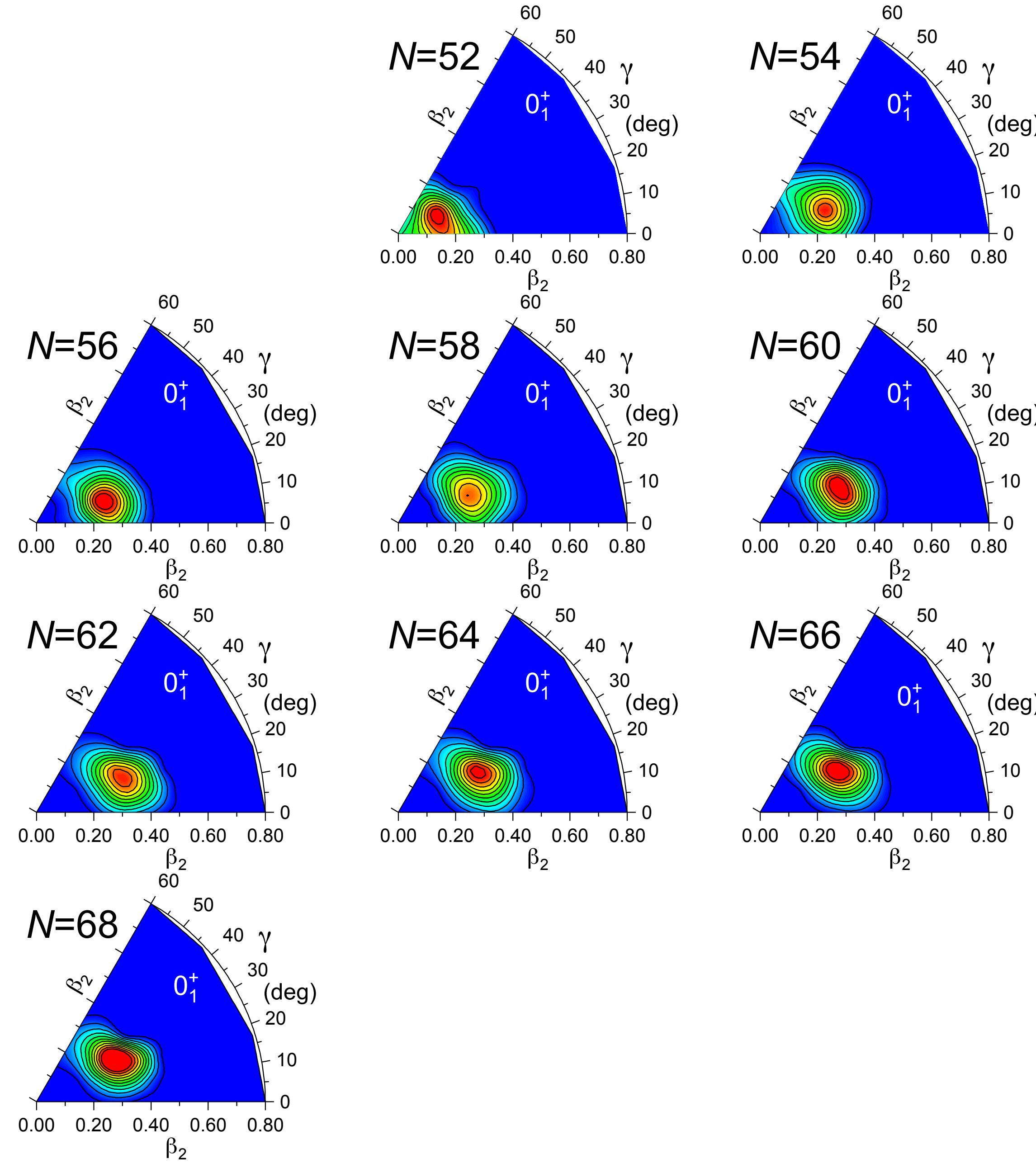
D. Ralet et al., Physical Review C 95, 034320 (2017)

Ruthenium (Z=44)

Total PN-VAP Energy Surfaces

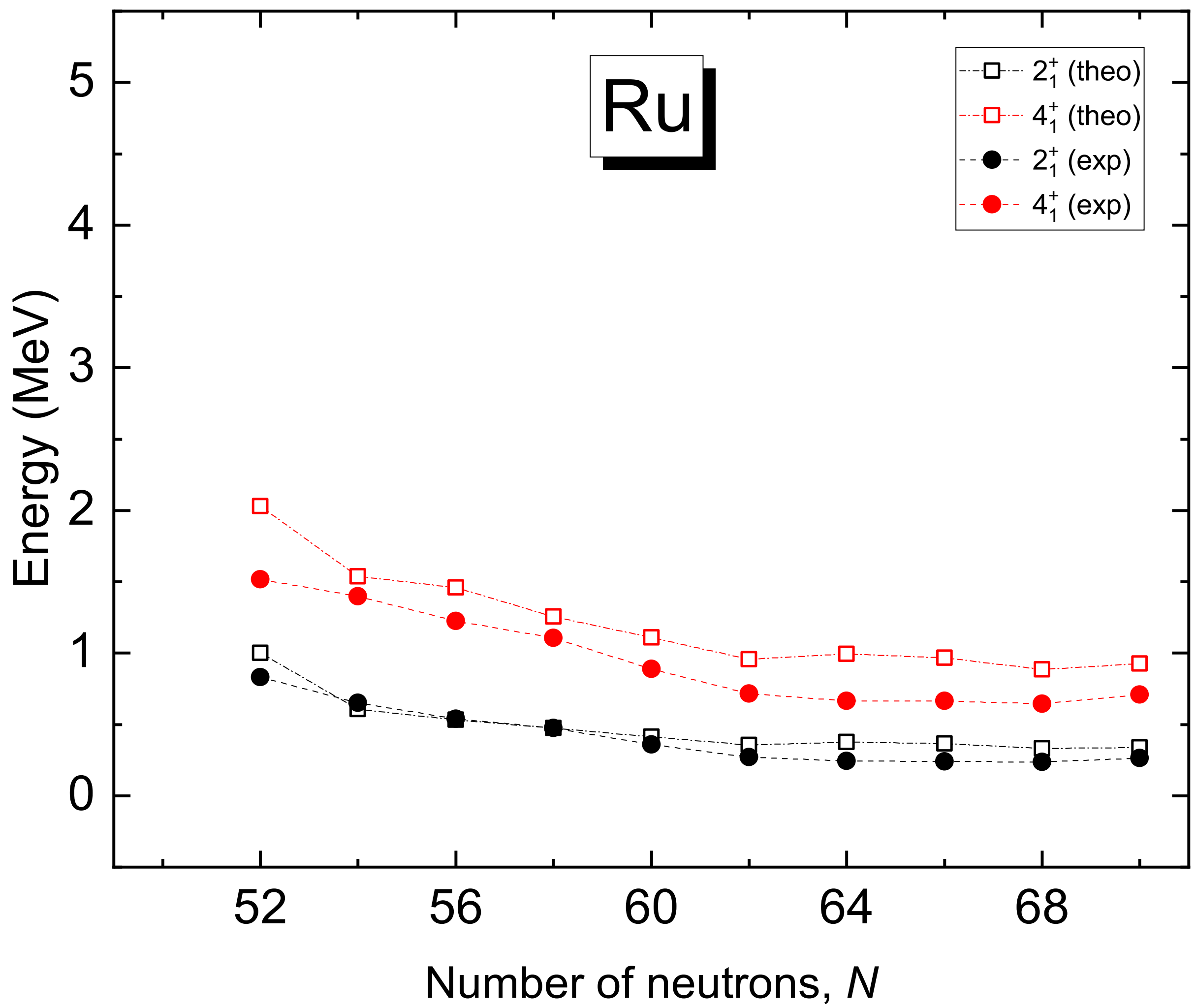


Ground state collective wave functions

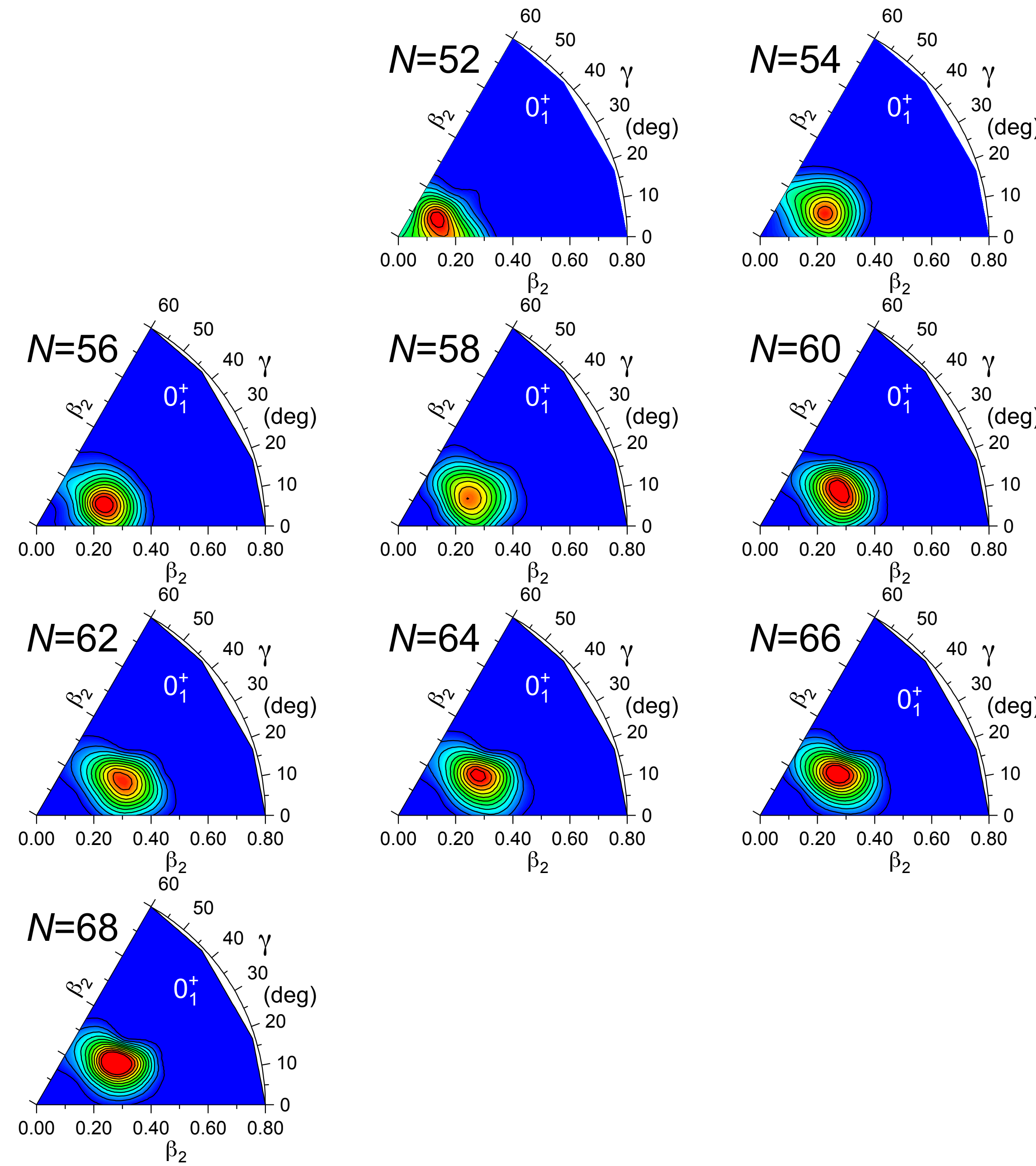


Ruthenium (Z=44)

Excitation energies



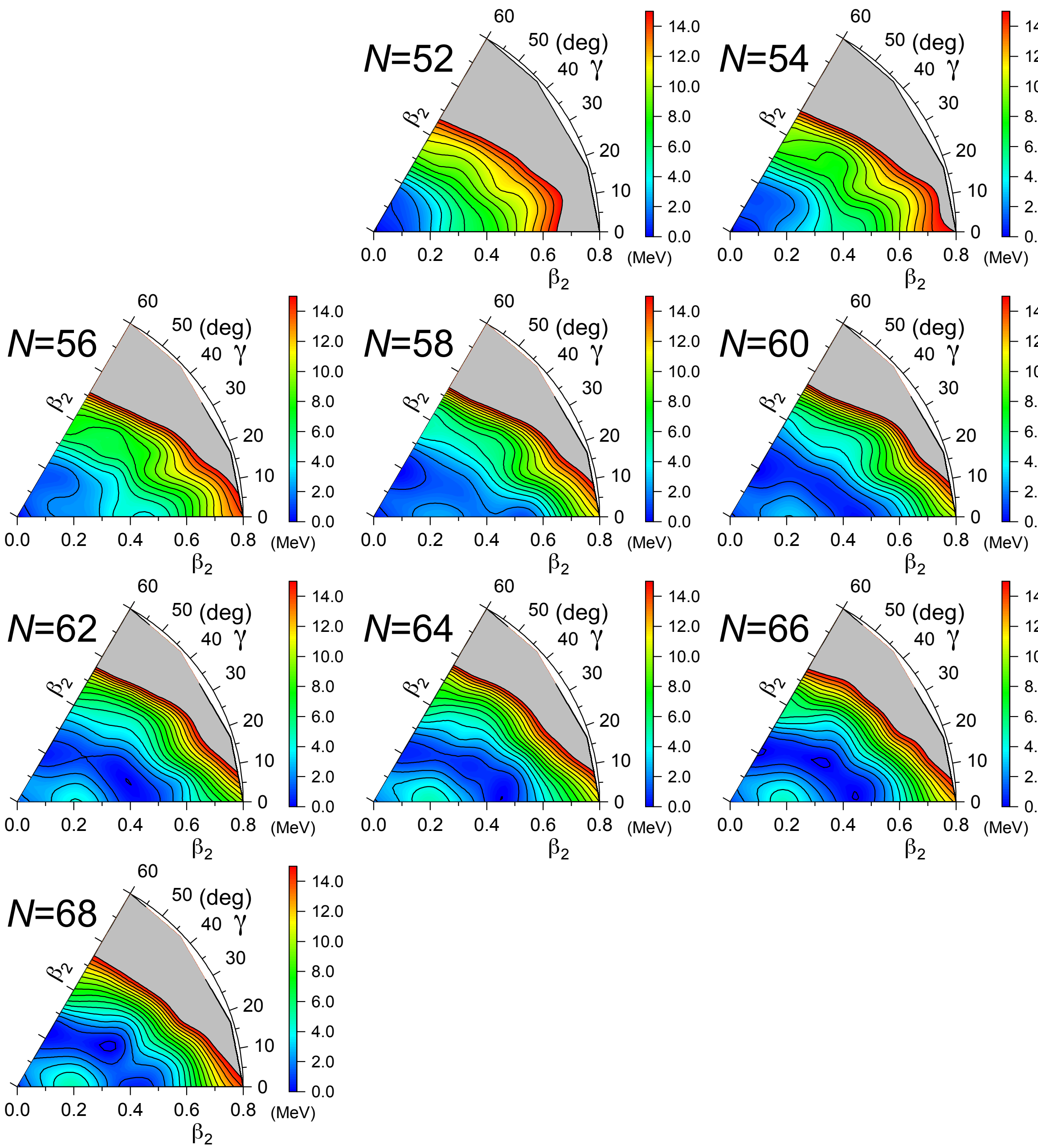
Ground state collective wave functions



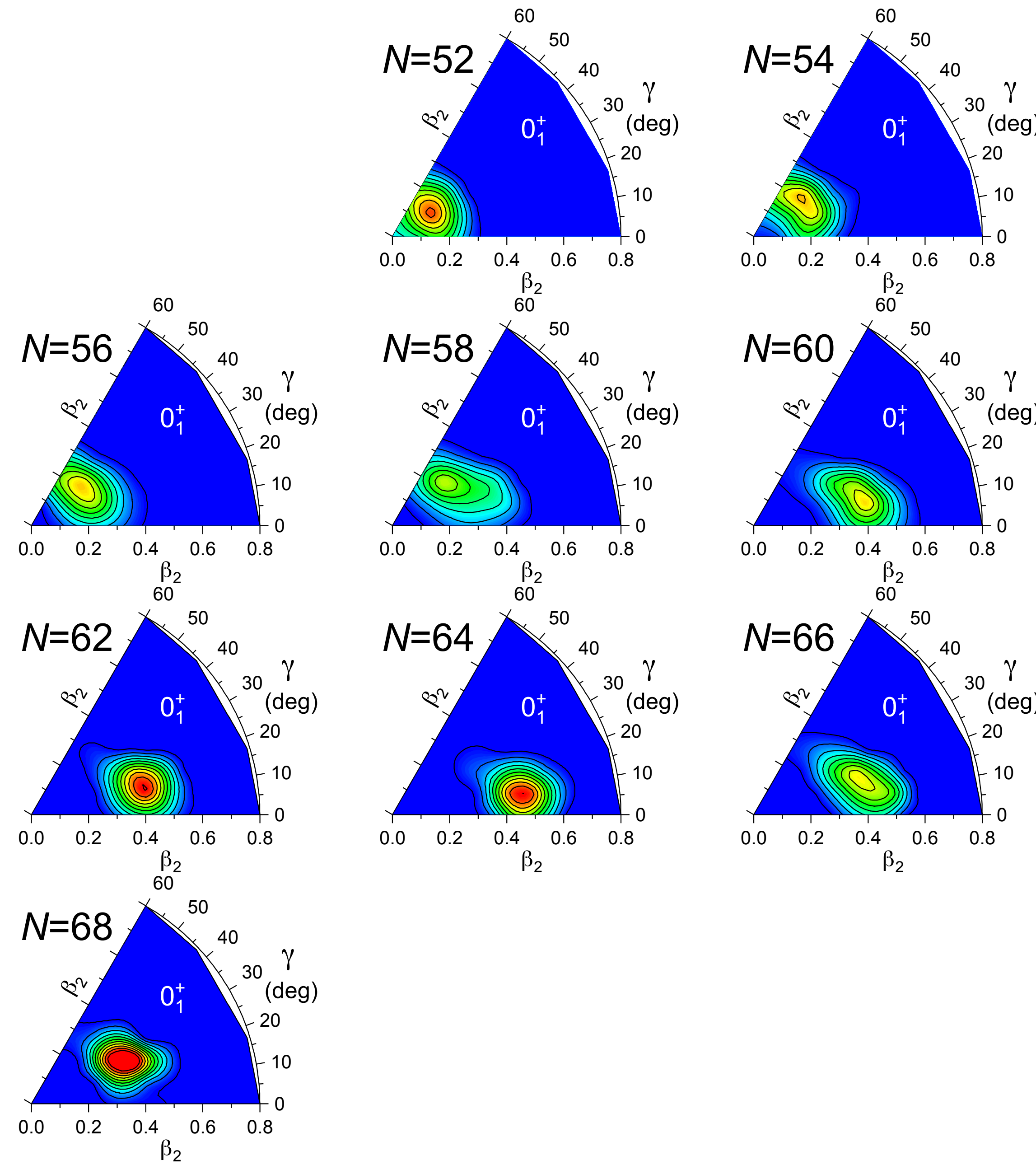
P. Garrett et al., PLB 809, 135762 (2020)

Zirconium's puzzle (Z=40)

Total PN-VAP Energy Surfaces

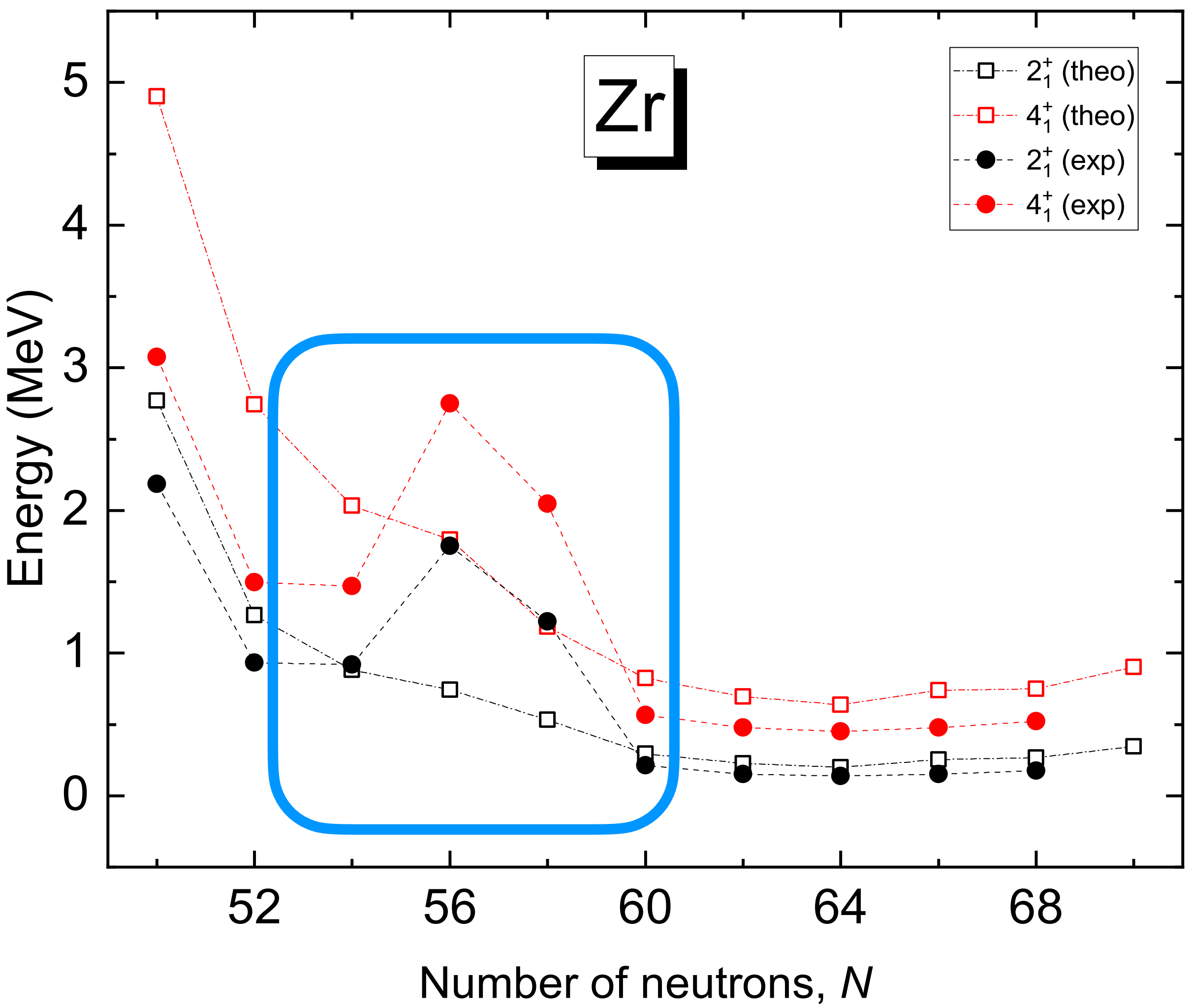


Ground state collective wave functions

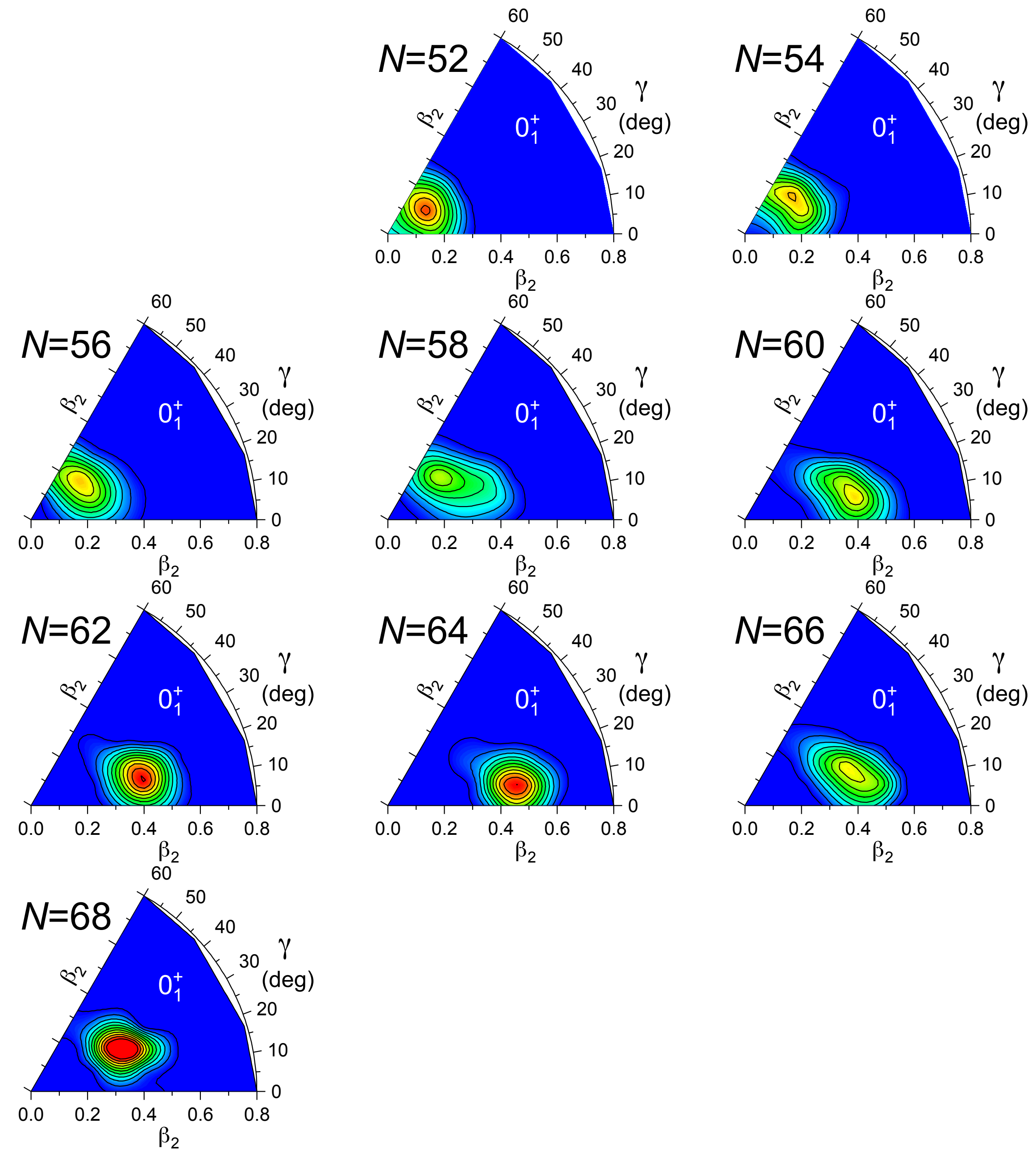


Zirconium's puzzle (Z=40)

Excitation energies



Ground state collective wave functions



Other degrees of freedom (octupolarity?)

Outline

1. Introduction. Theoretical framework

2. Multiple shapes in ^{84}Mo, ^{80}Zr and ^{110}Cd

3. Shape evolution and systematics

4. Summary and outlook

Summary and Outlook

SUMMARY

- SCCM/PGCM methods provide a reliable description of nuclear structure observables.

- It is a very flexible method to approach exact solutions although the present implementation tends to favor correlations in the ground state (stretched spectra).

- The region *Z*=30-48 is rich in triaxial nuclei and shape-coexistent nuclei.

- Shape coexistence can be visible in the TES (several minima) and/or in the GCM calculation (bands with different collective wave functions)

- The 2^+ excitation energies of $^{96-98}$Zr cannot be reproduced with the present SCCM calculations

OUTLOOK (and work in progress)

- Include additional degrees of freedom (cranking, 2qp-excitations, triaxial octupoles)

- Extend PGCM techniques to nuclear Hamiltonians (ab-initio, shell model, …)

Thank you!!