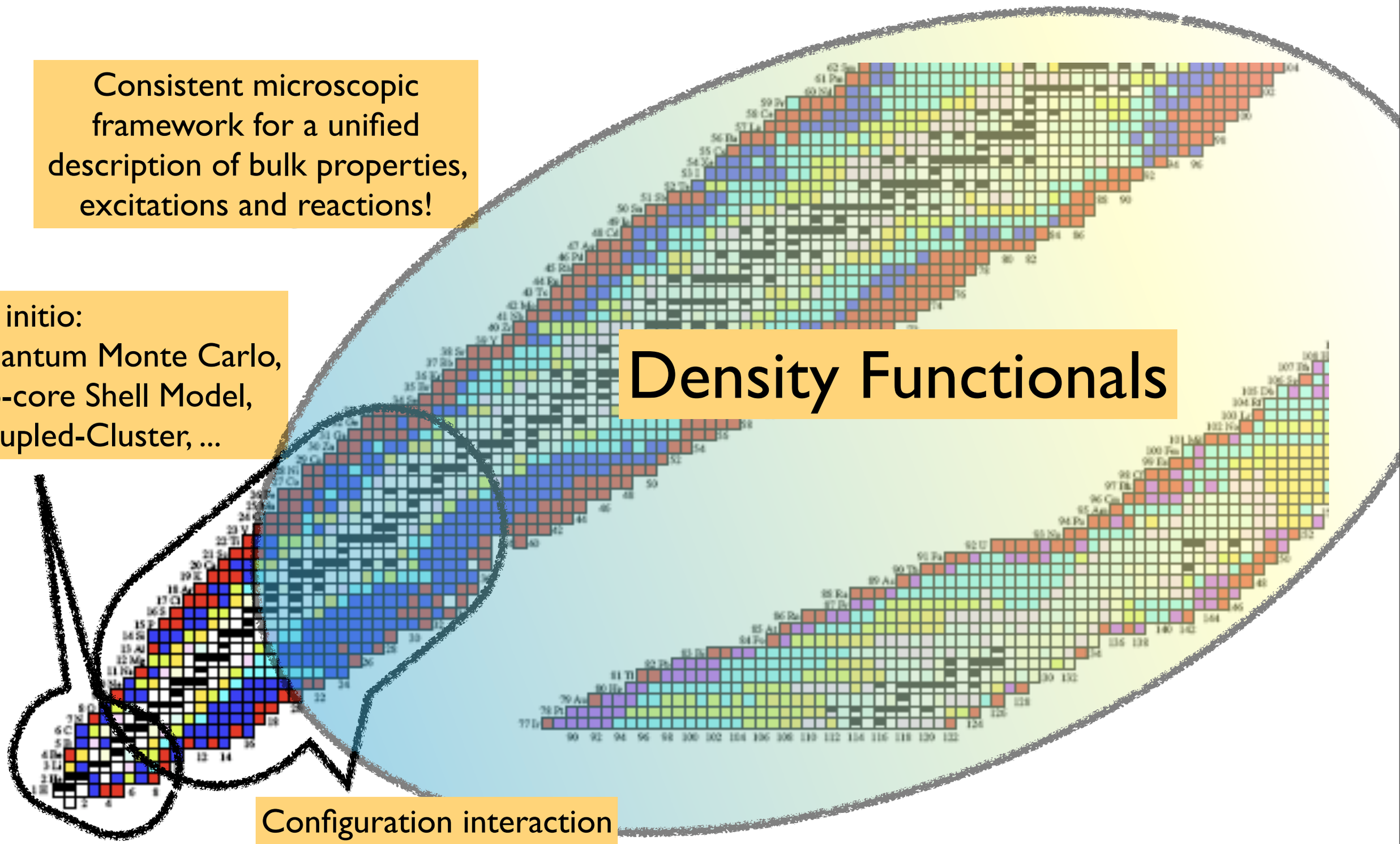
Relativistic Nuclear Energy Density Functionals

Dario Vretenar
University of Zagreb

Energy Density Functionals

Consistent microscopic framework for a unified description of bulk properties, excitations and reactions!

Ab initio:
Quantum Monte Carlo,
No-core Shell Model,
Coupled-Cluster, ...



Configuration interaction
(Interacting Shell-Model)

Kohn-Sham Density Functional Theory:

For any interacting system, there exists a **local single-particle potential $v_s(\mathbf{r})$**, such that the **exact** ground-state density of the interacting system equals the ground-state density of the auxiliary non-interacting system:

$$\rho(\mathbf{r}) = \rho_s(\mathbf{r}) \equiv \sum_{i}^{occ} |\phi_i(\mathbf{r})|^2$$

... there exists a unique energy functional:

$$E_s[\rho] = T_s[\rho] + \int d^3r \; v_s(\mathbf{r})\rho(\mathbf{r})$$

for which the variational equation yields the exact ground-state density n_s.
$T_s[n]$ - universal kinetic energy functional of non-interacting particles.

$$v_s[\rho(\mathbf{r})] = v(\mathbf{r}) + U[\rho(\mathbf{r})] + v_{xc}[\rho(\mathbf{r})]$$

external potential

Hartree term

exchange-correlation

Self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the Hartree-Fock. It has the advantage of being a **local scheme**.

$$v_{xc}[\rho(\mathbf{r})] = \frac{\delta E_{xc}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})}$$

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found!

Nuclear Energy Density Functionals: the many-body problem is mapped onto a one body problem without explicitly involving inter-nucleon interactions!

The exact density functional is approximated with **powers and gradients of ground-state nucleon densities and currents.**

Local densities and currents:

T=0 density:

$$\rho_0(\mathbf{r}) \quad = \quad \rho_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)$$

T=1 density:

$$\rho_1(\mathbf{r}) \quad = \quad \rho_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)\,\tau$$

T=0 spin density:

$$\mathbf{s}_0(\mathbf{r}) \quad = \quad \mathbf{s}_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}$$

T=1 spin density:

$$\mathbf{s}_1(\mathbf{r}) \quad = \quad \mathbf{s}_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}\,\tau$$

Current:

$$\mathbf{j}_T(\mathbf{r}) \quad = \quad \tfrac{i}{2}(\nabla' - \nabla)\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Spin-current tensor:

$$\mathcal{J}_T(\mathbf{r}) \quad = \quad \tfrac{i}{2}(\nabla' - \nabla) \otimes \mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic density:

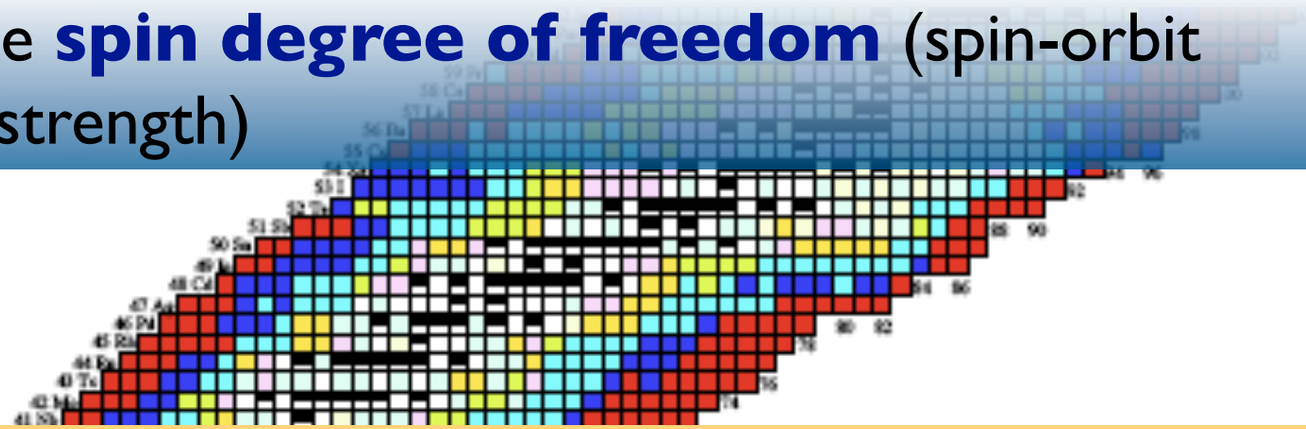
$$\tau_T(\mathbf{r}) \quad = \quad \nabla \cdot \nabla'\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic spin-density:

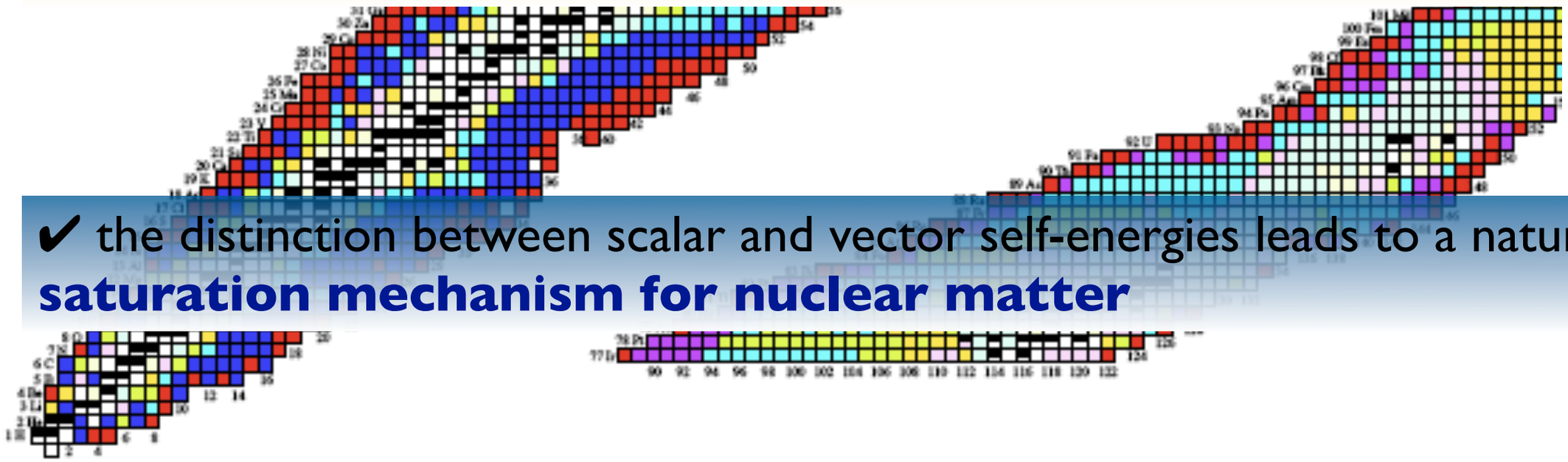
$$\mathbf{T}_T(\mathbf{r}) \quad = \quad \nabla \cdot \nabla'\,\mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

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.

"No-sea" approximation!

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.

Advantages of the Energy Density Functional approach to nuclear structure

✔ an intuitive interpretation of mean-field results in terms of ***intrinsic shapes*** and ***single-particle states***

✔ the ***full model space*** of occupied states can be used; no distinction between core and valence nucleons, ***no need for effective charges***

✔ the use of ***universal density functionals*** that can be applied to all nuclei throughout the periodic chart

Important for extrapolations to regions far from stability!

... microscopic foundation for a universal EDF framework, related to and constrained by low-energy QCD

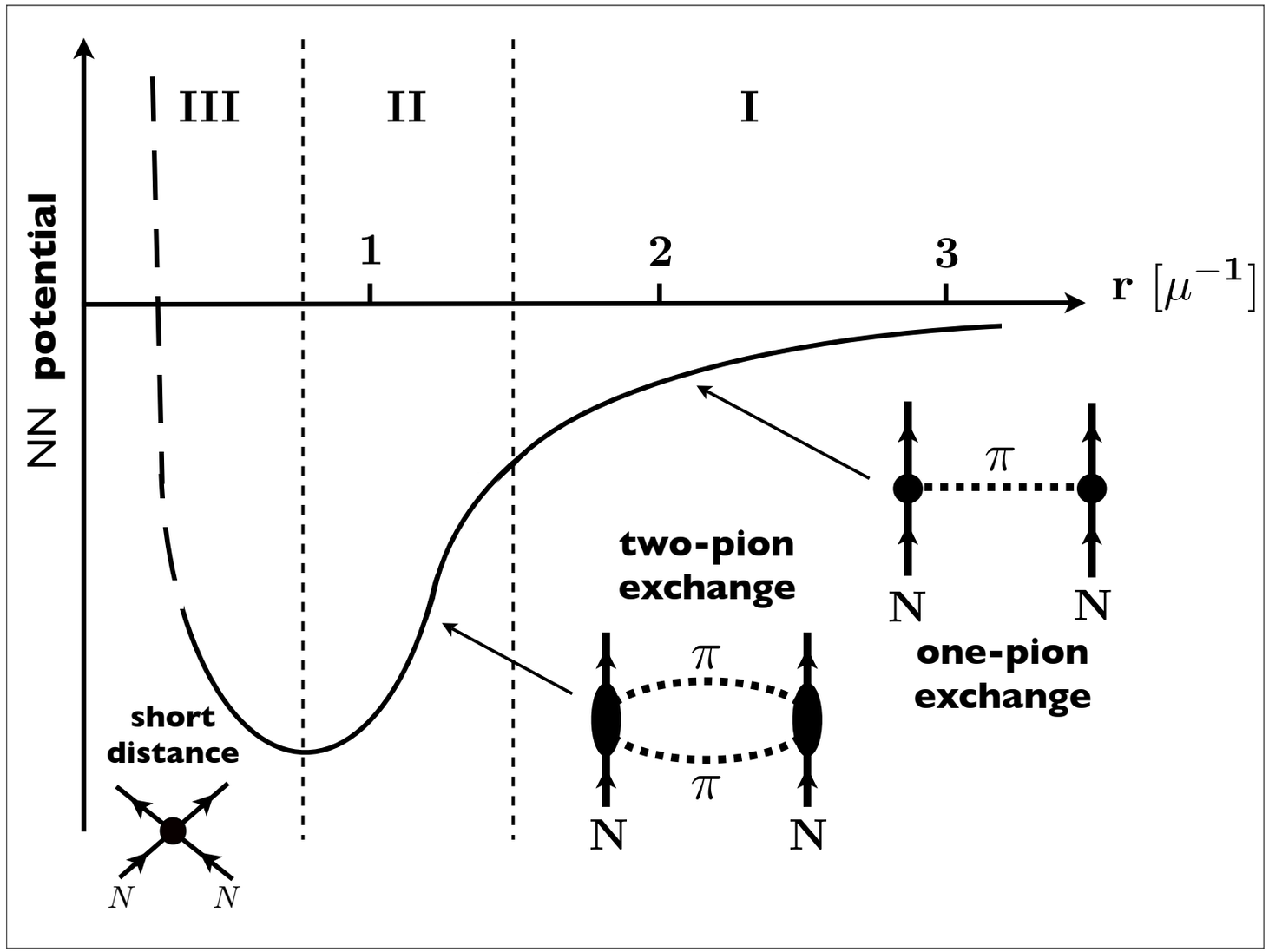
... accurate and controlled approximations for the nuclear exchange-correlation energy functional

... correlations related to restoration of broken symmetries and fluctuations of collective coordinates

The description of **nuclear many-body systems** must be related to and constrained by **low-energy, non-perturbative QCD.**

A **microscopic nuclear energy density functional** must include the **exchange-correlation part**, starting from the relevant active degrees of freedom at low energy:

PIONS & NUCLEONS



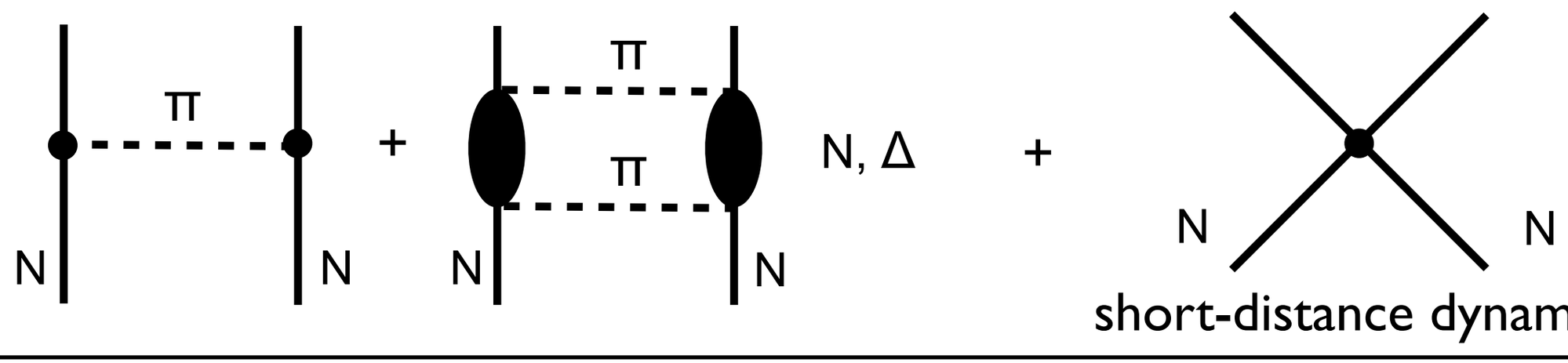
An **effective field theory (EFT)** of low-energy in-medium NN interactions can be used to construct approximations to **the exact exchange-correlation functional.**

In the nuclear medium:

relevant scale:
Fermi momentum

$$k_f \approx 2m_\pi << 4\pi f_\pi$$

pion-exchange processes in the presence of a filled Fermi sea:



The density functional involves an expansion of nucleon self-energies in **powers of the Fermi momentum.**

Model for Finite Nuclei

P. Finelli, N. Kaiser, D. Vretenar, W. Weise, Nucl. Phys. A **735** (2004) 449, A **770** (2006) 1.

Chiral (pionic) fluctuations in combination with three-nucleon (3N) interactions are responsible for **nuclear binding and saturation.**

...exchange-correlation functional $E_{xc}[\rho]$

1st step: **Local Density Approximation**

$$E_{xc}^{LDA} \equiv \int \varepsilon^{ChPT}[\rho(\mathbf{r})]\rho(\mathbf{r})d^3r$$

2nd step: **second-order gradient correction to the LDA**

ChPT calculations for inhomogeneous nuclear matter:

$$\mathcal{E}(\rho, \nabla\rho) = \rho\,\overline{E}(k_f) + (\nabla\rho)^2\, F_{\nabla}(k_f) + \ldots$$

Semi-empirical functionals

Infinite nuclear matter cannot determine the density functional on the level of accuracy that is needed for a quantitative description of structure phenomena in finite nuclei.

... start from a favorite microscopic nuclear matter EOS

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

DD-PC1

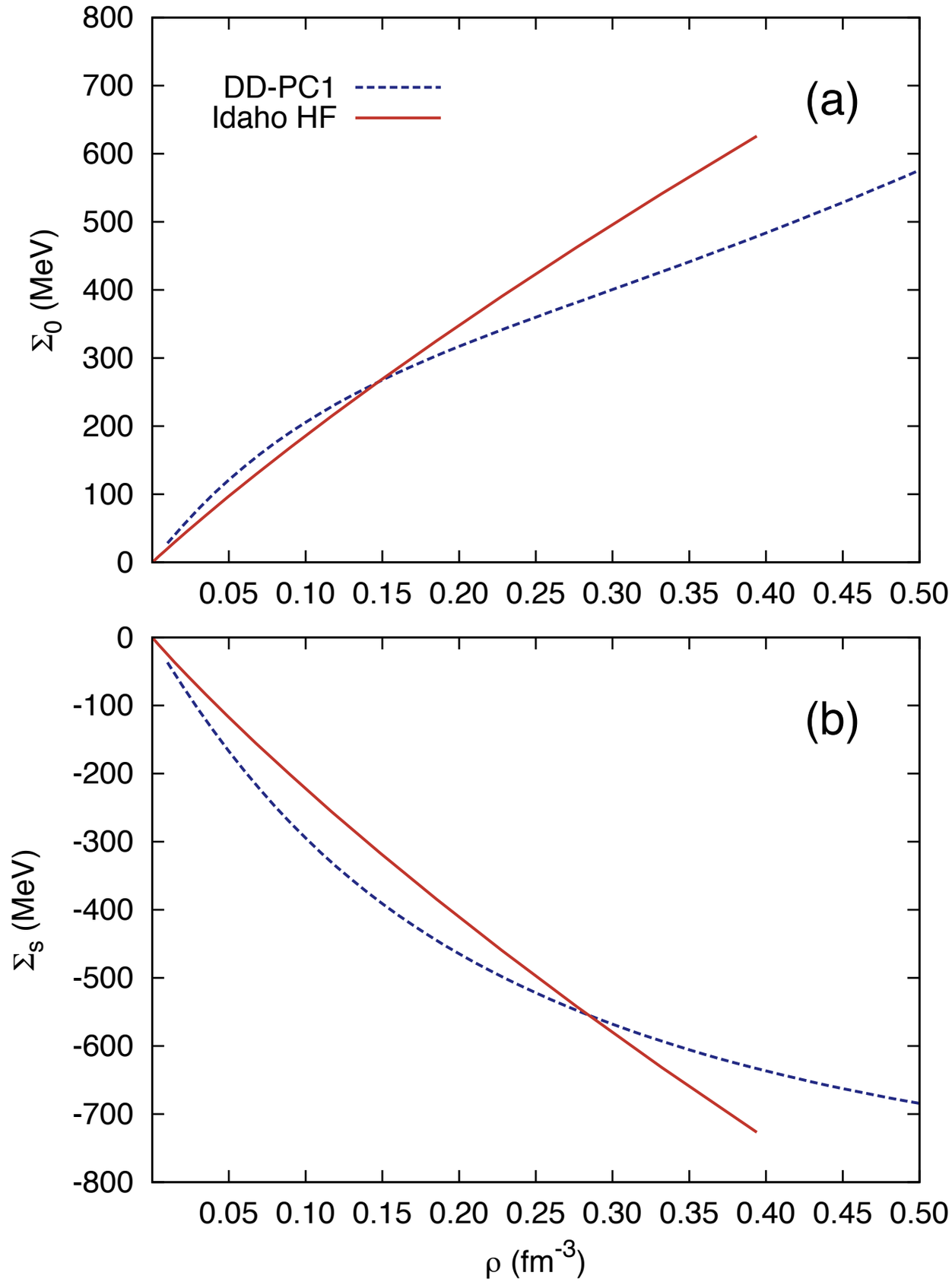
Nikšić, Vretenar, and Ring, Phys. Rev. C **78**, 034318 (2008)

... 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.

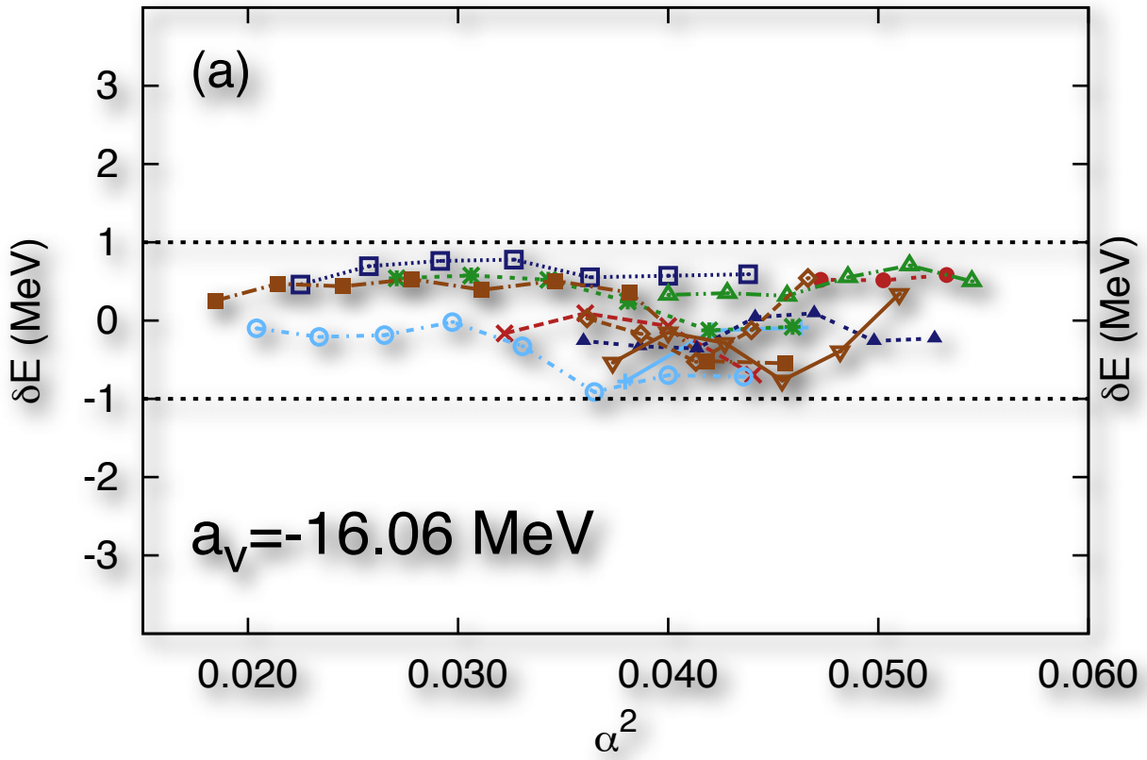
Starting approximation: Hartree-Fock self-energies calculated from the Idaho N^3LO NN-potential.

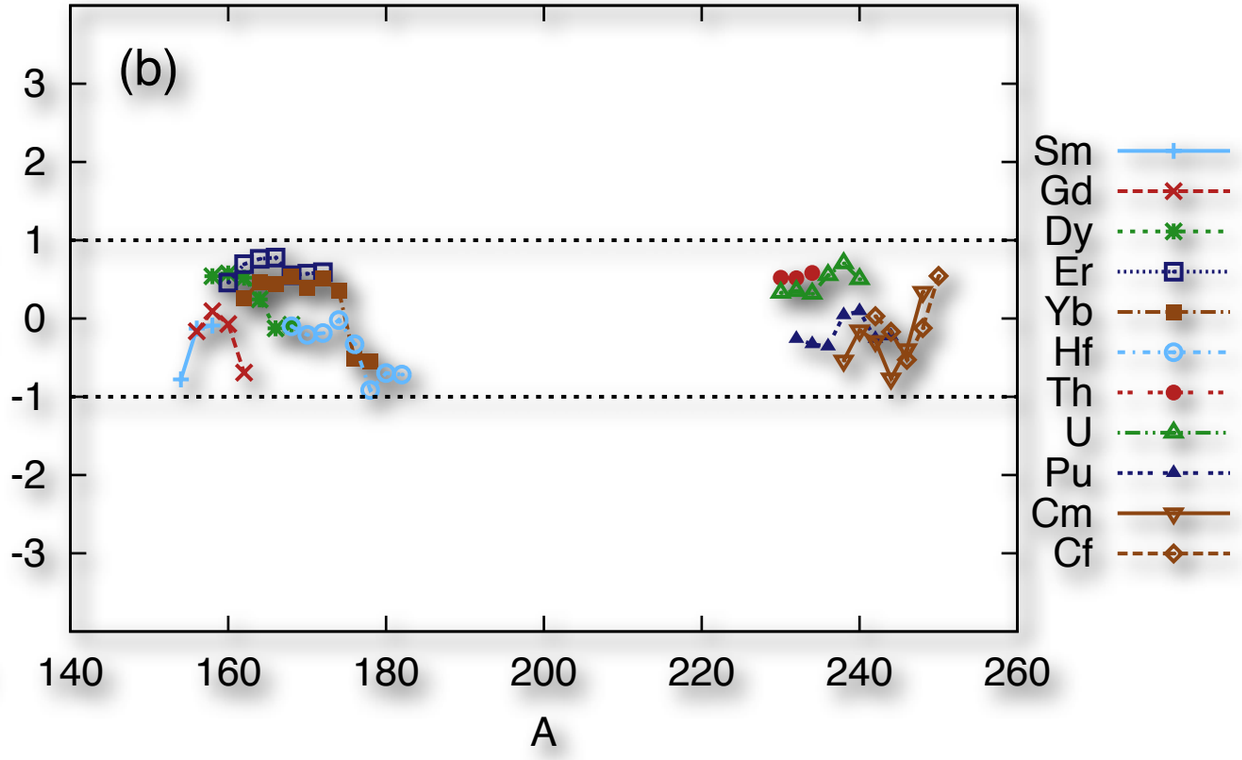


Deformed nuclei

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

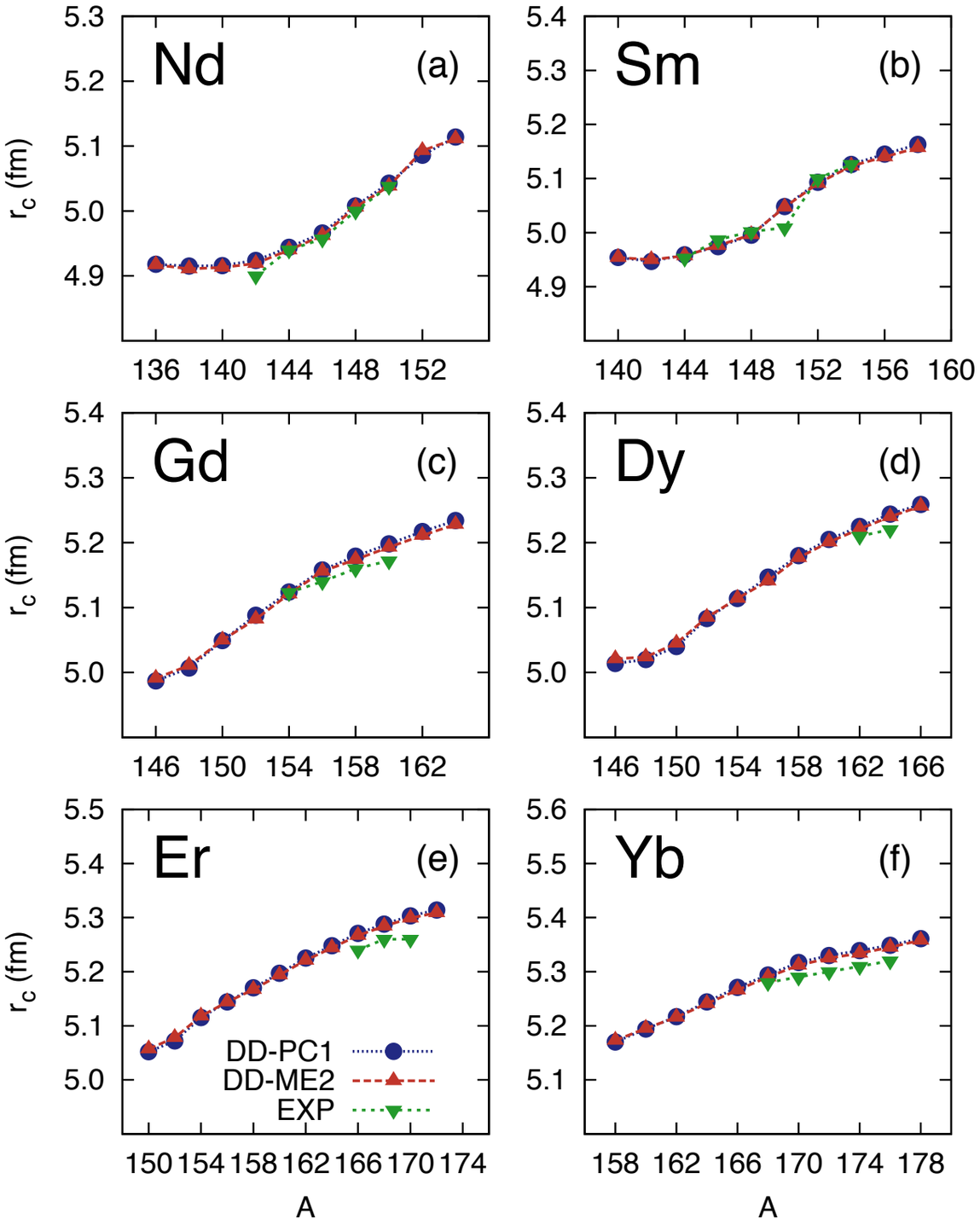




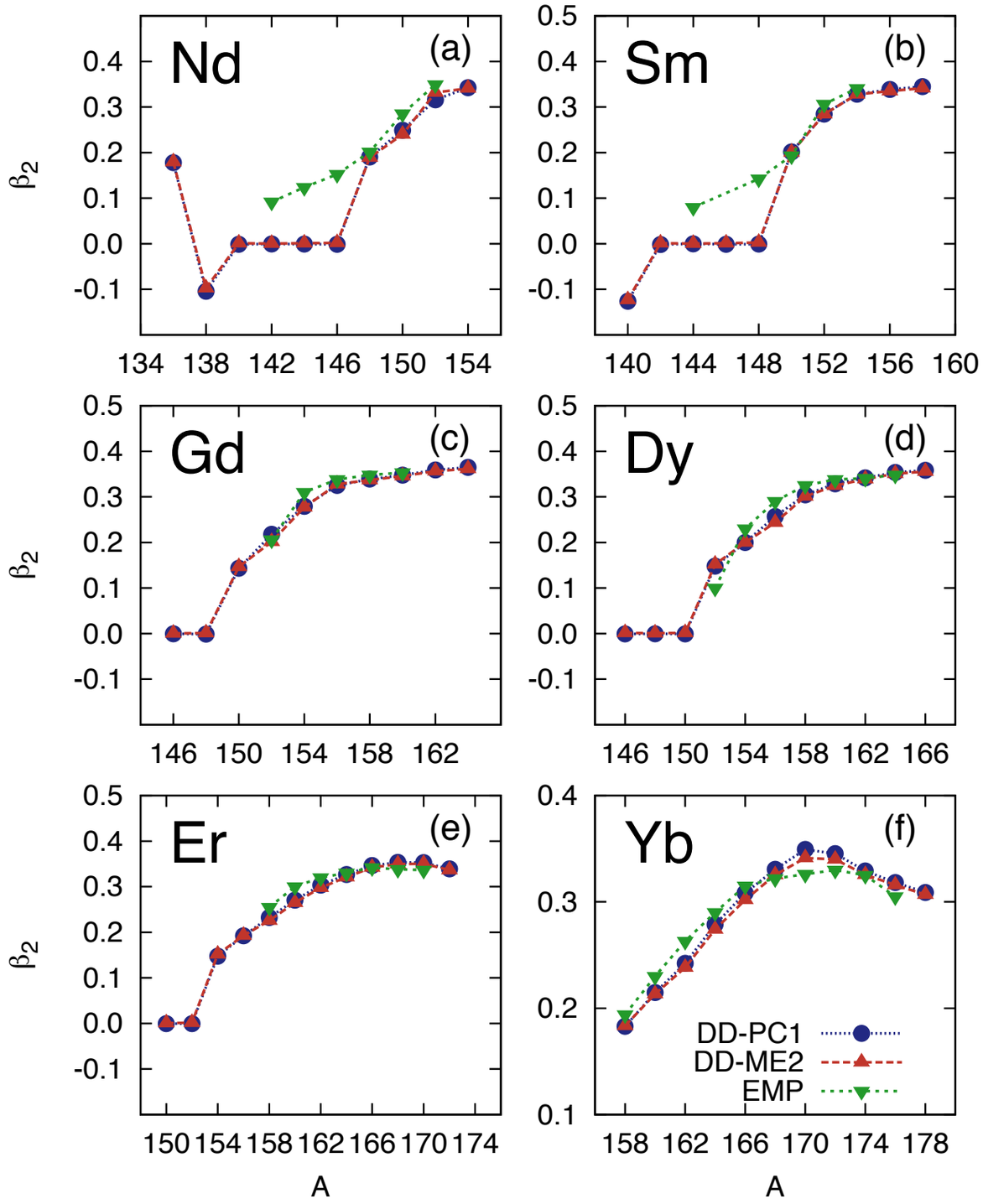
Nikšić, Vretenar, and Ring, Phys. Rev. C **78**, 034318 (2008)

Systematic calculation of ground-state properties:

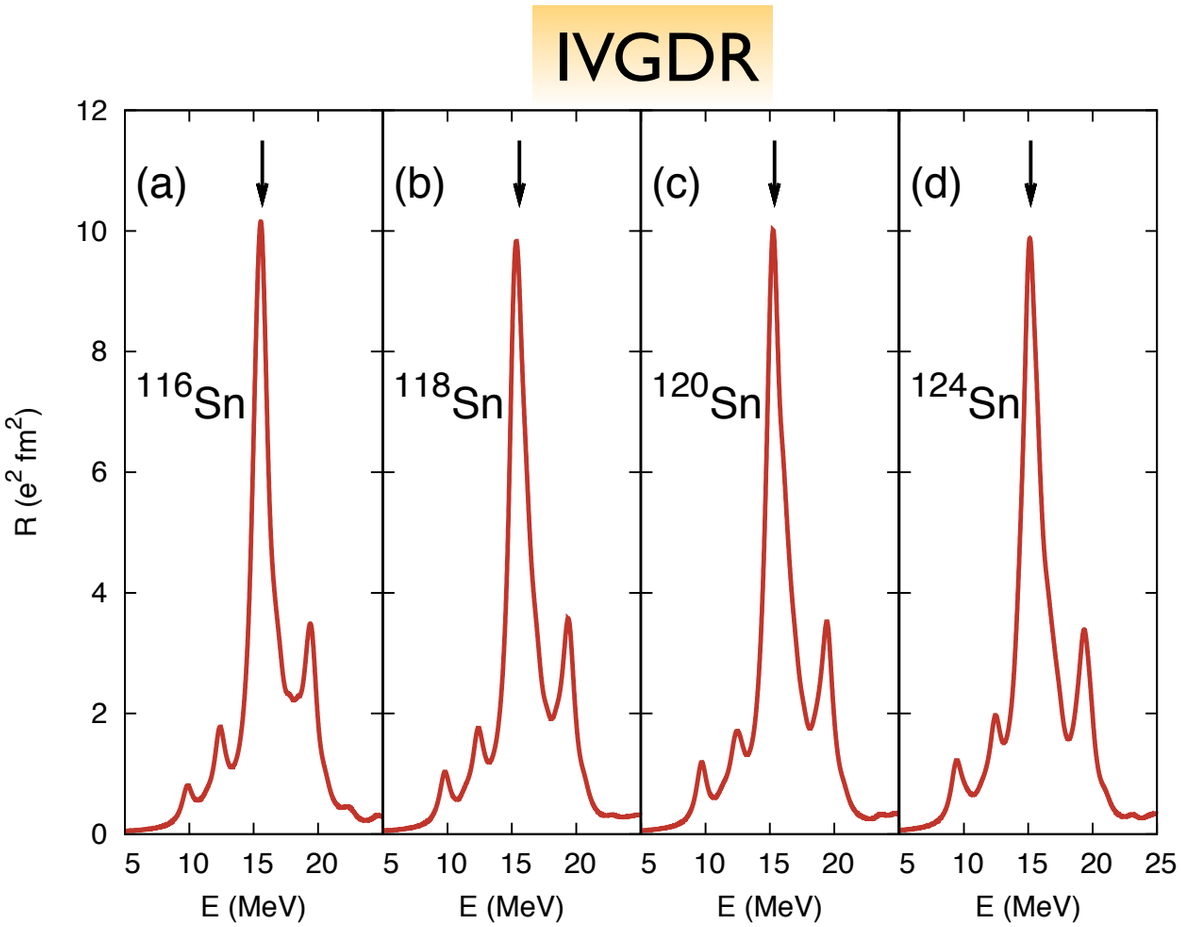
Charge radii

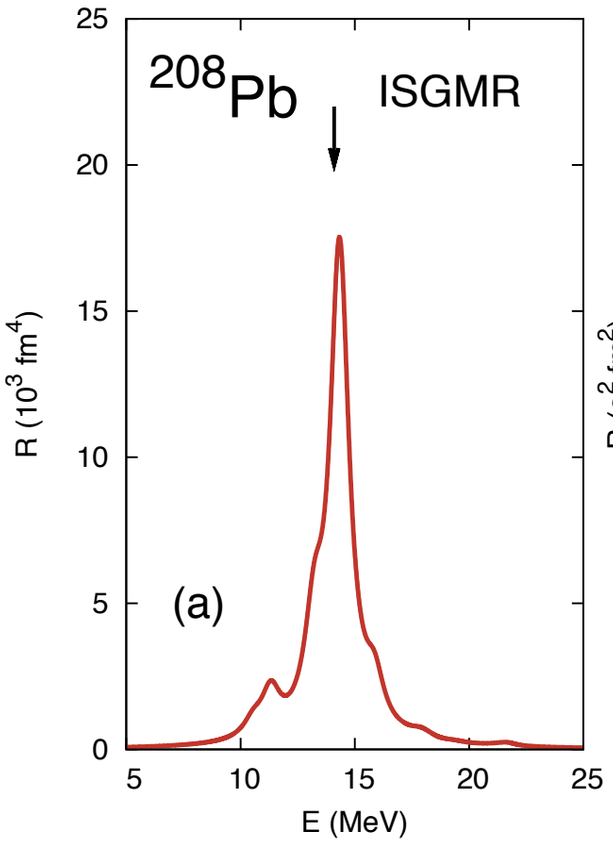


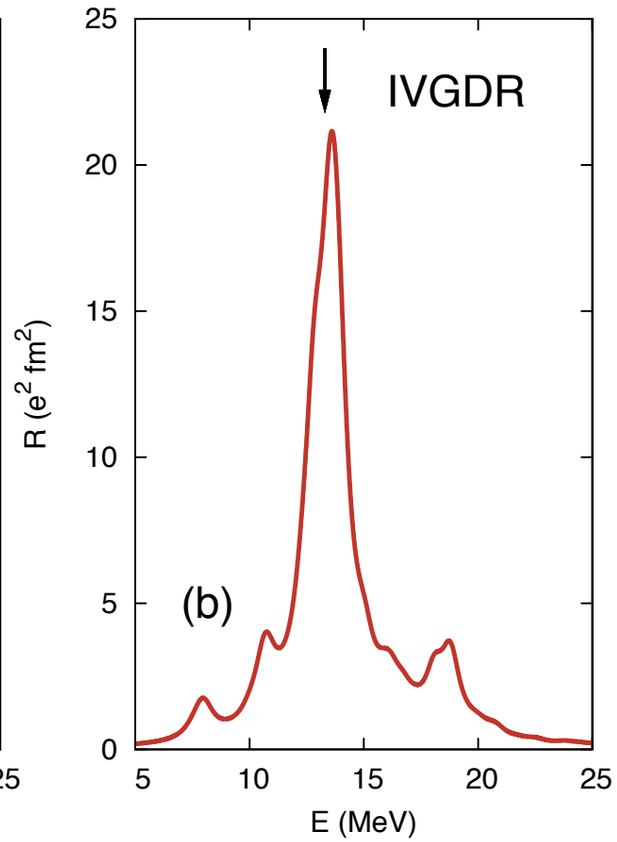
Quadrupole deformations



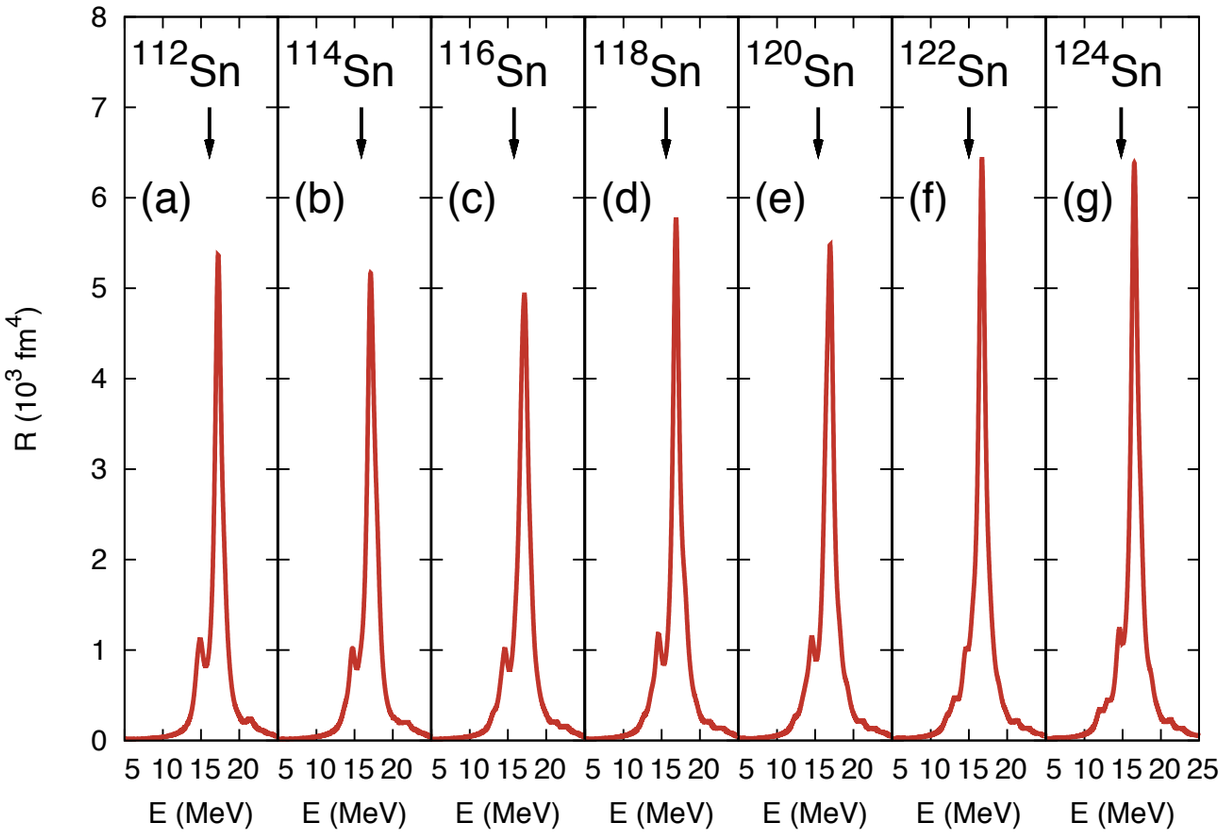
Excitation energies of collective modes:







ISGMR



Nuclear Many-Body Correlations

short-range
(hard repulsive core of the NN-interaction)

long-range
nuclear resonance modes

collective correlations
large-amplitude soft modes:
(center of mass motion, rotation, low-energy quadrupole vibrations)

...vary smoothly with nucleon number!
Implicitly included in the universal EDF.

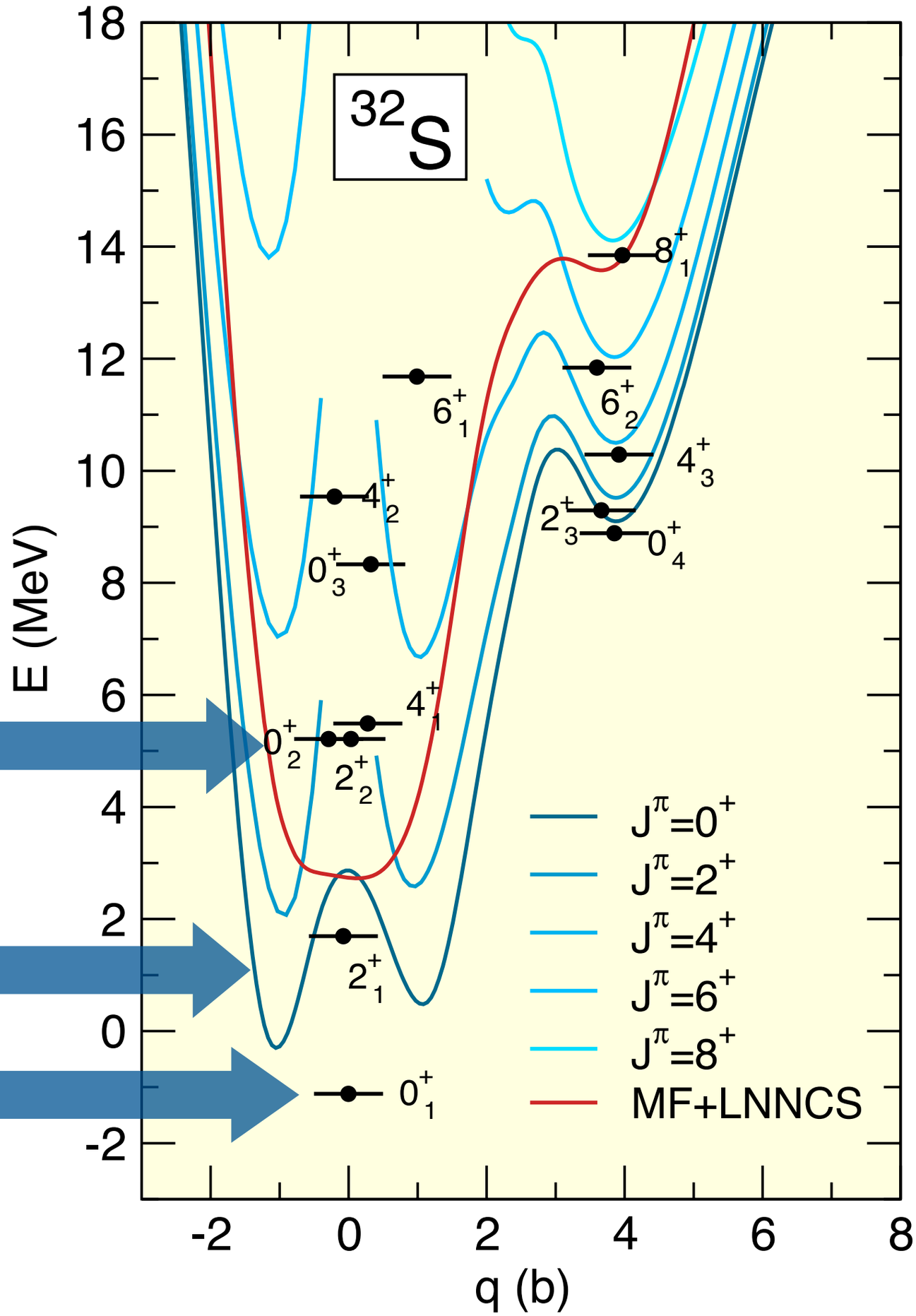
...sensitive to shell-effects and strong variations with nucleon number!
Cannot be included in a simple EDF framework.

Restoration of broken symmetries and fluctuations of collective variables

1. Mean-field + Lipkin-Nogami BCS equations, with a constraint on the quadrupole moment.

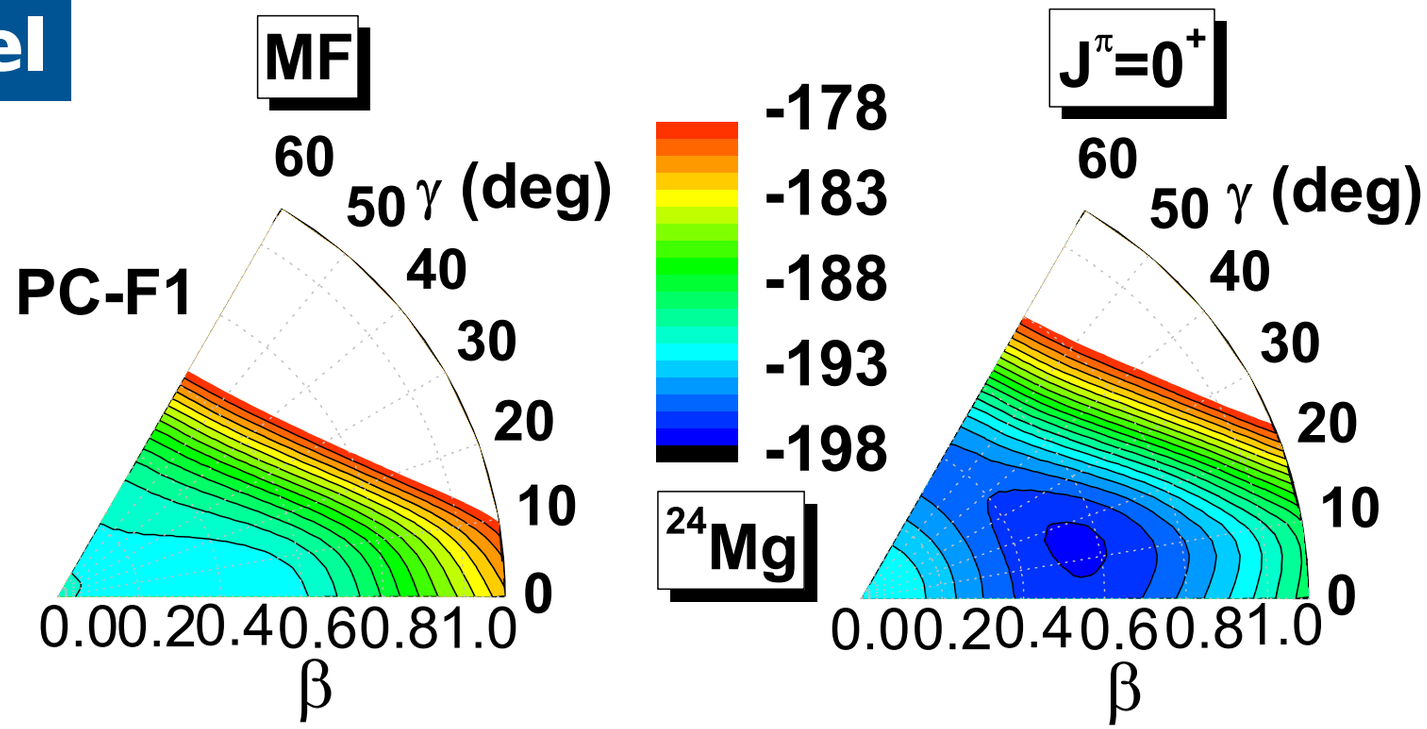
2. Angular-momentum and particle-number projection.

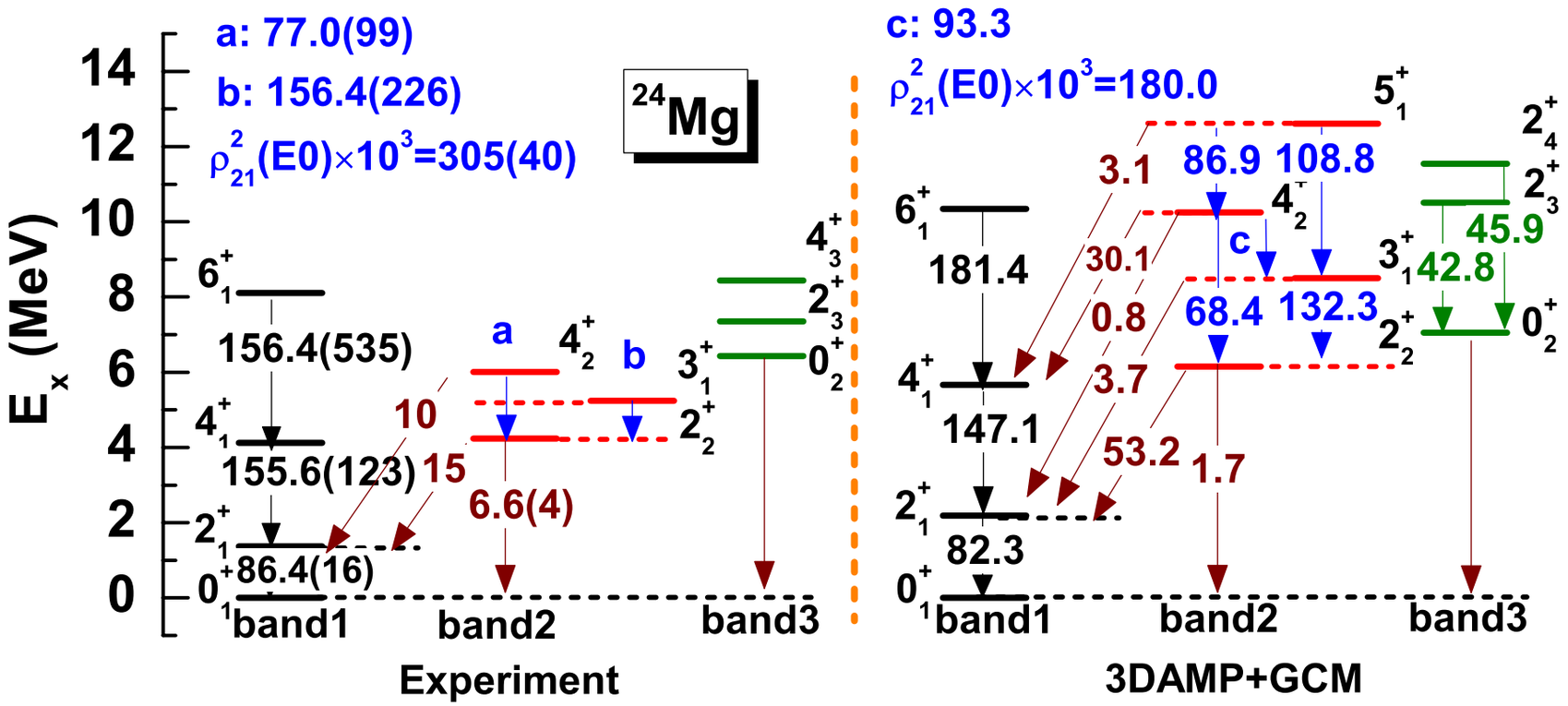
3. Generator Coordinate Method
⇒ configuration mixing



... larger variational space for projected GCM calculations!

3D AMP + GCM model





Yao, Meng, Ring, Vretenar,
Phys. Rev. C **81**, 044311 (2010)

Five-dimensional collective Hamiltonian

Nikšić, Li, Vretenar, Prochniak, Meng, Ring, Phys. Rev. C **79**, 034303 (2009)

... 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.

The quantized collective Hamiltonian: $\hat{H} = \hat{T}_{\rm vib} + \hat{T}_{\rm rot} + V_{\rm coll}$

$$\begin{aligned}\hat{T}_{\rm vib} &= -\frac{\hbar^2}{2\sqrt{wr}}\left\{\frac{1}{\beta^4}\left[\frac{\partial}{\partial\beta}\sqrt{\frac{r}{w}}\beta^4 B_{\gamma\gamma}\frac{\partial}{\partial\beta} - \frac{\partial}{\partial\beta}\sqrt{\frac{r}{w}}\beta^3 B_{\beta\gamma}\frac{\partial}{\partial\gamma}\right]\right. \\ &\left. + \frac{1}{\beta\sin 3\gamma}\left[-\frac{\partial}{\partial\gamma}\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\gamma}\frac{\partial}{\partial\beta} + \frac{1}{\beta}\frac{\partial}{\partial\gamma}\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\beta}\frac{\partial}{\partial\gamma}\right]\right\}\end{aligned}$$

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

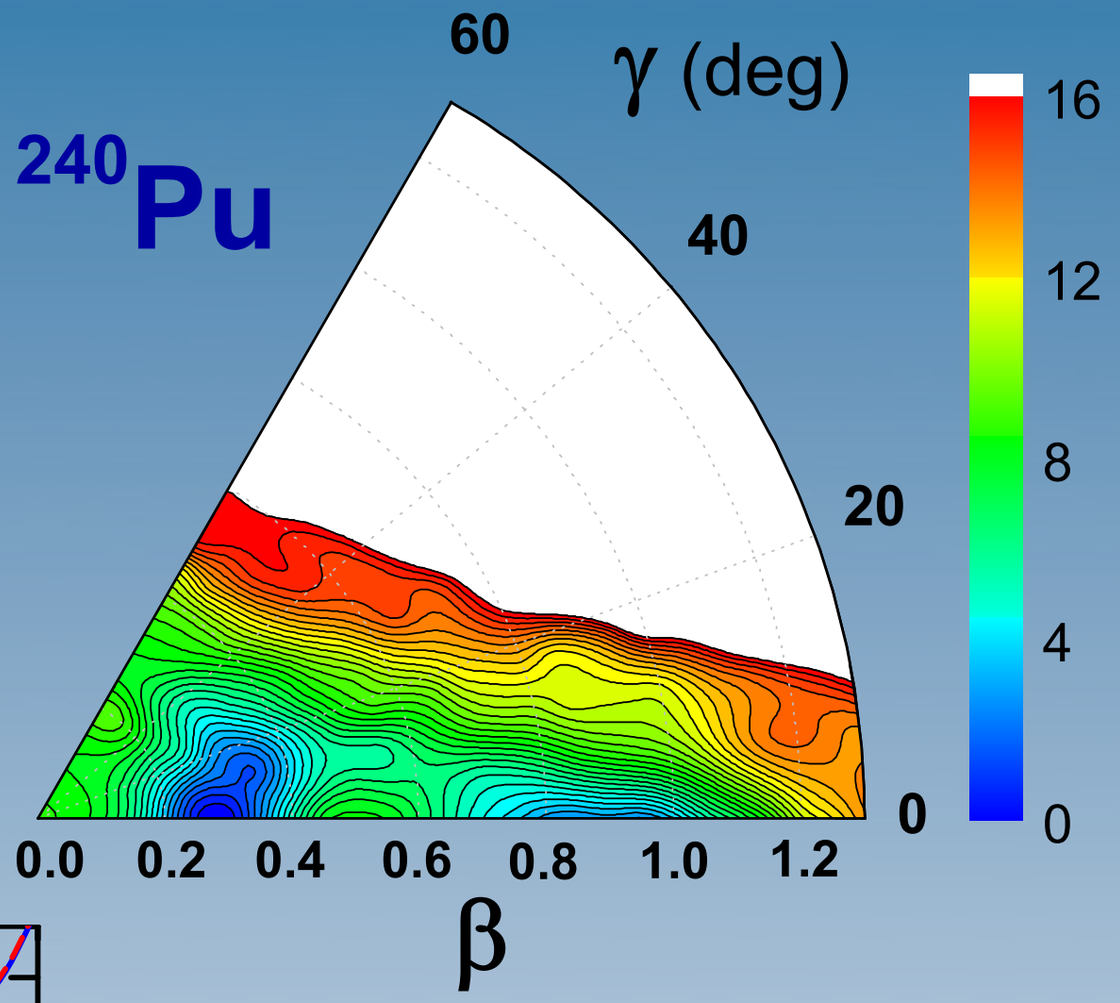
$$V_{\rm coll}(q_0, q_2) = E_{\rm tot}(q_0, q_2) - \Delta V_{\rm vib}(q_0, q_2) - \Delta V_{\rm rot}(q_0, q_2)$$

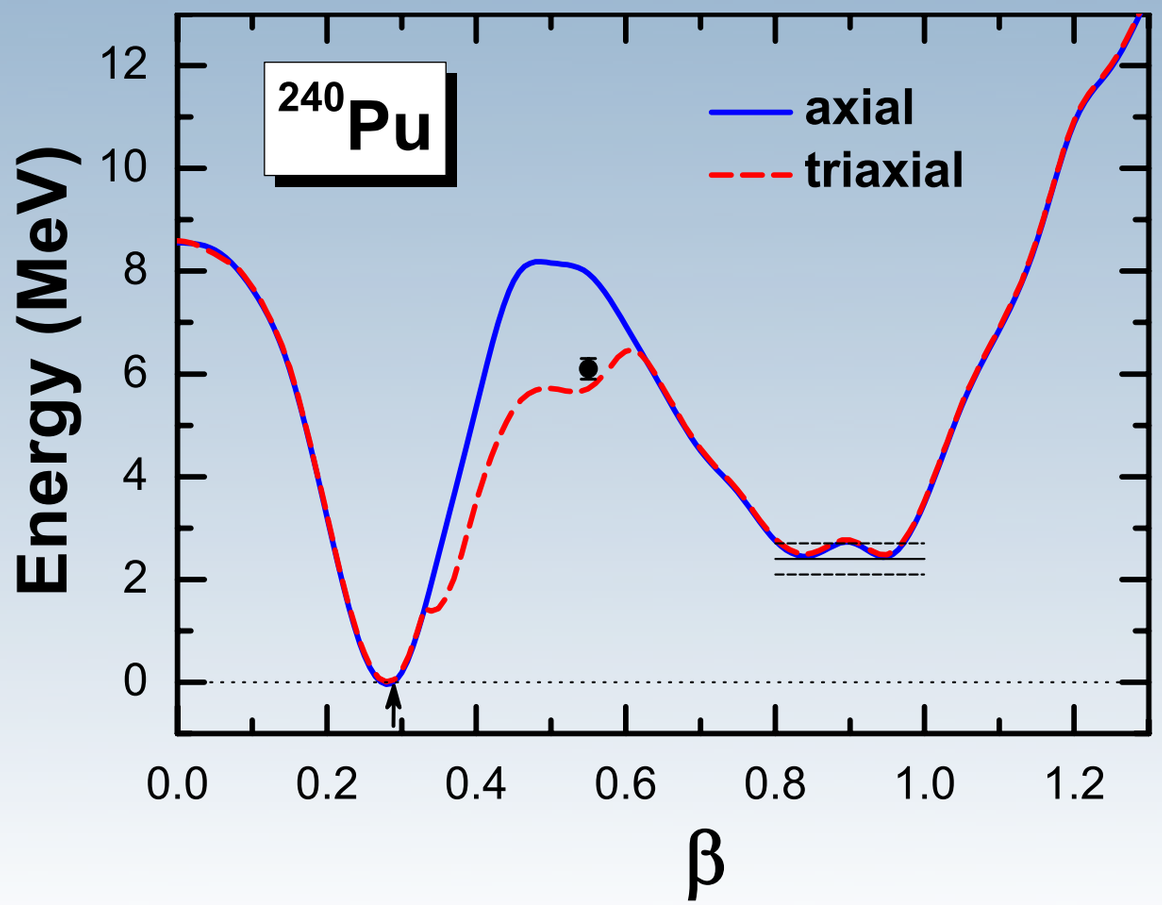
...collective wave functions: $\Psi_\alpha^{IM}(\beta,\gamma,\Omega) = \sum_{K\in\Delta I}\psi_{\alpha K}^I(\beta,\gamma)\Phi_{MK}^I(\Omega)$

$$\Phi_{MK}^I(\Omega) = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}}\left[D_{MK}^{I*}(\Omega) + (-1)^I D_{M-K}^{I*}(\Omega)\right]$$

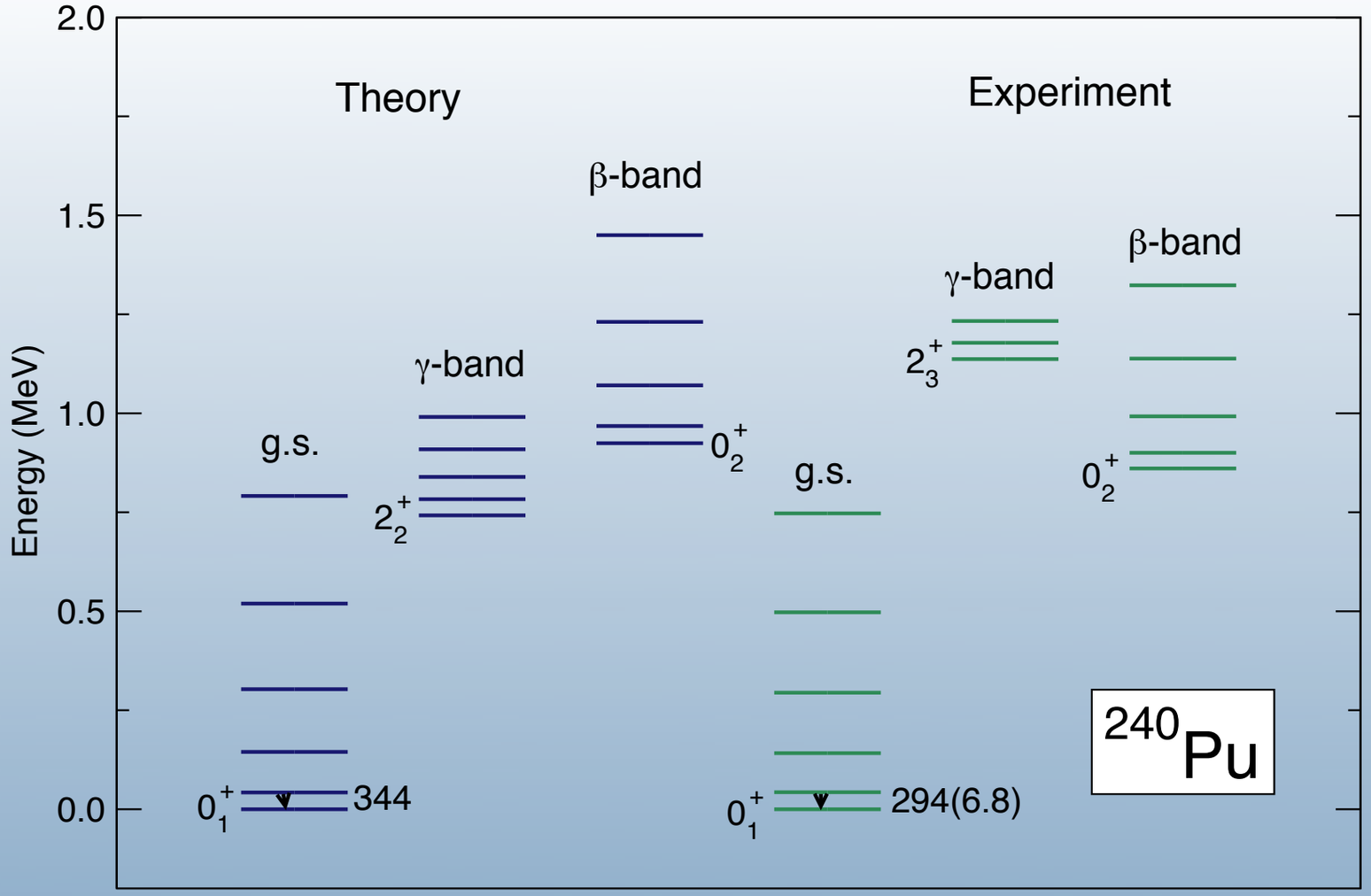
Test of DD-PC1:

Fission path and barriers:





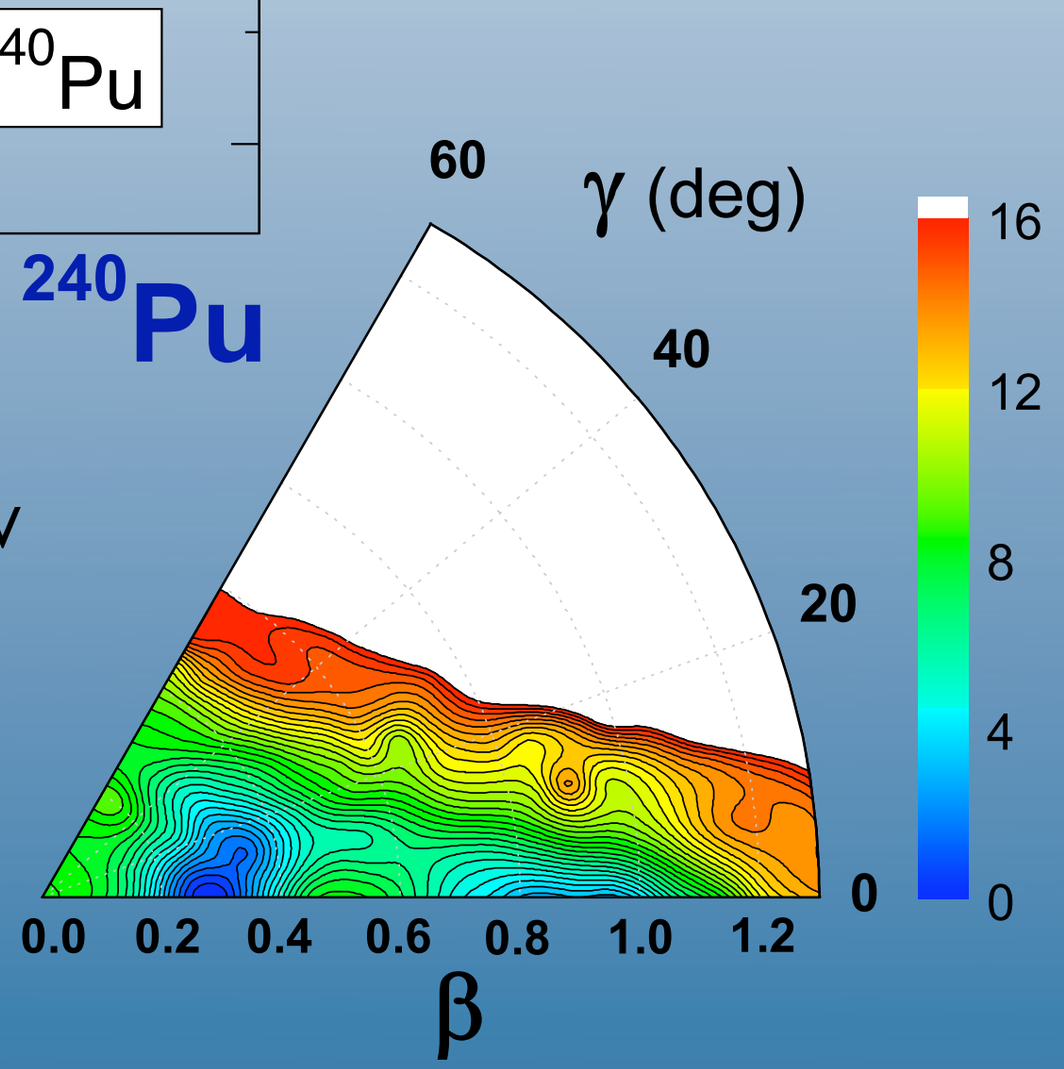
Li, Nikšić, Vretenar, Ring, Meng, Phys. Rev. C (2010)



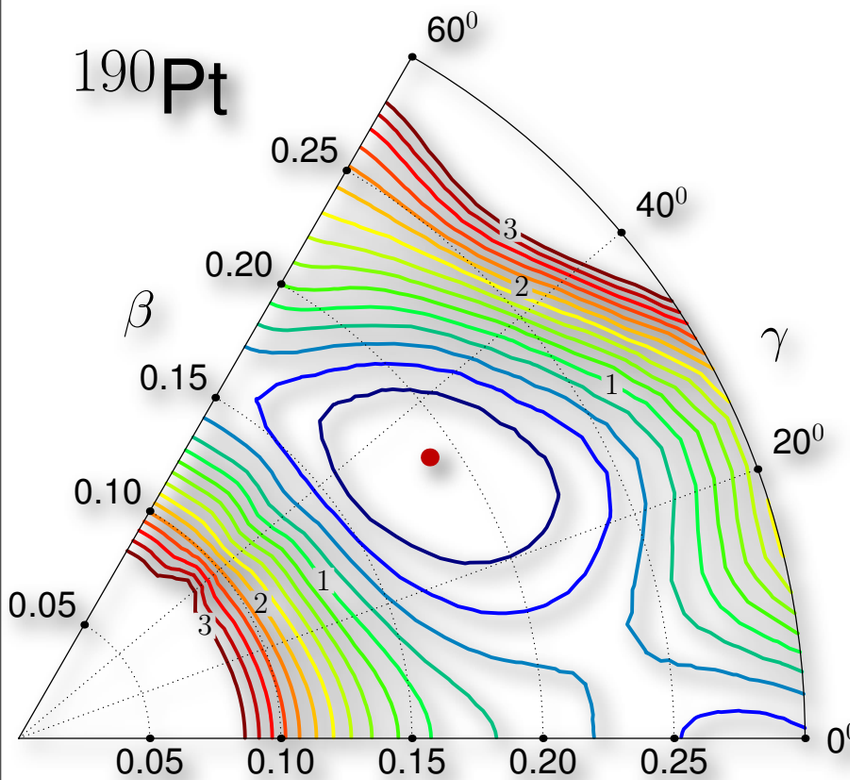
$$E^{th}_{4^+_1}/E^{th}_{2^+_1} = 3.33$$

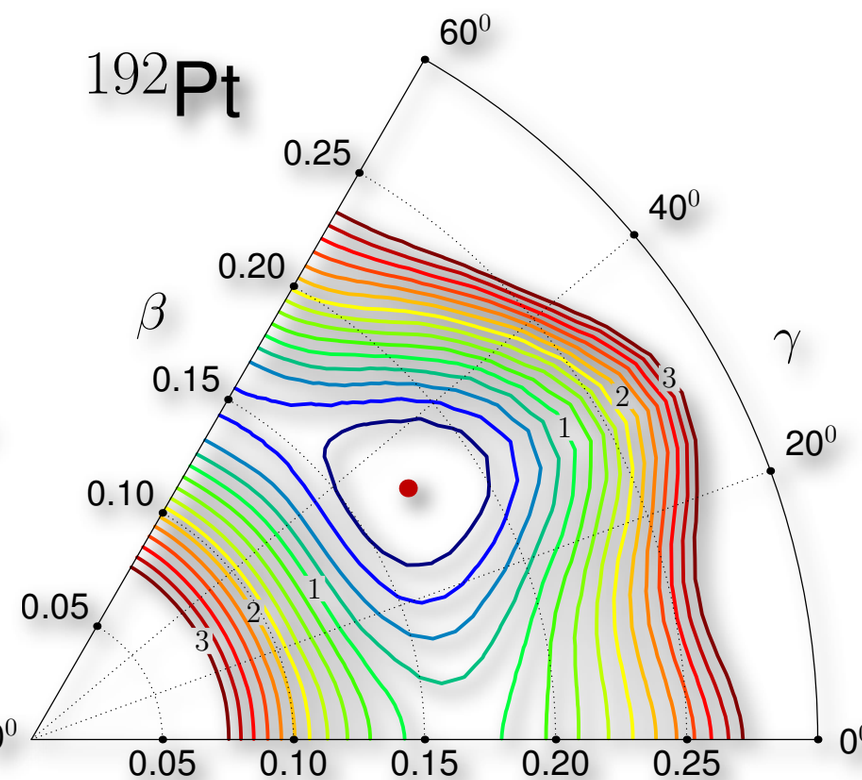
$$E^{exp}_{4^+_1}/E^{exp}_{2^+_1} = 3.31$$

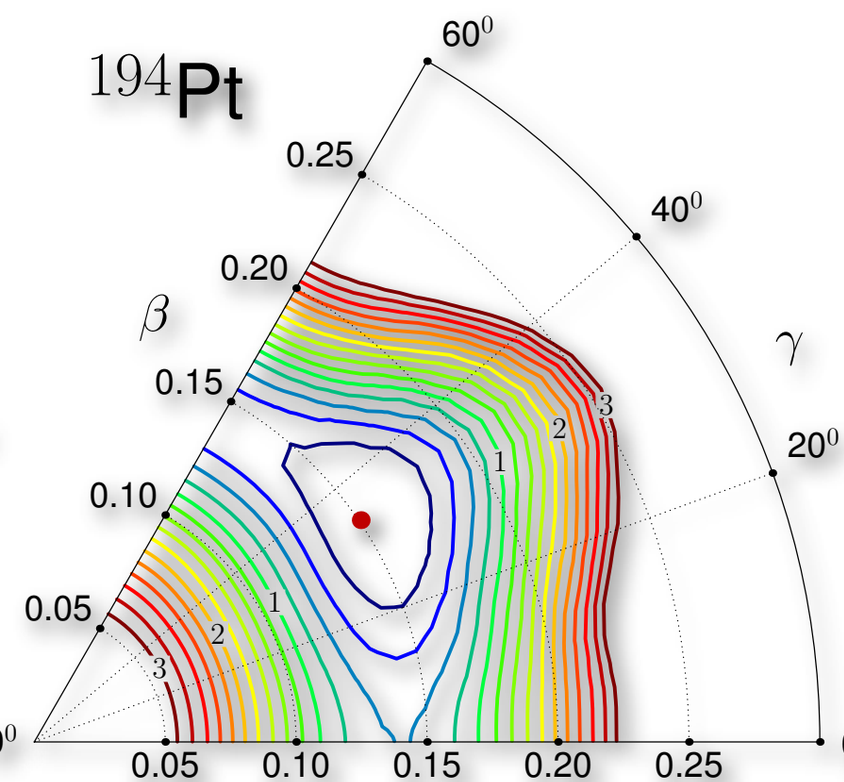
The moments of inertia are renormalized by a factor ≈ 1.3 (difference between the IB and TV moments of inertia).

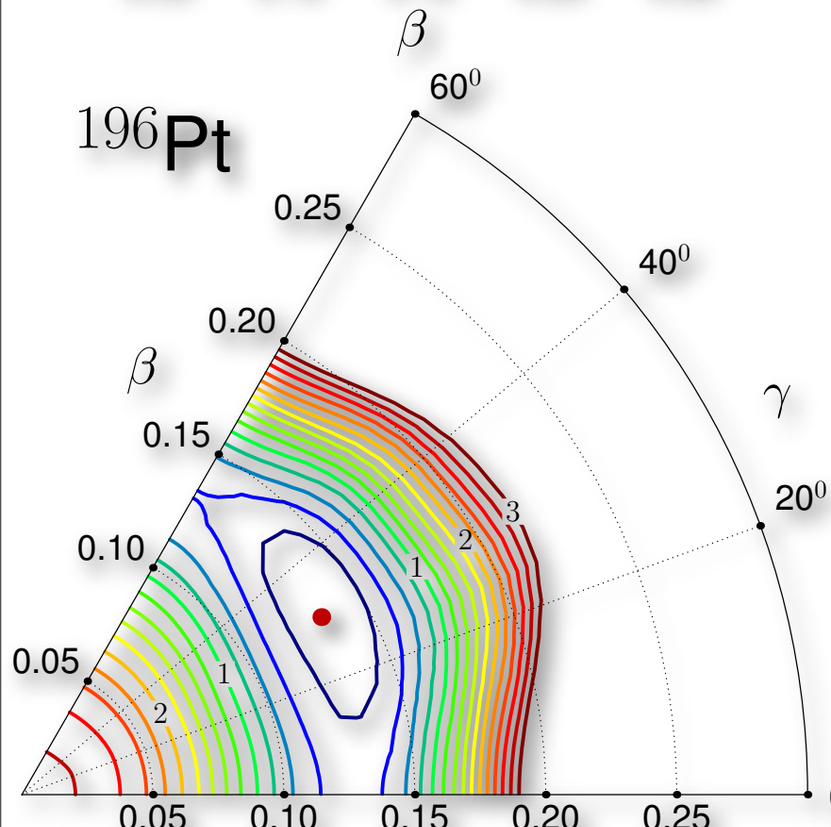


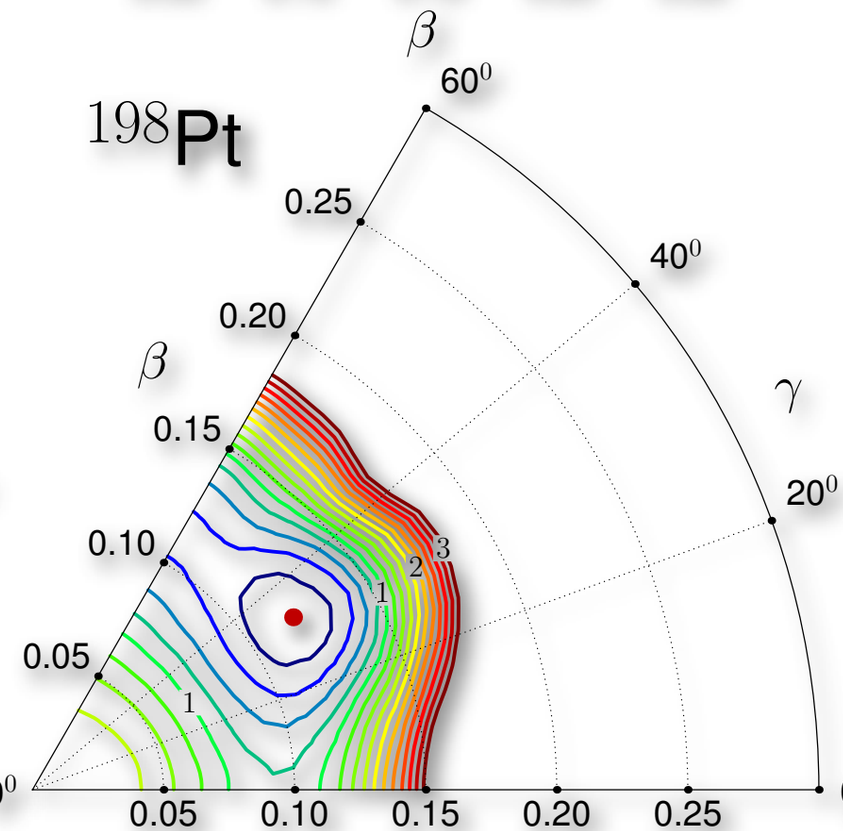
Evolution of triaxial shapes in Pt nuclei:

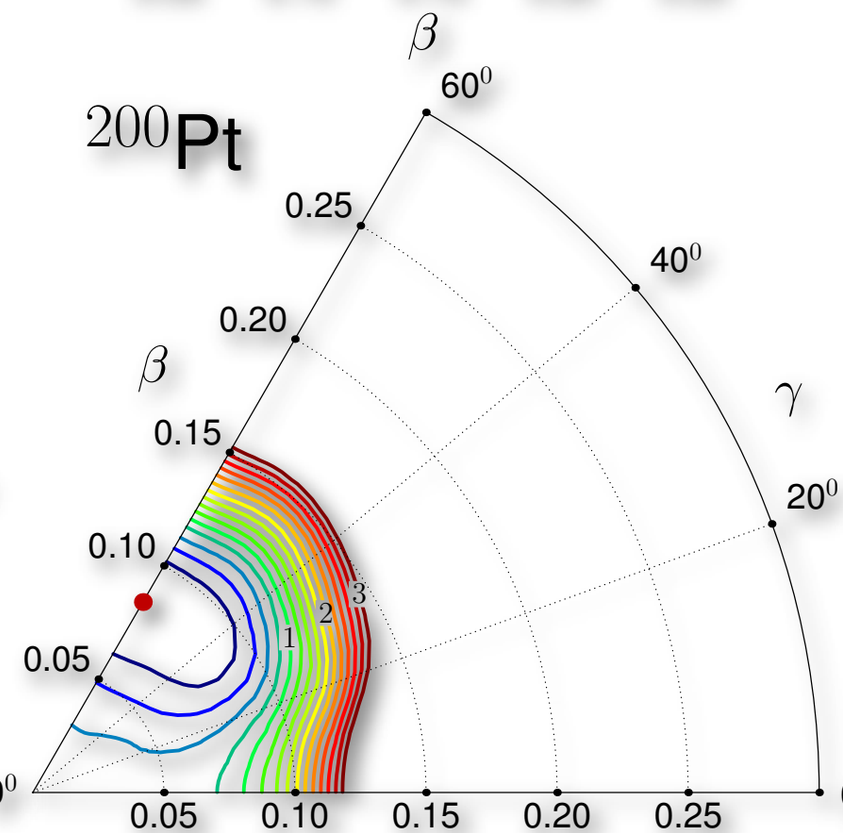


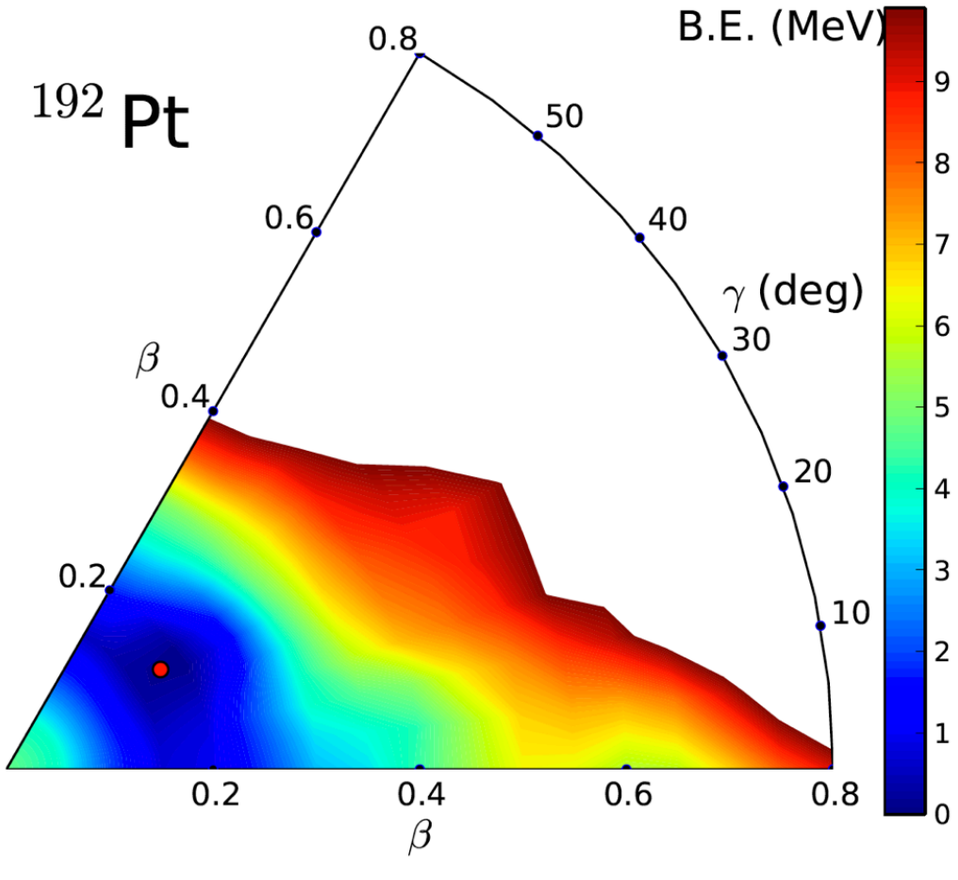






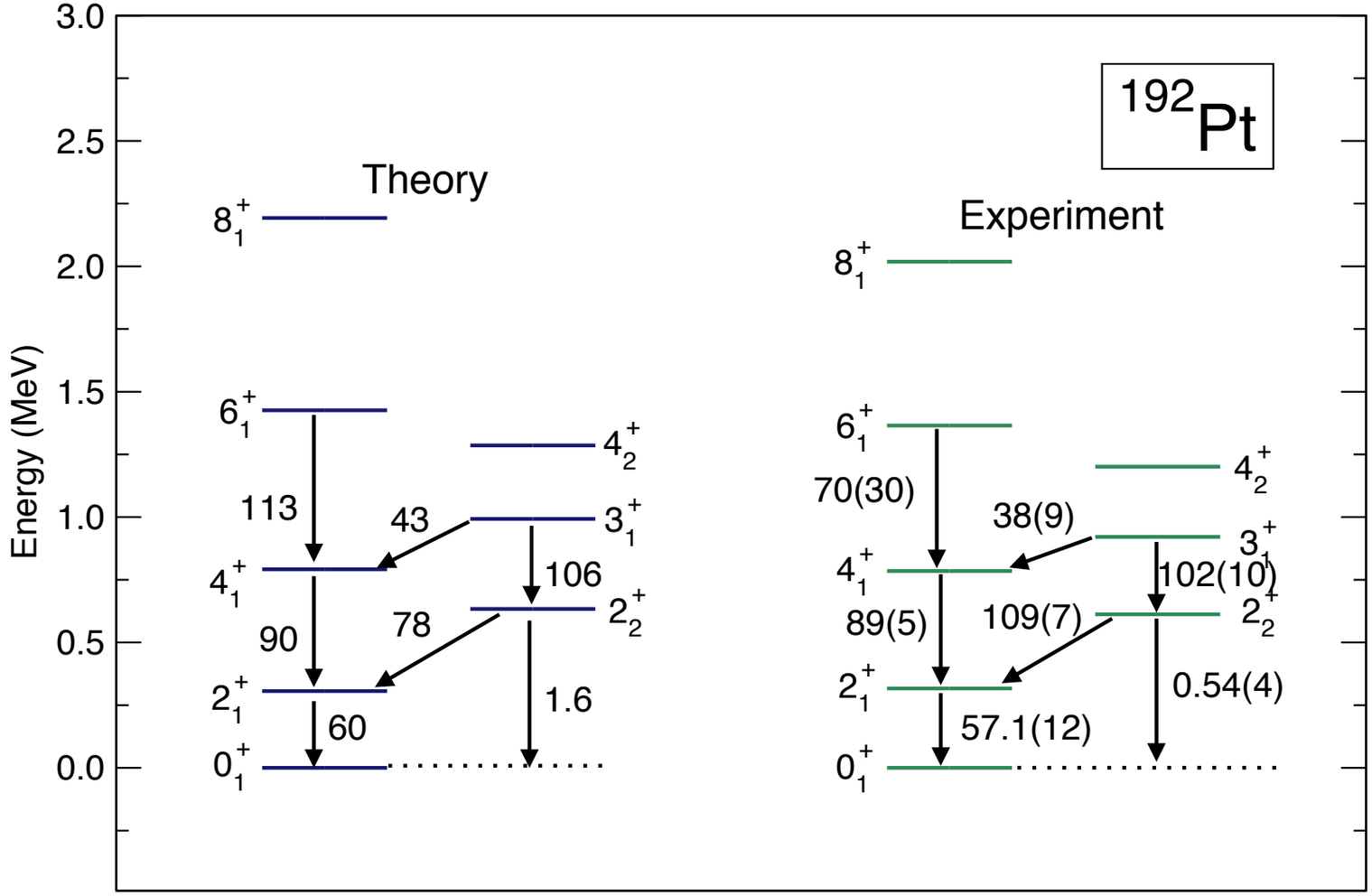






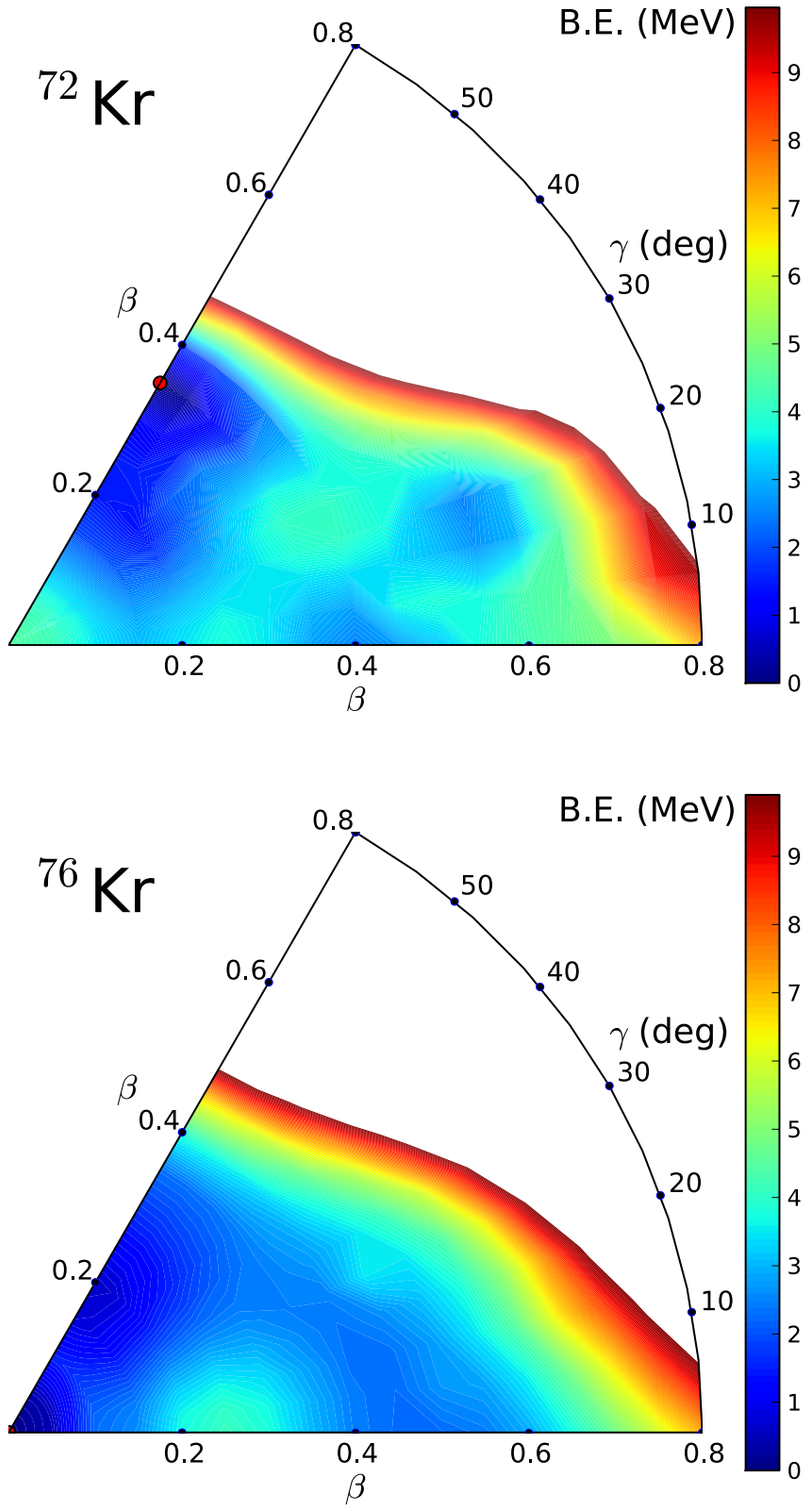
$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 2.58$$

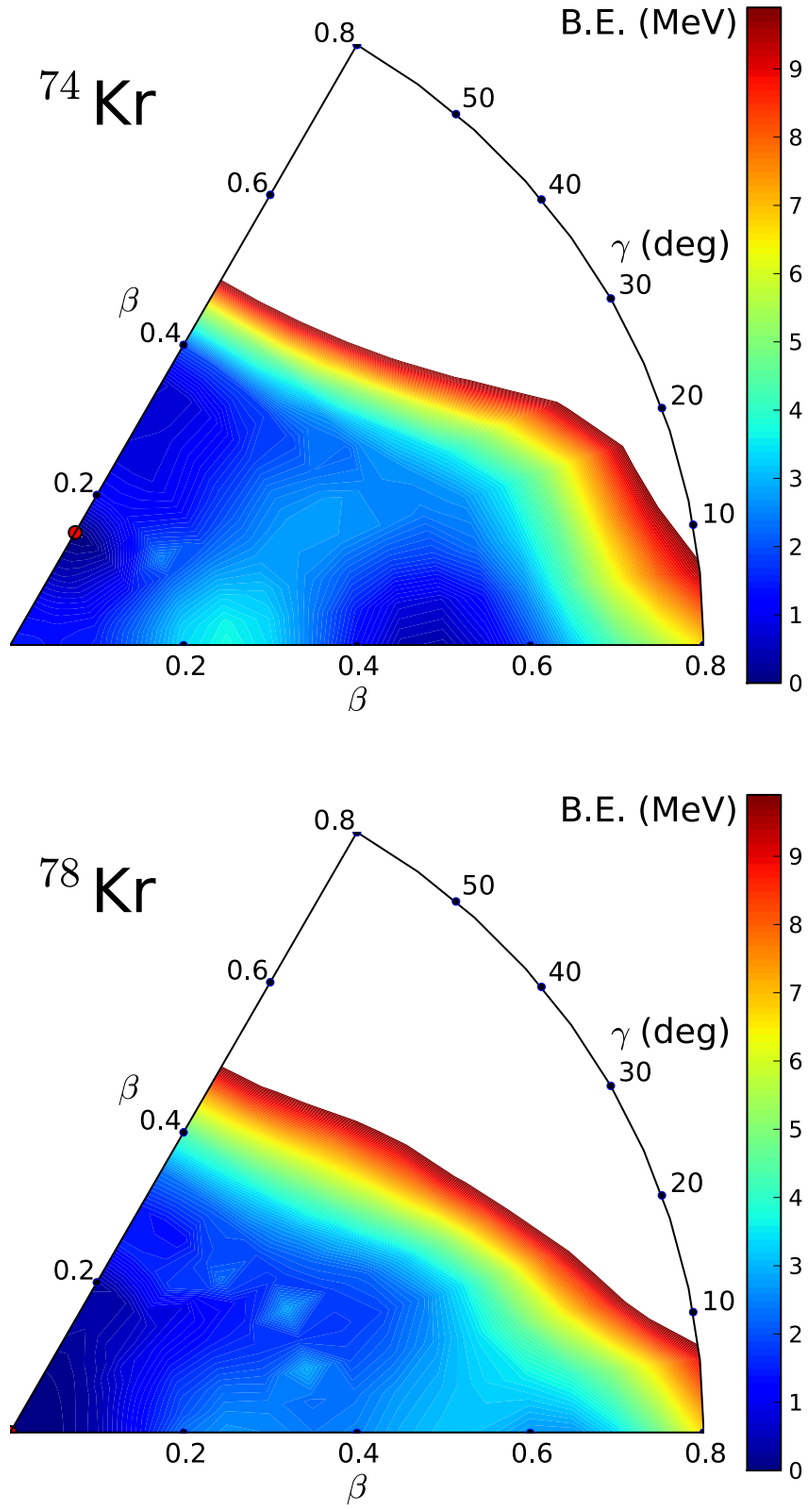
$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 2.48$$

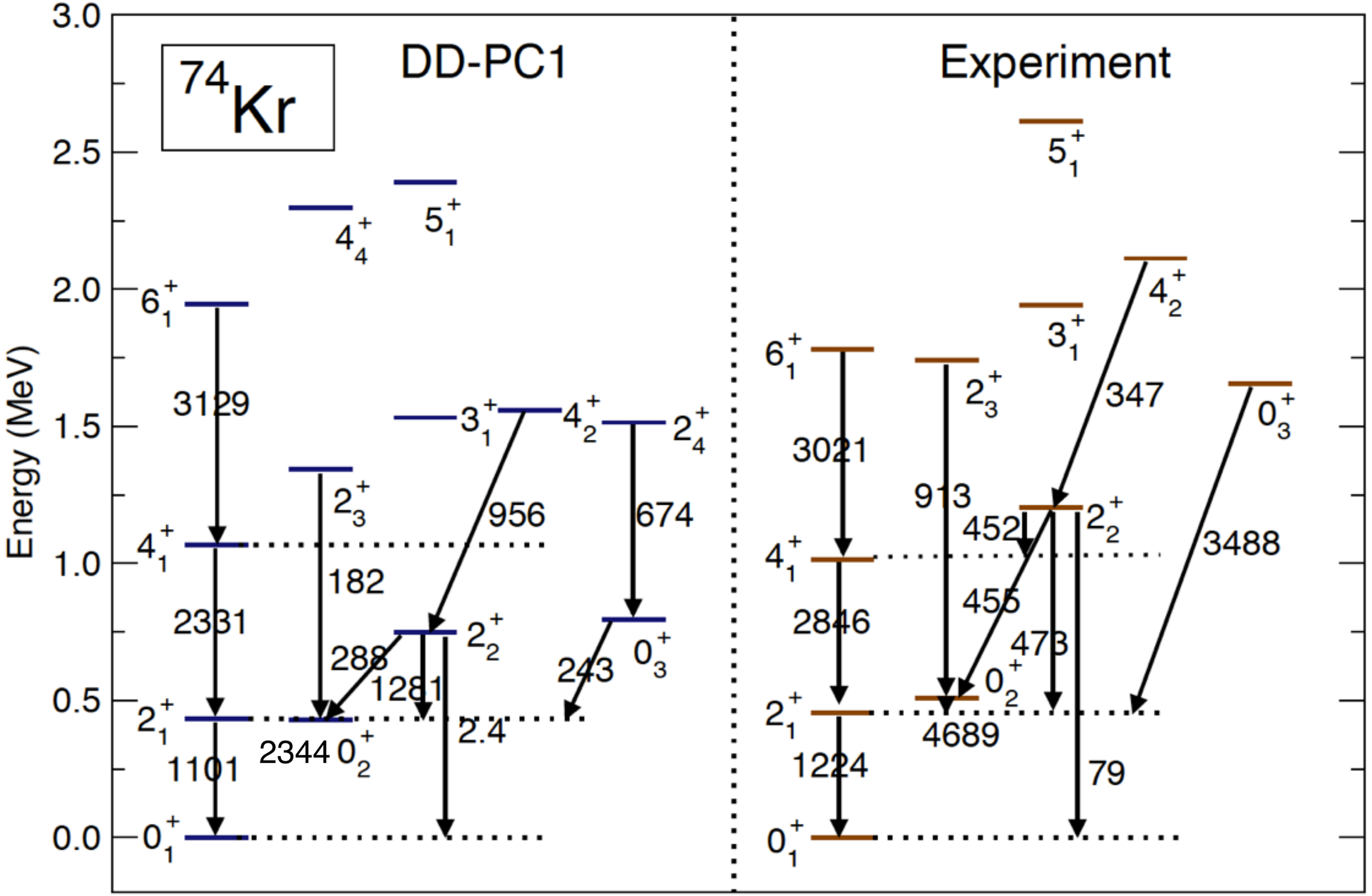


How does the functional DD-PC1 extrapolate to other mass regions?

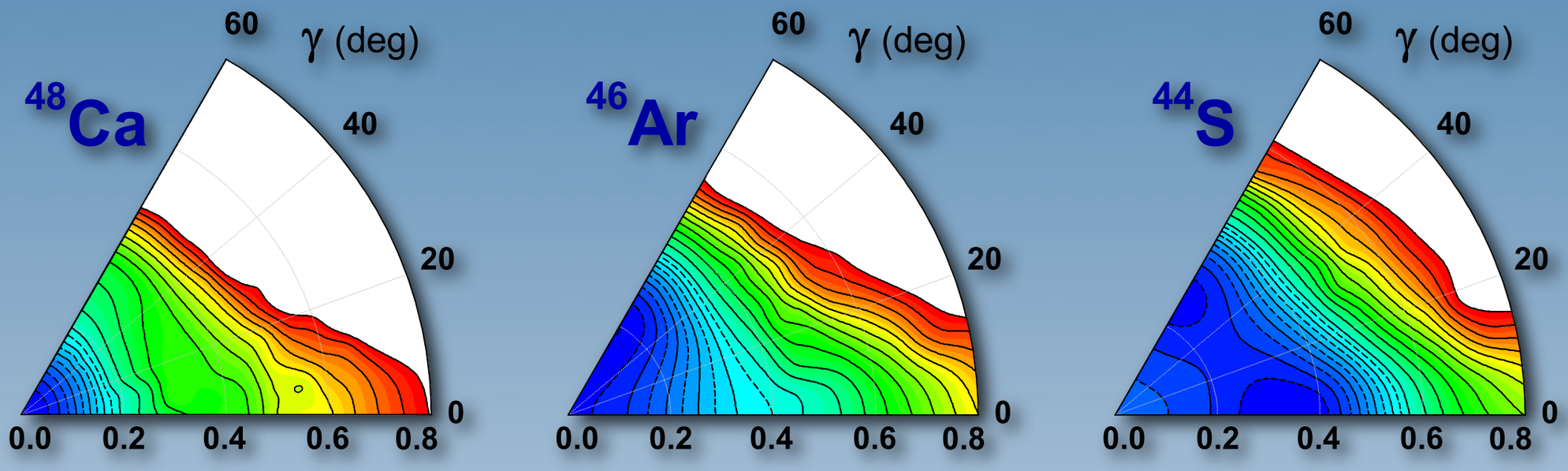
Shape-coexistence in neutron-deficient Kr isotopes

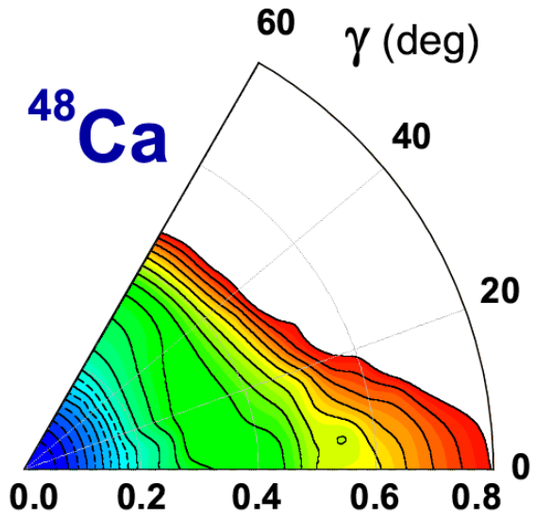


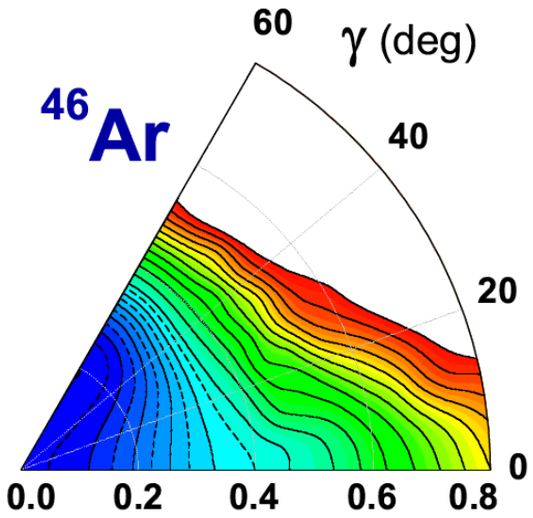


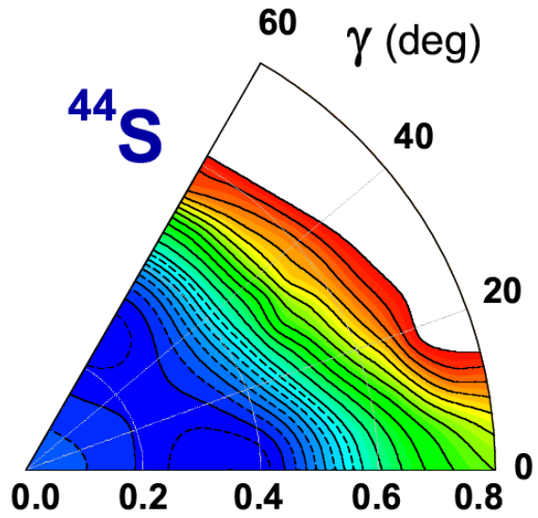

^{74}Kr
DD-PC1
Experiment
Energy (MeV)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
6_1^+
4_4^+
5_1^+
3_1^+
4_2^+
2_4^+
2_3^+
4_1^+
2_2^+
0_3^+
2_1^+
0_2^+
0_1^+
3129
2331
1101
182
288
2344
956
1281
2.4
674
243
5_1^+
6_1^+
3_1^+
4_2^+
2_3^+
0_3^+
2_2^+
4_1^+
0_2^+
2_1^+
0_1^+
3021
2846
1224
913
455
4689
347
452
473
79
3488

Coexisting shapes in the N=28 isotones









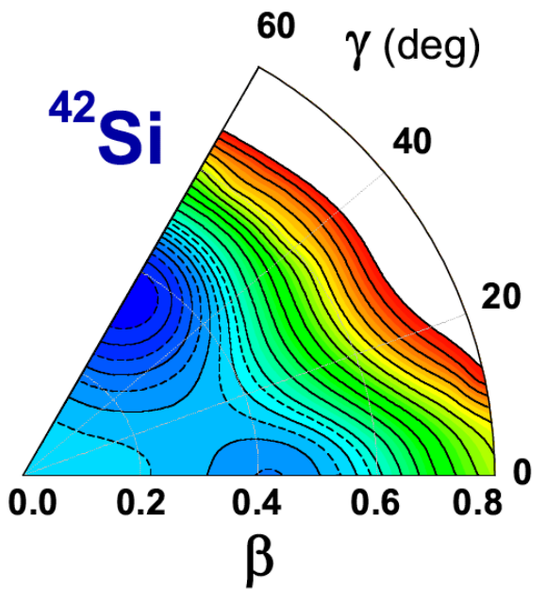
Neutron N=28 spherical energy gaps

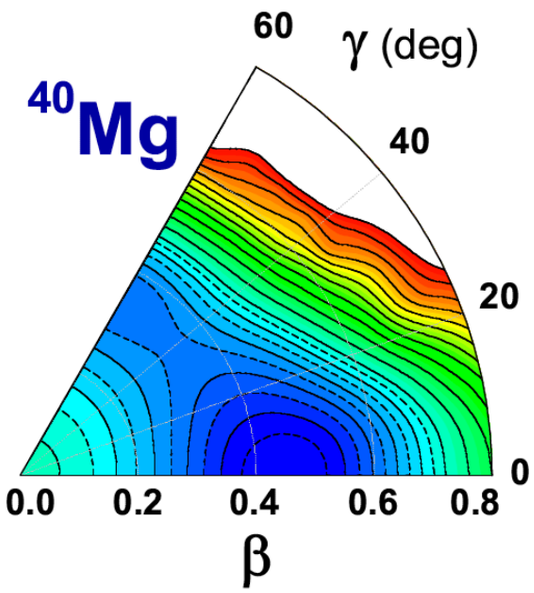
	$\Delta^{\text{sph.}}_{N=28}$	β_{min}
^{48}Ca	4.73	0.00
^{46}Ar	4.48	-0.19
^{44}S	3.86	0.34
^{42}Si	3.13	-0.35
^{40}Mg	2.03	0.45

<u>Experimental values:</u>

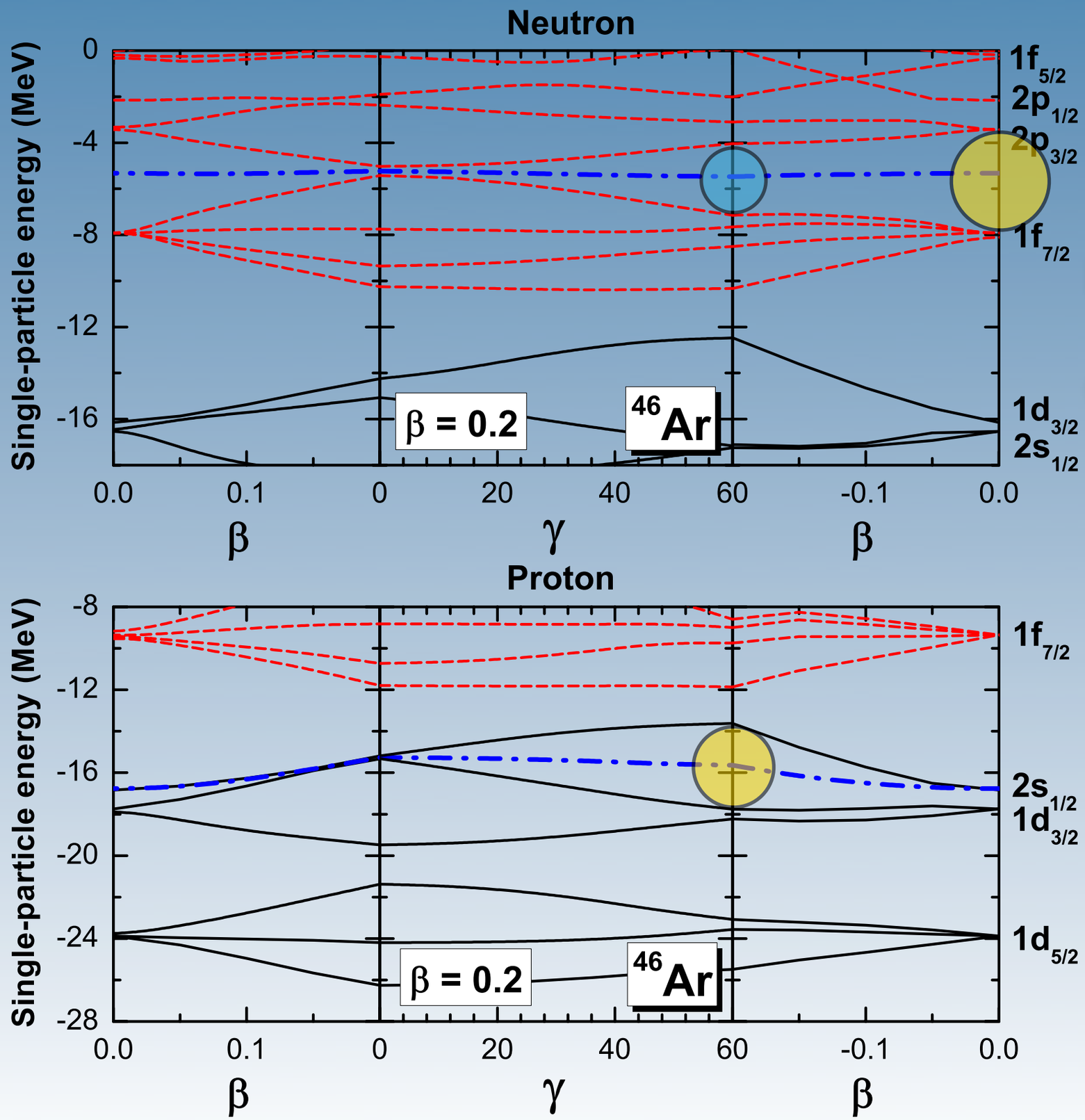
4.80 MeV

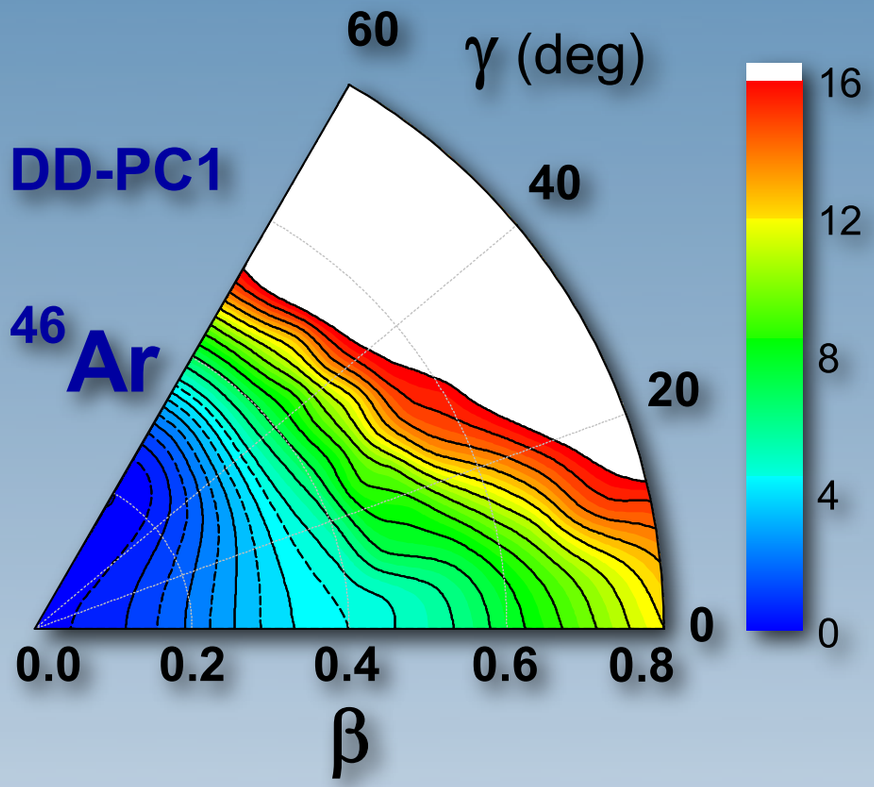
4.47 MeV



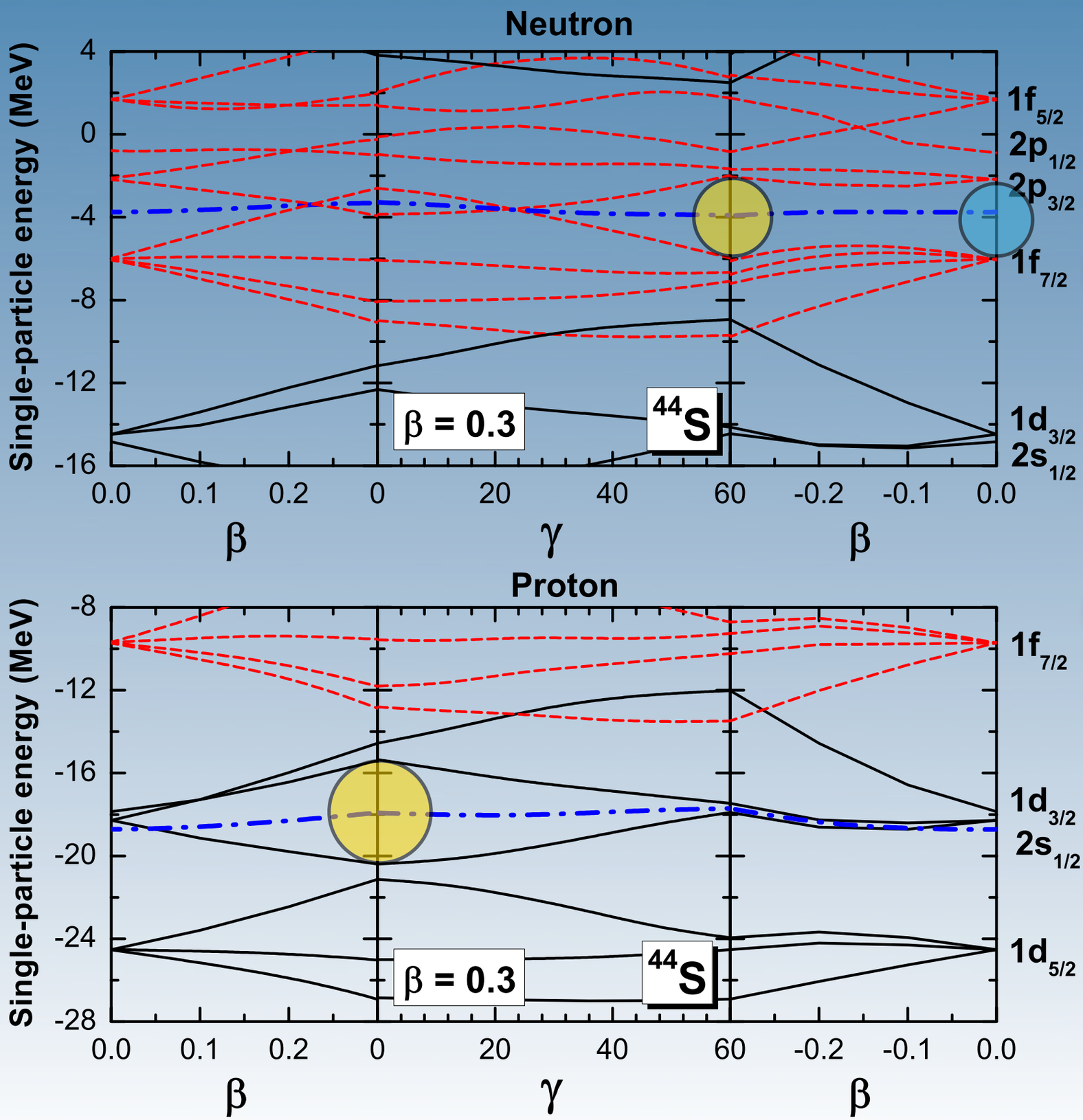


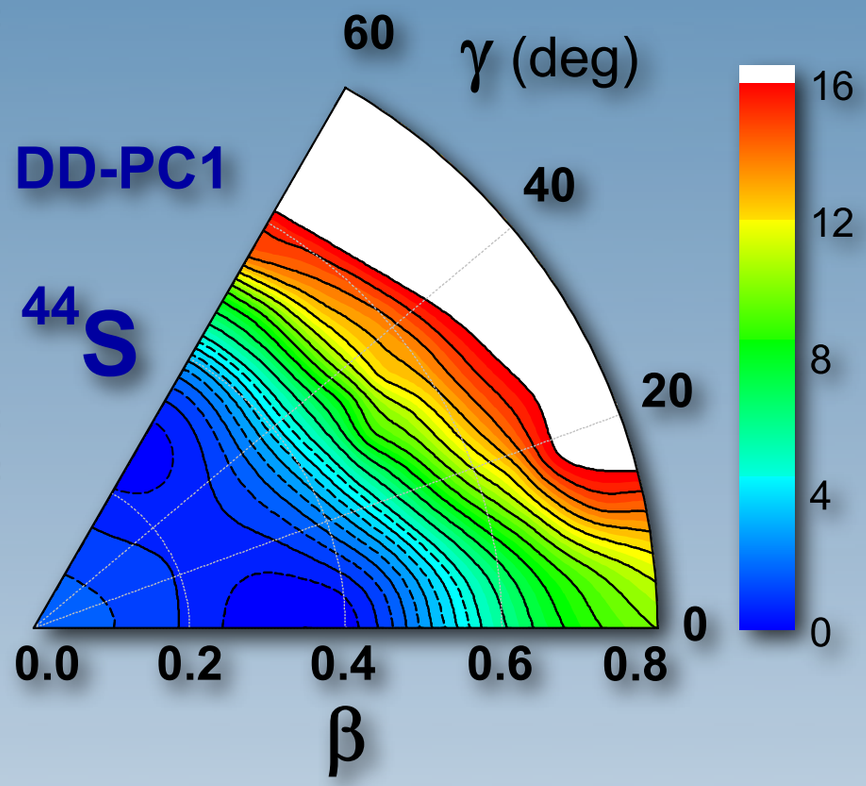
^{46}Ar: single-particle levels



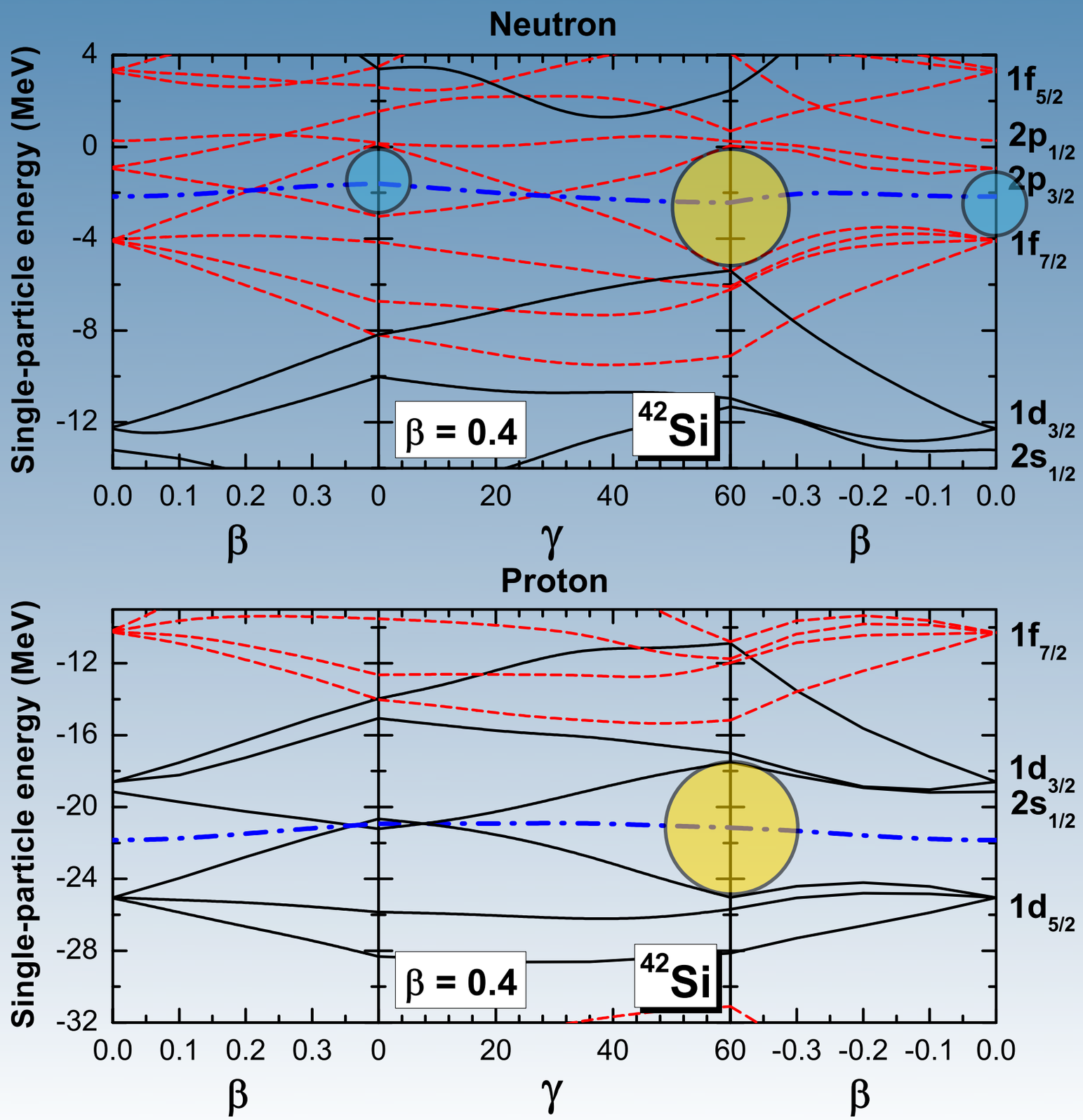


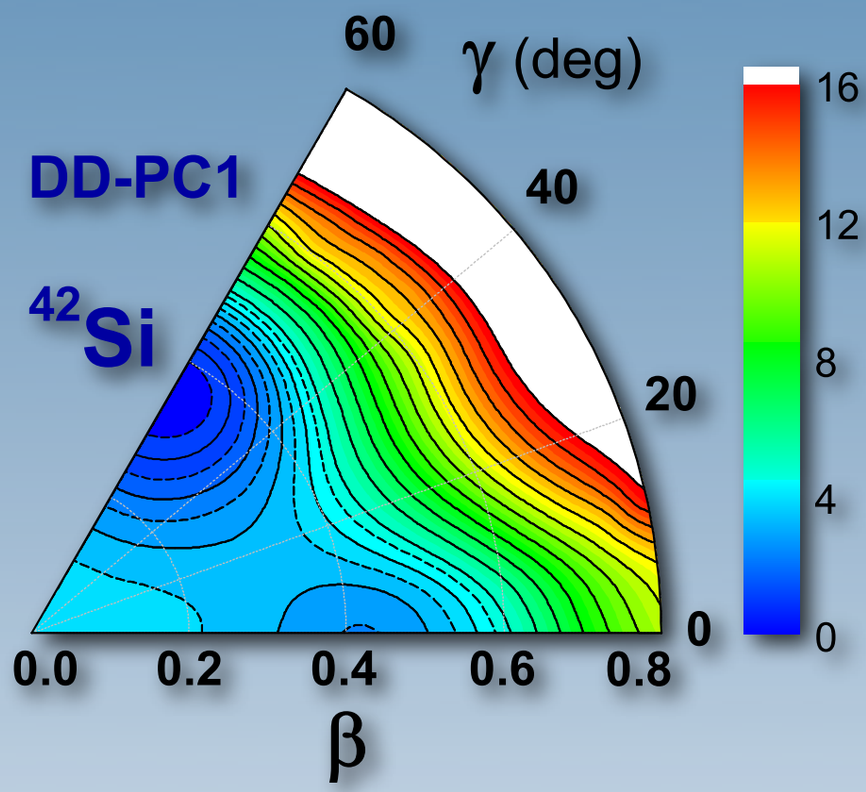
^{44}S: single-particle levels



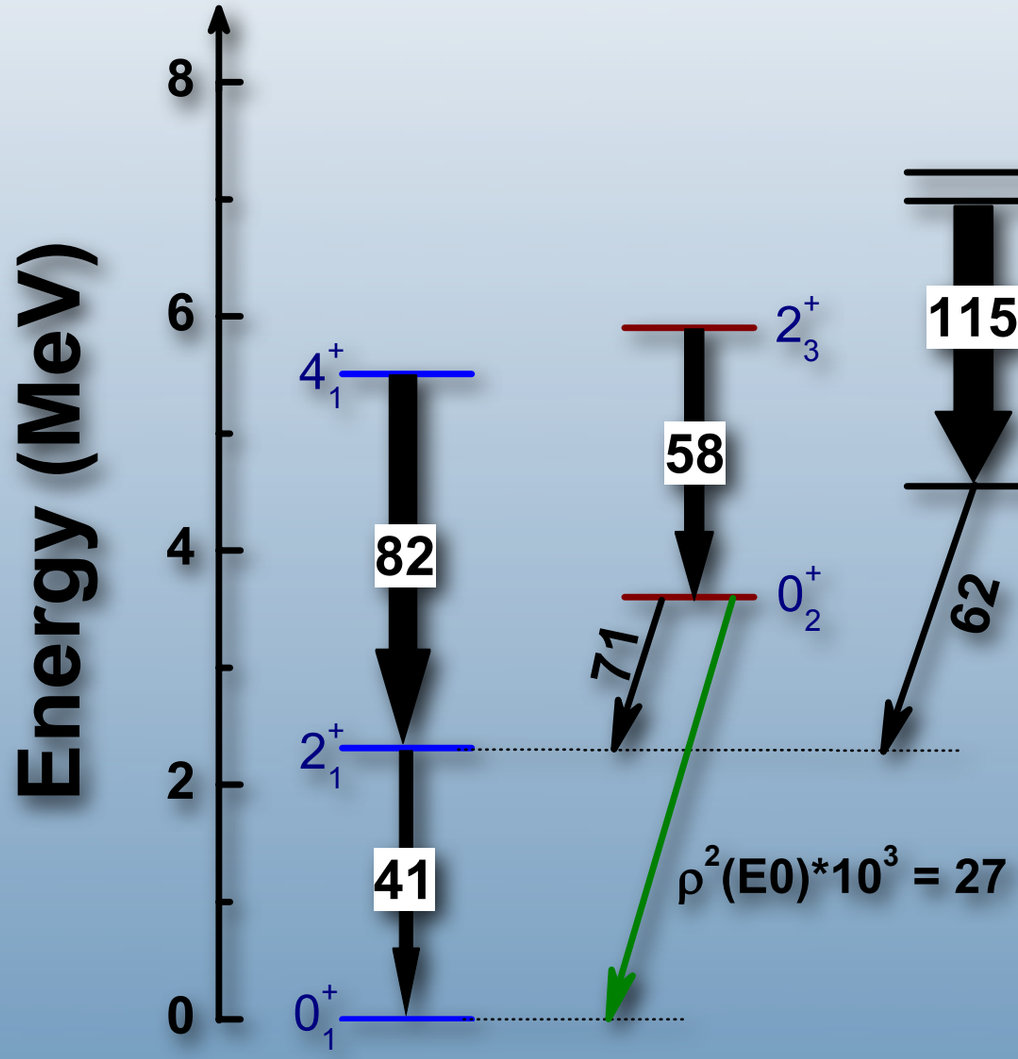


^{42}Si: single-particle levels

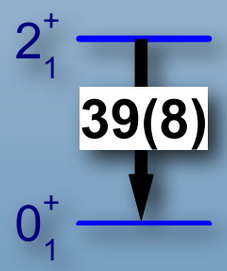




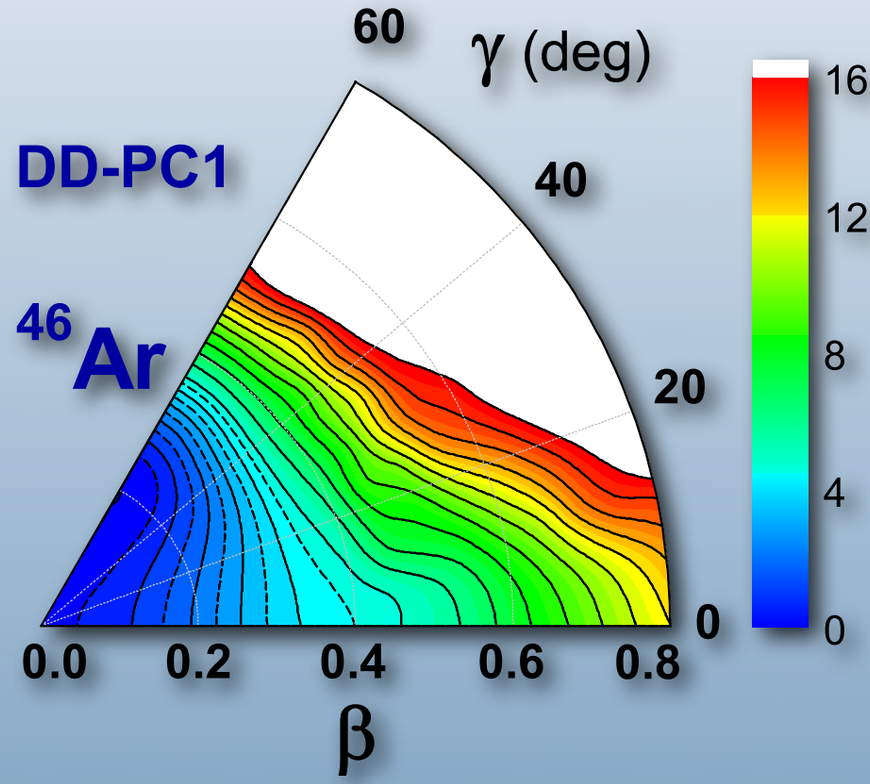
^{46}Ar

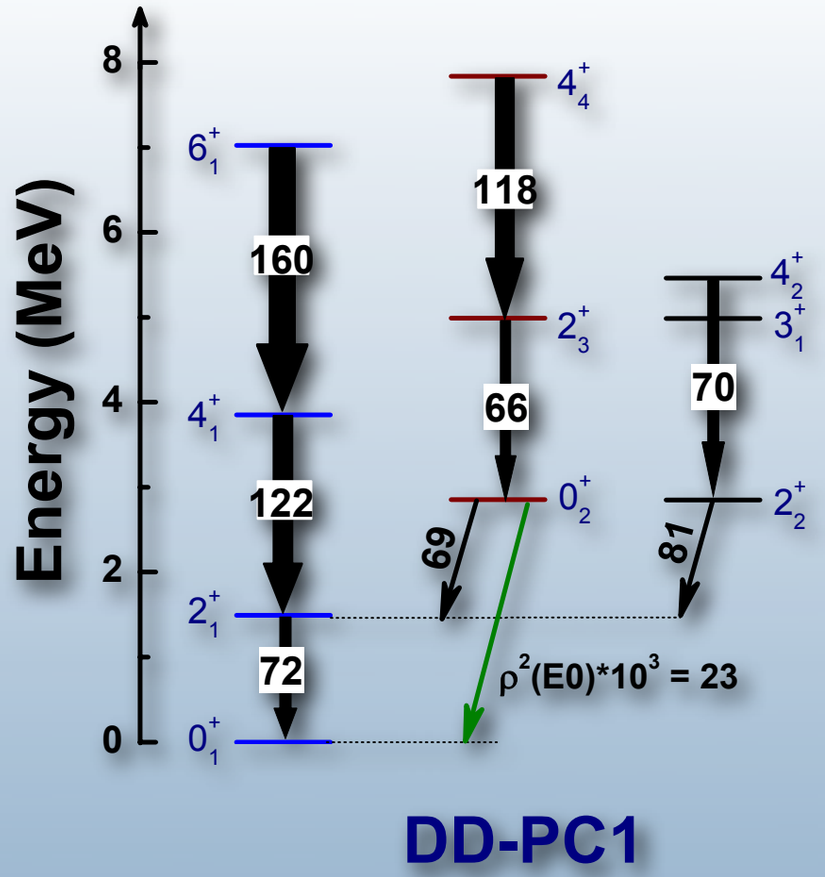


DD-PC1

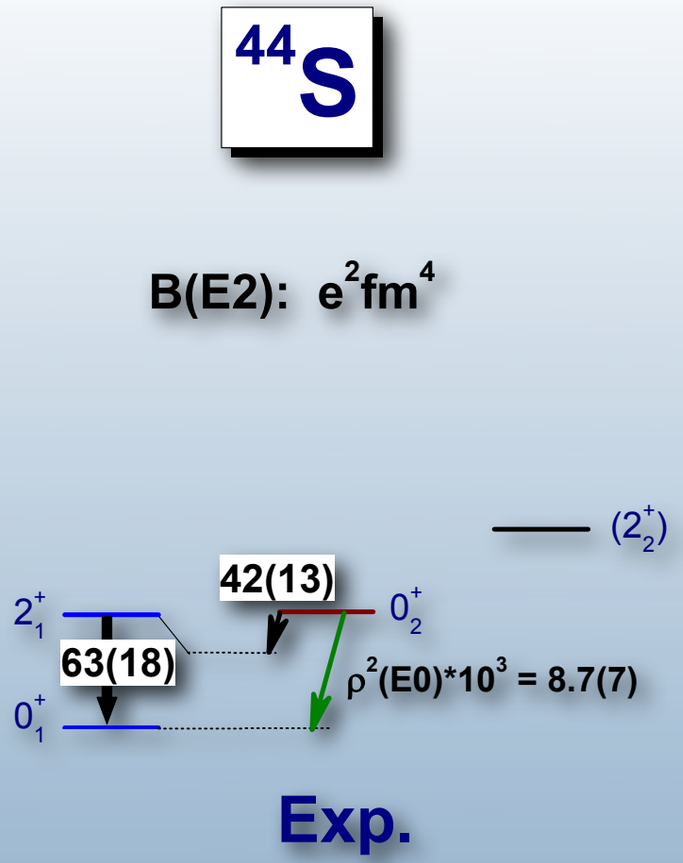


Exp.

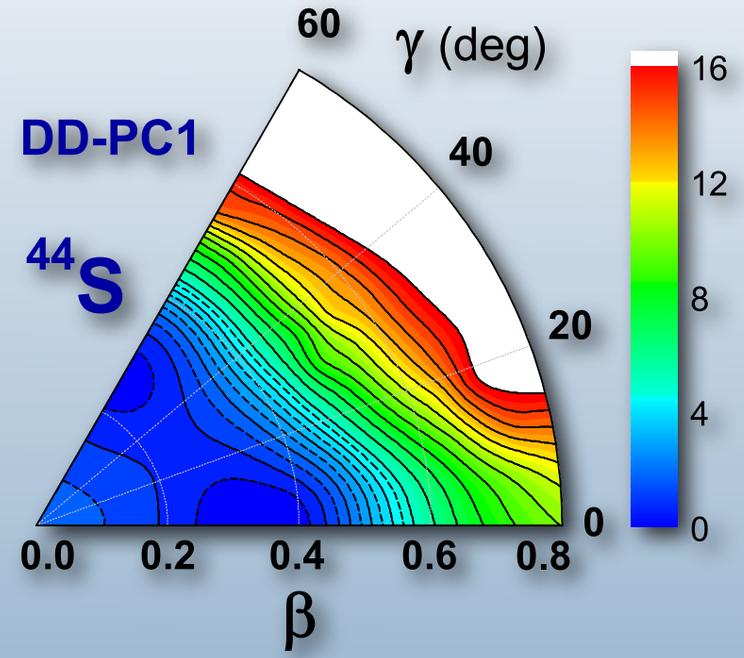




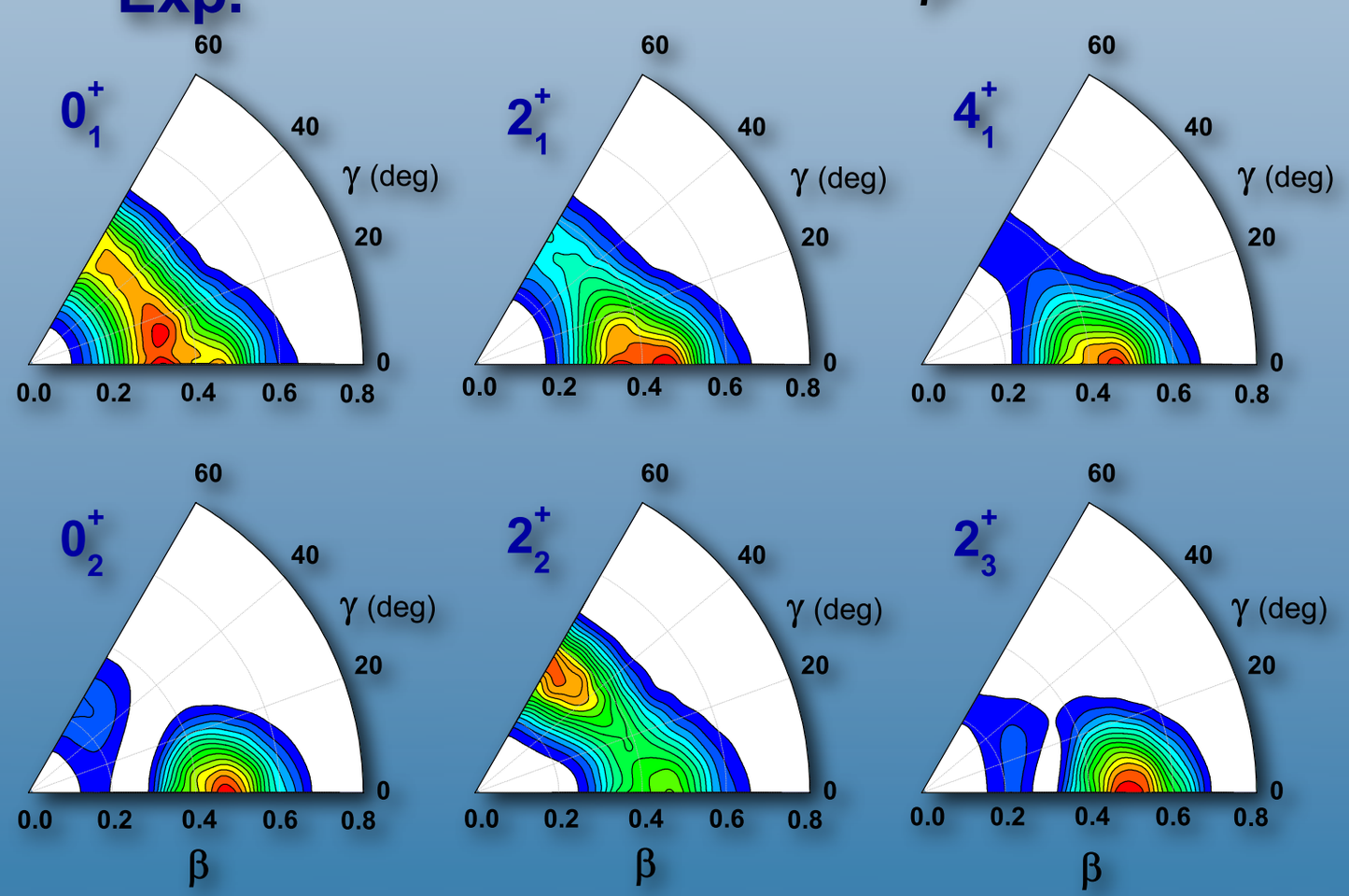
DD-PC1

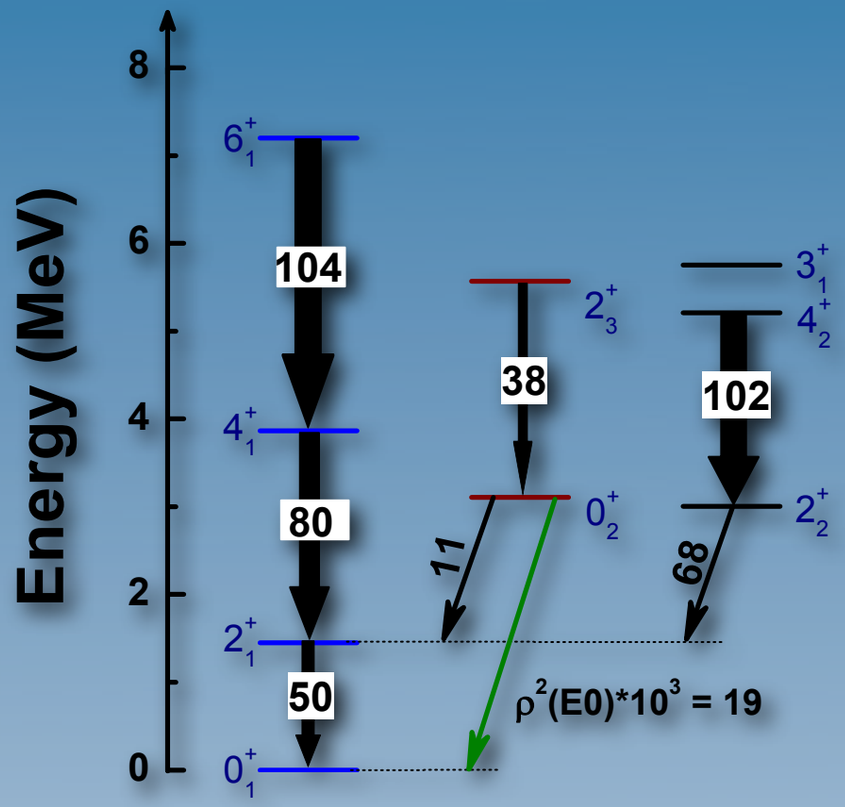


Exp.

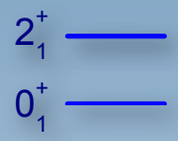


Probability density distributions:

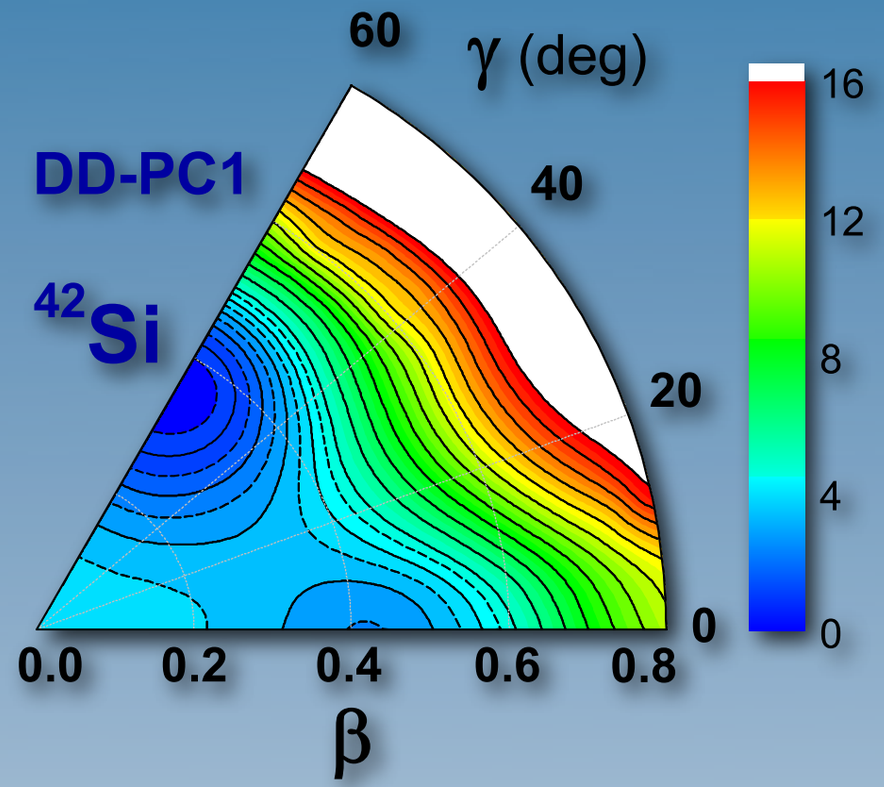




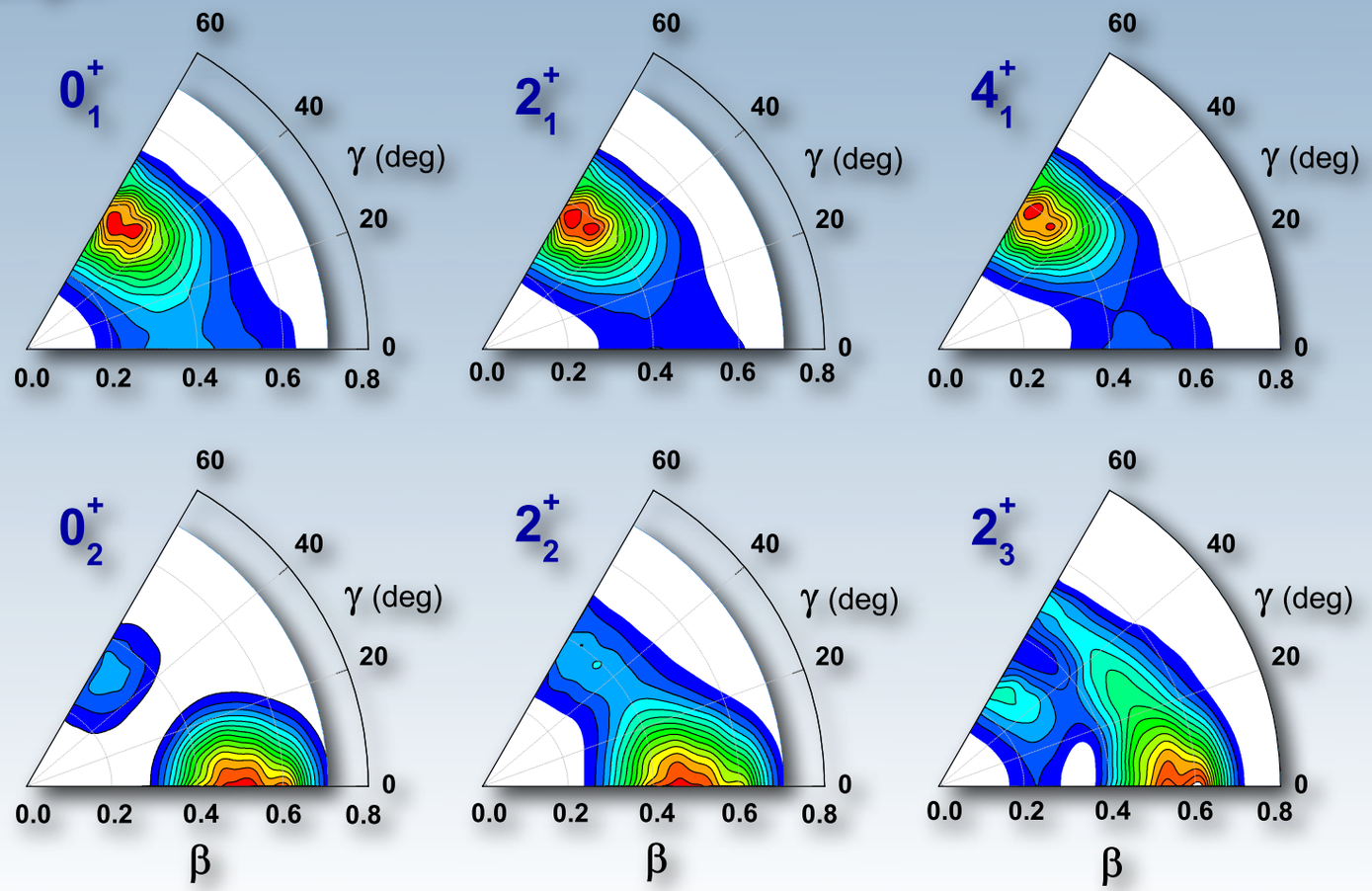
DD-PC1



Exp.



Probability density distributions:



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.

✔ fully self-consistent (Q)RPA analysis of giant resonances, low-energy multipole response in weakly-bound nuclei, dynamics of exotic modes of excitation.

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

Zagreb T. Nikšić
N. Paar
T. Marketin
D. Vretenar

Thessaloniki G.A. Lalazissis
V. Prassa

Beijing Jie Meng
Yifei Niu
Chunyan Song

München P. Ring
N. Kaiser
W. Weise

Bologna P. Finelli

Chongqing Zhipan Li
Jiang-Ming Yao