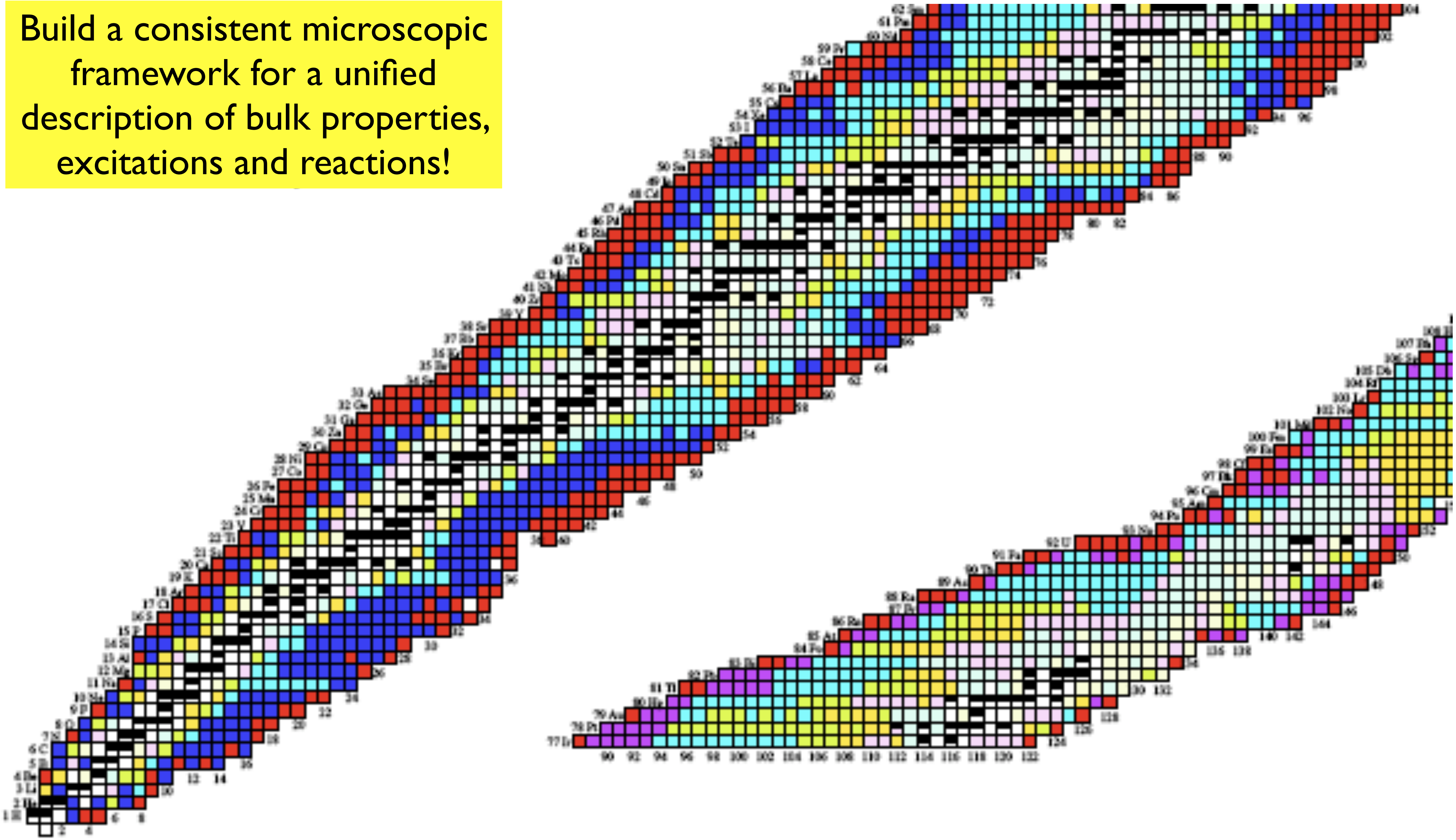
Nuclear Energy Density Functionals

Dario Vretenar
University of Zagreb

Energy Density Functionals

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



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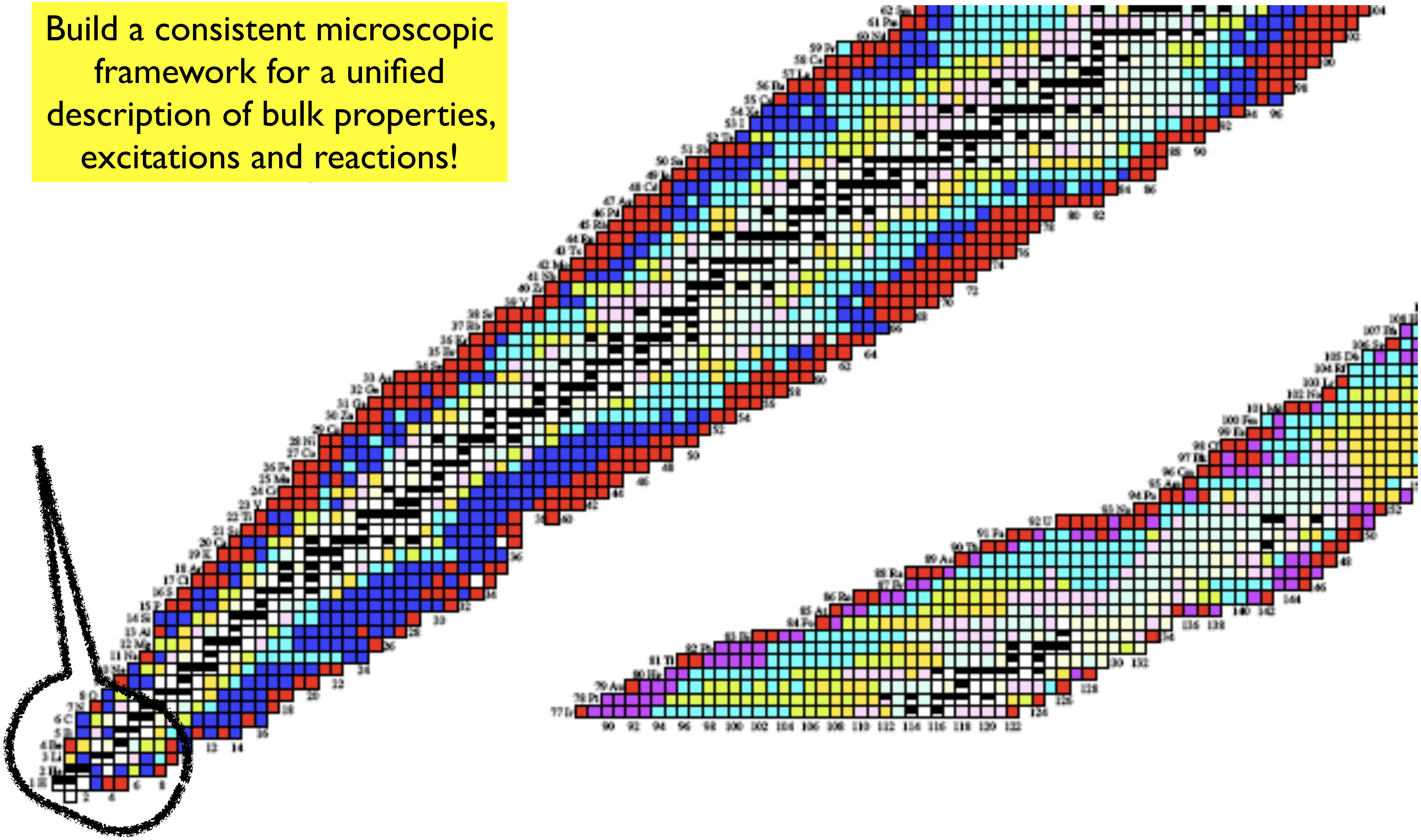

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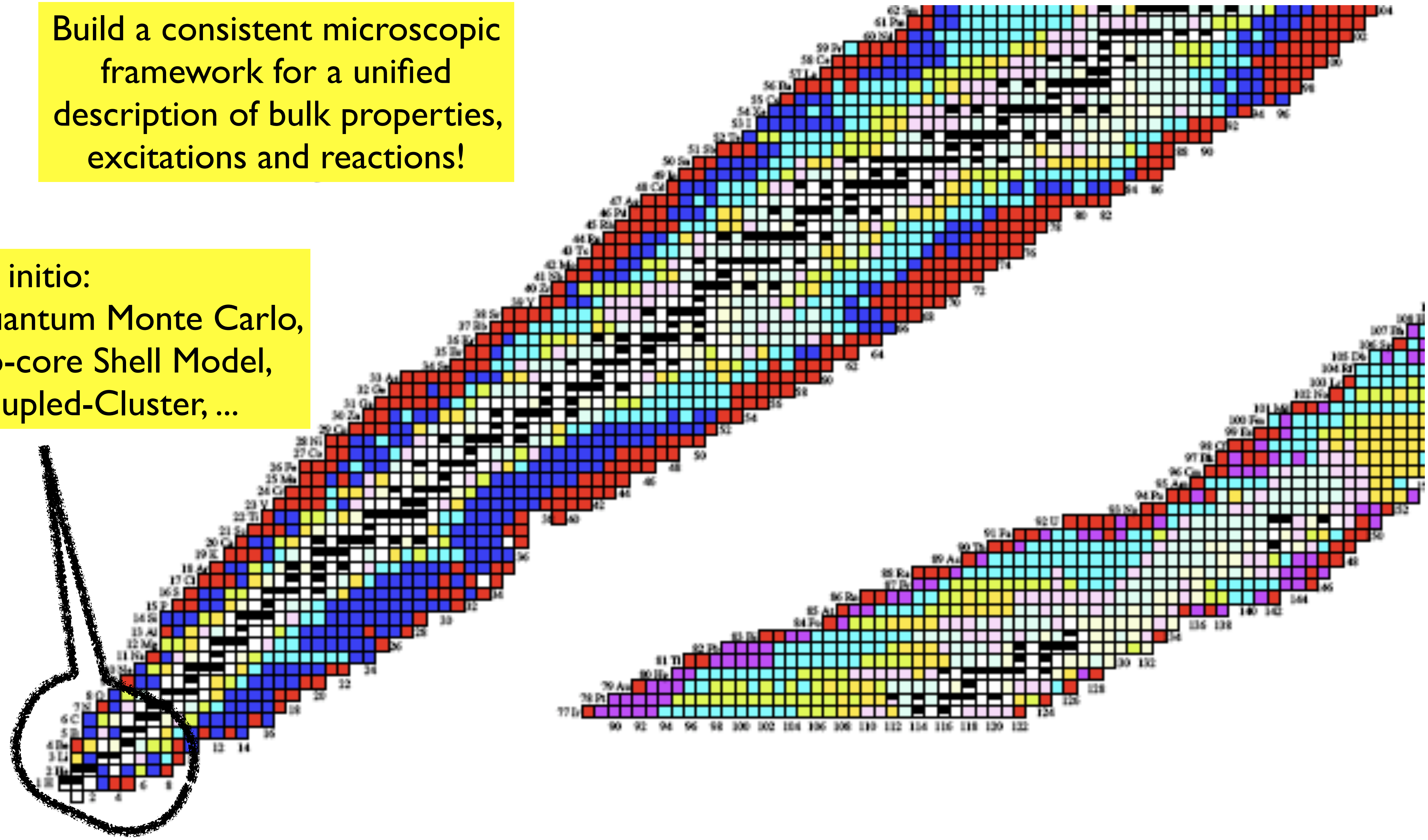
Quantum Monte Carlo,
No-core Shell Model,
Coupled-Cluster, ...



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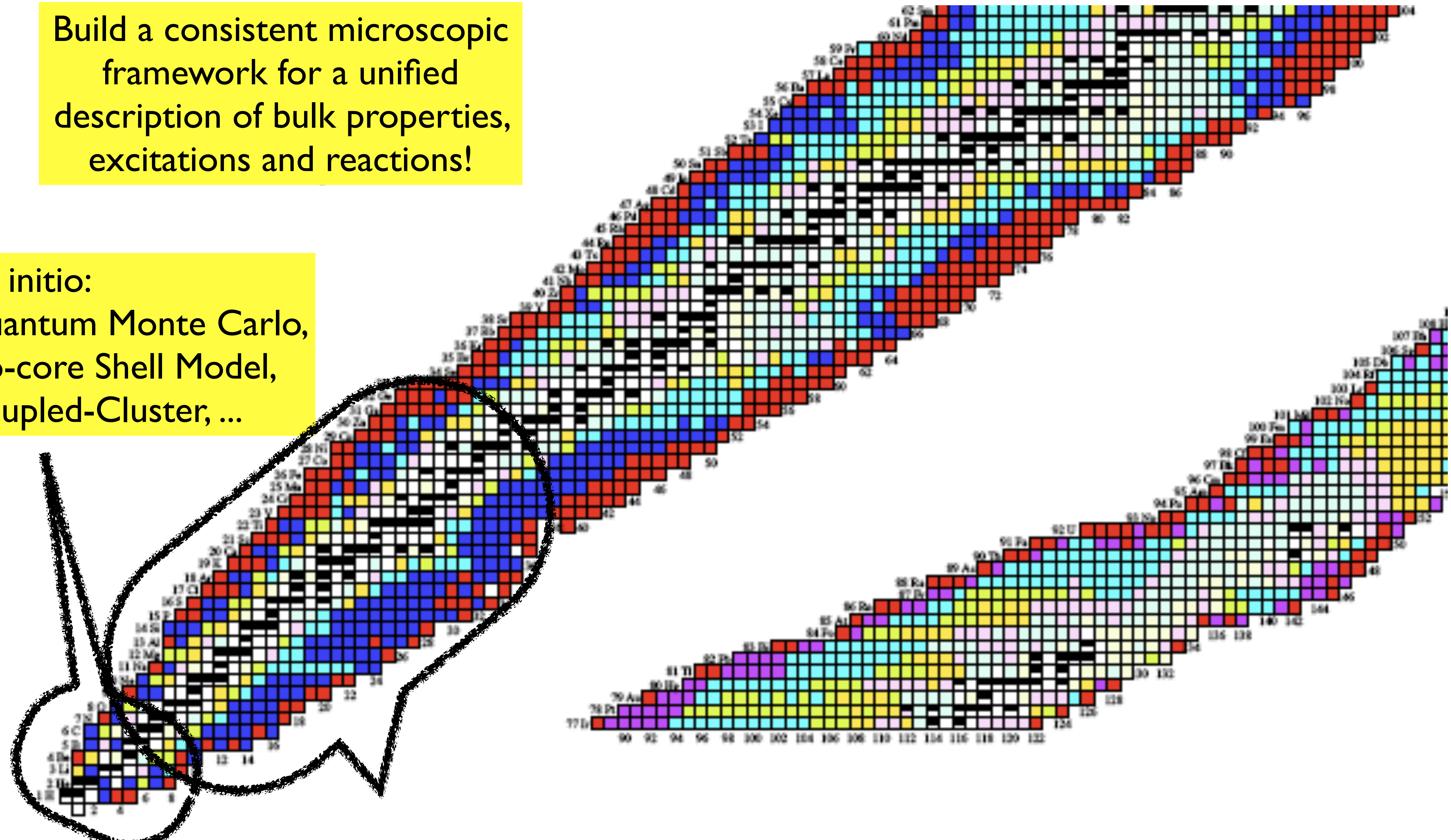

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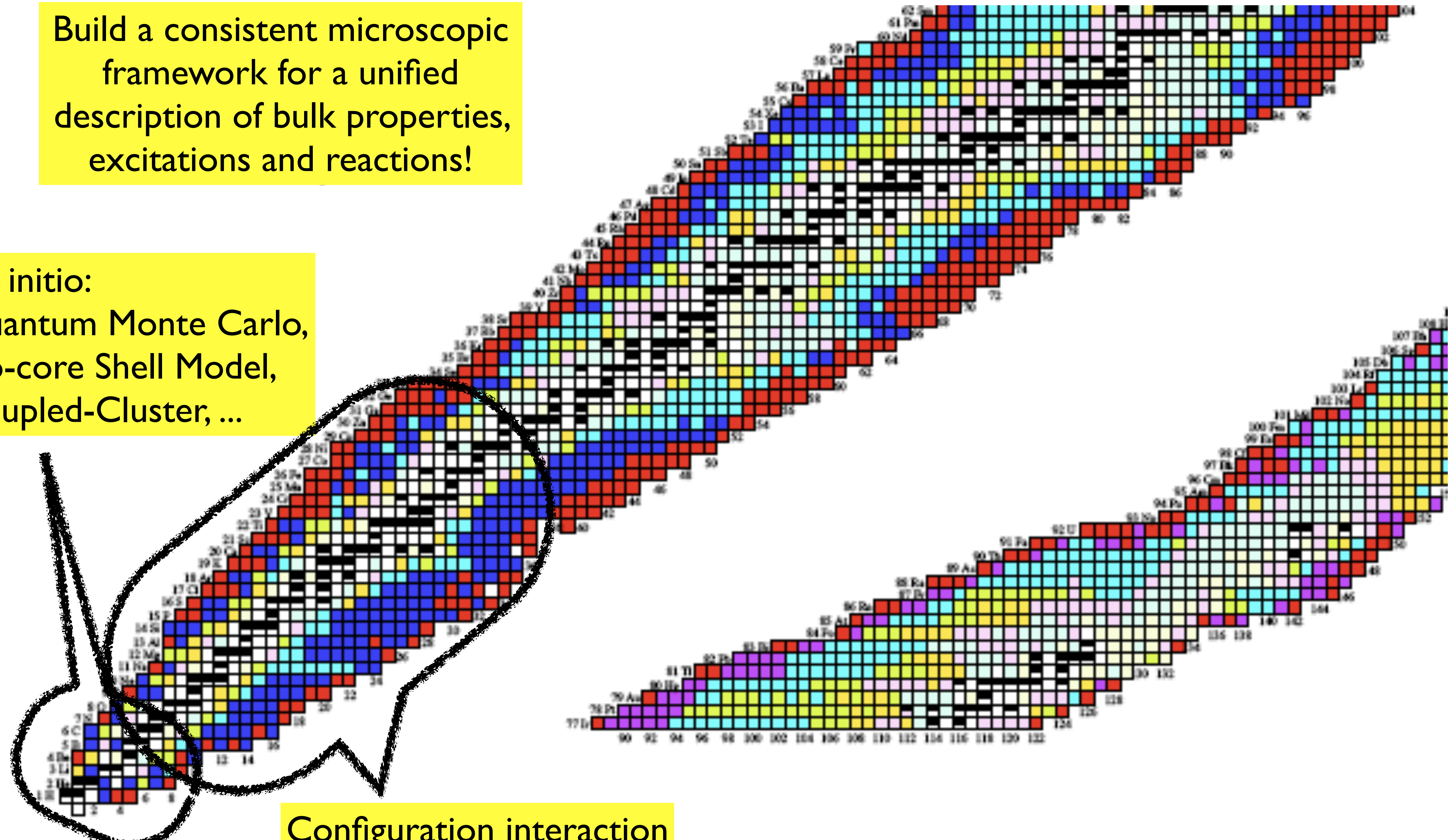

Configuration interaction
(Interacting Shell-Model)

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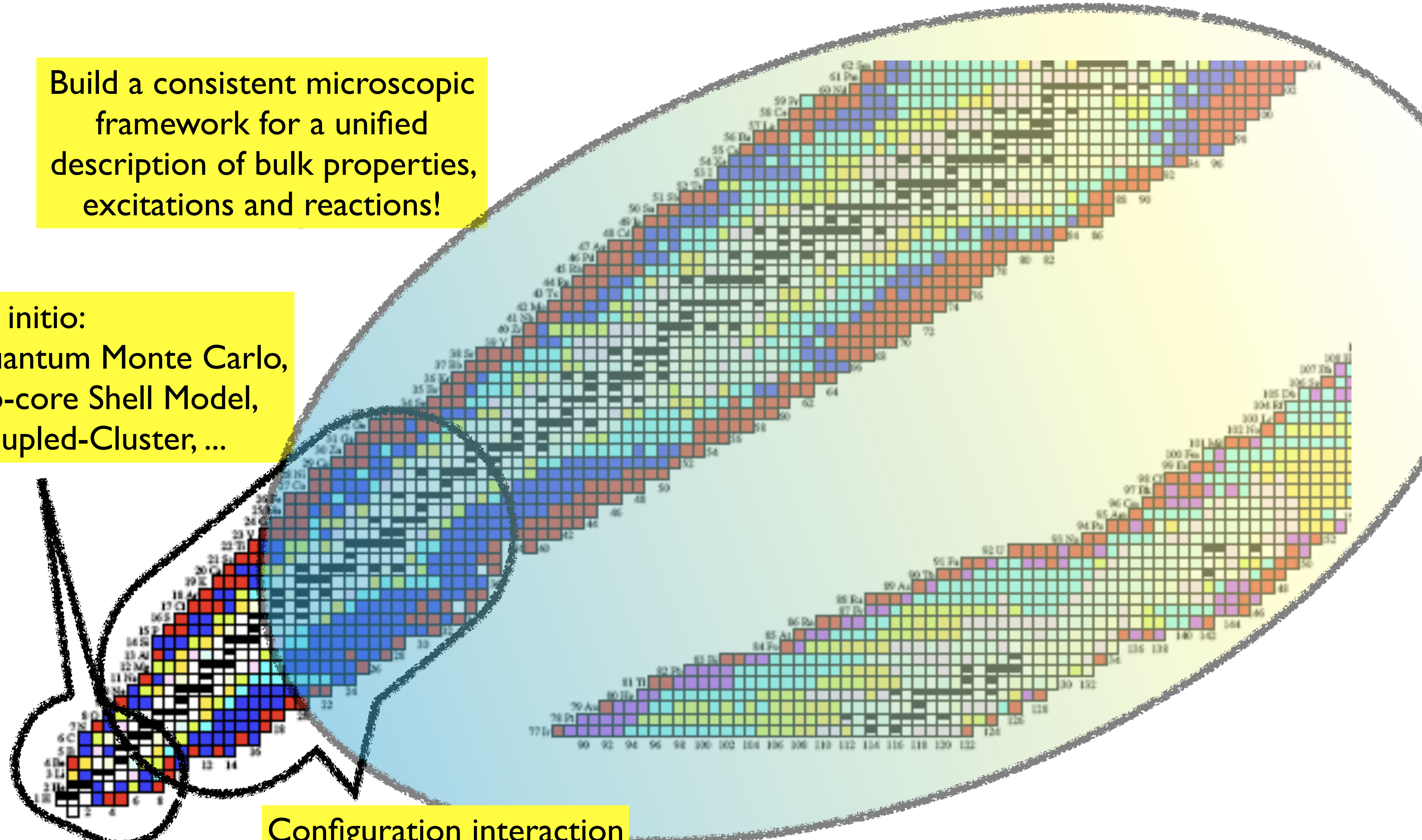

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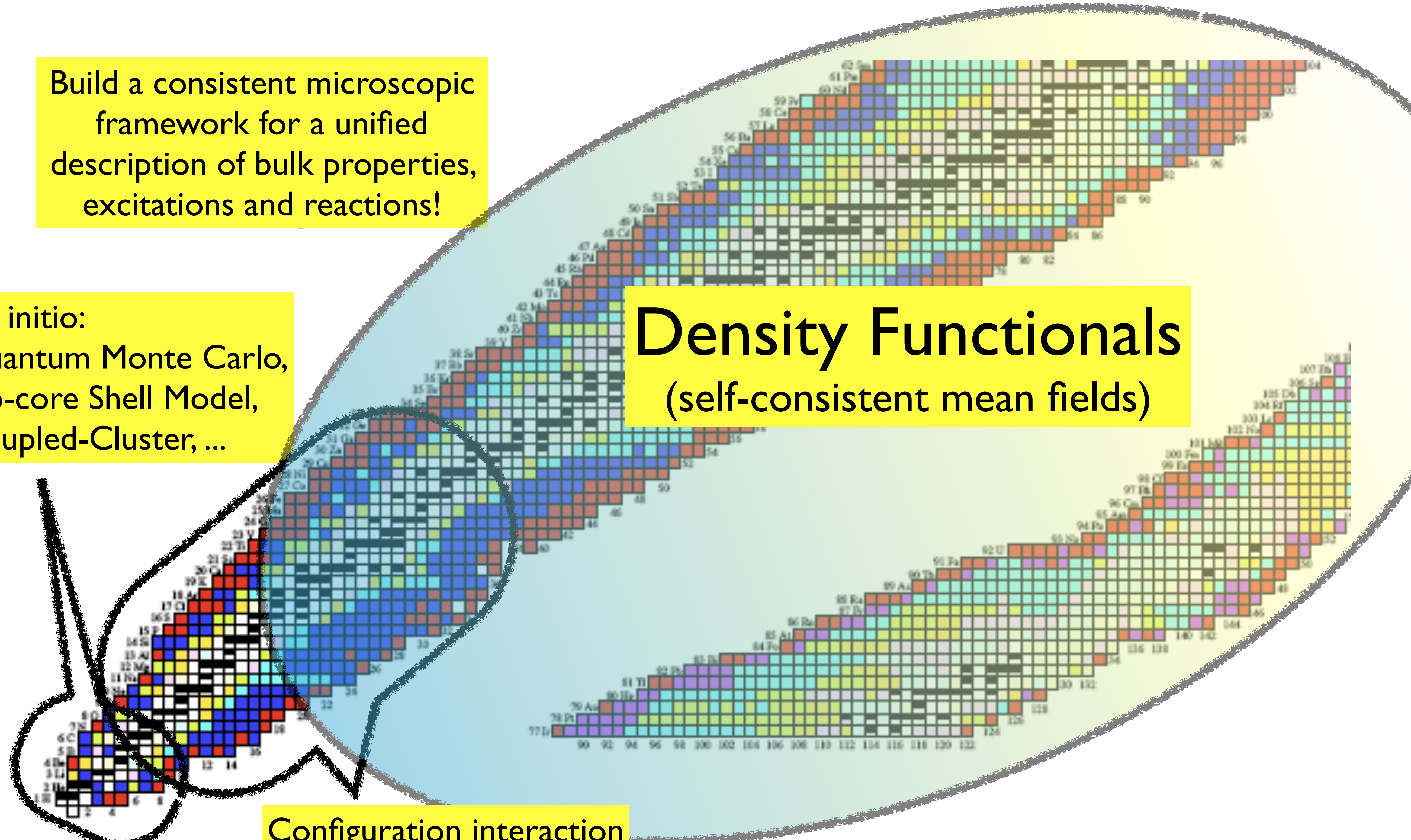

Density Functionals
(self-consistent mean fields)

Configuration interaction
(Interacting Shell-Model)

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

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

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

external potential — Hartree term — exchange-correlation

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

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

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

Local densities and currents:

T=0 density:

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

T=1 density:

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

T=0 spin density:

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

T=1 spin density:

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

Current:

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

Spin-current tensor:

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

Kinetic density:

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

Kinetic spin-density:

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

Advantages of the Energy Density Functional approach to nuclear structure

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✔ 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!

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

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DD-PC1

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DD-PC1

... 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.

... calculated masses of finite nuclei are primarily sensitive to the three leading terms in the empirical mass formula:

$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

... generate families of effective interactions characterized by different values of $\mathbf{a_v}$, $\mathbf{a_s}$ and $\mathbf{a_4}$, and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

DD-PC1

volume energy: $a_v = -16.06 \text{ MeV}$

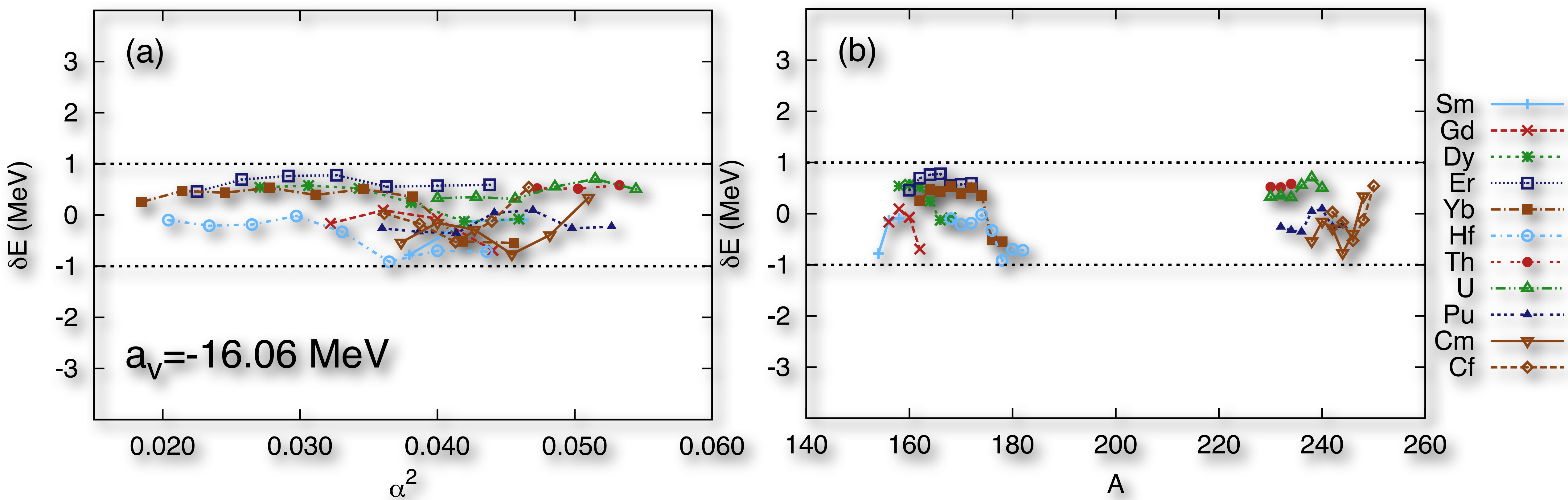
surface energy: $a_s = 17.498 \text{ MeV}$

symmetry energy: $\langle S_2 \rangle = 27.8 \text{ MeV} \quad (a_4 = 33 \text{MeV})$

Deformed nuclei

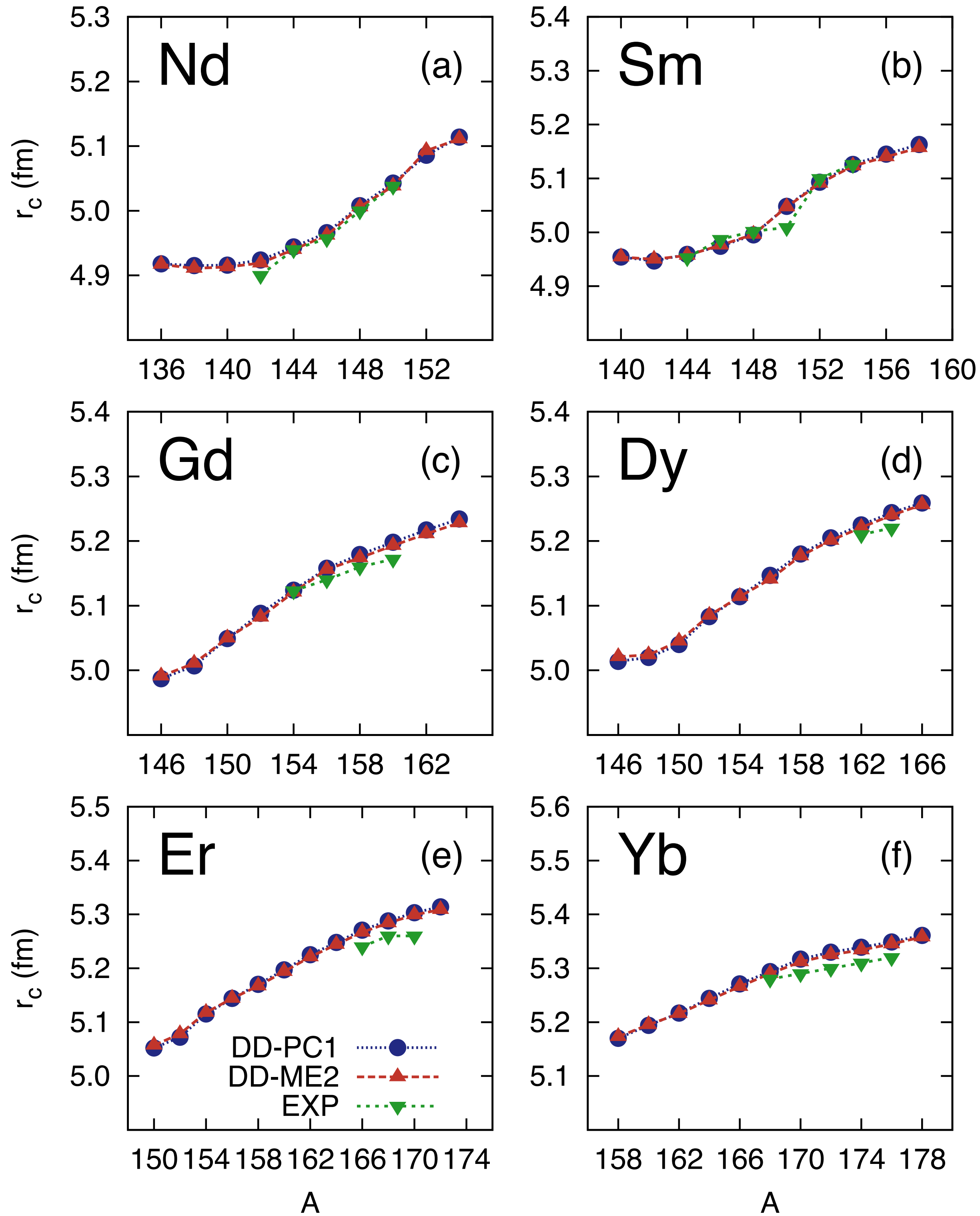
Binding energies used to adjust the parameters of the functional:

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

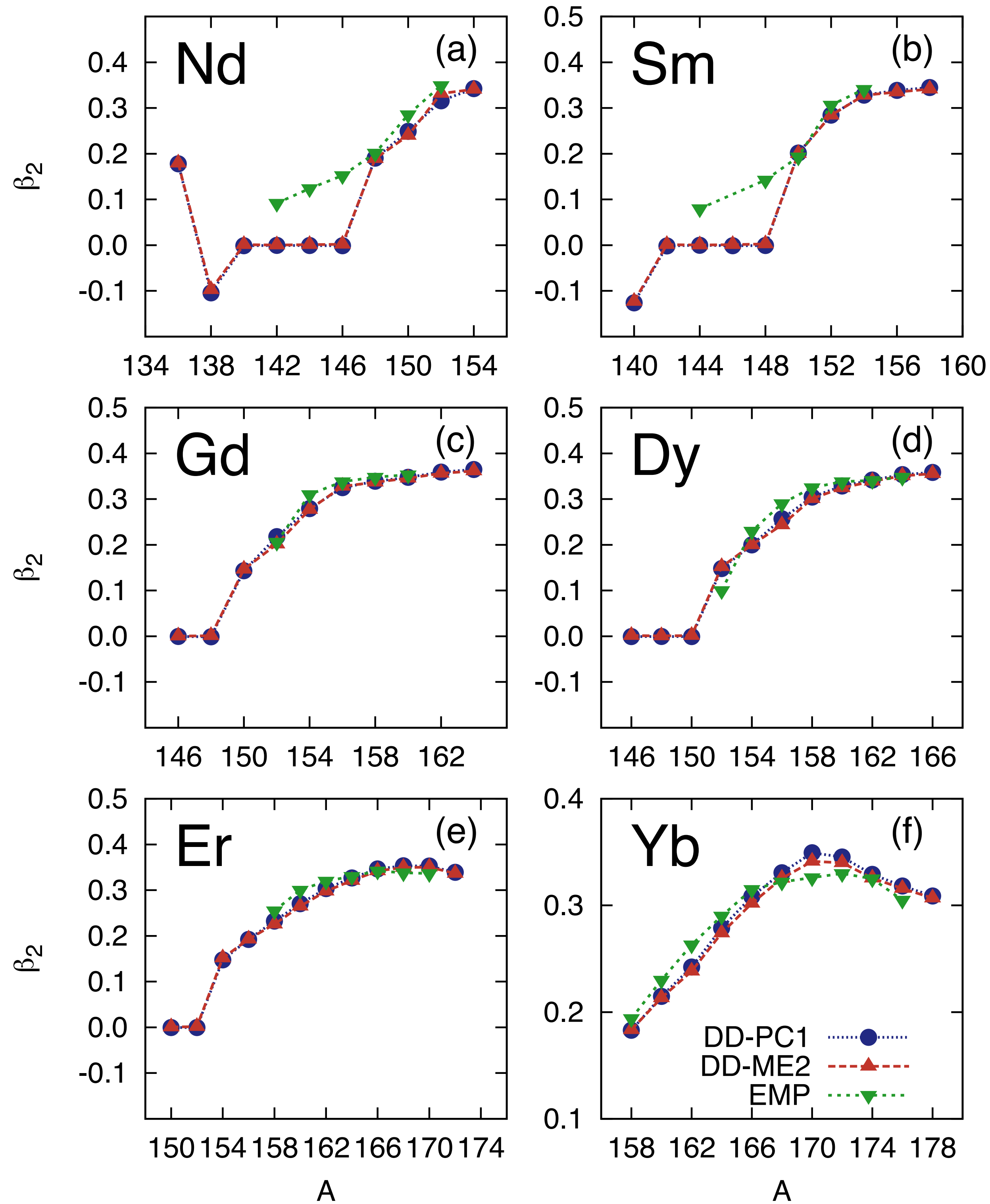


Systematic calculation of ground-state properties:

Charge radii



Quadrupole deformations



Excitation energies of collective modes:

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IVGDR

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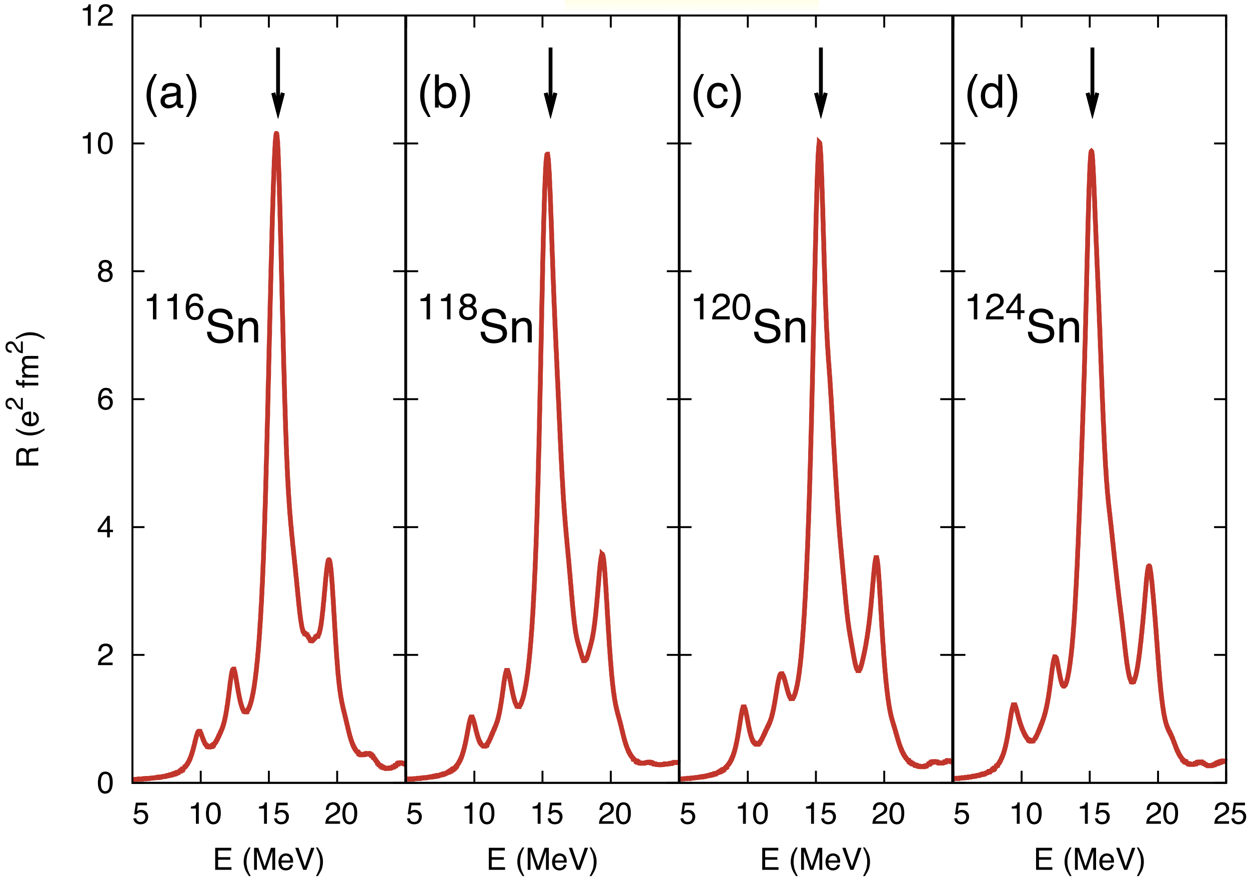

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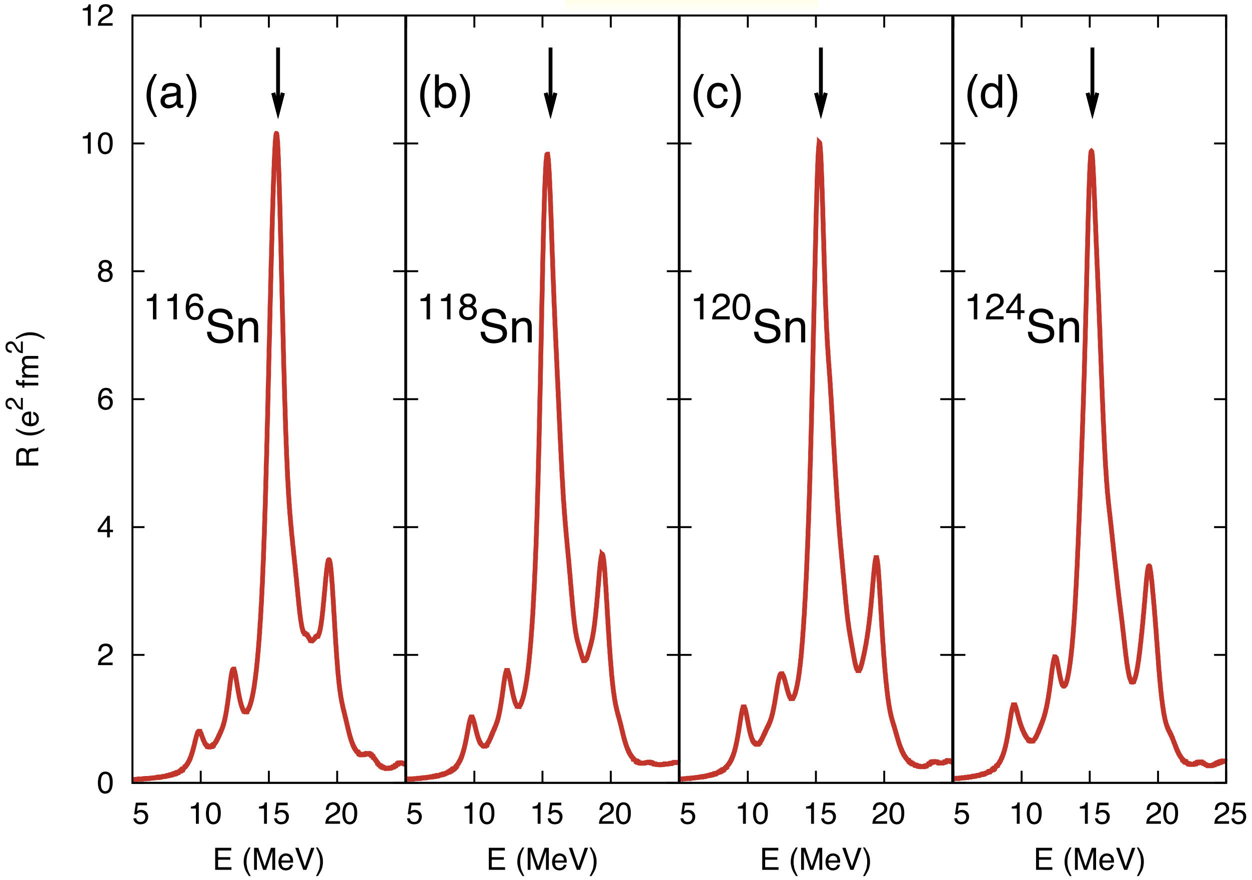

ISGMR

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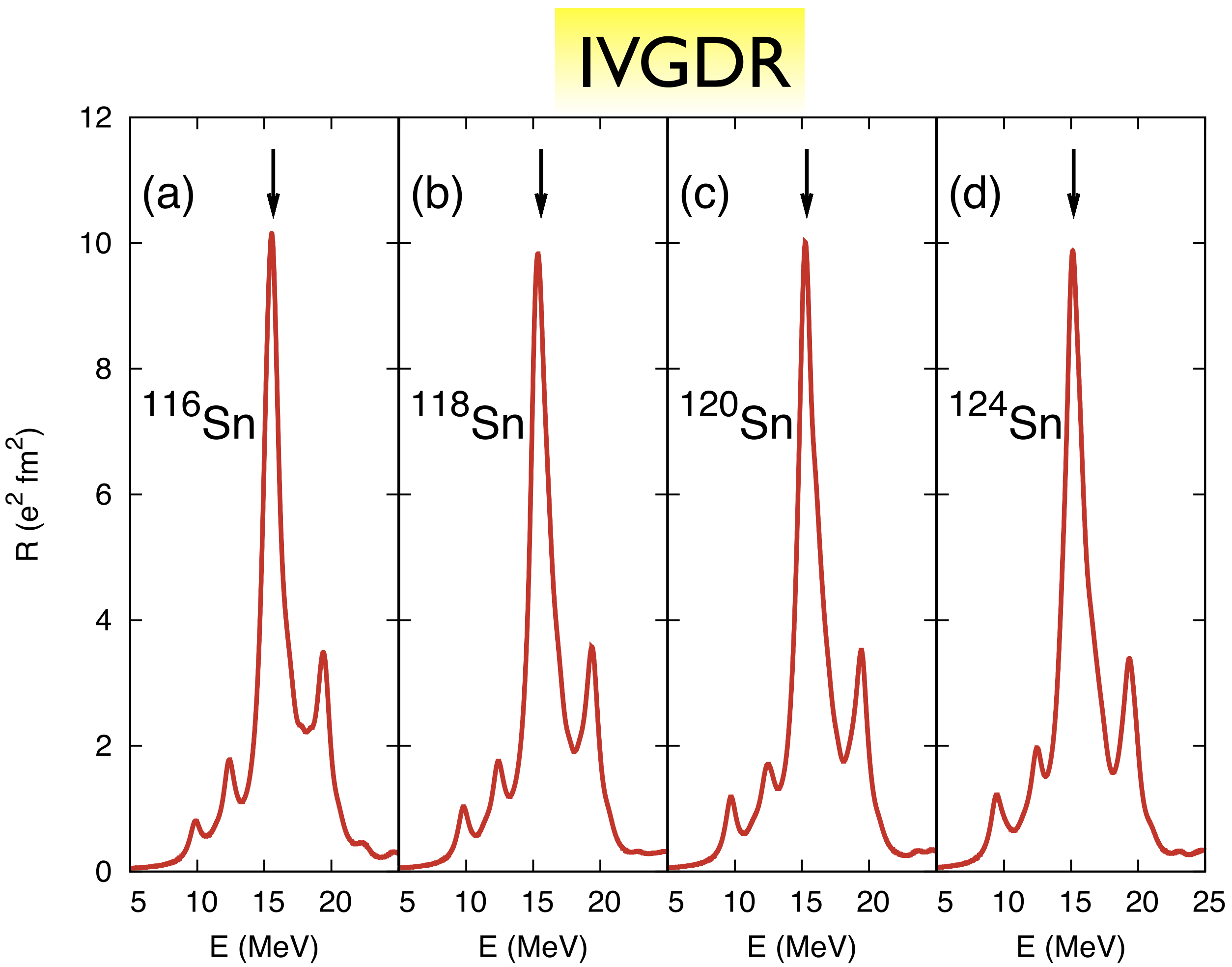

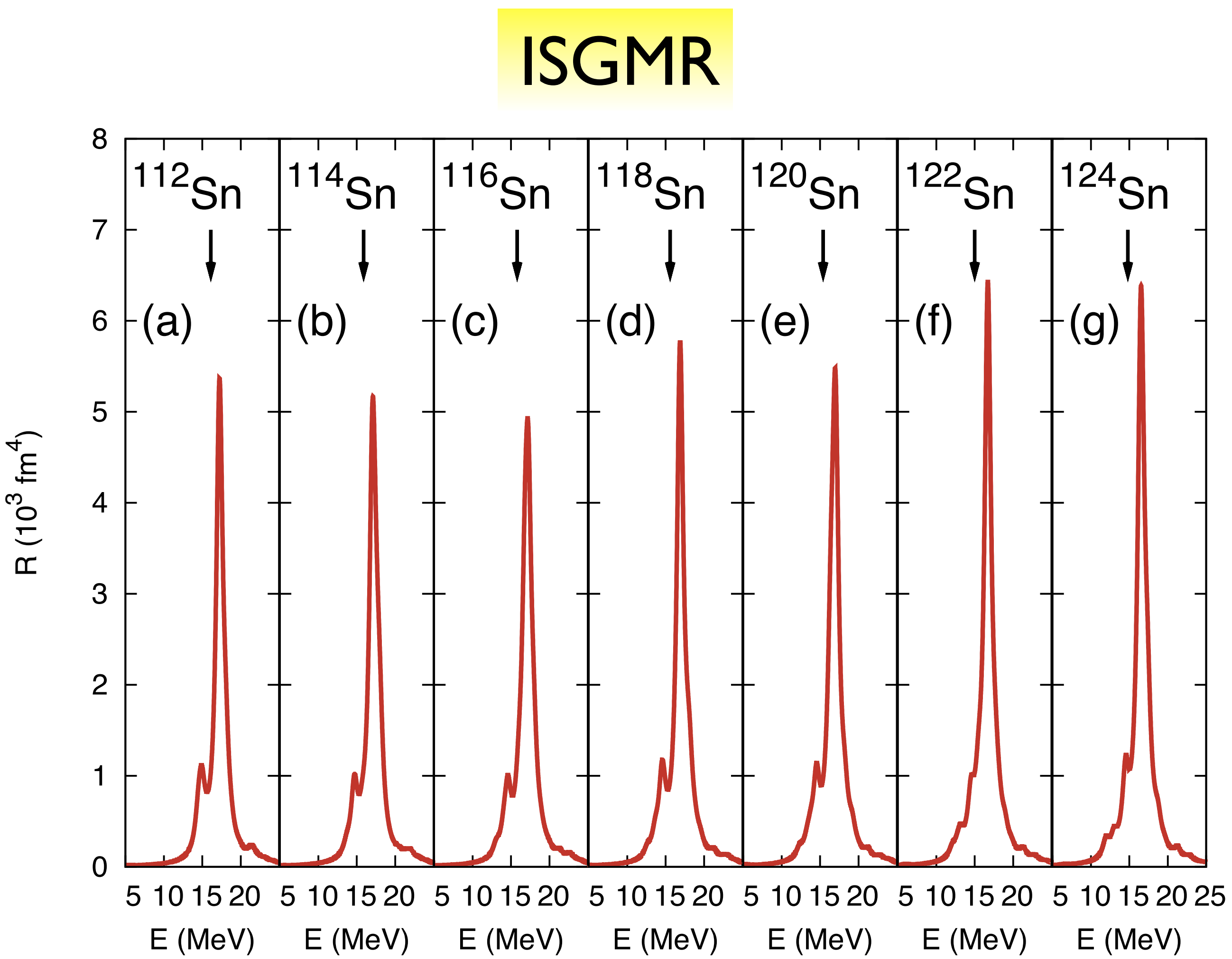

Nuclear Many-Body Correlations

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

long-range
nuclear resonance modes
(giant resonances)

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

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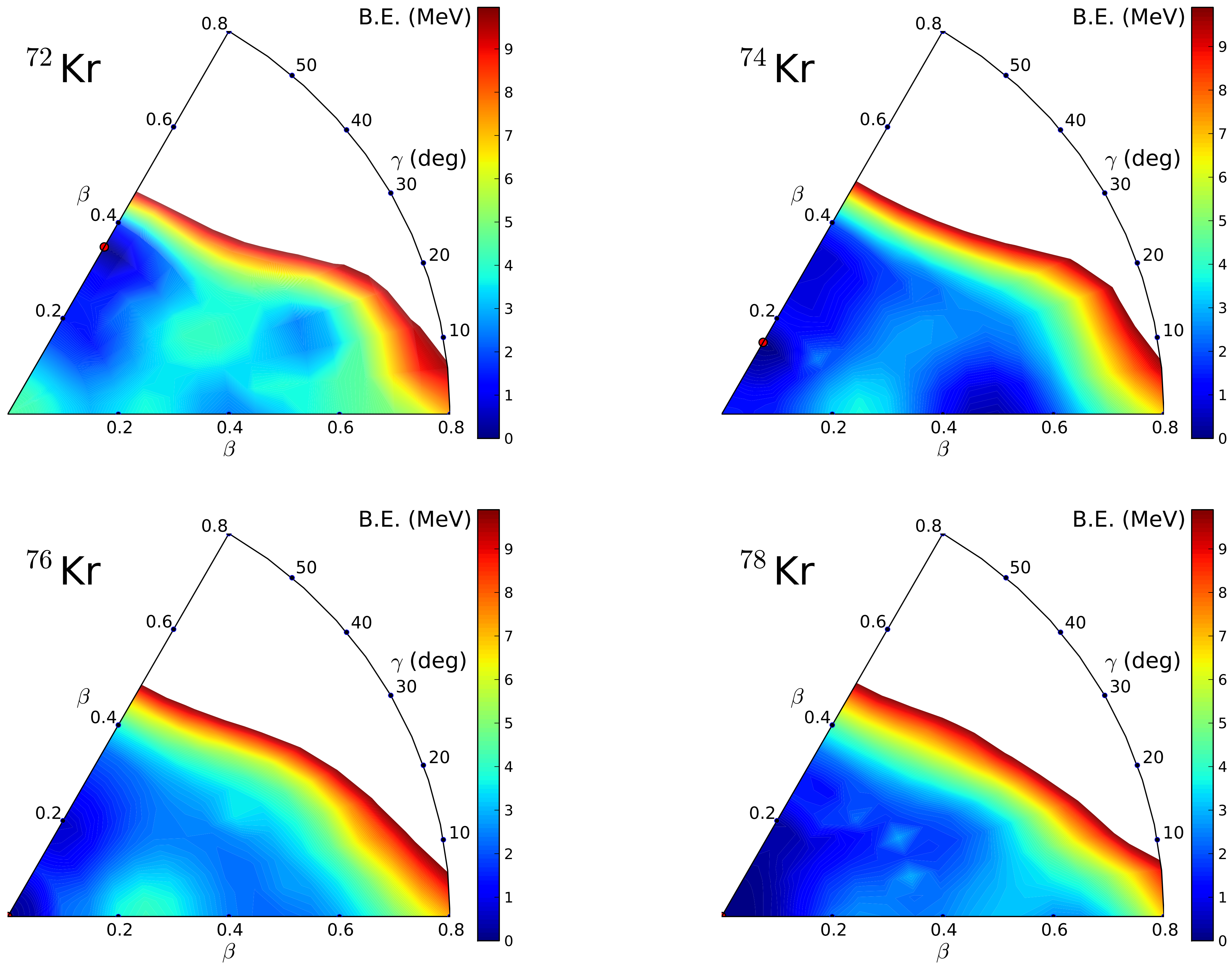
...vary smoothly with nucleon number!
Can be included implicitly in an effective Energy Density Functional.

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

Shape-coexistence in neutron-deficient Kr isotopes



Five-dimensional collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

$$H_{\rm coll} = \mathcal{T}_{\rm vib}(\beta, \gamma) + \mathcal{T}_{\rm rot}(\beta, \gamma, \Omega) + \mathcal{V}_{\rm coll}(\beta, \gamma)$$

$$\mathcal{T}_{\rm vib} = \frac{1}{2} B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

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

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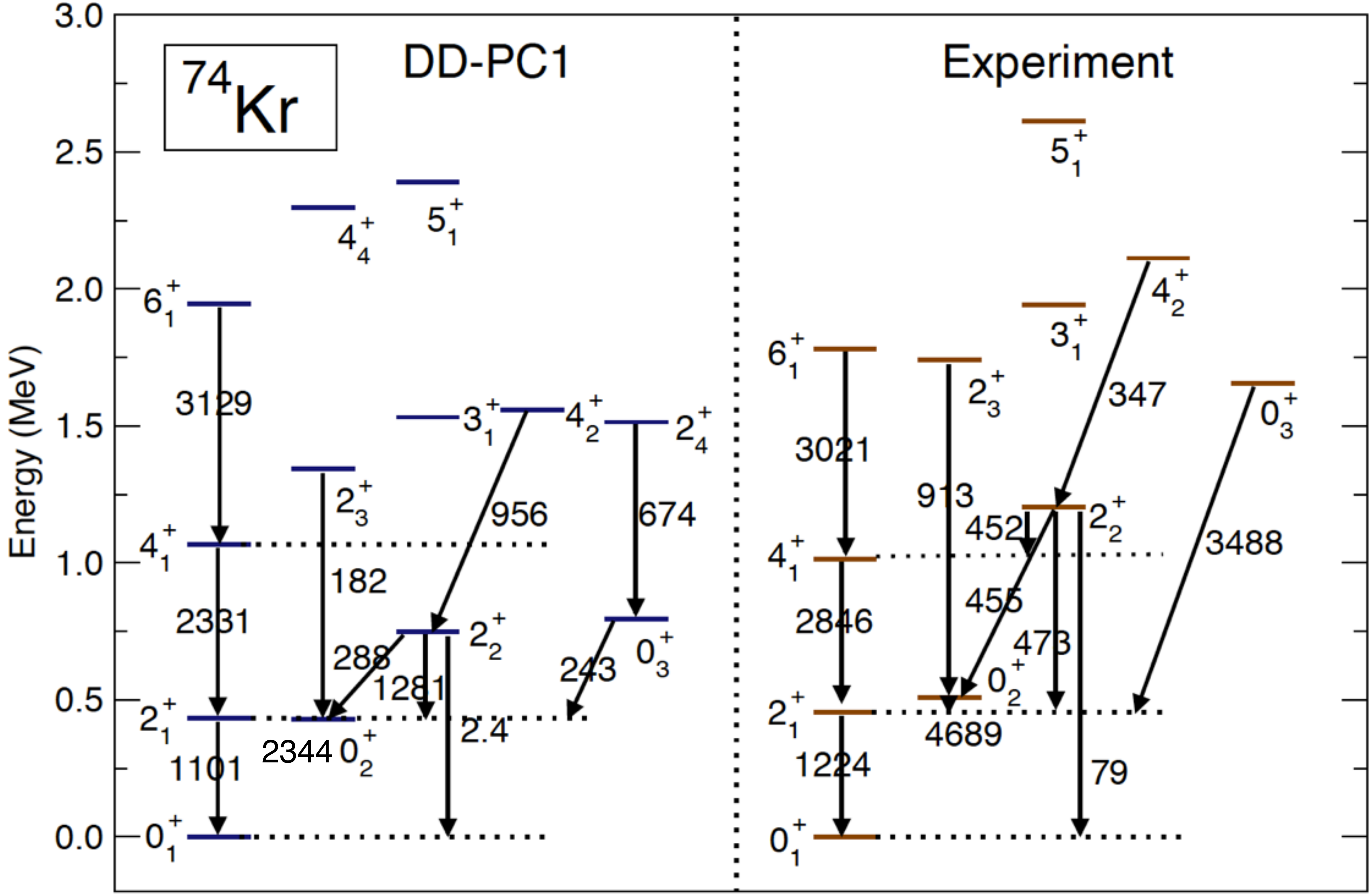
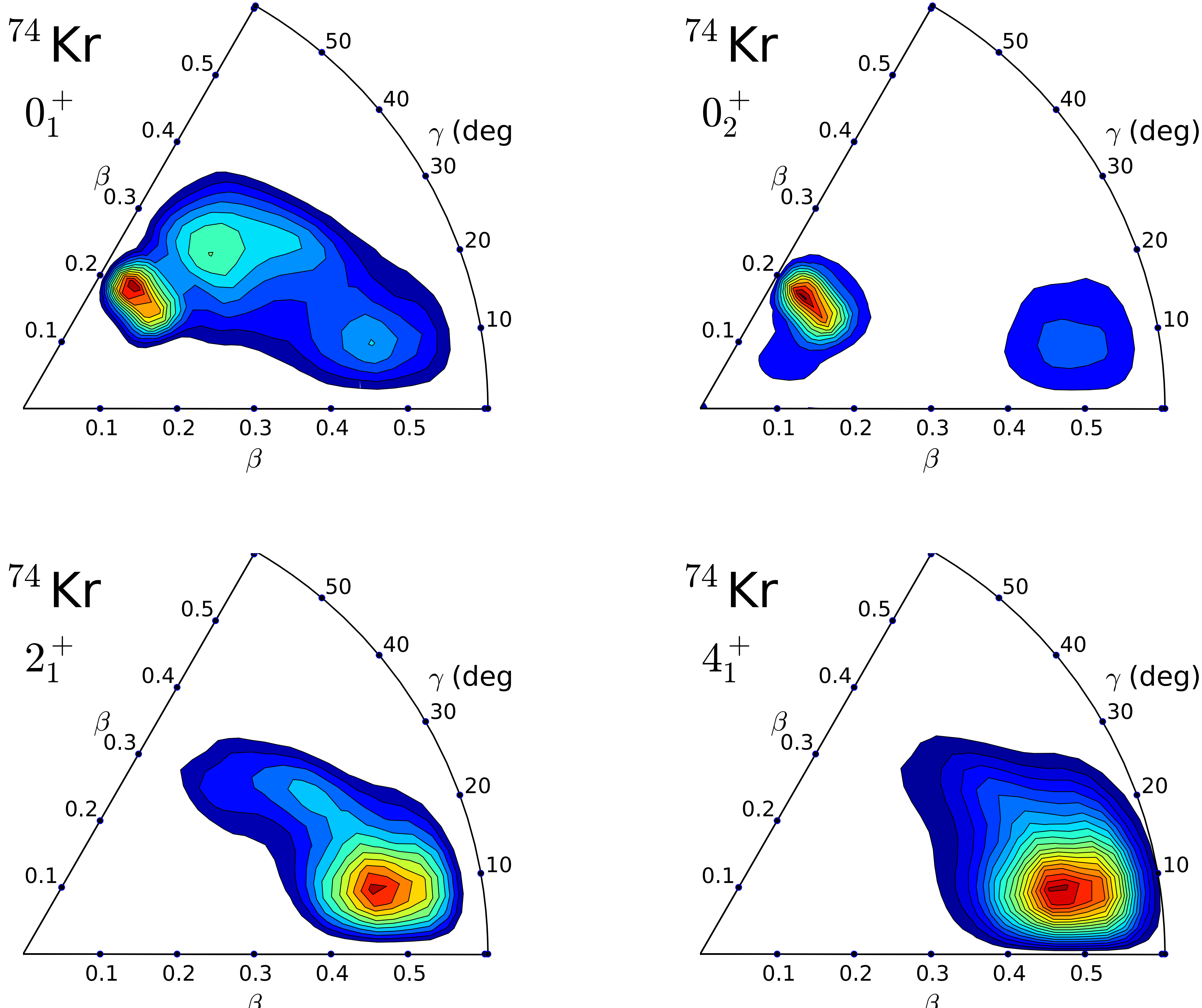
$$\mathcal{T}_{\mathrm{rot}} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

The quasiparticle wave functions and energies generated from constrained self- consistent solutions of the RHB model, provide the microscopic input for the parameters of the collective Hamiltonian.

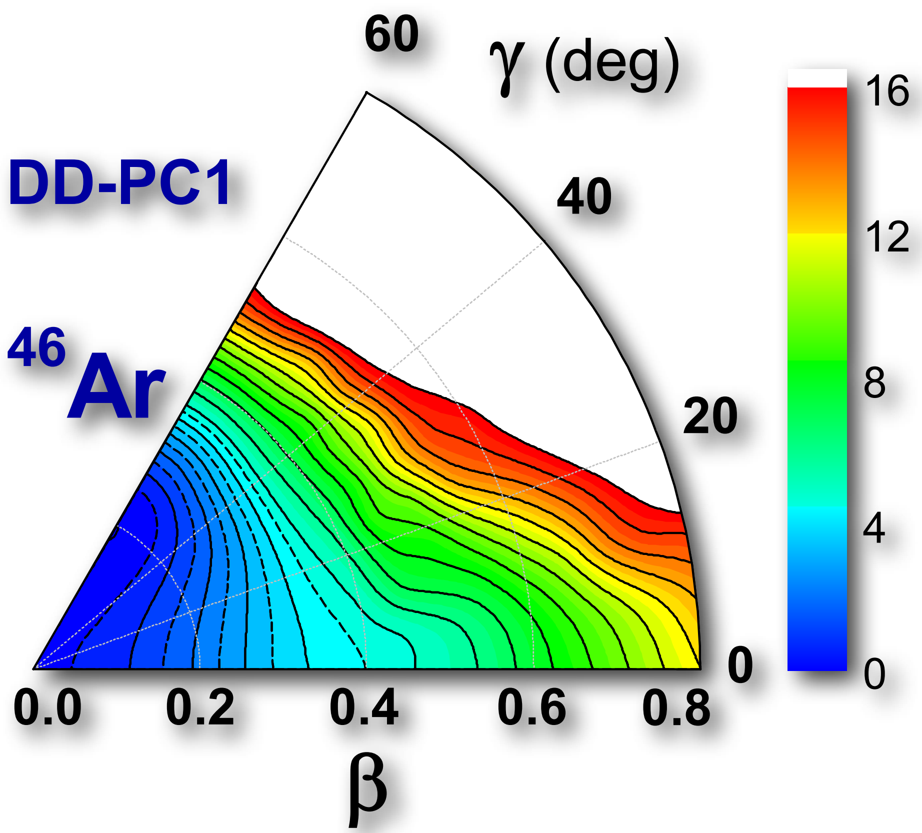


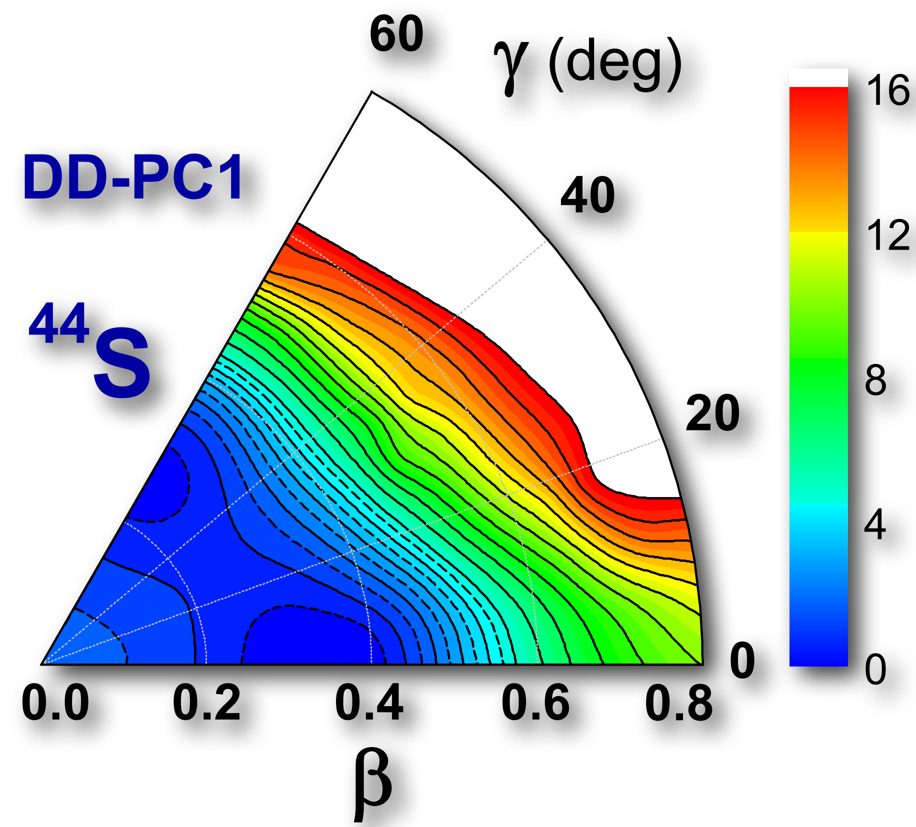
74Kr
DD-PC1
Experiment
Energy (MeV)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3129
2331
1101
182
288
2344
1281
2.4
956
674
243
3021
2846
1224
913
452
455
473
4689
79
347
3488

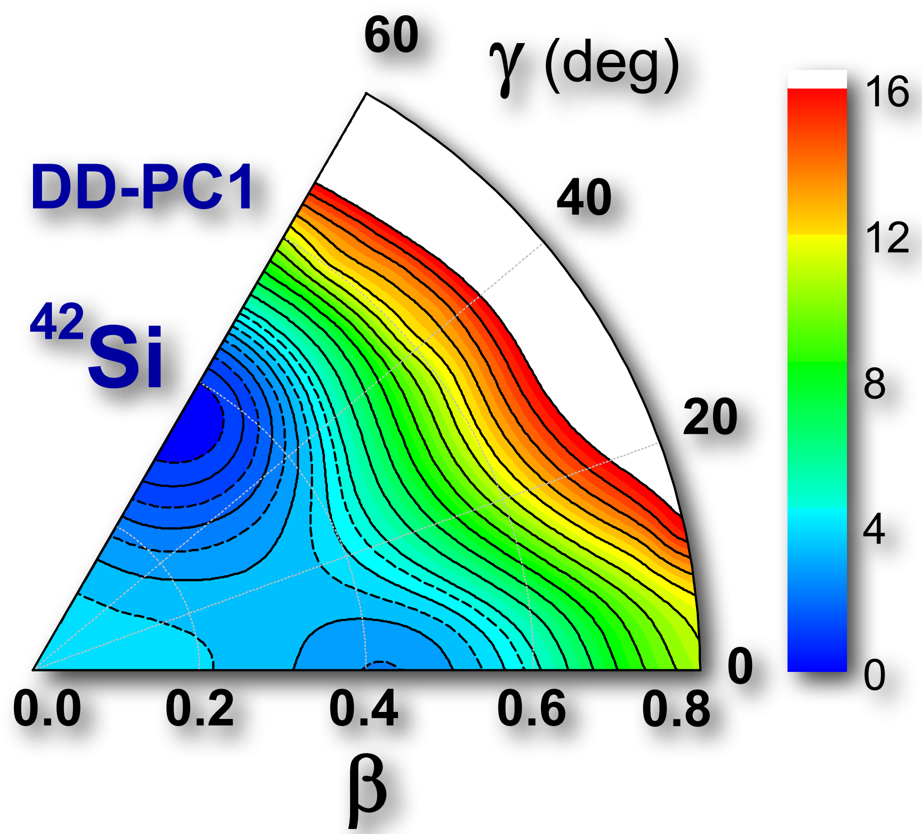


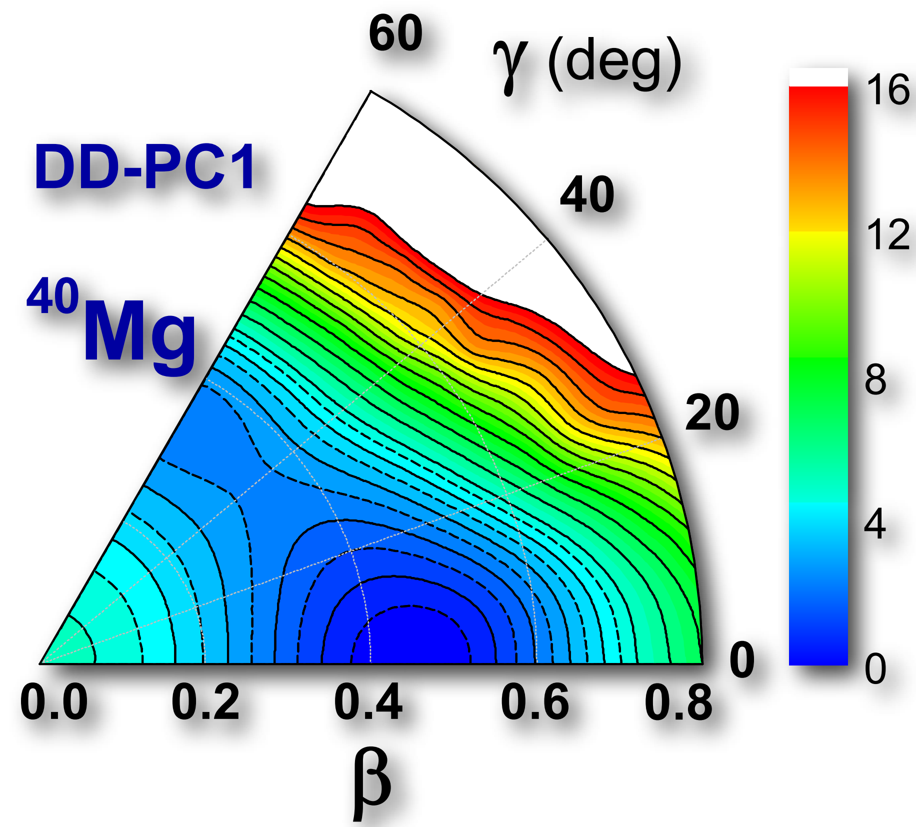
^{74}Kr
0_1^+
^{74}Kr
0_2^+
^{74}Kr
2_1^+
^{74}Kr
4_1^+
γ (deg
γ (deg)
β
0.1
0.2
0.3
0.4
0.5
10
20
30
40
50

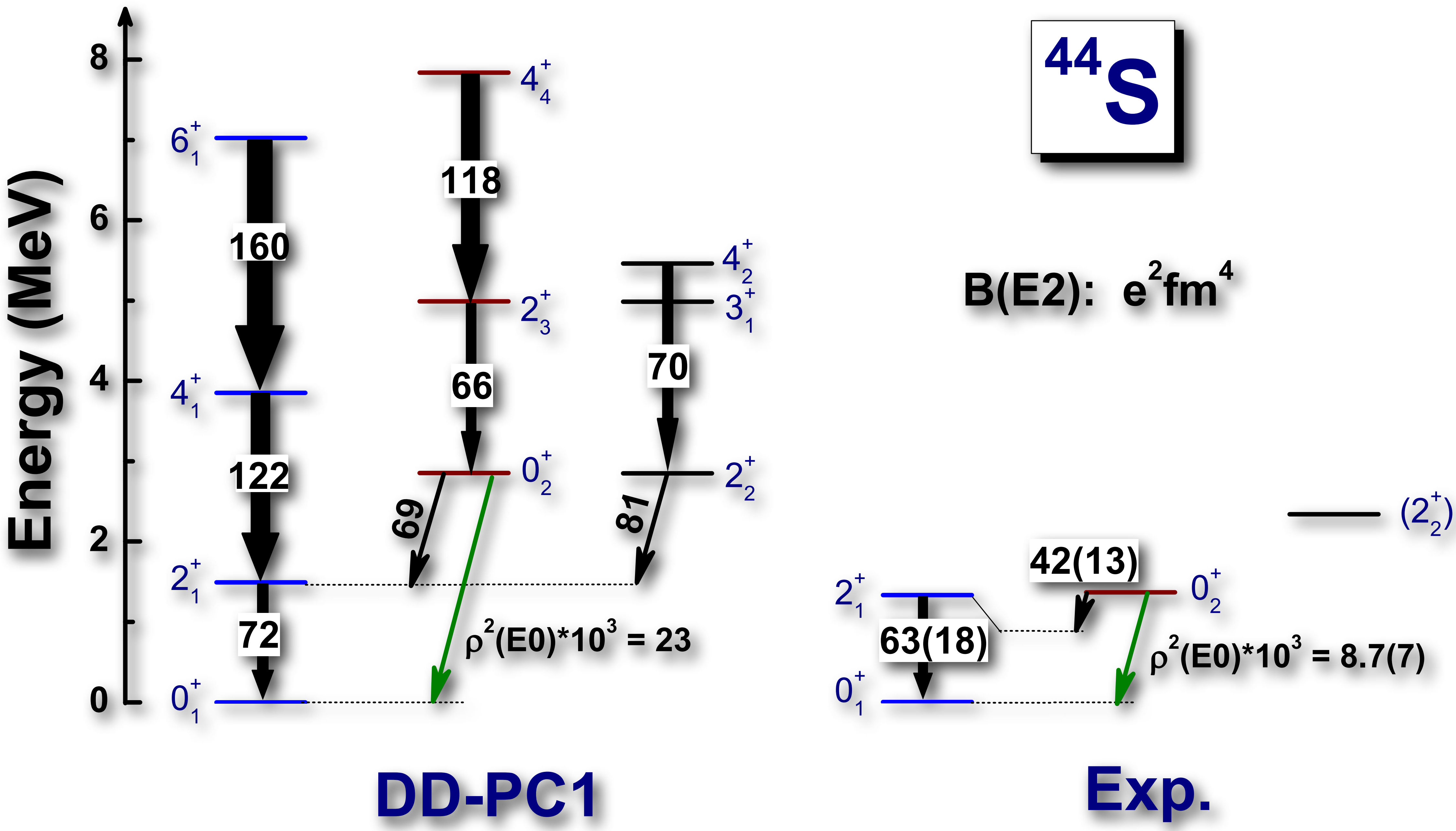
Rapidly-changing shapes in the N=28 isotones



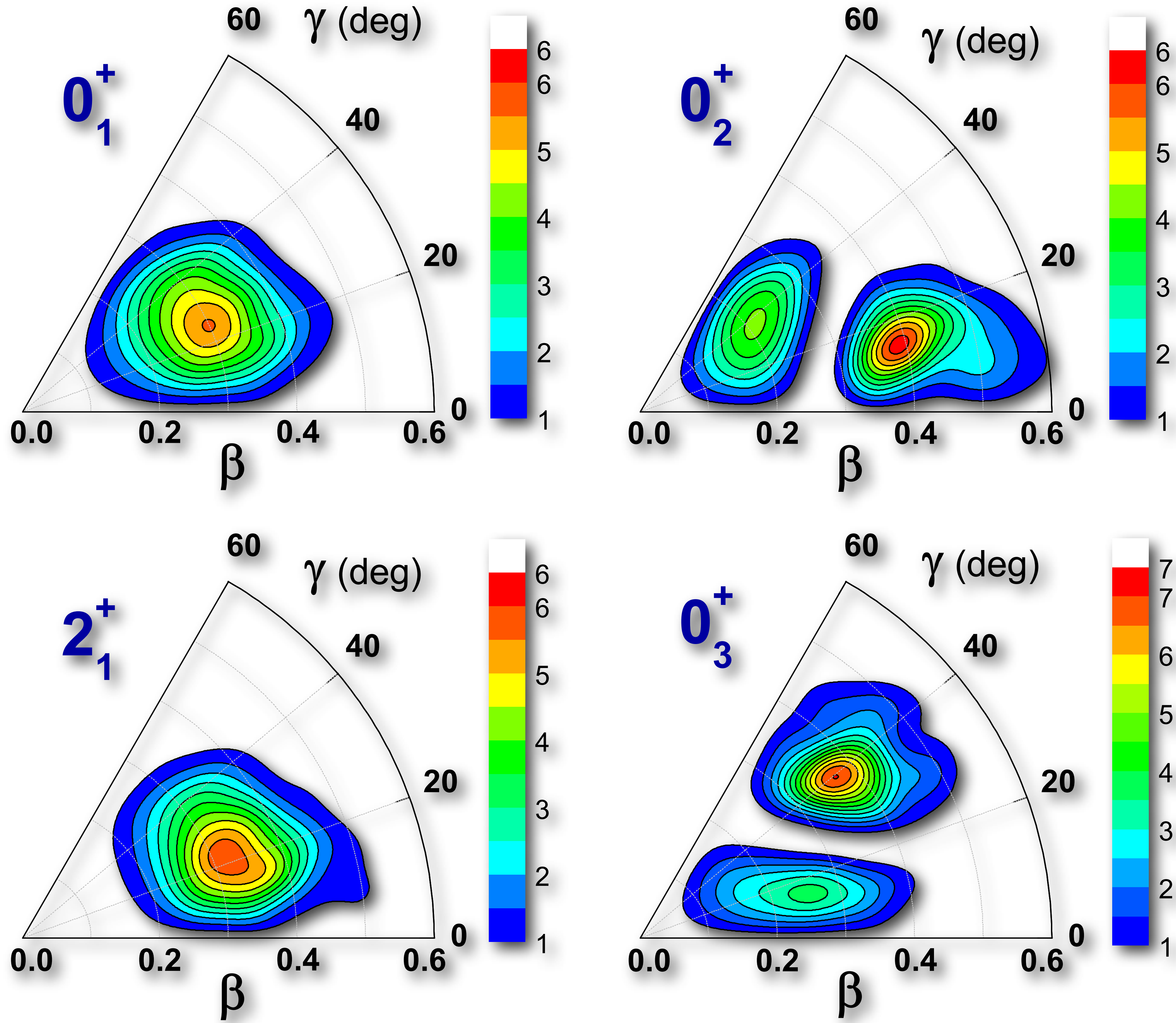




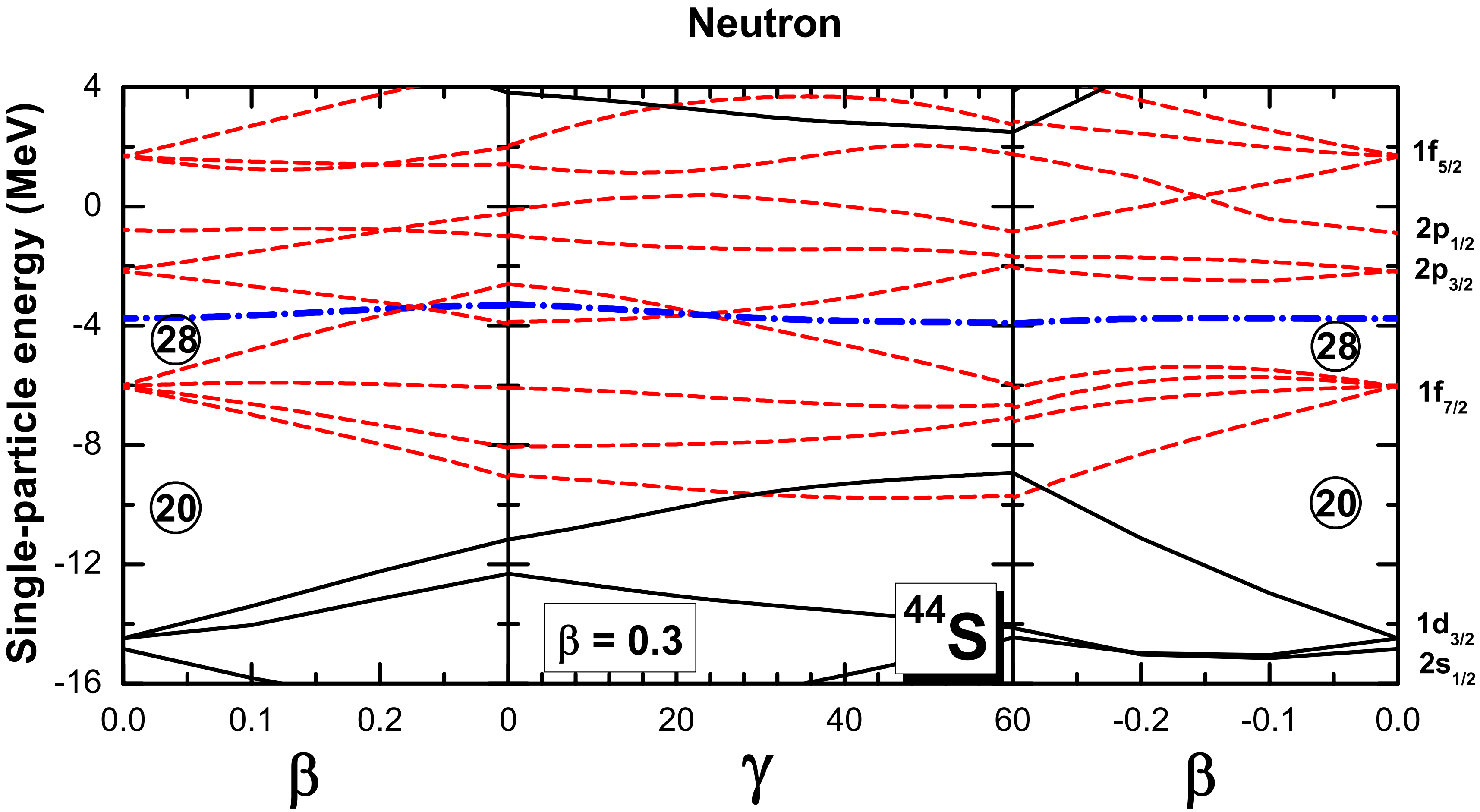


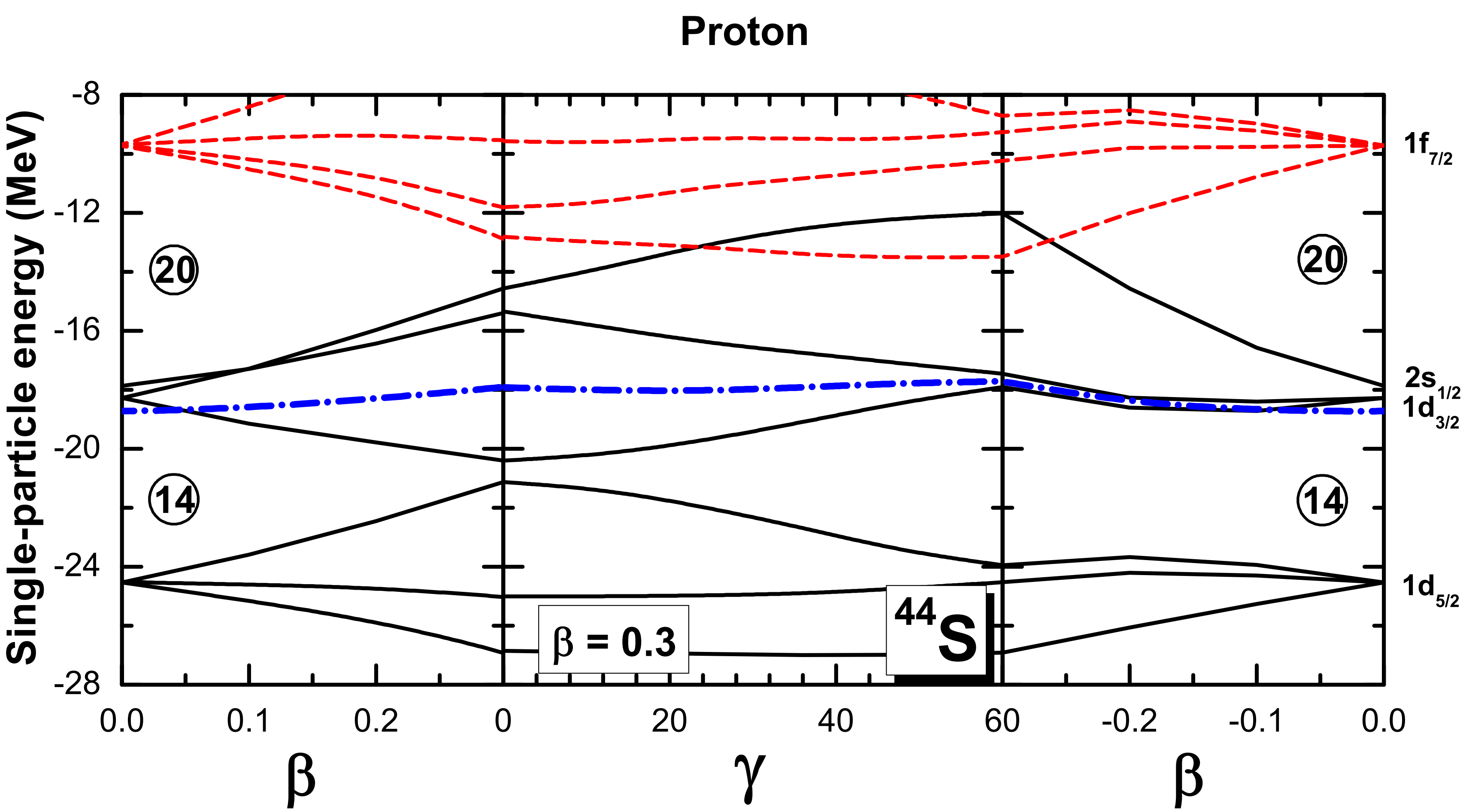


44S
B(E2): e2fm4
Energy (MeV)
8
6
4
2
0
6+1
4+1
2+1
0+1
4+4
2+3
0+2
4+2
3+1
2+2
160
122
72
118
66
69
70
81
ρ2(E0)*103 = 23
DD-PC1
(2+2)
42(13)
63(18)
ρ2(E0)*103 = 8.7(7)
Exp.

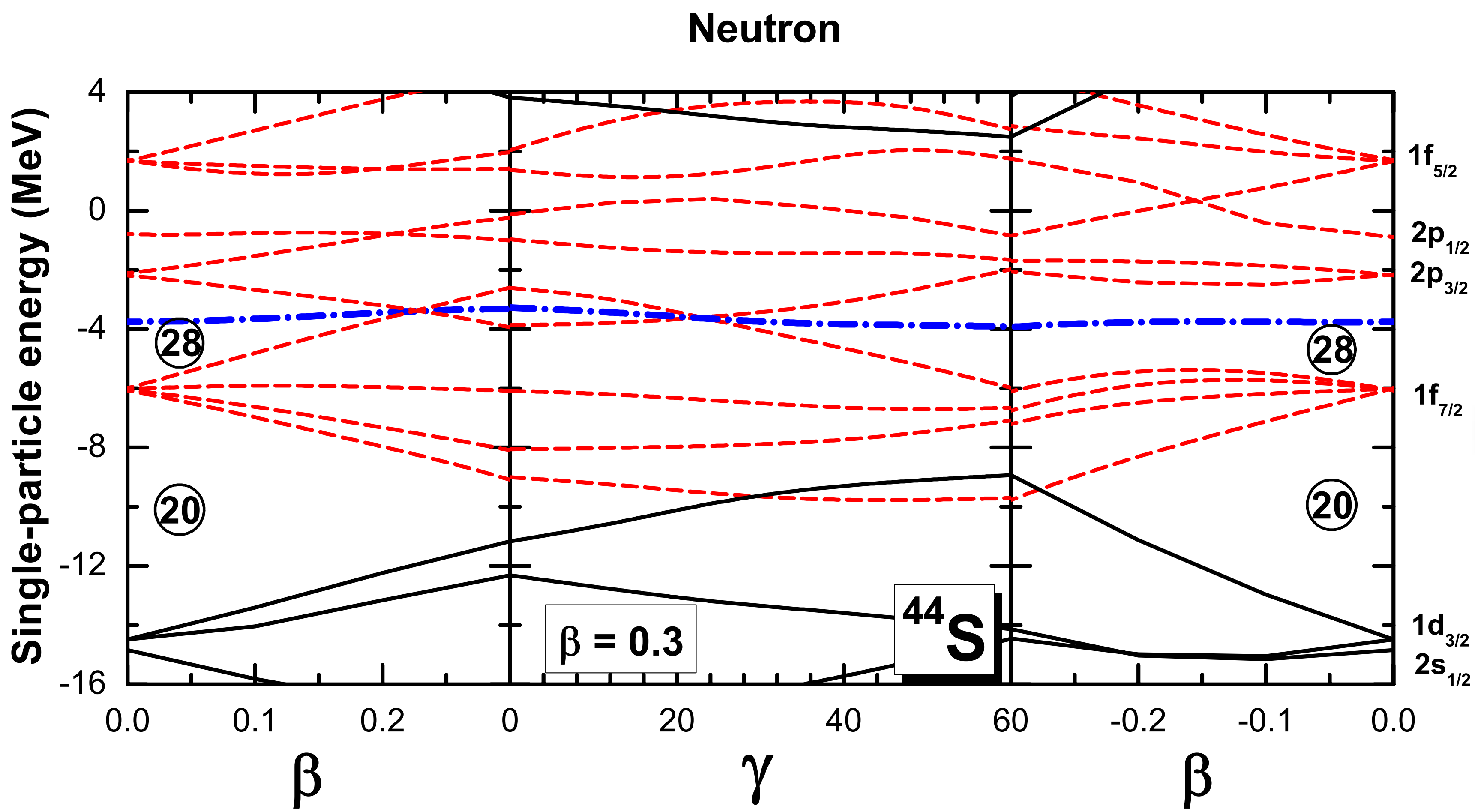


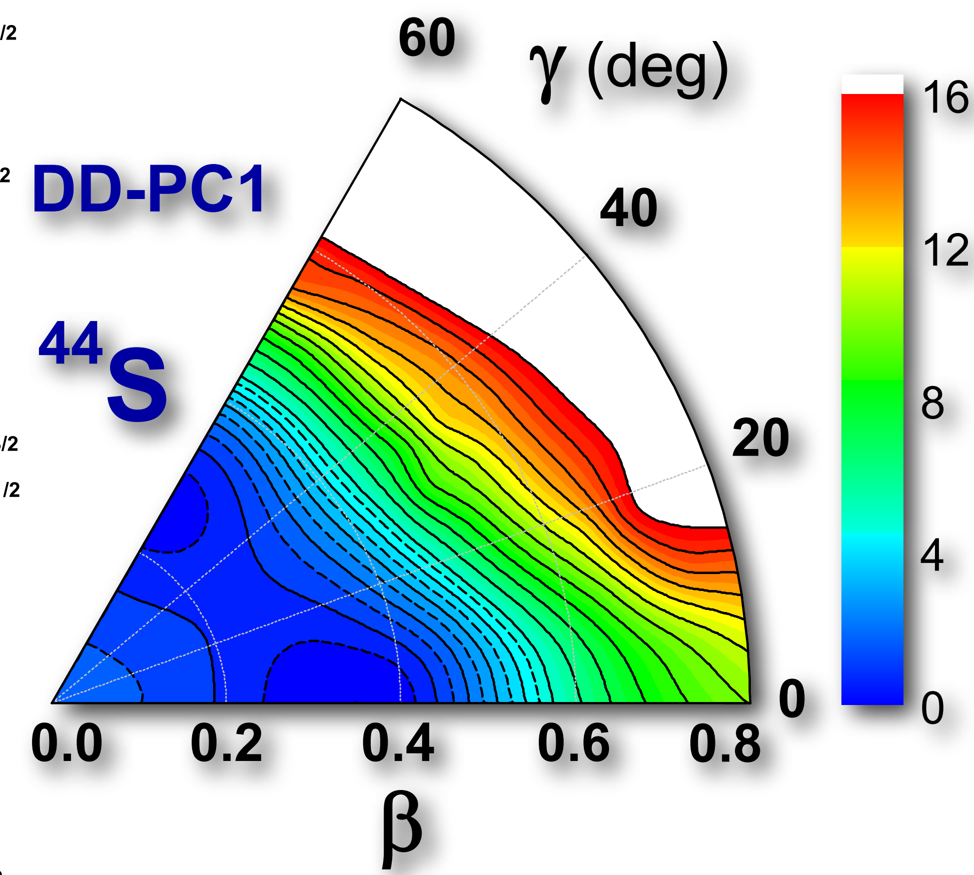
0_1^+
60
γ (deg)
40
20
0
0.0
0.2
0.4
0.6
β
6
6
5
4
3
2
1
0_2^+
2_1^+
0_3^+
7
7
6
5
4
3
2
1

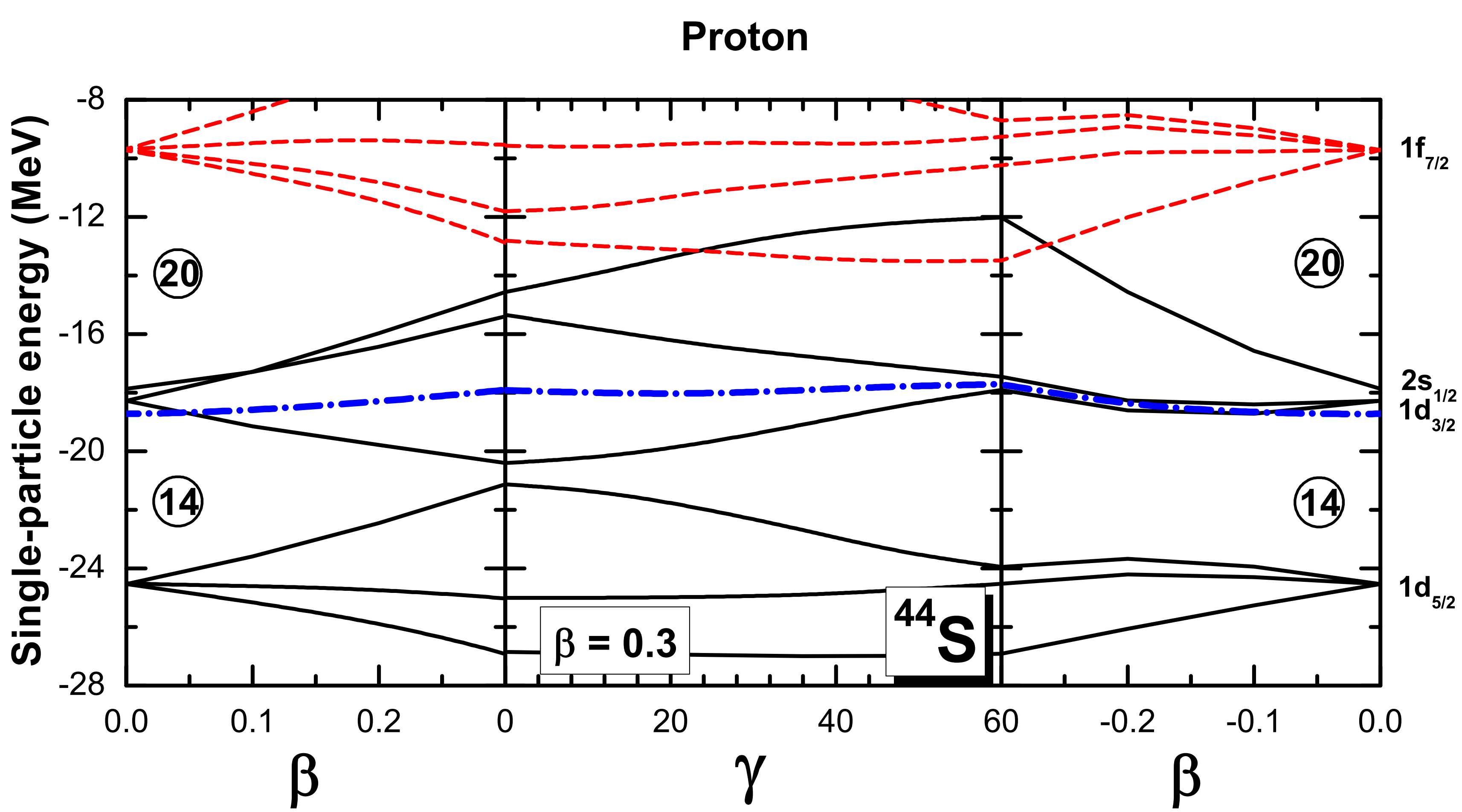


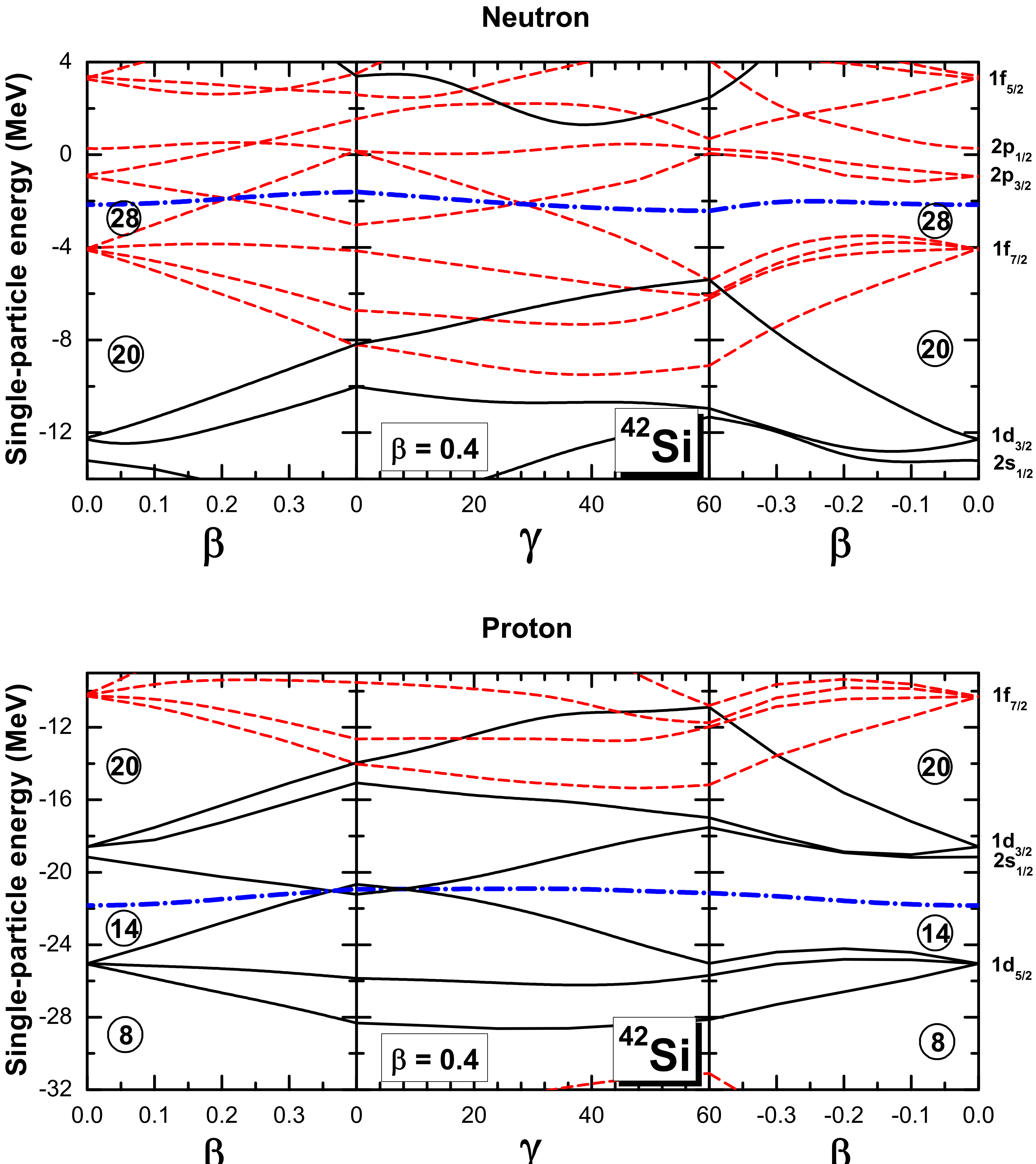


Monday, November 15, 2010

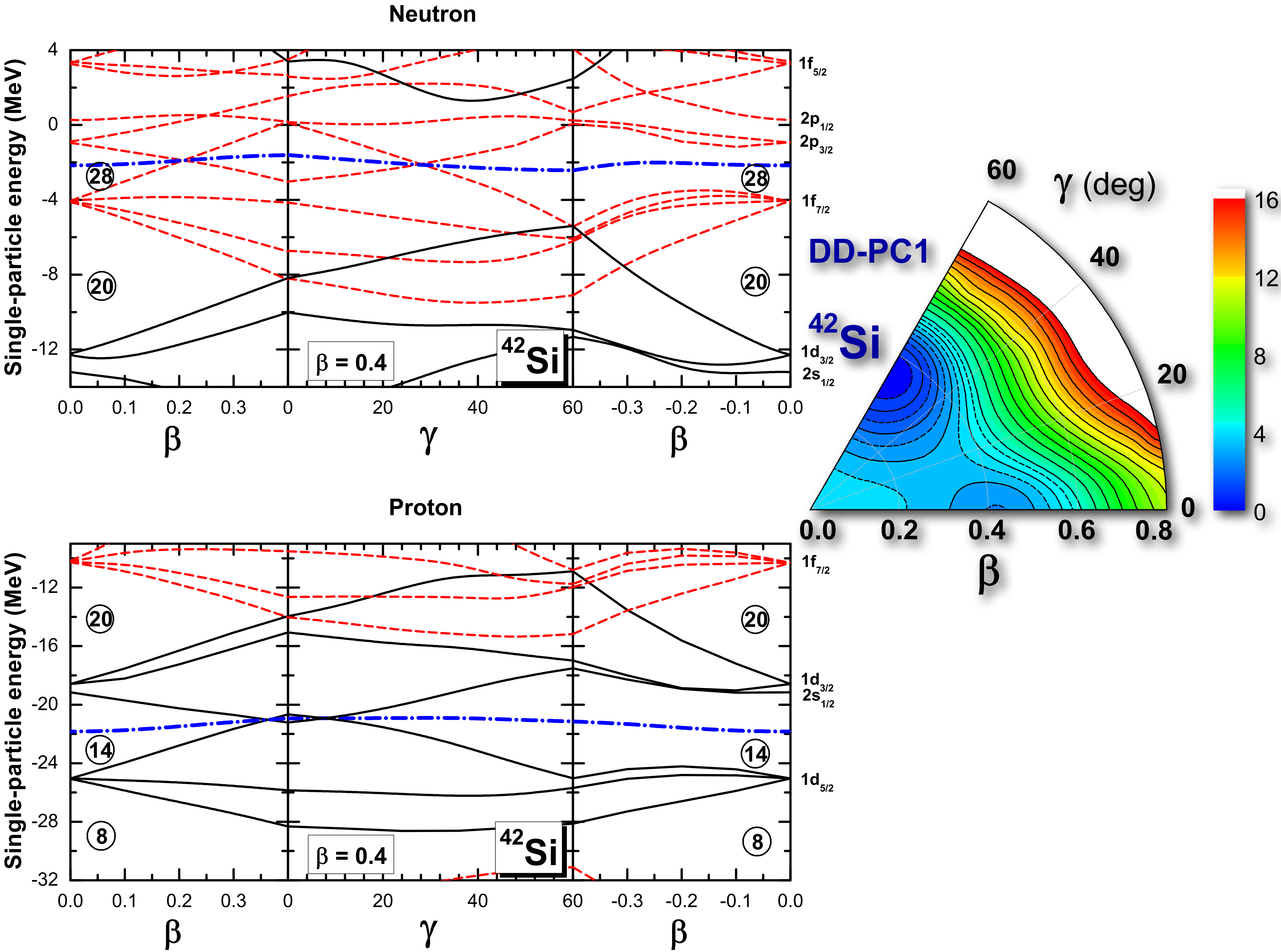

Neutron
Single-particle energy (MeV)
1f5/2
2p1/2
2p3/2
1f7/2
1d3/2
2s1/2
28
20
β = 0.3
44S
β
γ
β


γ (deg)
DD-PC1
44S
β


Proton
Single-particle energy (MeV)
1f7/2
2s1/2
1d3/2
1d5/2
20
14
β = 0.3
44S
β
γ
β



Neutron
Single-particle energy (MeV)
1f5/2
2p1/2
2p3/2
1f7/2
1d3/2
2s1/2
28
20
β = 0.4
42Si
β
γ
β
Proton
Single-particle energy (MeV)
1f7/2
1d3/2
2s1/2
1d5/2
20
14
8
β = 0.4
42Si
β
γ
β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Single-particle energy (MeV)
1f5/2
2p1/2
2p3/2
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1d3/2
2s1/2
28
20
β = 0.4
42Si
β
γ
Proton
1f7/2
1d3/2
2s1/2
1d5/2
20
14
8
DD-PC1
42Si
γ (deg)
0.0
0.2
0.4
0.6
0.8
60
40
20
0
16
12
8
4
0

EDF description of nuclear Quantum Phase Transitions

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Atomic nuclei → first- and second-order QPT occur between systems characterized by **different ground-state shapes**. Control parameter → **number of nucleons.**

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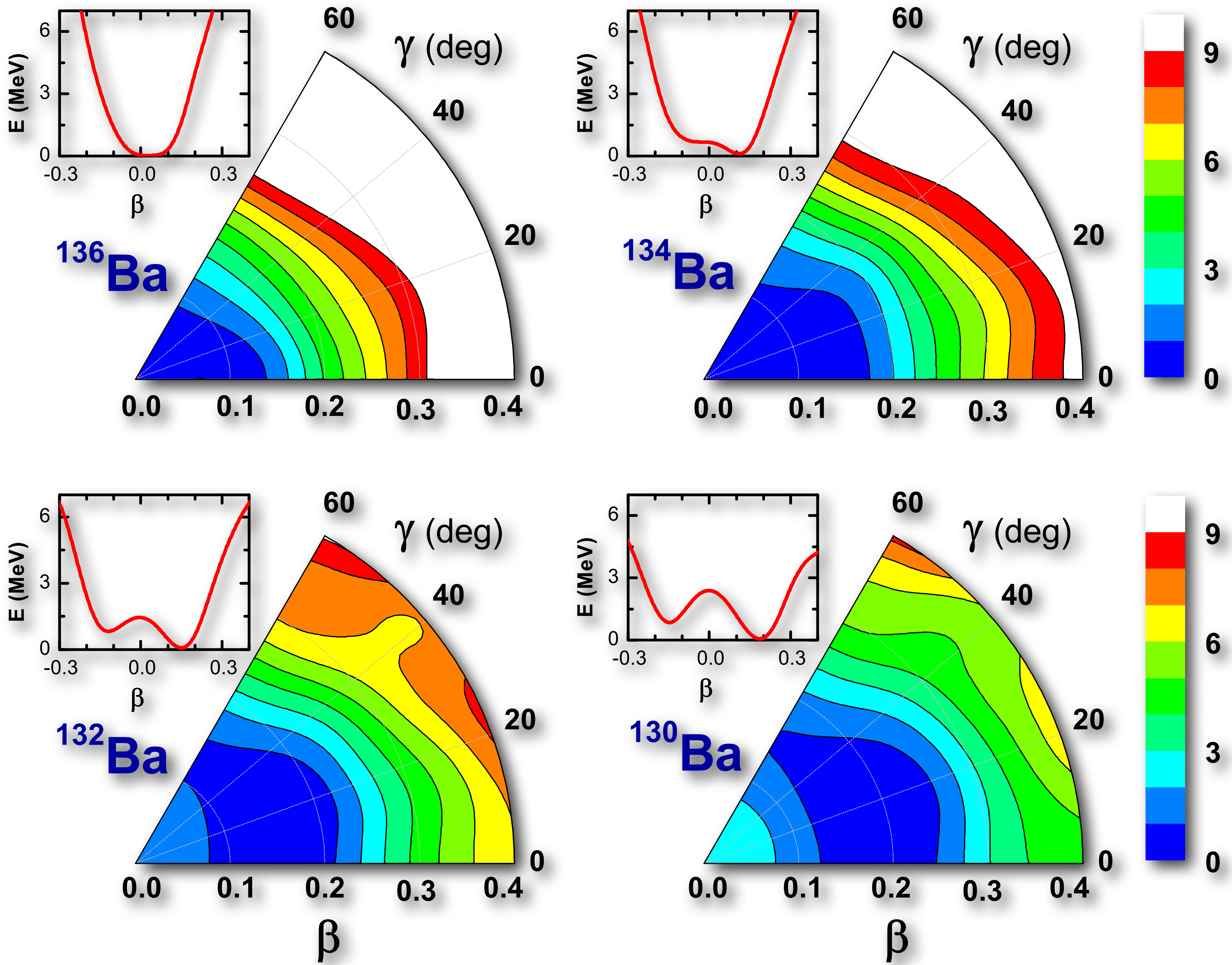
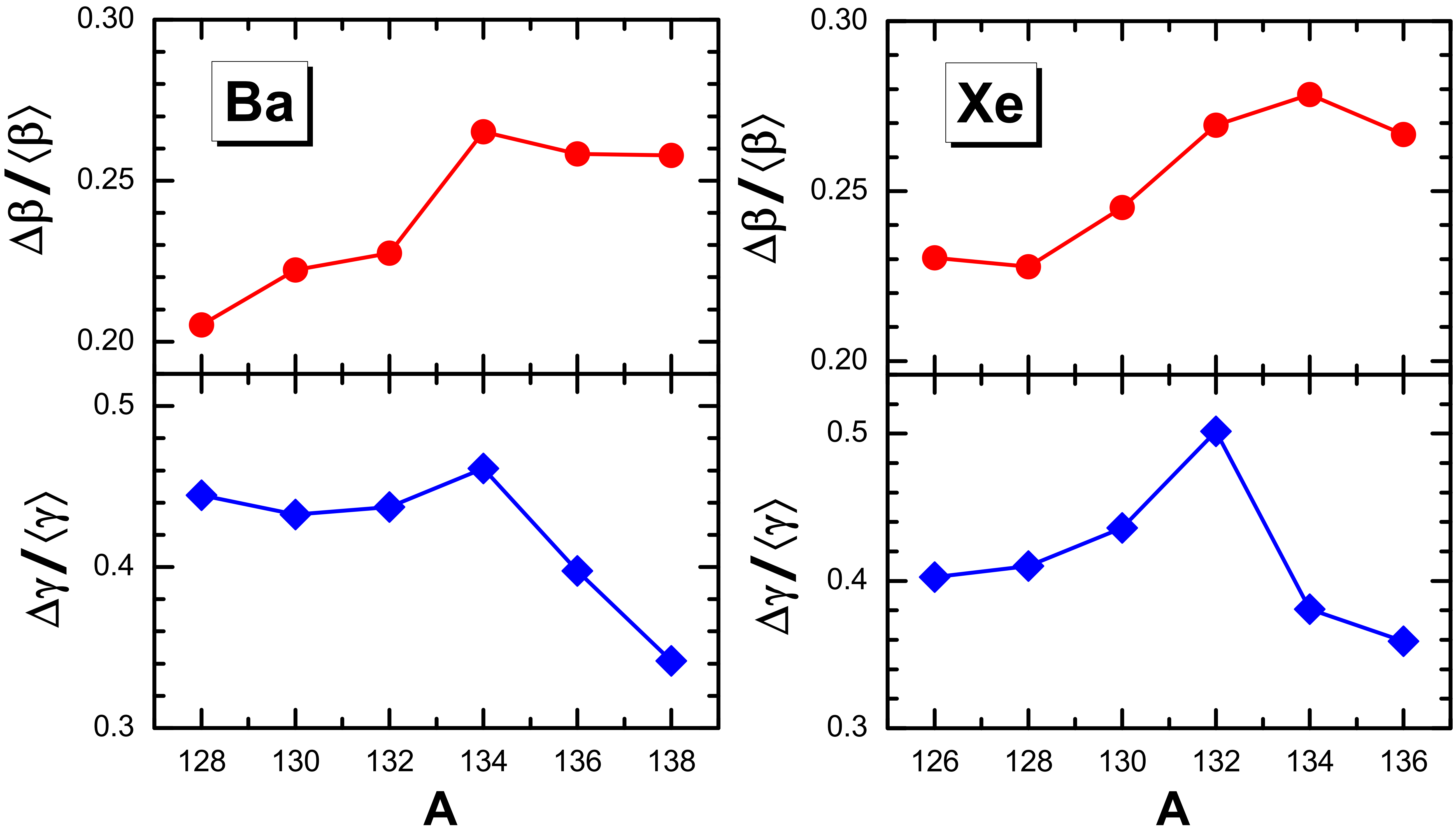
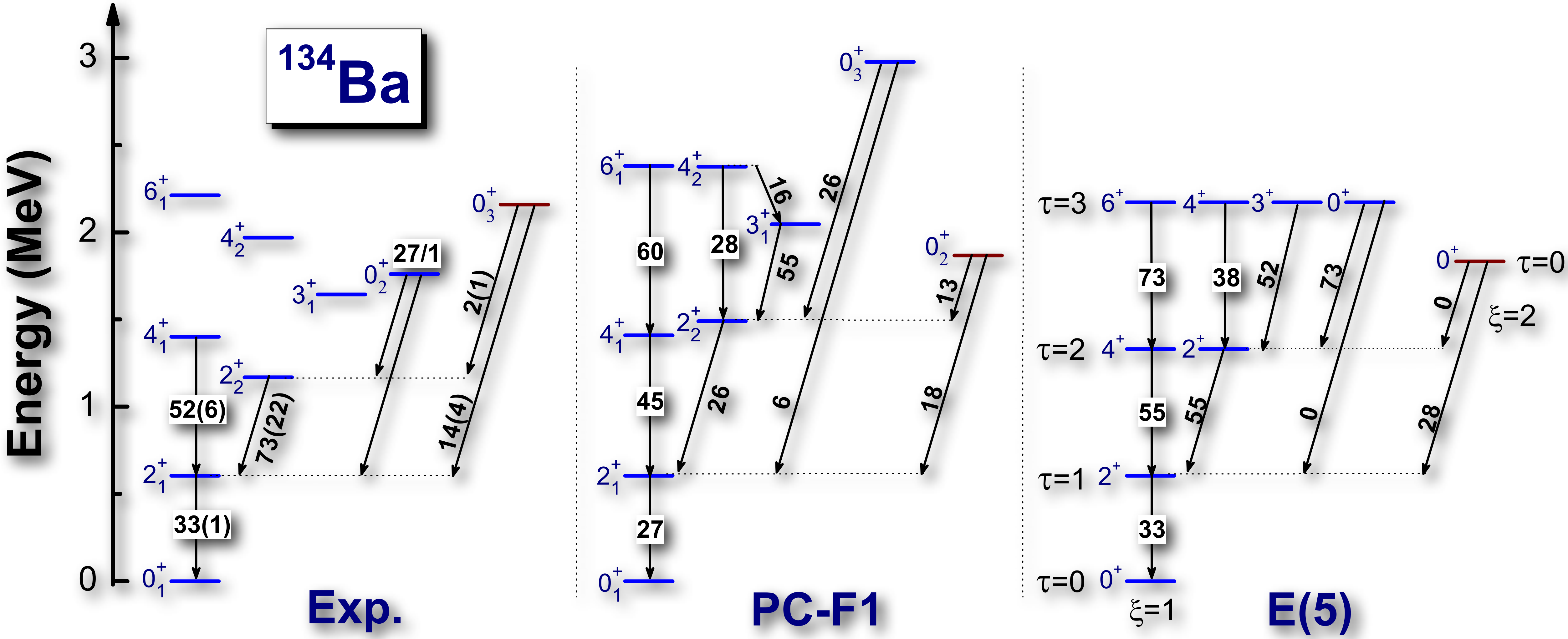
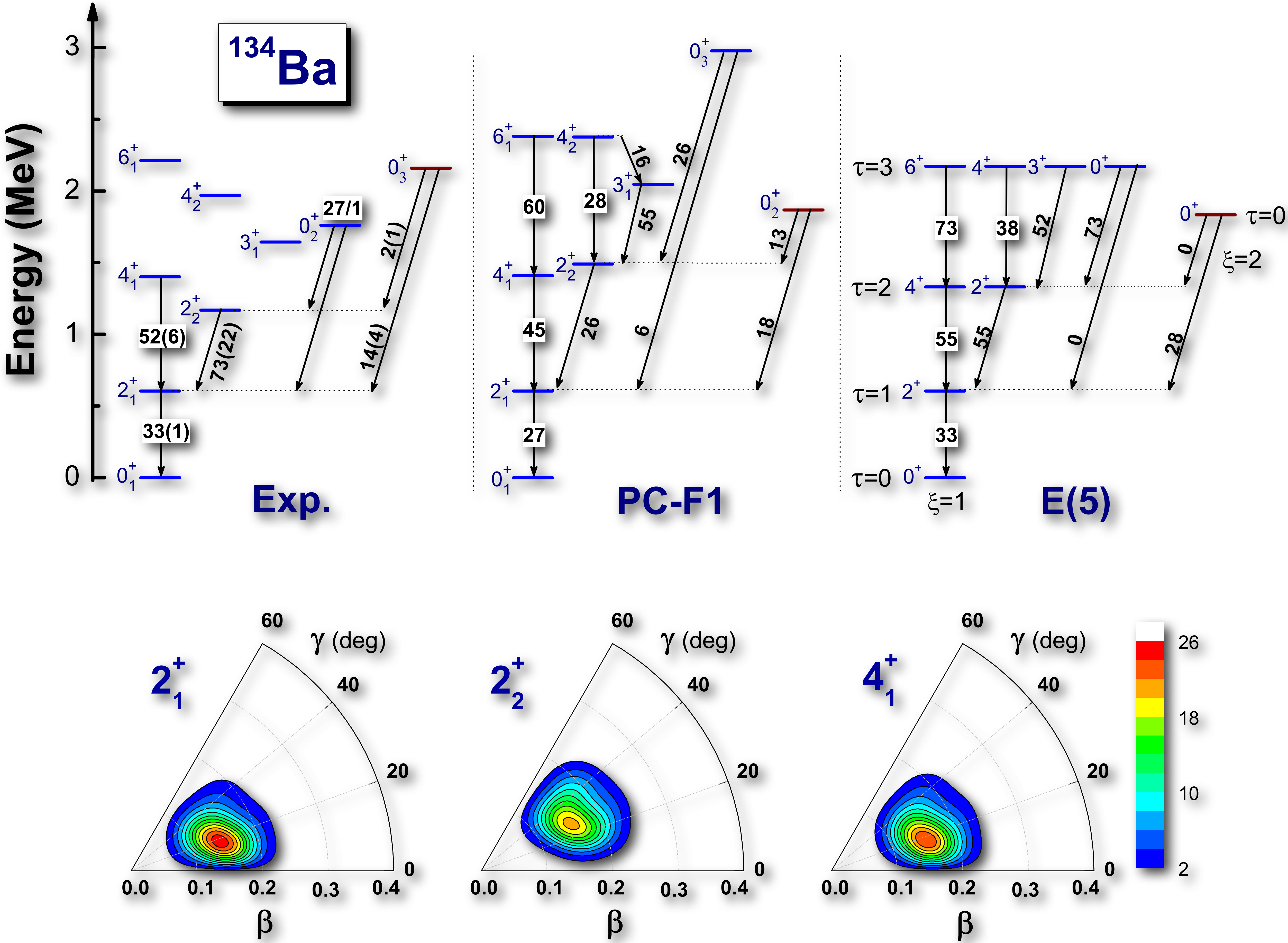


Fluctuations of quadrupole deformation parameters

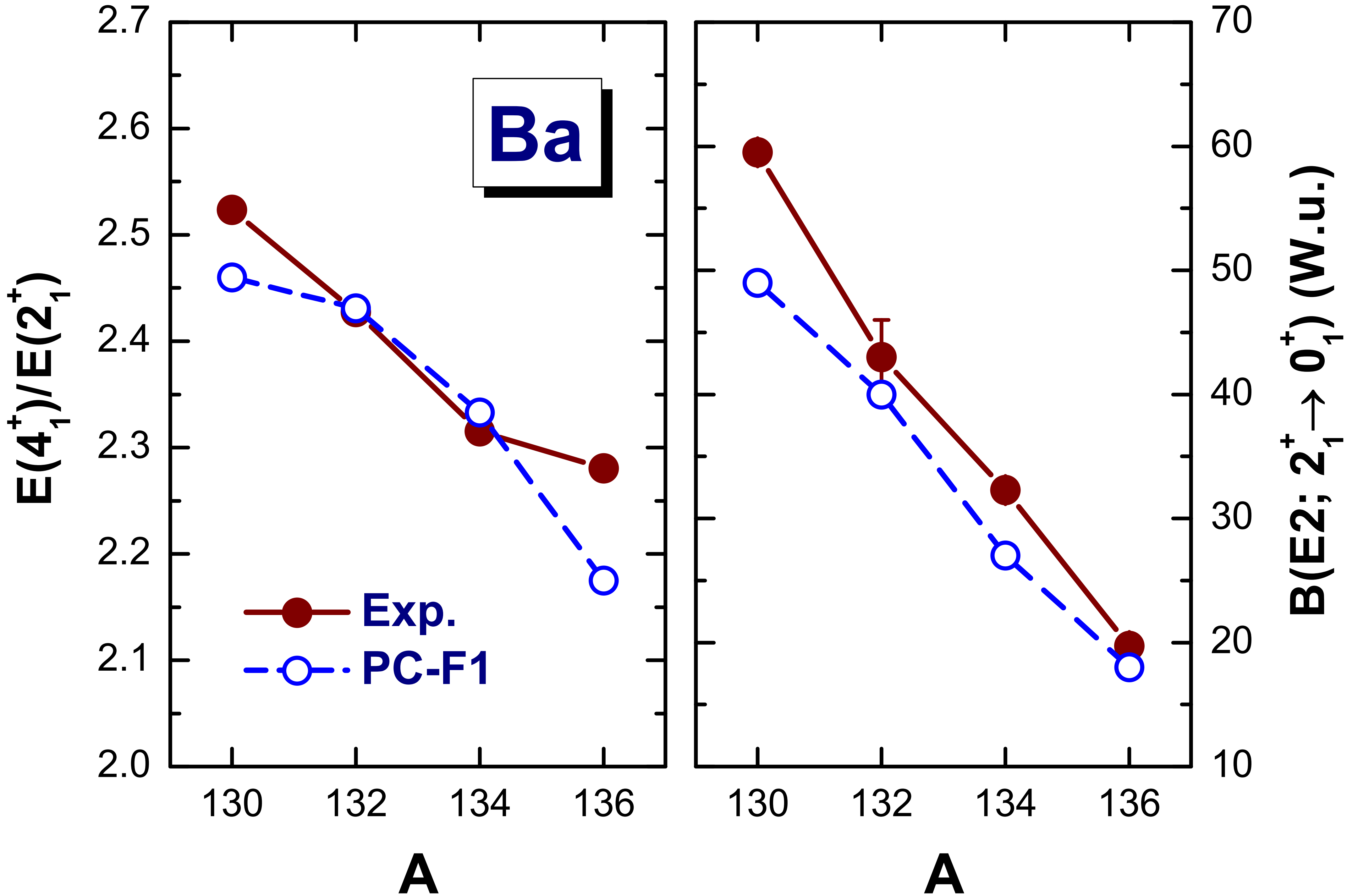




134Ba
Energy (MeV)
Exp.
PC-F1
E(5)
τ=0
τ=1
τ=2
τ=3
ξ=1
ξ=2
52(6)
33(1)
73(22)
27/1
2(1)
14(4)
60
45
27
28
26
16
55
6
13
18
73
38
52
0
55
33
28

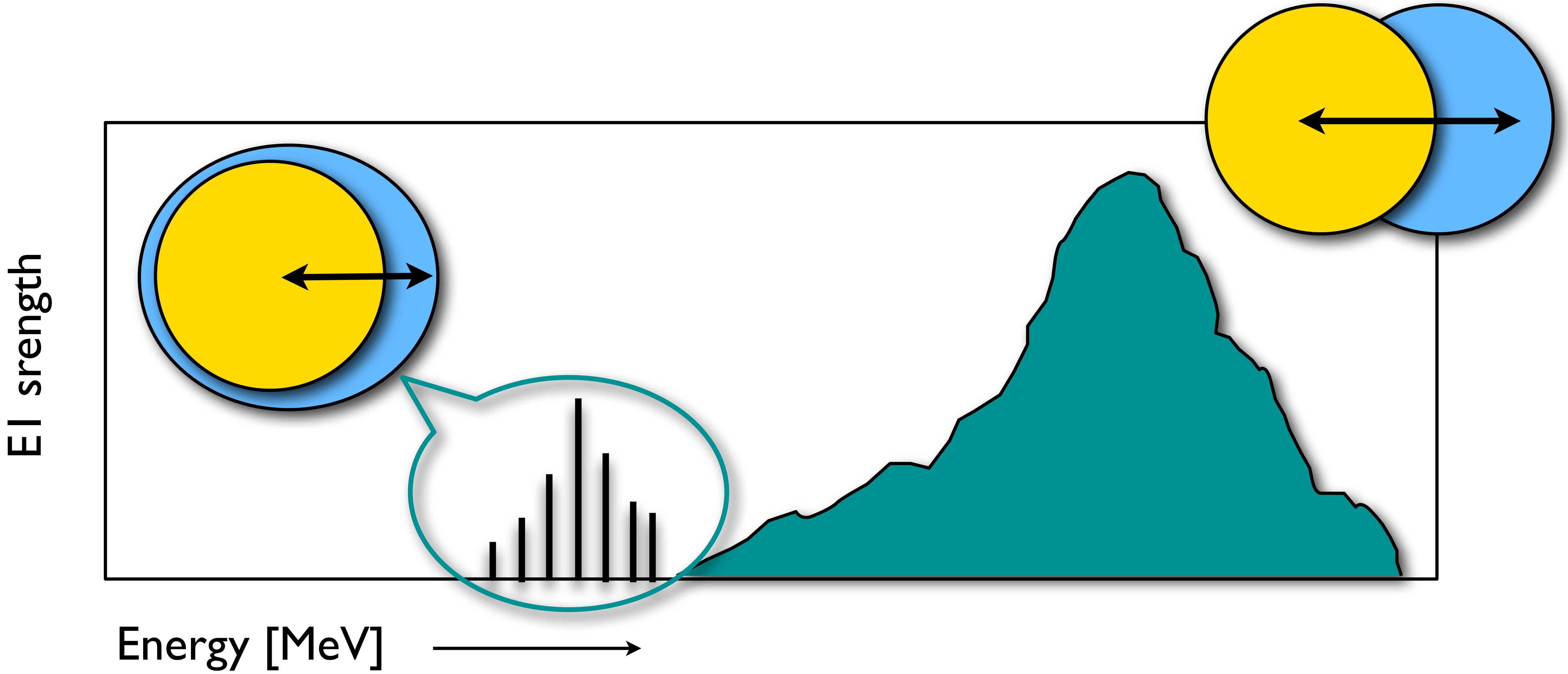


134Ba
Energy (MeV)
Exp.
PC-F1
E(5)
52(6)
33(1)
73(22)
27/1
2(1)
14(4)
60
28
19
26
55
45
26
6
13
18
27
τ=3
τ=2
τ=1
τ=0
ξ=1
ξ=2
73
38
52
73
0
55
55
0
28
33
γ (deg)
β



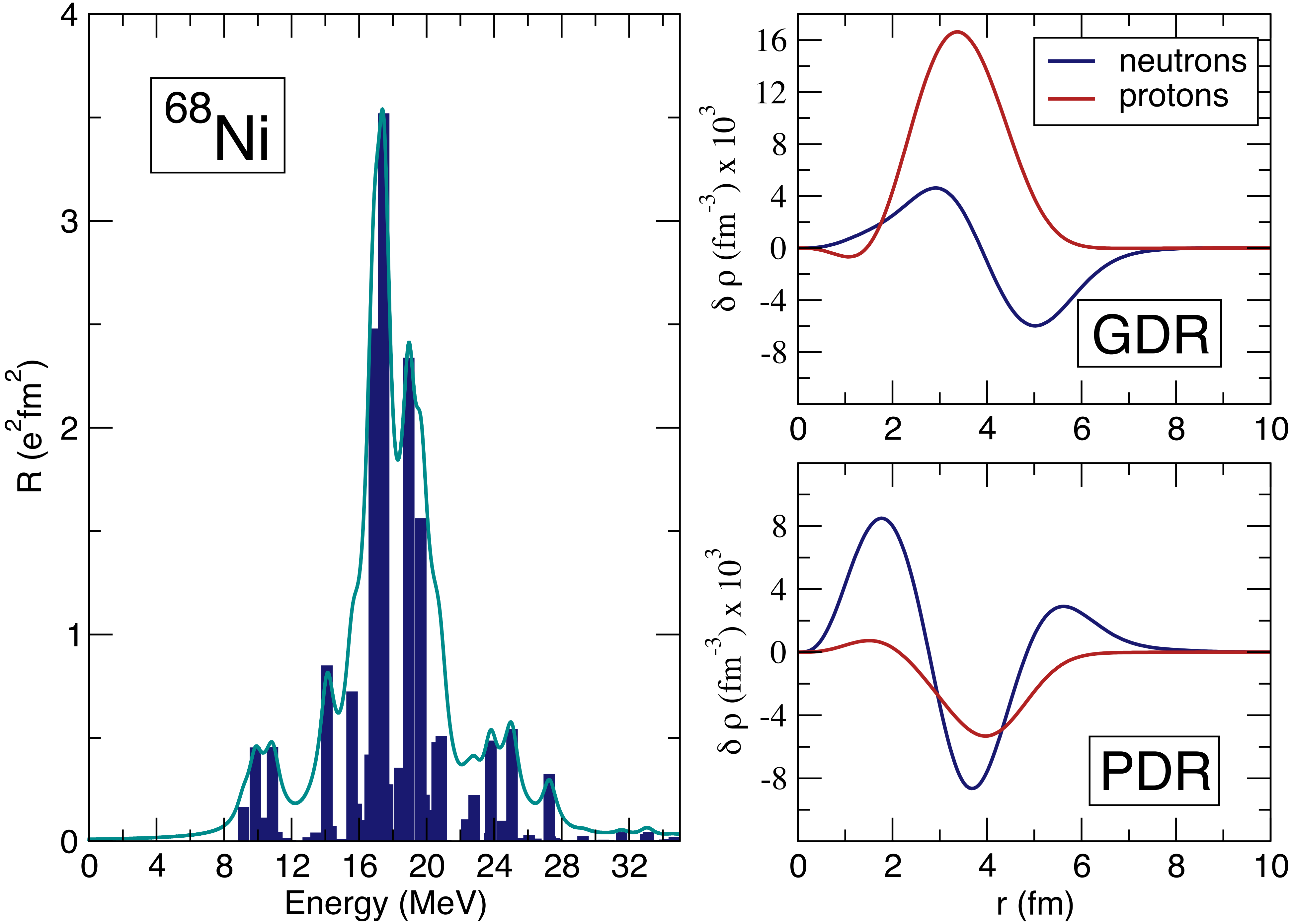
Ba
Exp.
PC-F1
$E(4^+_1)/E(2^+_1)$
$B(E2; 2^+_1 \to 0^+_1)$ (W.u.)
A
A
2.0
2.1
2.2
2.3
2.4
2.5
2.6
2.7
10
20
30
40
50
60
70
130
132
134
136

Exotic modes of excitations
Evolution of low-lying collective modes

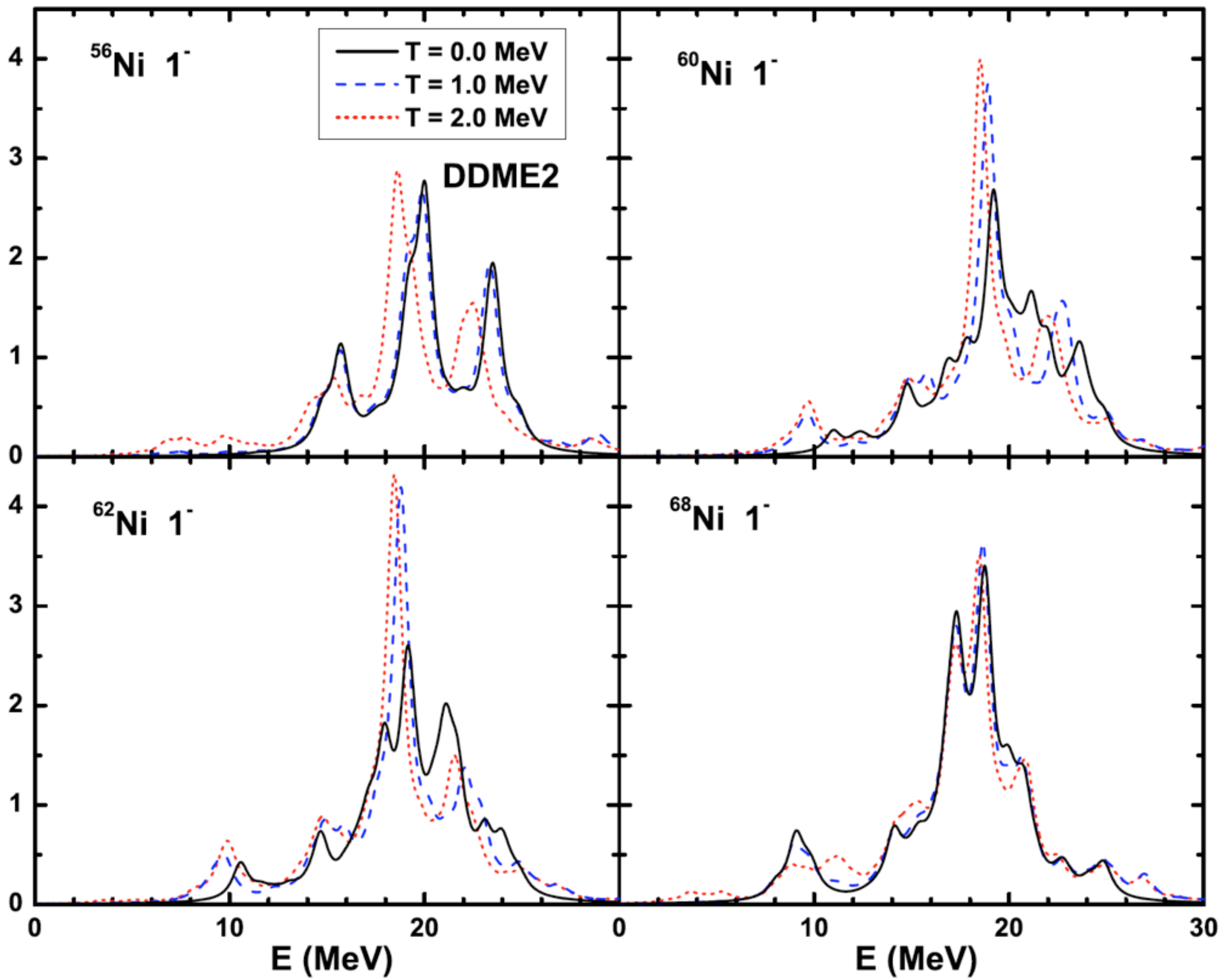


Neutron-rich nuclei → predicted occurrence of a collective soft dipole mode (**Pygmy Dipole Resonance**)

Low-lying E1 strength in Ni isotopes



Low-energy dipole response at finite temperature



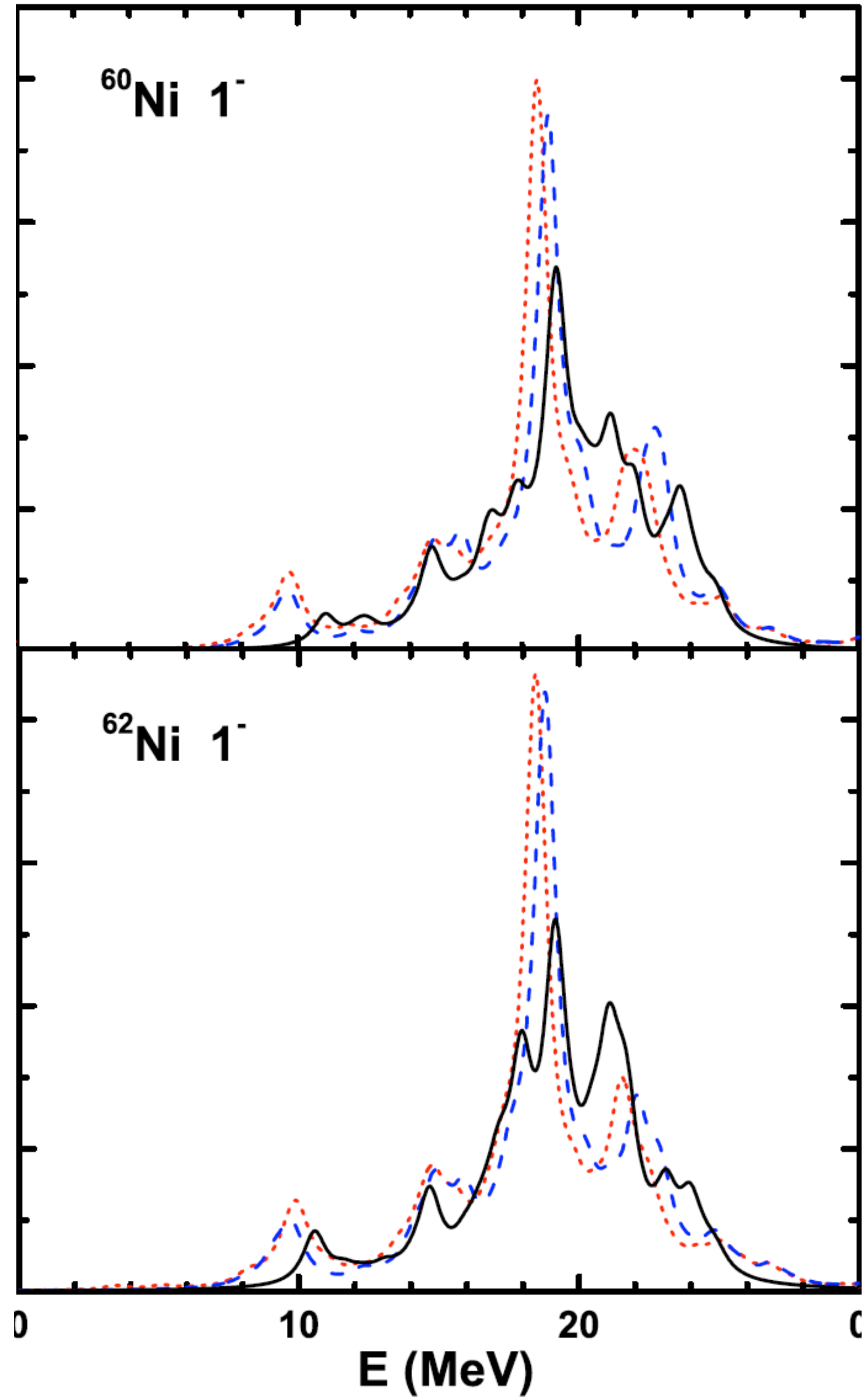
Thermal unblocking of single-particle orbitals close to the Fermi level.

FTRRPA transition amplitudes at temperature $T = 2$ MeV for the dipole state at $E = 9.71$ MeV in ^{60}Ni. Included are the contributions (in % in the second column) of the dominant configurations to the total sum of FTRRPA amplitudes: $\sum_{mi}(X_{mi}^2 - Y_{mi}^2)(n_i - n_m)$.

$\nu 2p_{3/2} \to \nu 2d_{5/2}$	45.87
$\nu 1f_{5/2} \to \nu 2d_{3/2}$	13.92
$\nu 2p_{3/2} \to \nu 3s_{1/2}$	8.43
$\nu 1f_{7/2} \to \nu 1g_{9/2}$	3.58
$\nu 2p_{1/2} \to \nu 2d_{3/2}$	1.30
$\pi 2p_{3/2} \to \pi 2d_{3/2}$	7.89
$\pi 2p_{3/2} \to \pi 2d_{5/2}$	6.32
$\pi 1f_{5/2} \to \pi 2d_{3/2}$	3.62
$\pi 1f_{7/2} \to \pi 1g_{9/2}$	1.21

Same as in Table 1, but for the dipole states at 9.78 and 10.03 MeV in ^{62}Ni.

$E = 9.78$ MeV	
$\pi 2p_{3/2} \to \pi 2d_{5/2}$	48.02
$\pi 1f_{5/2} \to \pi 2d_{3/2}$	20.99
$\pi 2p_{3/2} \to \pi 3s_{1/2}$	3.12
$\nu 2p_{3/2} \to \nu 2d_{5/2}$	17.06
$\nu 1f_{5/2} \to \nu 2d_{3/2}$	4.36
$\nu 1f_{7/2} \to \nu 1g_{9/2}$	1.22
$E = 10.03$ MeV	
$\nu 2p_{3/2} \to \nu 2d_{5/2}$	26.55
$\nu 2p_{3/2} \to \nu 3s_{1/2}$	3.59
$\pi 1f_{5/2} \to \pi 2d_{3/2}$	63.60
$\pi 2p_{3/2} \to \pi 2d_{5/2}$	2.55



Nuclear Energy Density Functional Framework

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✔ unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.

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