Relativistic Energy Density Functionals:
Beyond the mean-field approximation

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

Kohn-Sham Density Functional Theory

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

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

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

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**.

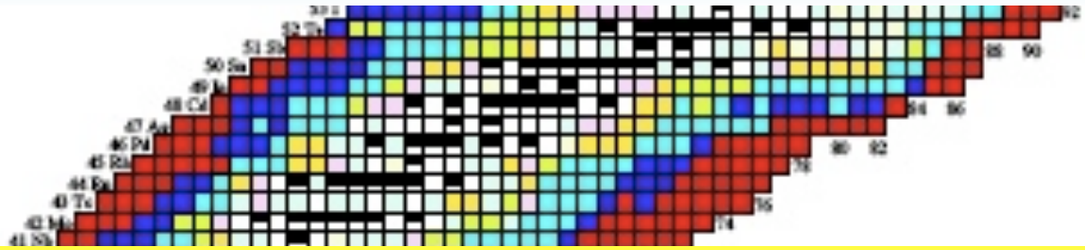
$$v_{xc}[\rho(\mathbf{r})] = \frac{\delta E_{xc}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})}$$

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

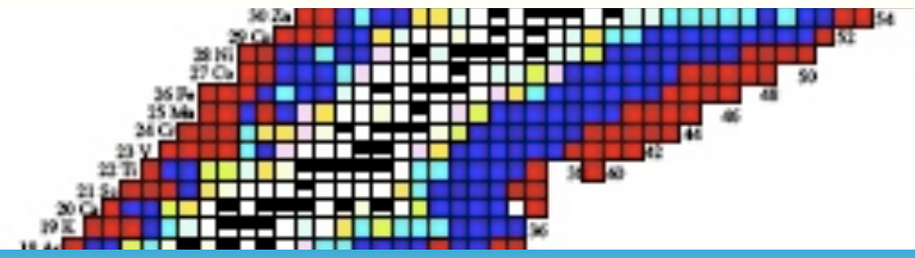
The exact density functional is approximated with **powers and gradients of ground-state nucleon densities and currents.**

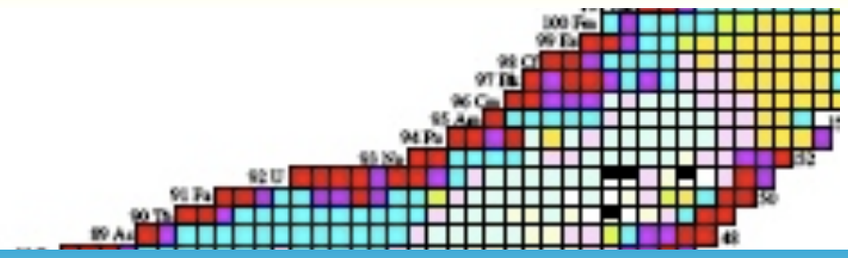
Relativistic Energy Density Functionals

✔ natural inclusion of the **spin degree of freedom** (spin-orbit potential with empirical strength)

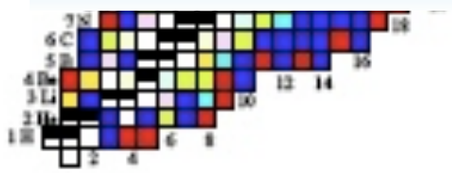


✔ unique parameterization of **time-odd components** (currents) of the nuclear mean-field





✔ 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.

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.

Effective Lagrangian:

$$
\begin{aligned}
\mathcal{L} \;=\; & \bar{\psi}(i\gamma\cdot\partial - m)\psi \\
& -\frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\
& -\frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\
& -\frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma\cdot A\frac{(1-\tau_3)}{2}\psi
\end{aligned}
$$

$$
\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} \qquad (i \equiv S, V, TV) \qquad x = \rho/\rho_{sat}
$$

Hartree

correlations

Only one isovector term and one derivative term can be constrained by data.

Microscopic functionals

... universal 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-phenomenological 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

... 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 **a_v, a_s** and **a_4**, and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

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

The nuclear matter saturation density, compression modulus, and Dirac mass are kept fixed:

$$\rho_{sat} = 0.152 \text{ fm}^{-3}$$

$$m_D^* = m + \Sigma_S = 0.58m$$

$$K_{nm} = 230 \text{ MeV}$$

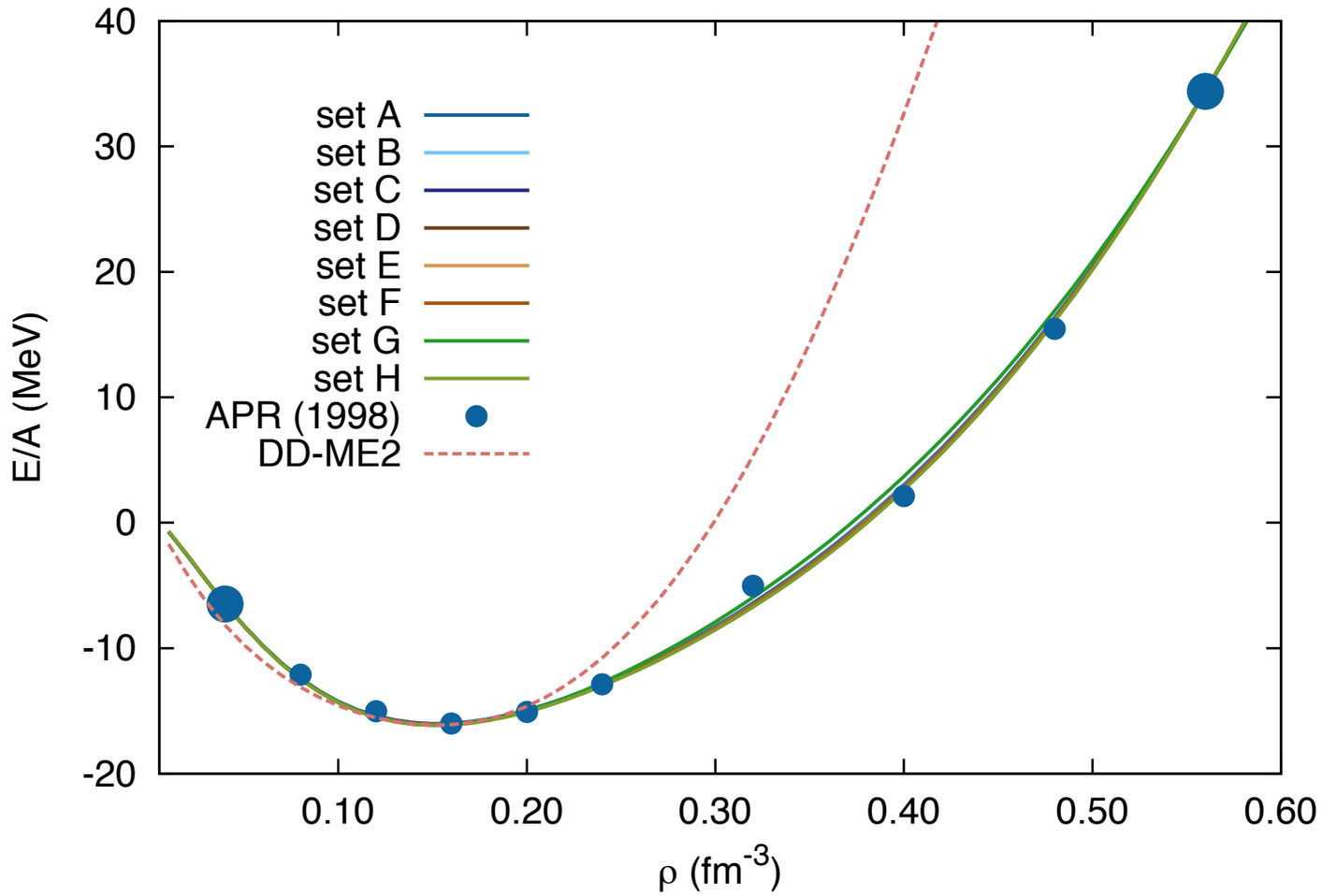
DD-ME1, DD-ME2

data on GMR

... plus two additional points on the microscopic EoS curve of Akmal, Pandharipande and Ravenhall:

$$\rho = 0.56 \text{ fm}^{-3} \quad E = 34.39 \text{ MeV}$$

$$\rho = 0.04 \text{ fm}^{-3} \quad E = -6.48 \text{ MeV}$$

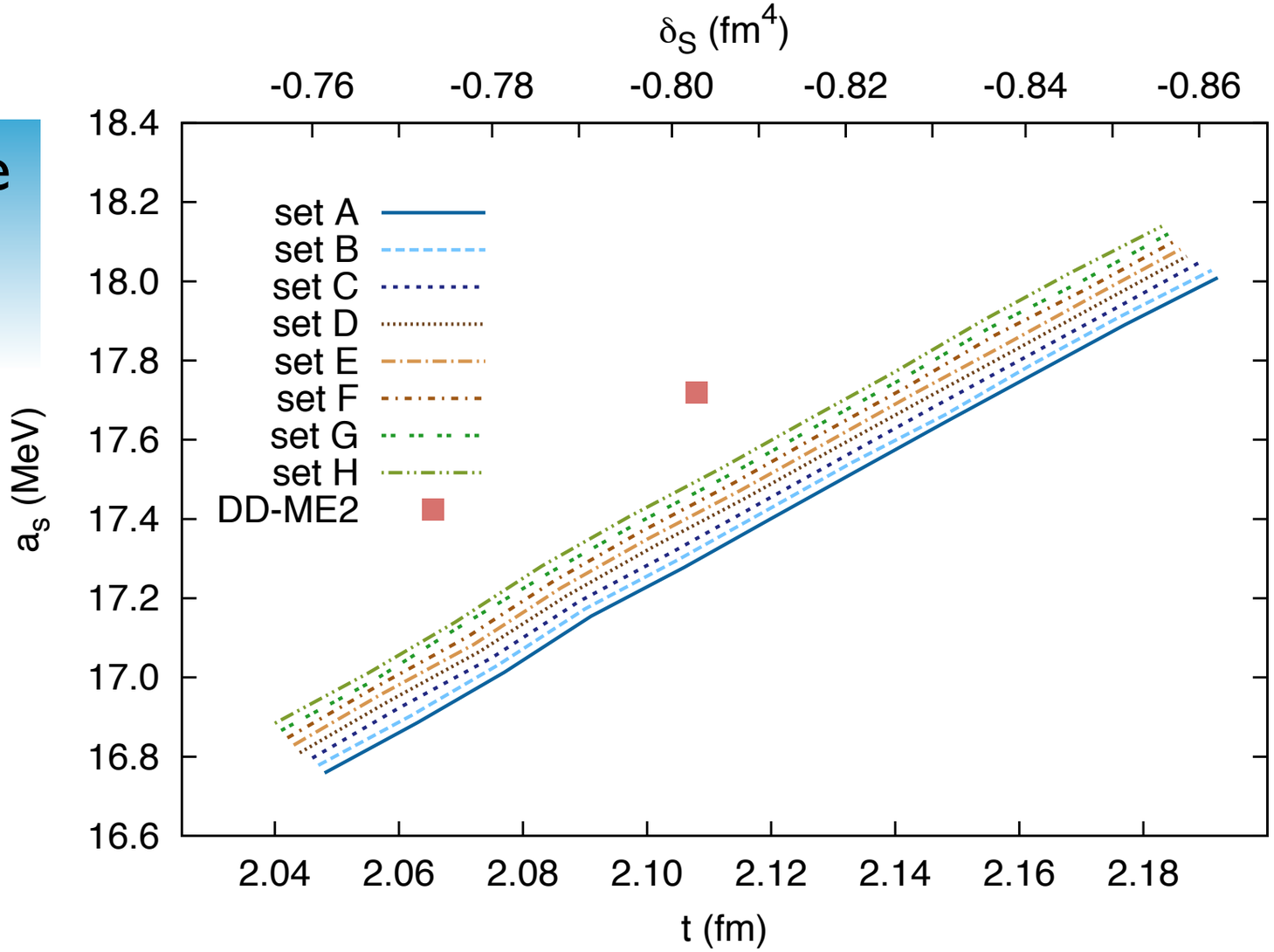


a_v = -16.02 (A), -16.04 (B), -16.06 (C), ...-16.14 (H) MeV

Isovector channel: $S_2(\rho) = a_4 + \frac{p_0}{\rho_{sat}^2}(\rho - \rho_{sat}) + \frac{\Delta K_0}{18\rho_{sat}^2}(\rho - \rho_{sat})^2 + \cdots$

... fix a_4 = 33 MeV and vary $S_2(\rho = 0.12\ \text{fm}^{-3})$

Surface energy of semi-infinite nuclear matter as a function of the surface thickness:



Deformed nuclei

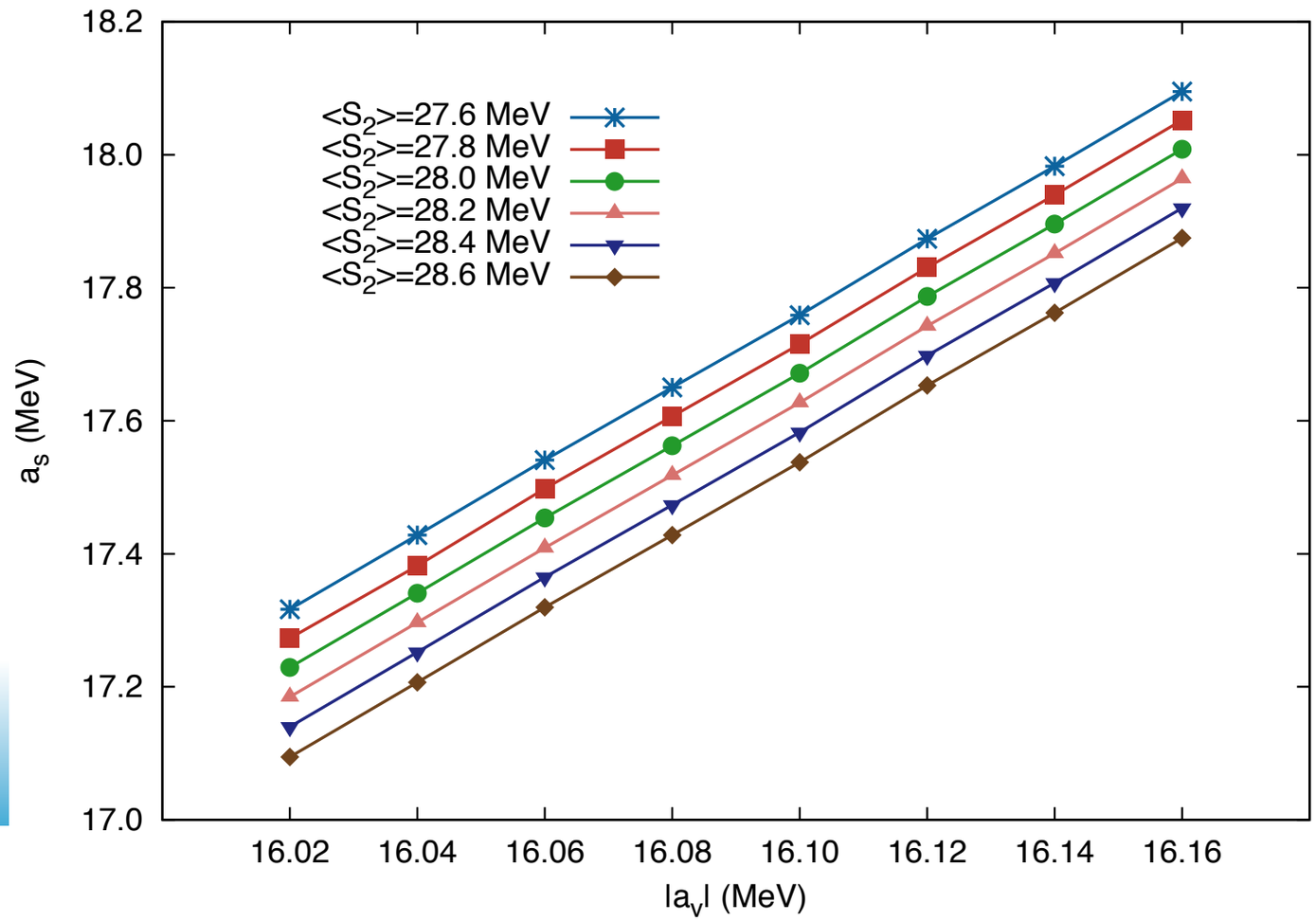
Binding energies used to adjust the parameters of the functional:

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

Pairing correlations:
BCS with empirical pairing gaps.

Surface energies of semi-infinite nuclear matter that minimize the deviation of the calculated binding energies from data.

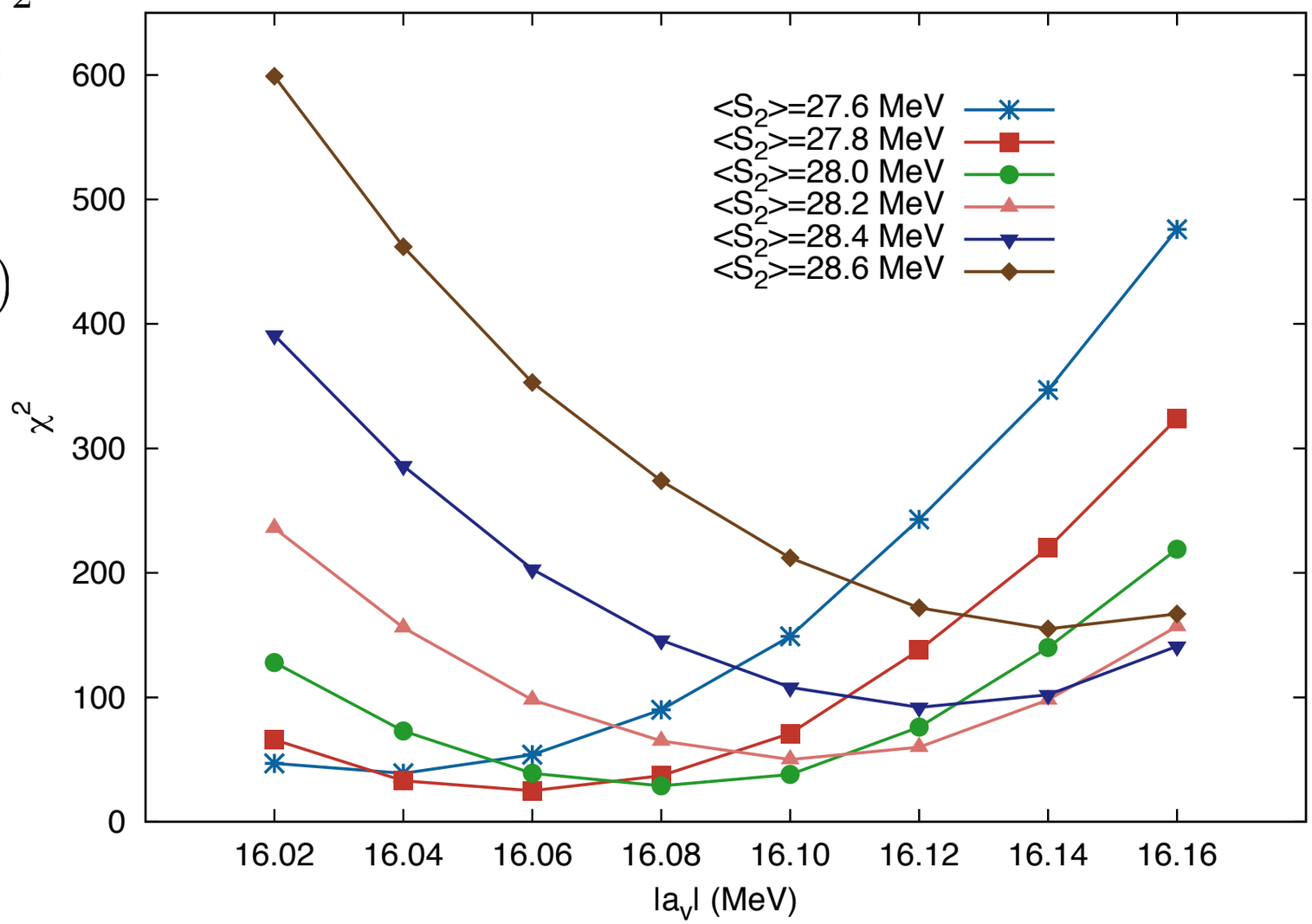
Required accuracy 0.05% ⇒ absolute error of ±1 MeV for the total binding energy



... 48 parameterizations of the energy density functional:

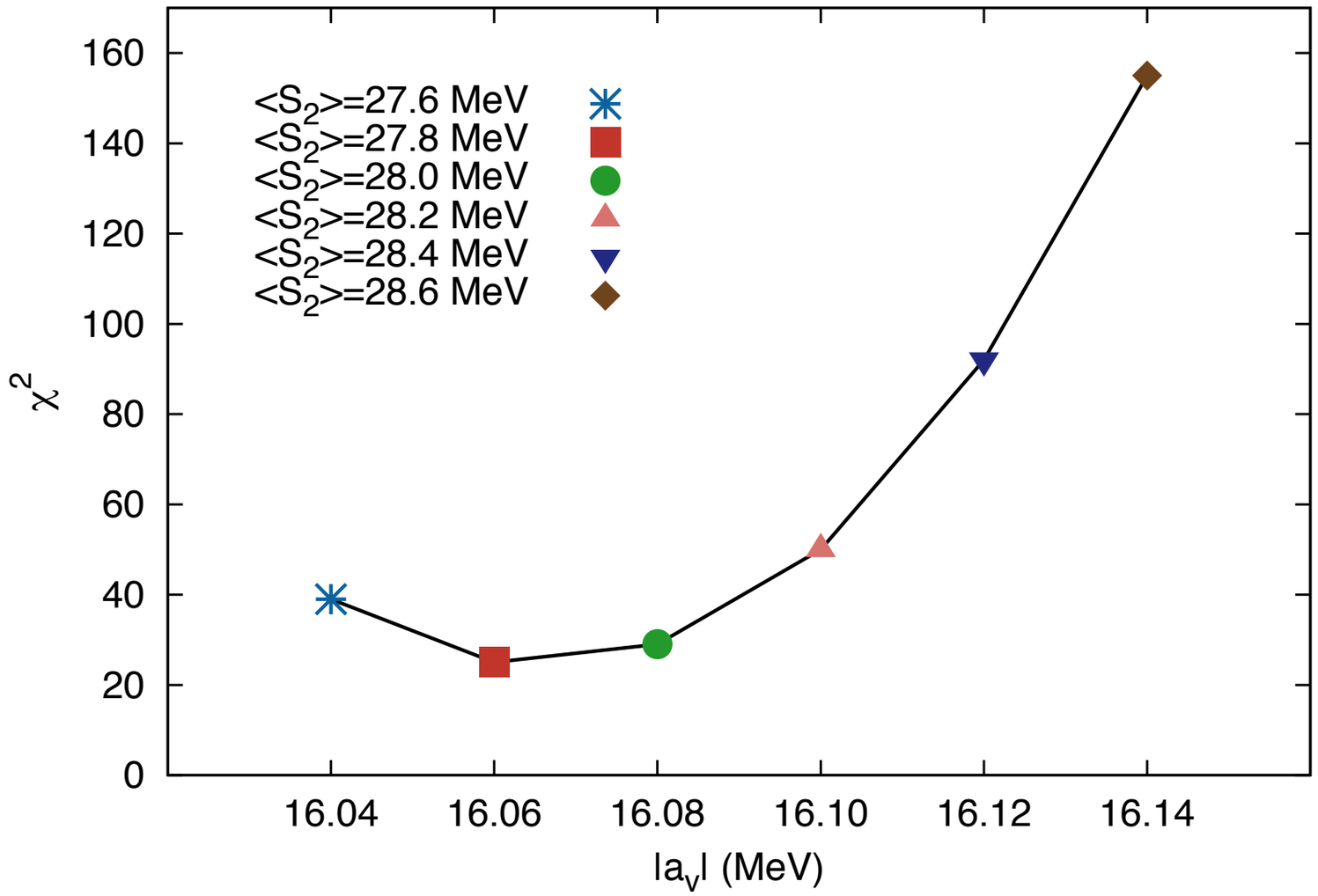
$$\chi^2 = \sum_i \left(\frac{E_B^{th}(i) - E_B^{exp}(i)}{\Delta E_B^{exp}(i)} \right)^2$$

$$\Delta E_B^{exp}(i) = 0.0005 \; E_B^{exp}(i)$$



For each value $\langle S_2 \rangle$ of the symmetry energy, there is a unique combination of volume and surface energies that minimizes χ^2.

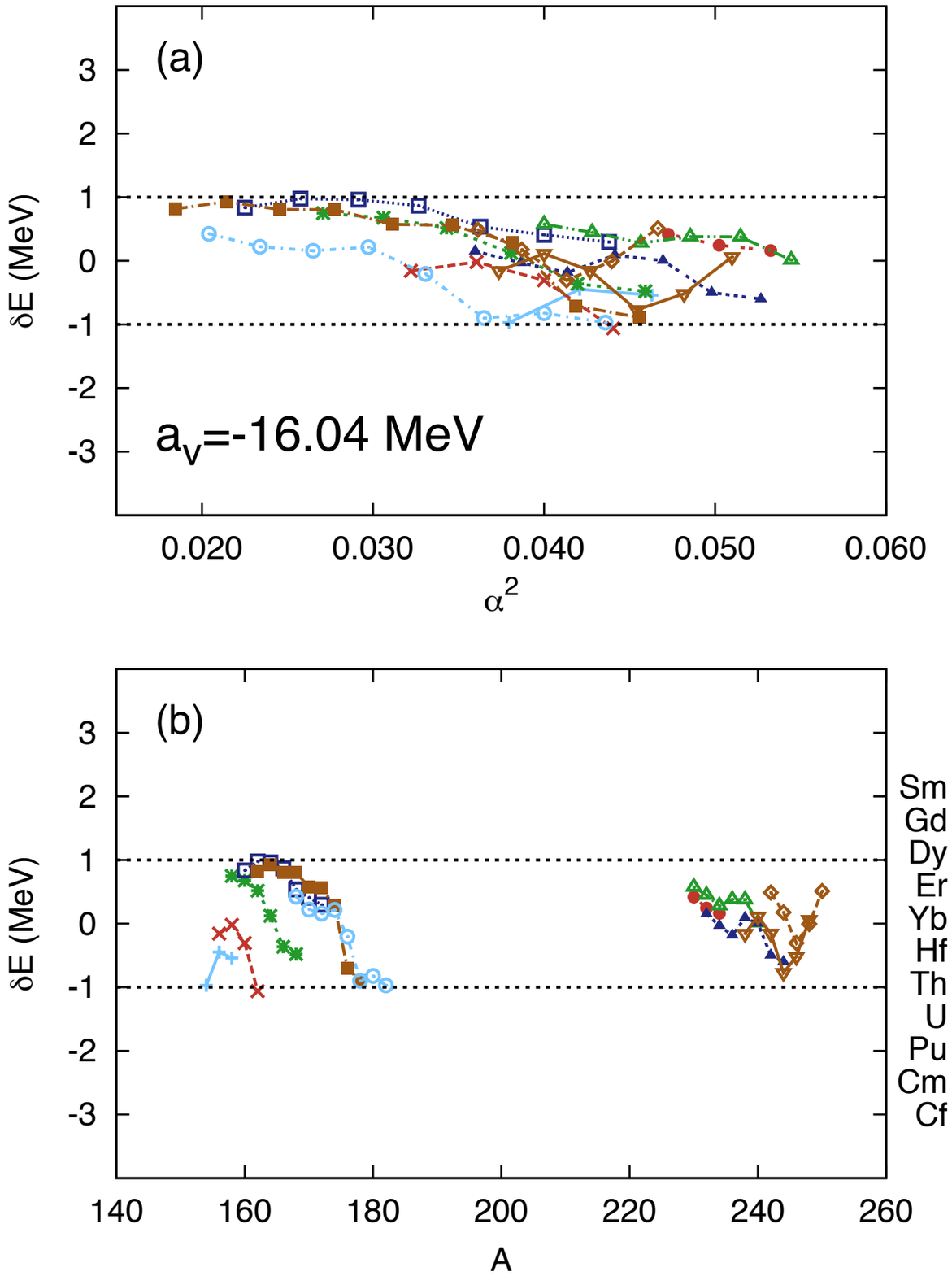
The minimum χ^2-deviation of the theoretical binding energies from data, as a function of the volume energy coefficient:

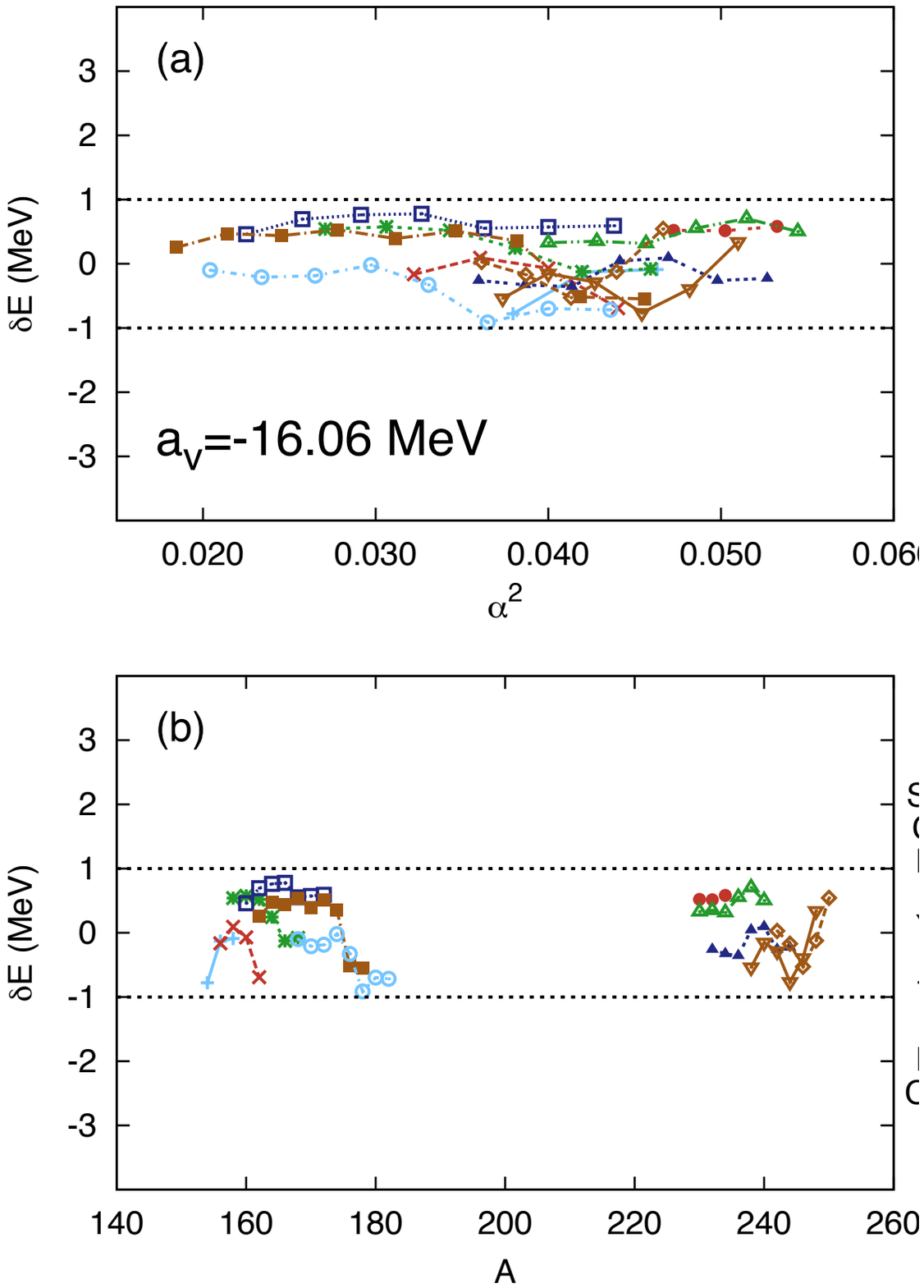


Absolute minimum:

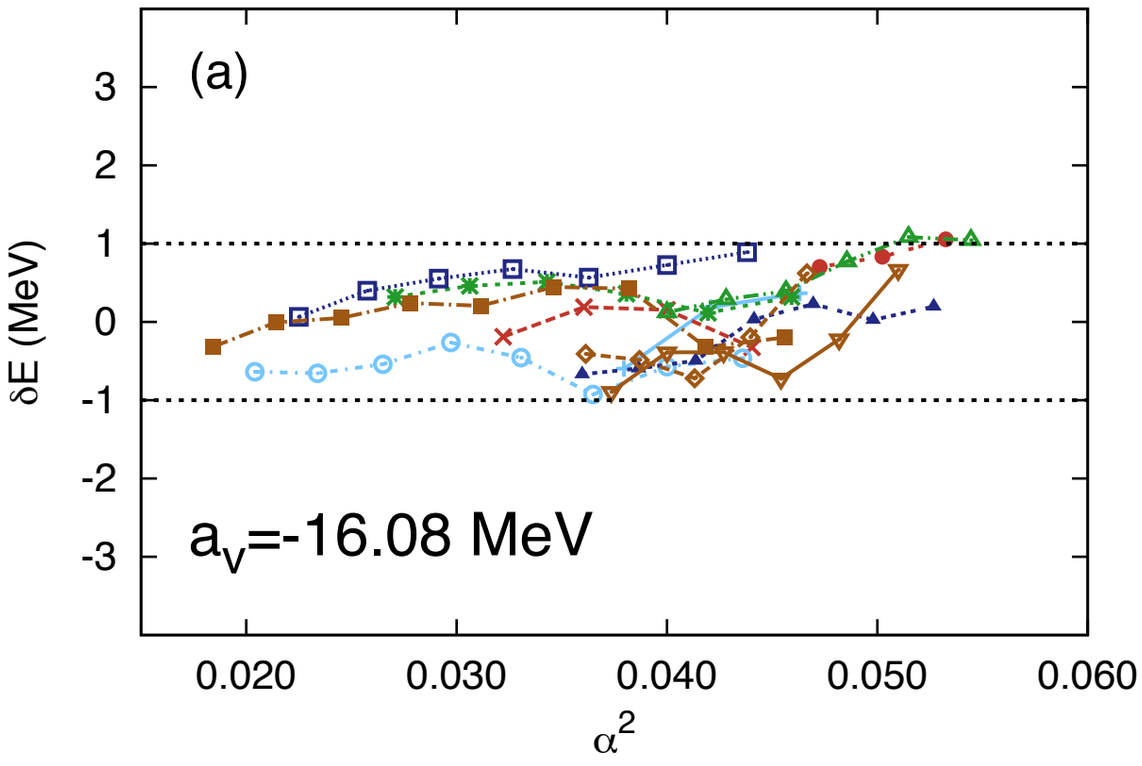
$$a_v = -16.06 \text{ MeV} \quad \langle S_2 \rangle = 27.8 \text{ MeV} \quad a_s = 17.498 \text{ MeV}$$

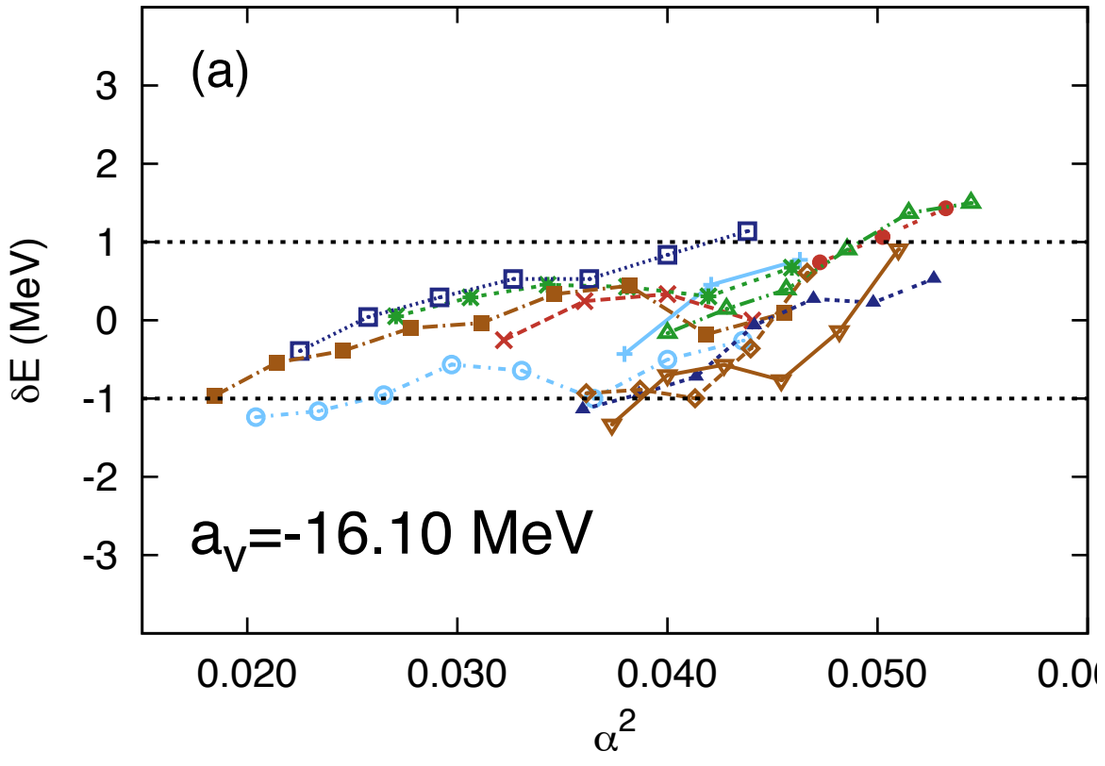
Absolute deviations of the calculated binding energies from data for 64 axially deformed nuclei:

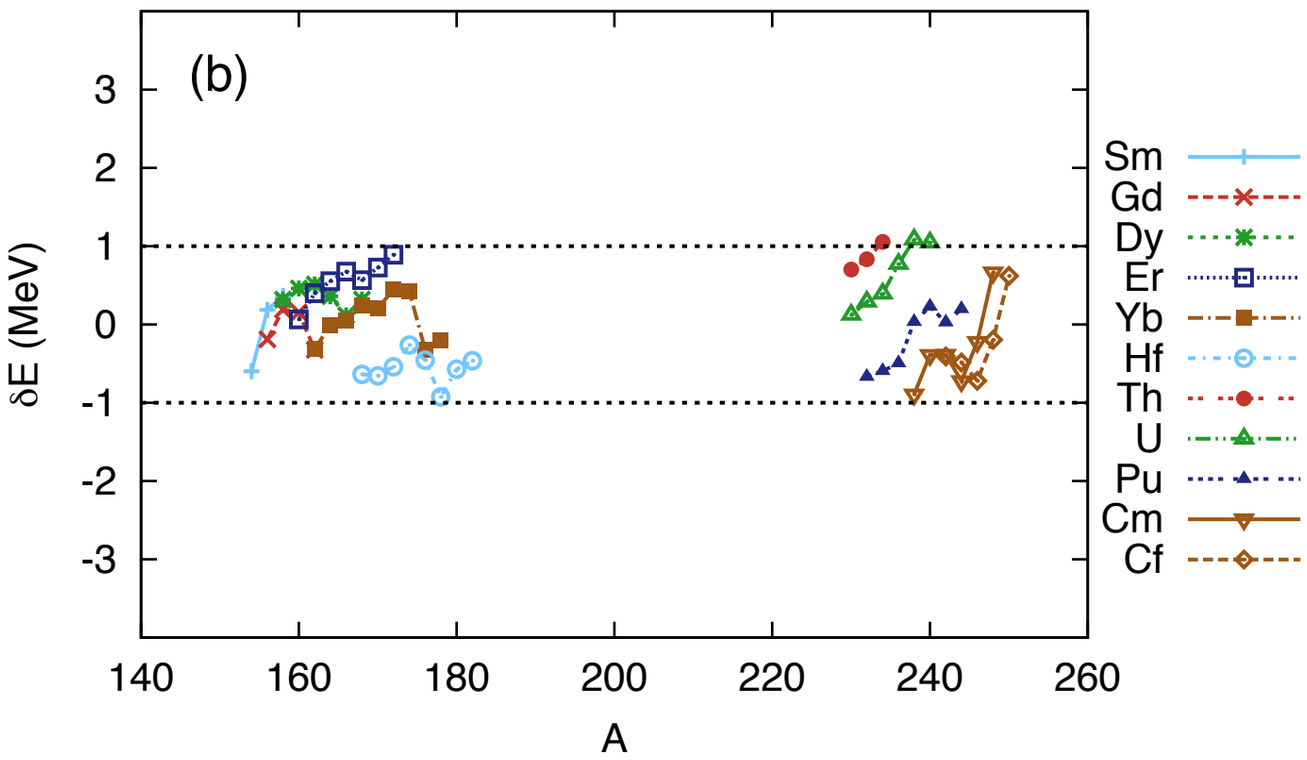


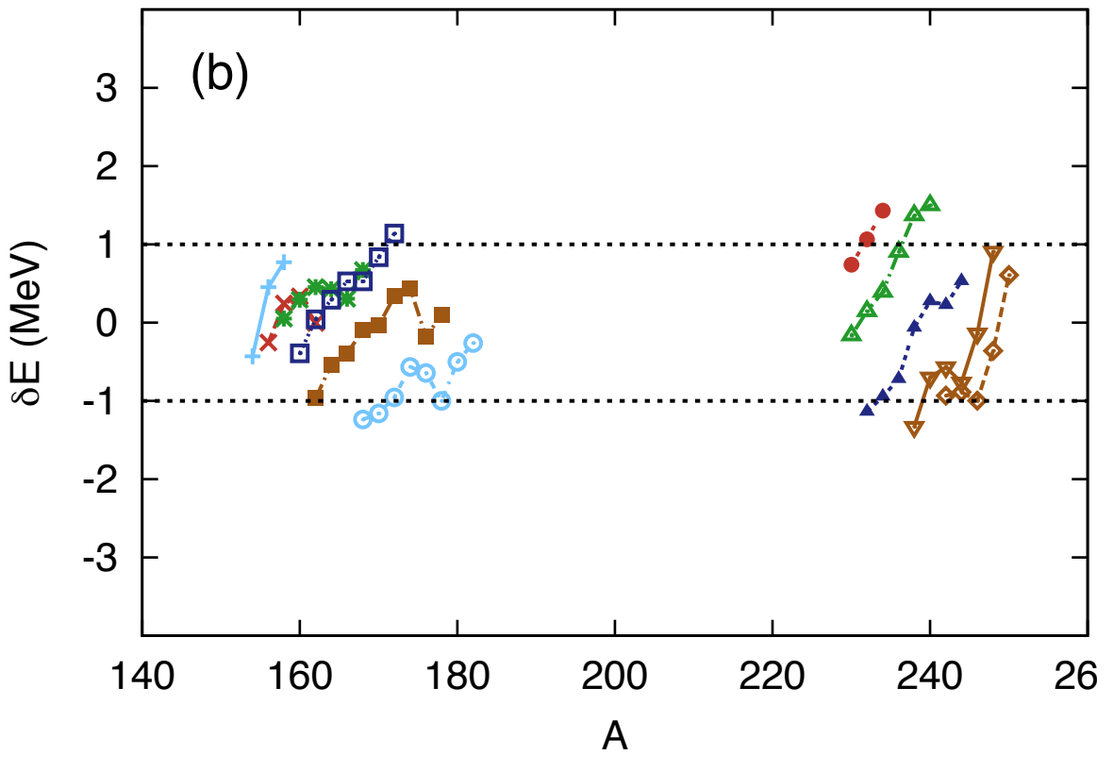


$$\alpha^2 = \frac{(N-Z)^2}{A^2}$$









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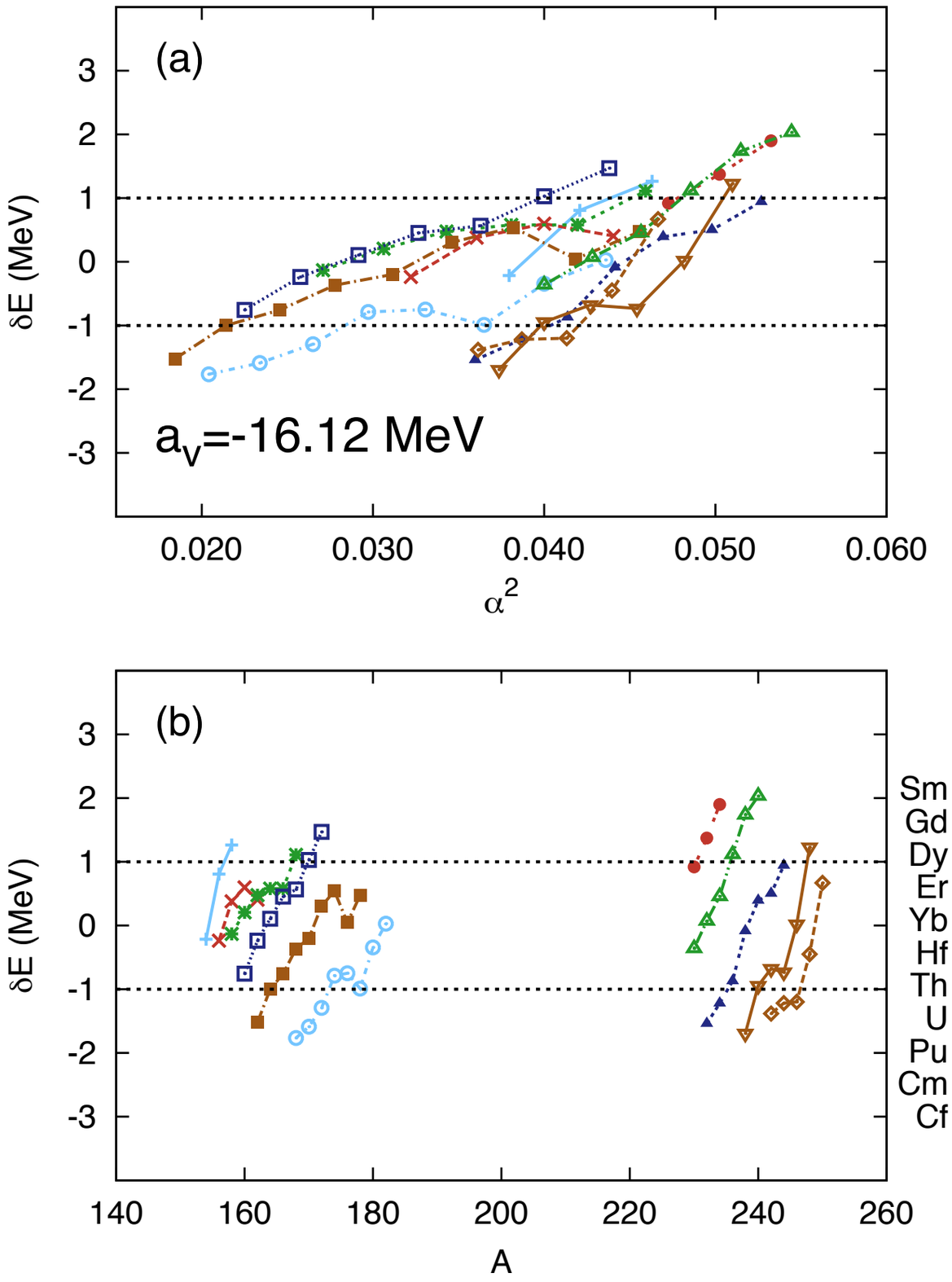
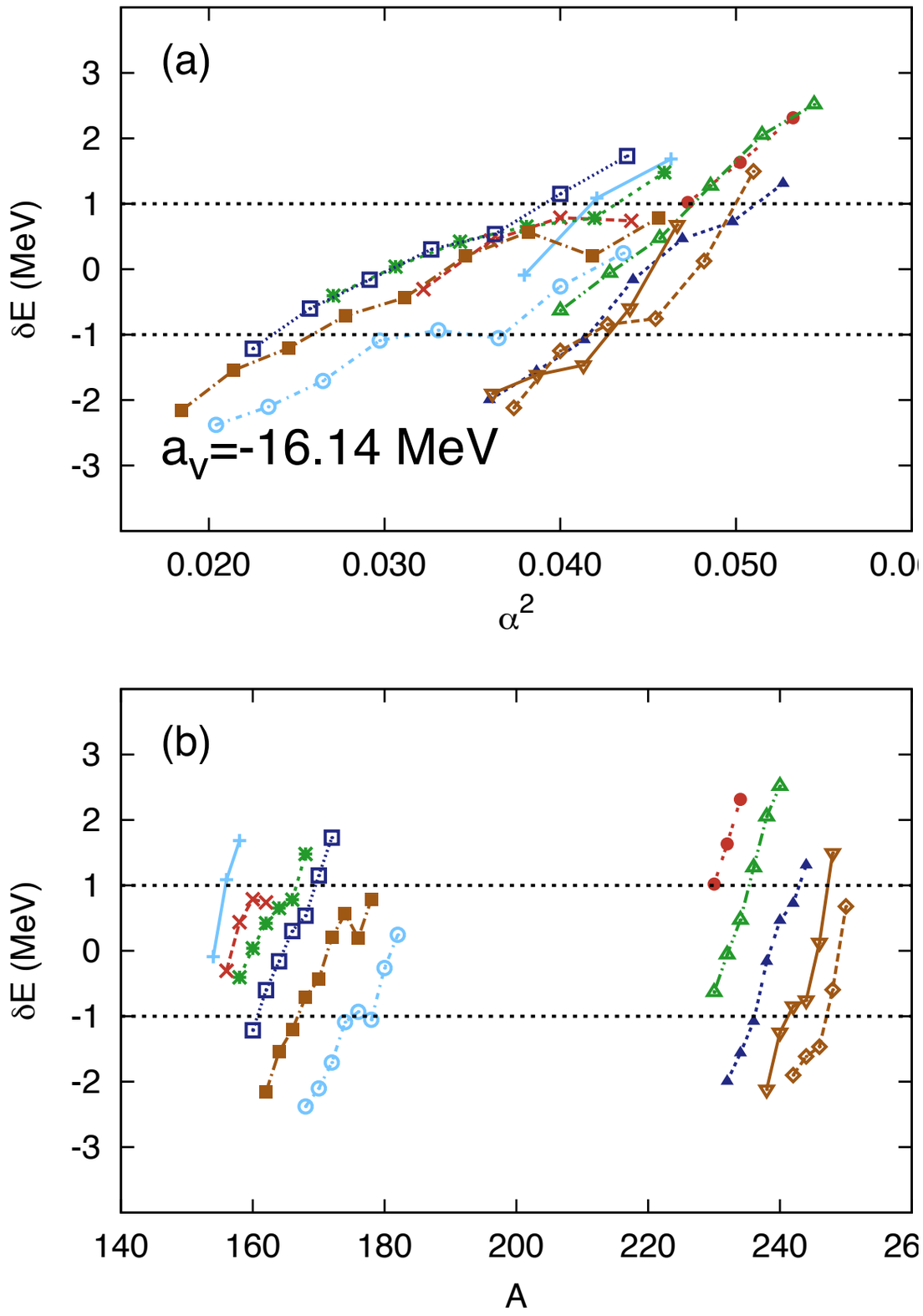




The calculated masses are very sensitive (isospin and mass dependence) to the choice of nuclear matter binding energy at saturation.

... not possible to determine the parameters of a density functional already at nuclear matter level, without additional adjustment to low-energy data on finite medium-heavy and heavy nuclei.

DD-PC1

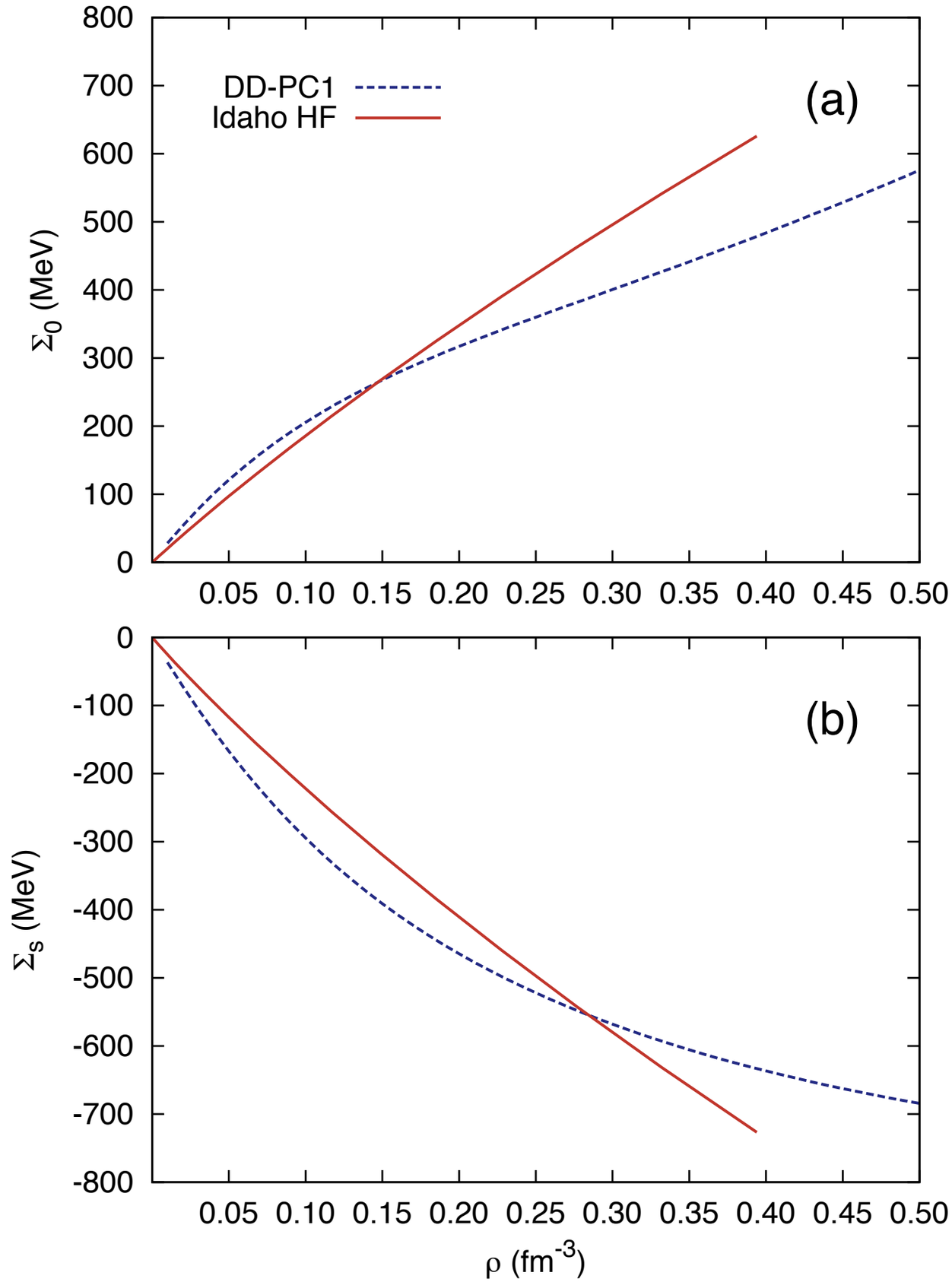
volume energy: $a_v = -16.06 \text{ MeV}$

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

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

The total number of parameters is 10.

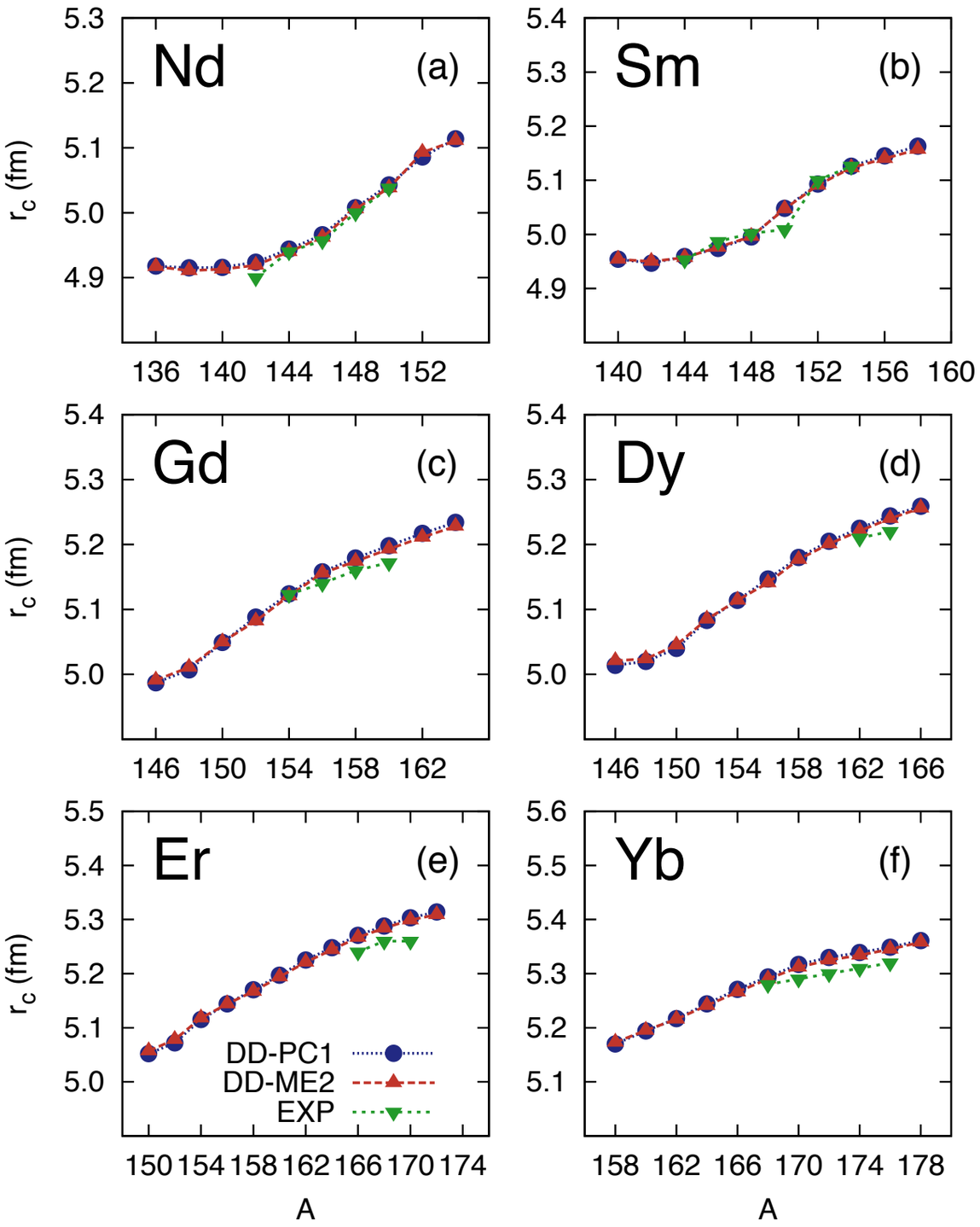
Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter, compared with the starting approximation:
the Hartree-Fock self-energies calculated from the Idaho N^3LO NN-potential.

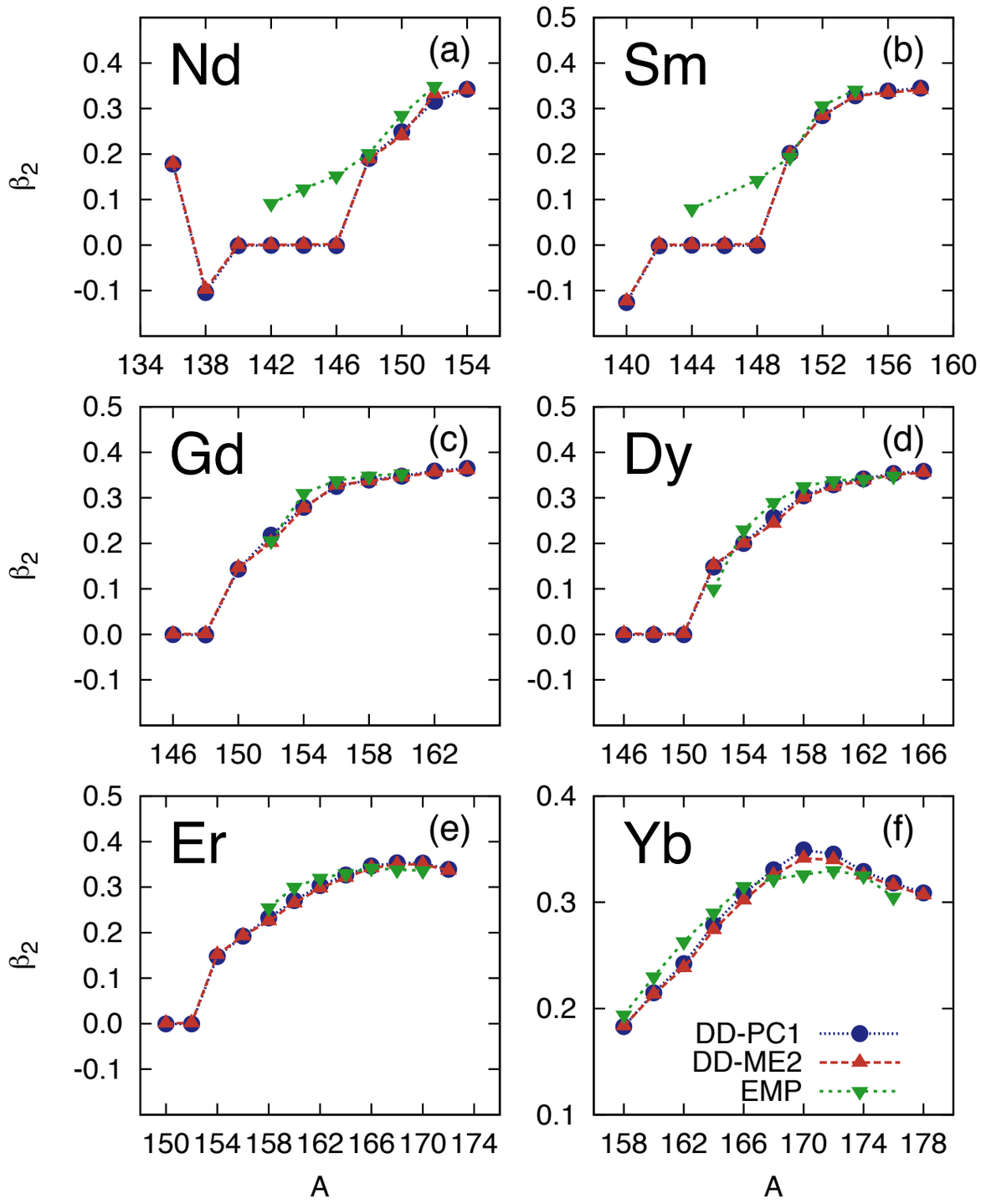


Illustrative calculations and predictions

Charge radii

Quadrupole deformations

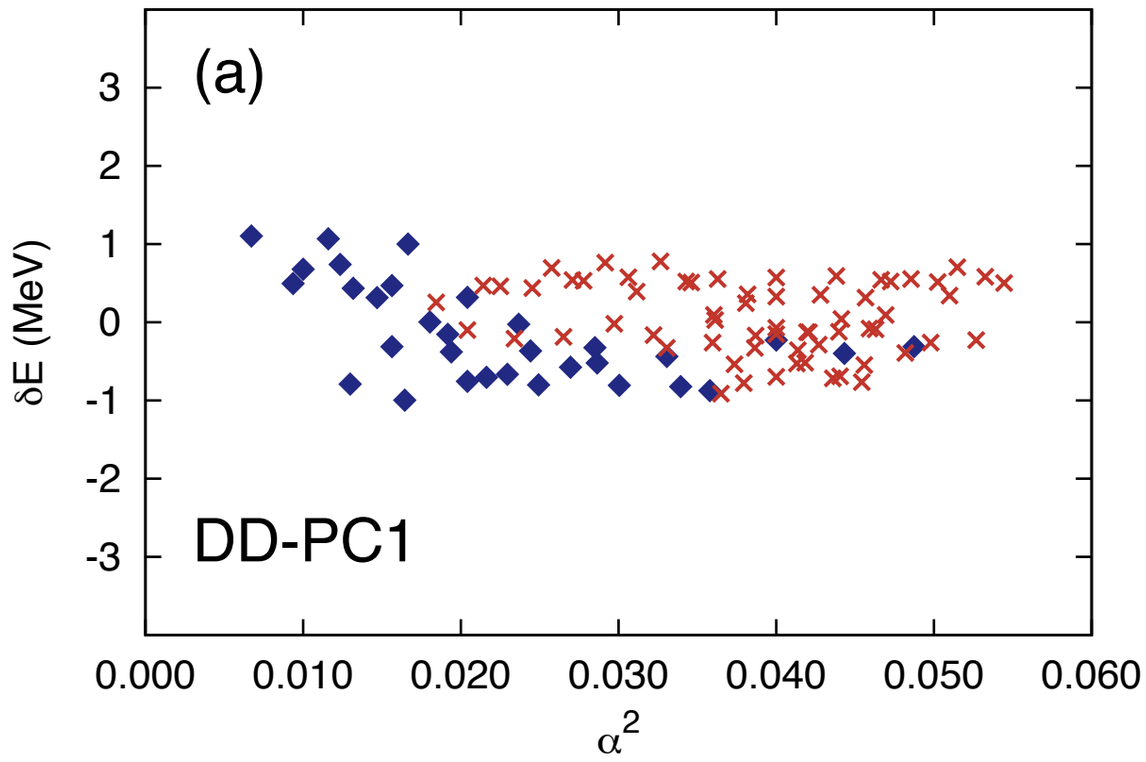


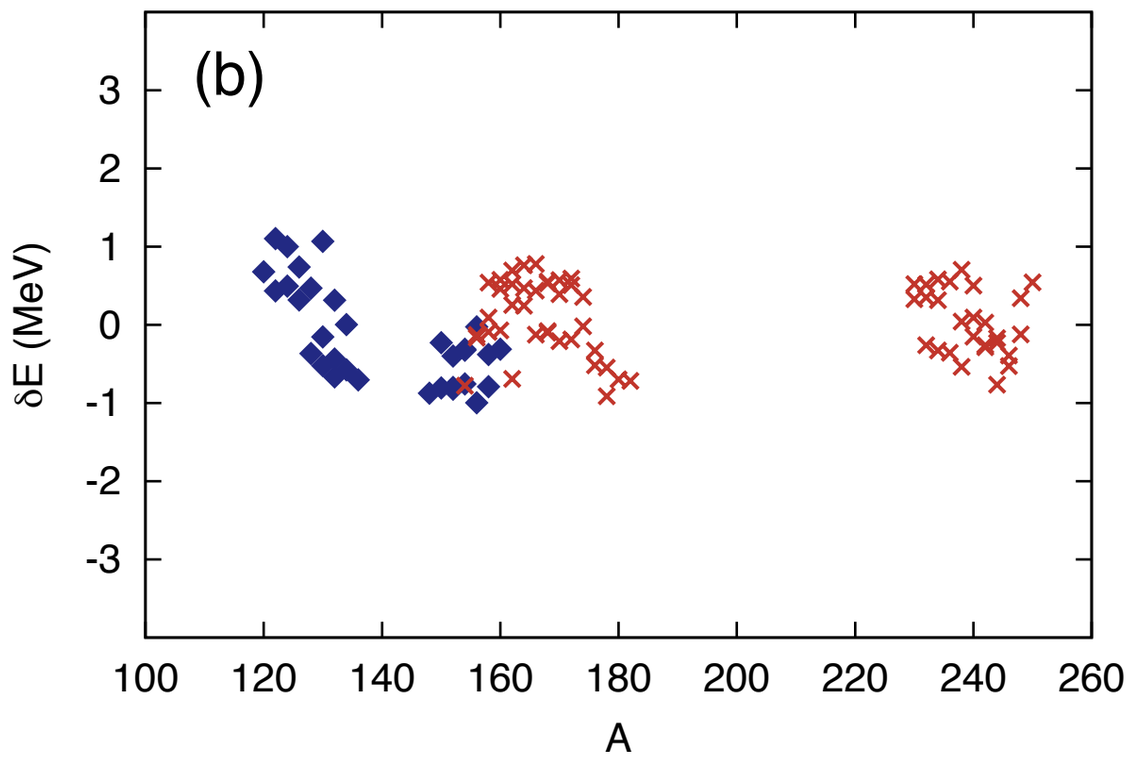


... calculated masses are extrapolated to a lower mass region not included in the fit and to lower values of the asymmetry parameter.

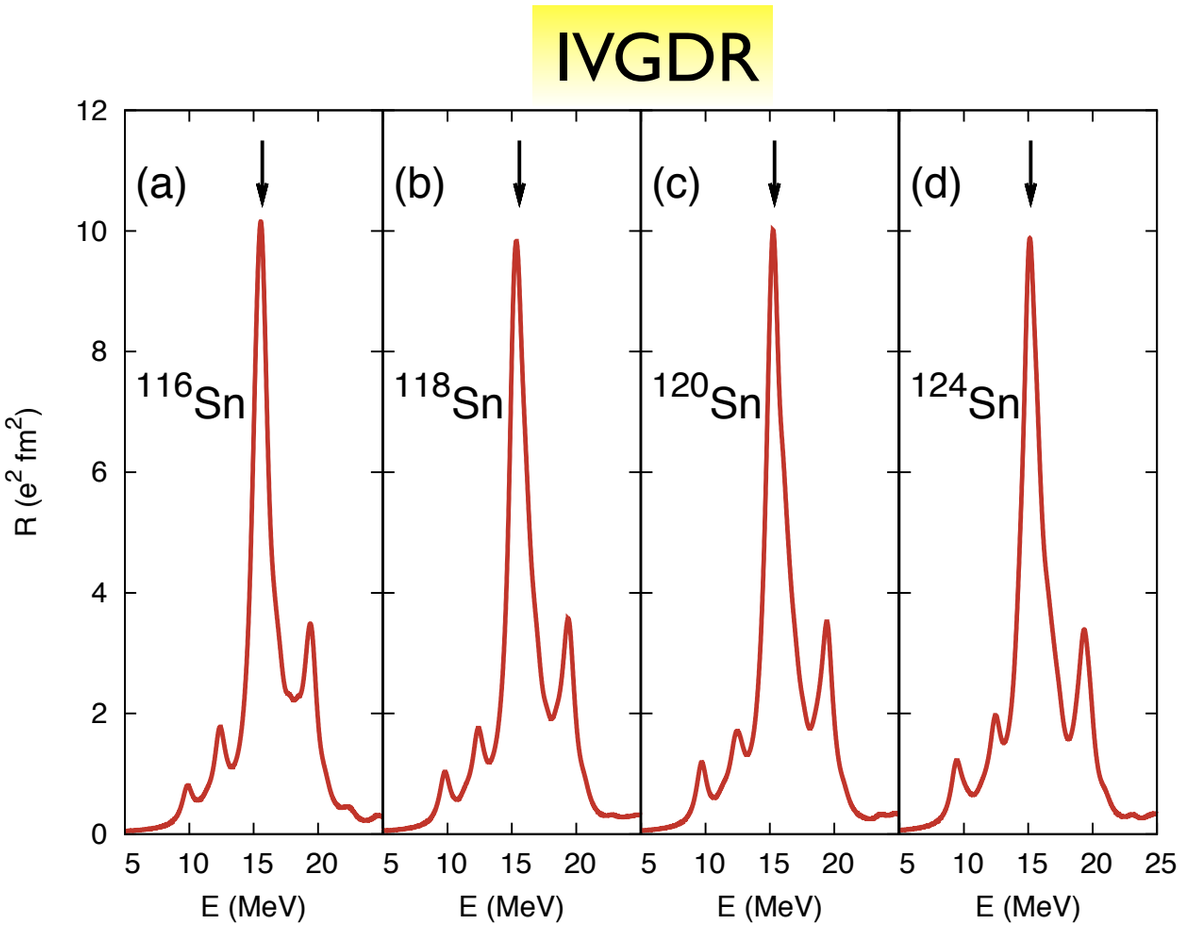
× fitted values

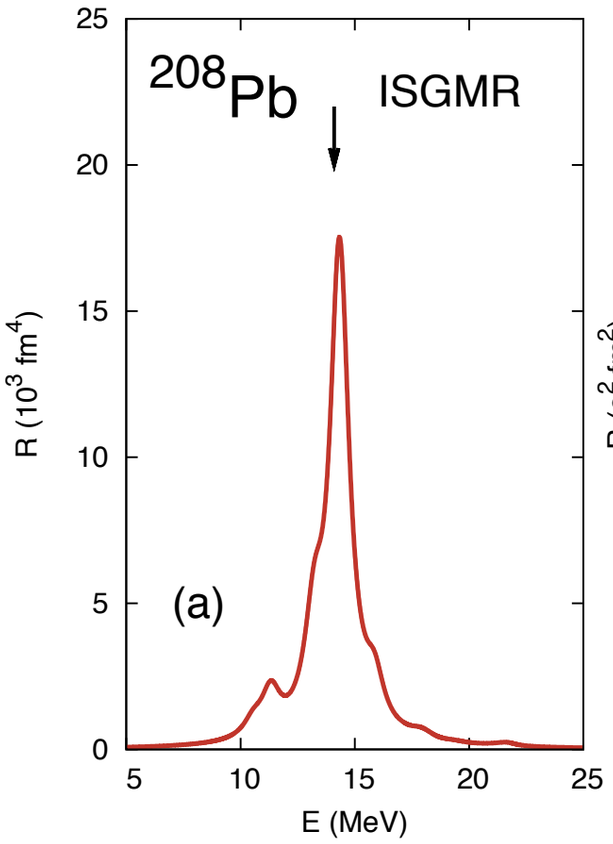
◆ extrapolated values

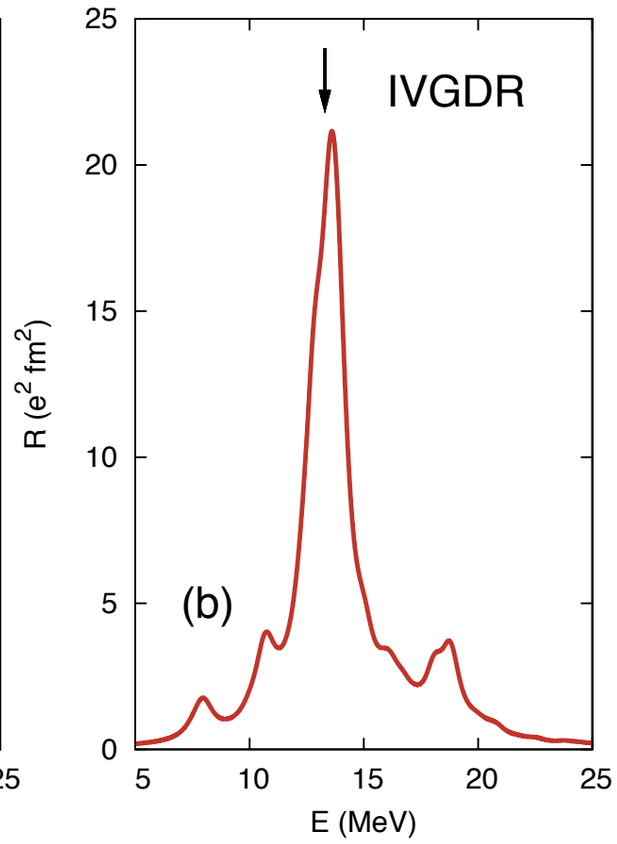




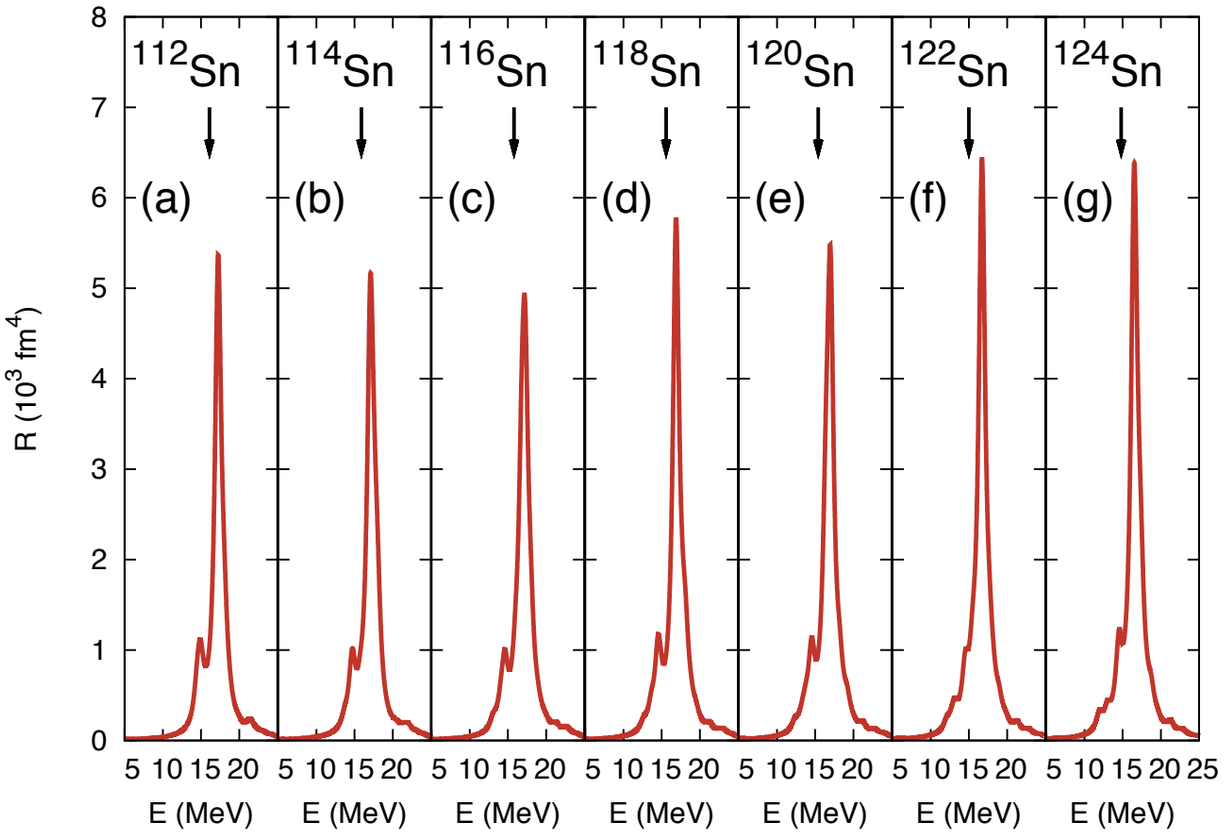
Excitation energies of collective modes:







ISGMR



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)

...vary smoothly with nucleon number!
Implicitly included in an effective EDF.

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

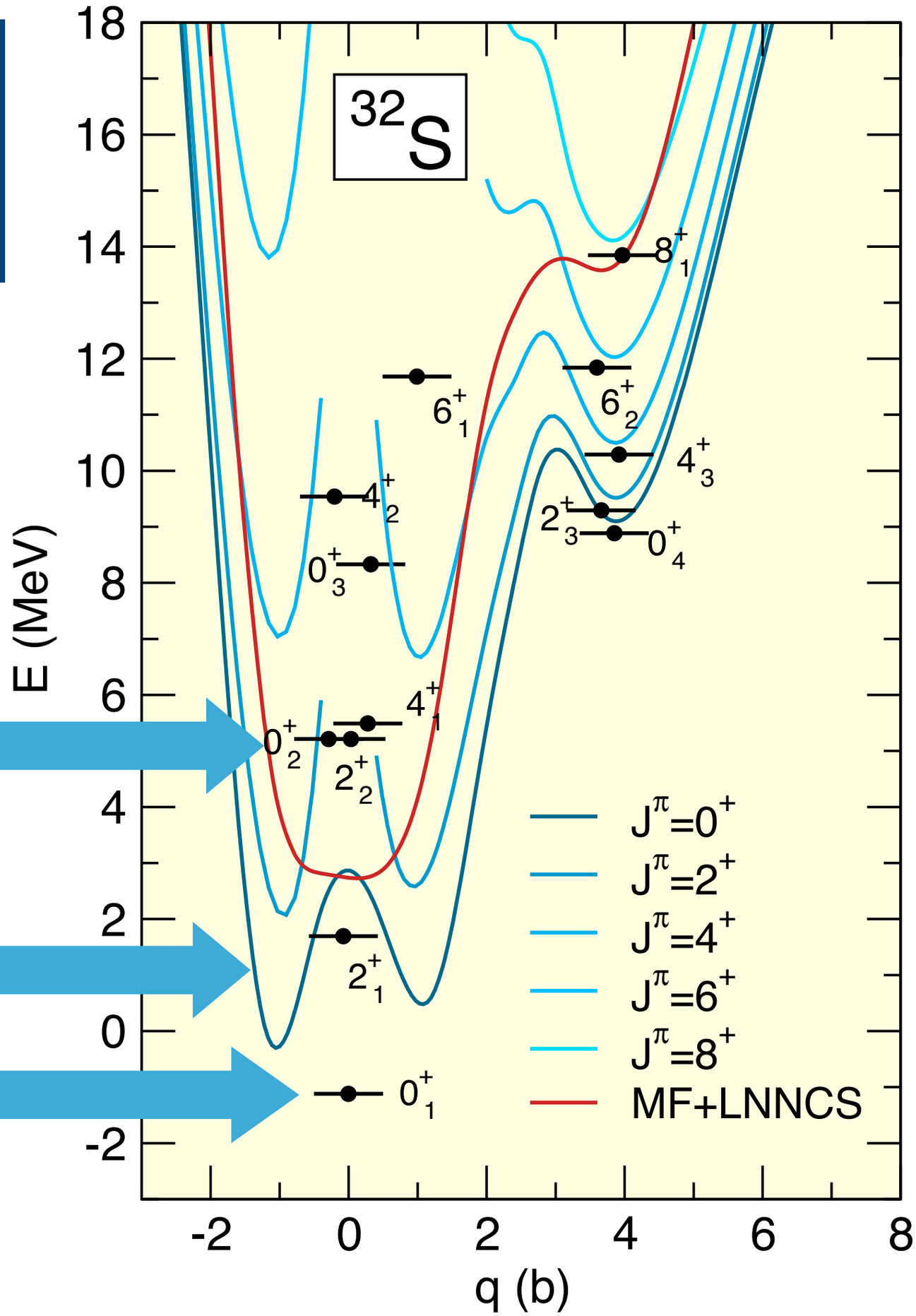
Restoration of broken symmetries (rotational, particle number) and fluctuations of collective variables (quadrupole deformation).

Nikšić, Vretenar, Ring
Phys. Rev. C **73**, 034308 (2006)
Phys. Rev. C **74**, 064309 (2006)

1. Mean-field calculations, with a constraint on the quadrupole moment.

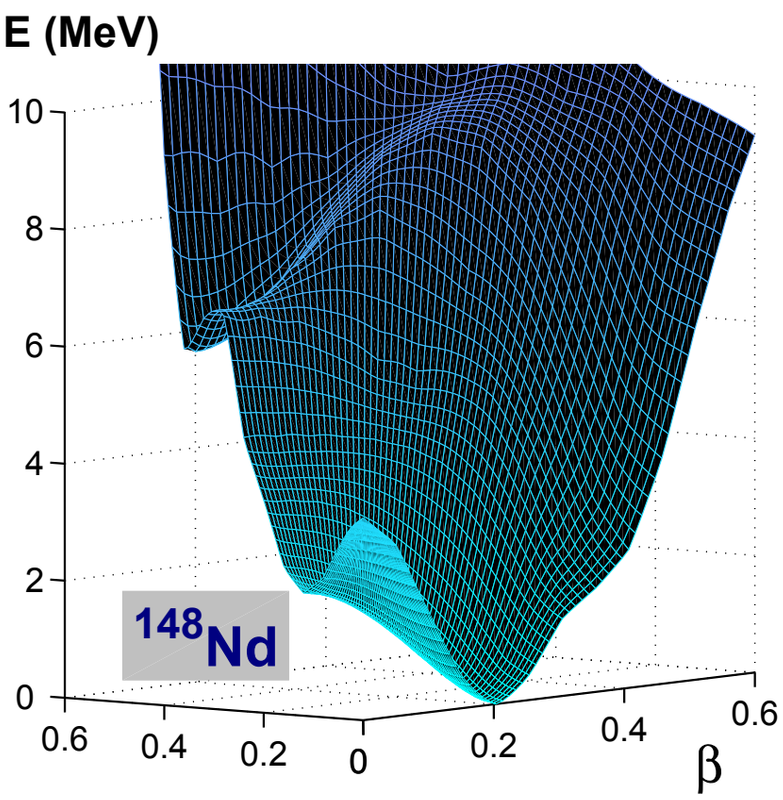
2. Angular-momentum and particle-number projection.

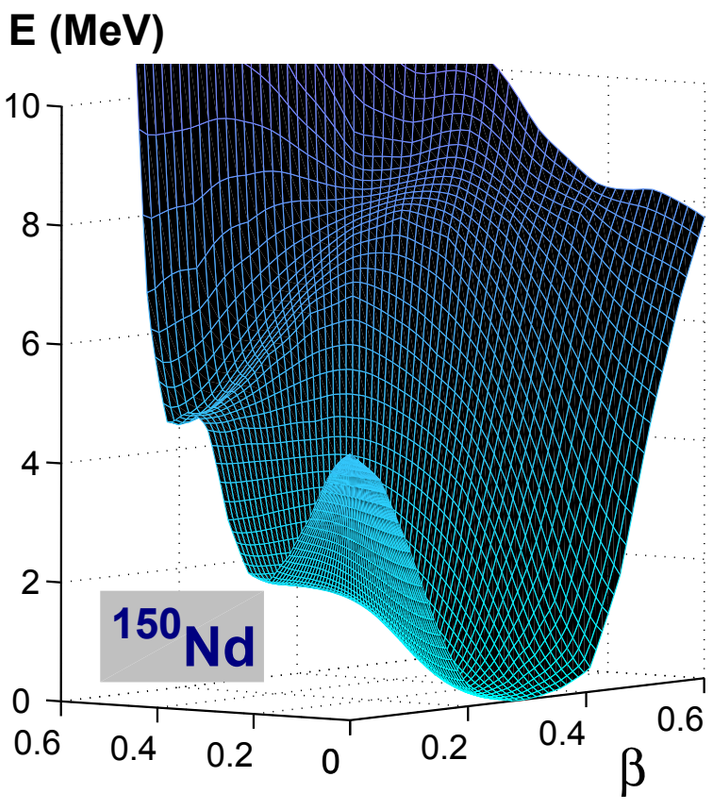
3. Generator Coordinate Method
⇒ configuration mixing

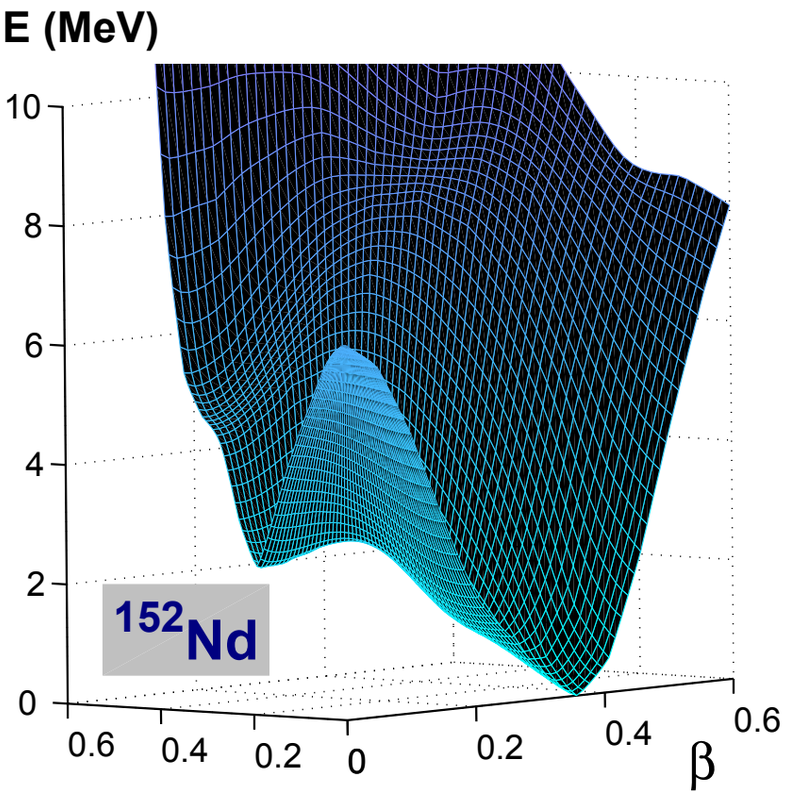


... larger variational space for projected GCM calculations!

triaxial shapes, breaking time-reversal invariance, different deformations for proton and neutron distributions, ...







Five-dimensional collective Hamiltonian

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

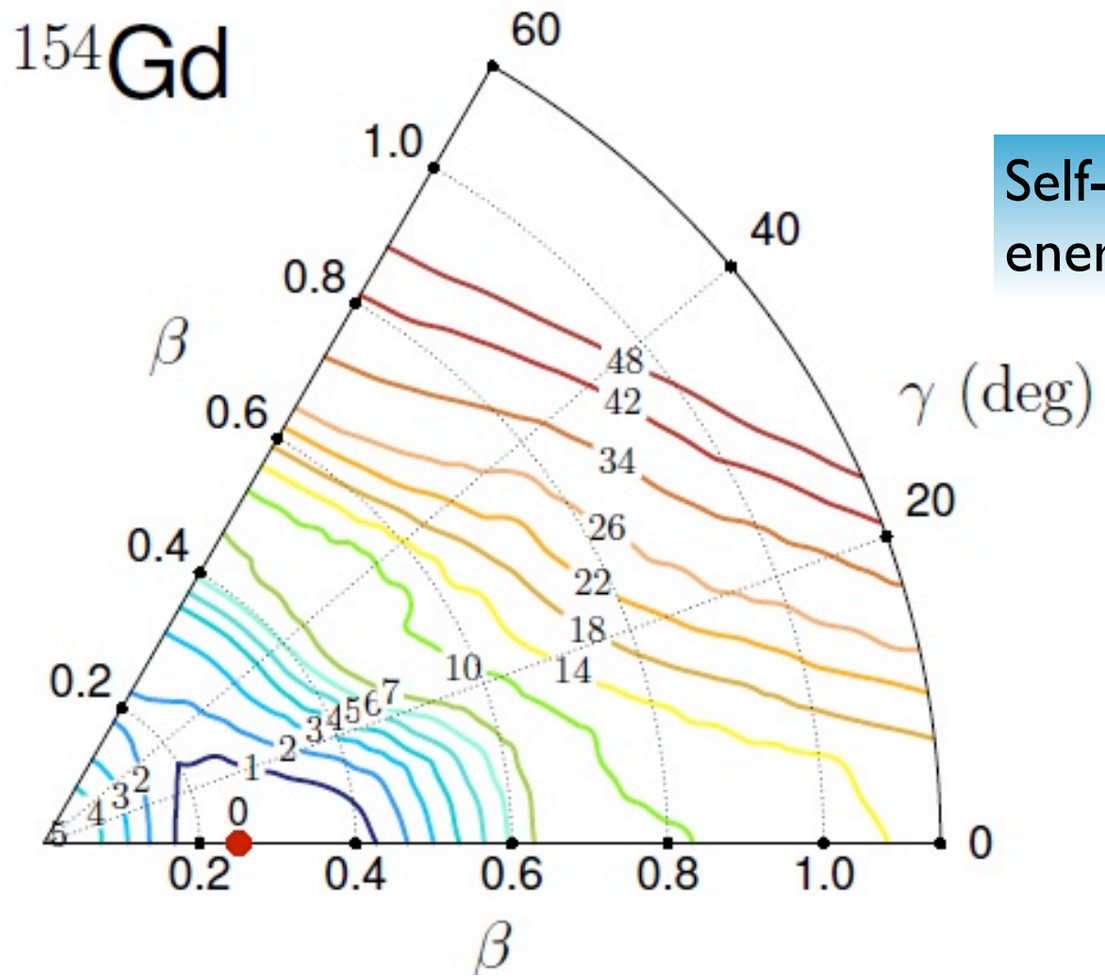
... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

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

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

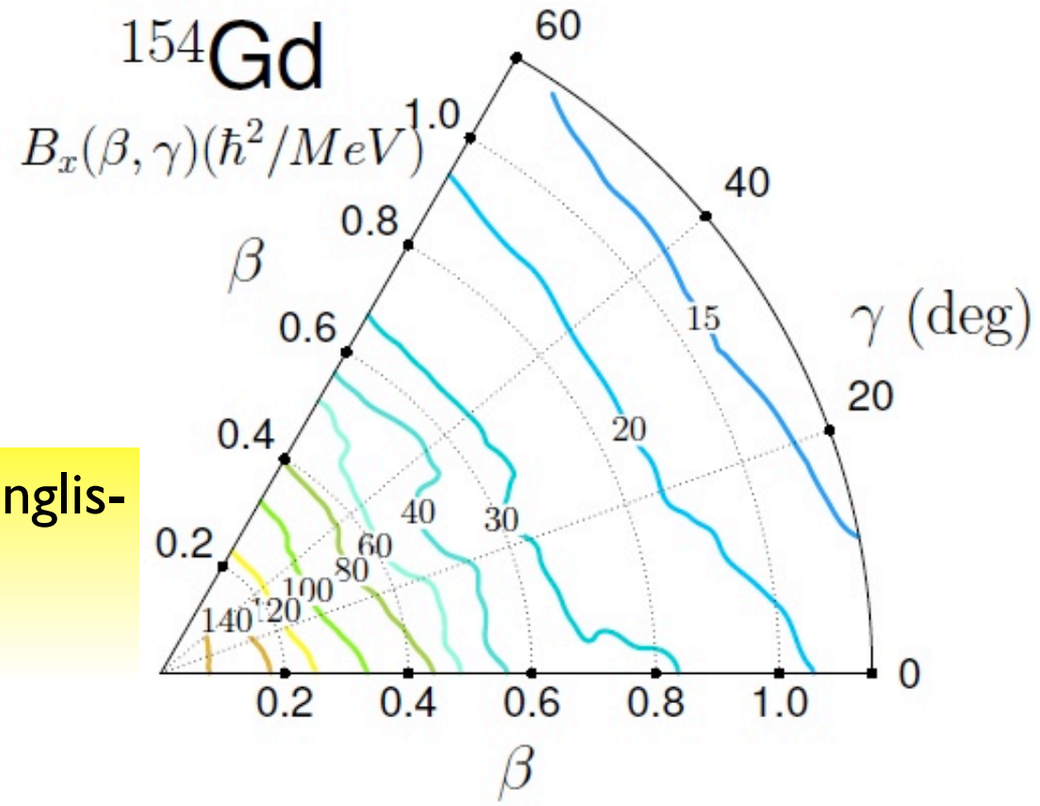
$$\mathcal{T}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

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.

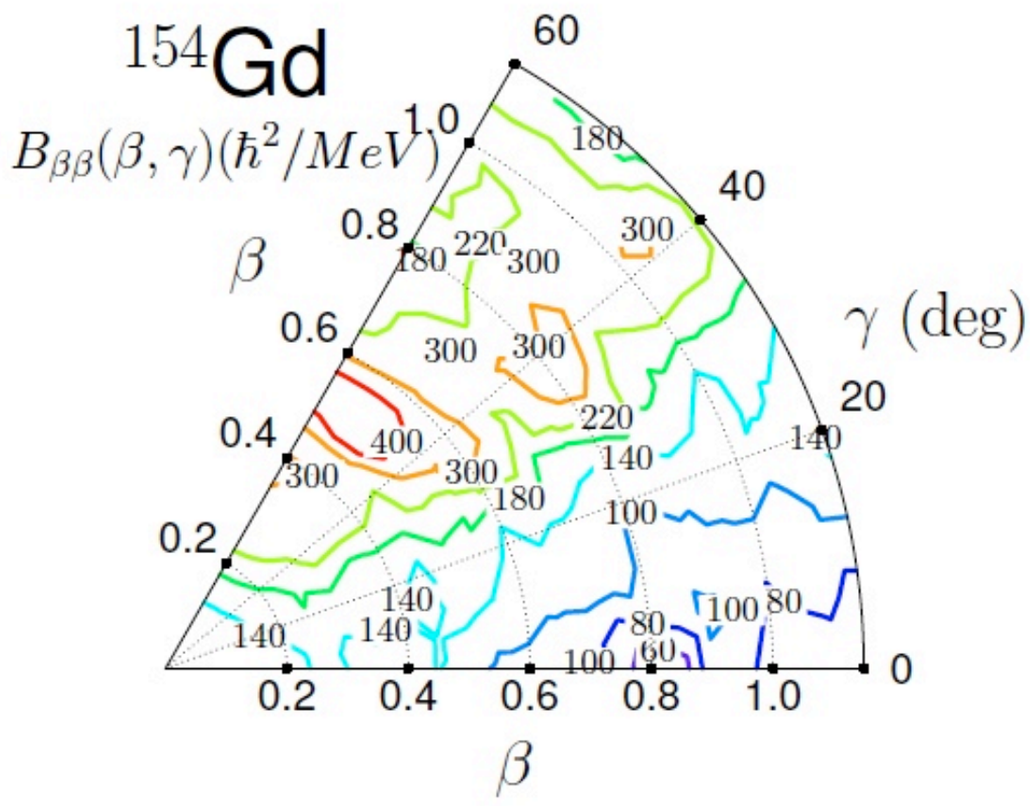


Self-consistent RMF+BCS triaxial quadrupole binding energy map of ^{154}Gd.

The cranking mass parameter $B_{\beta\beta}$

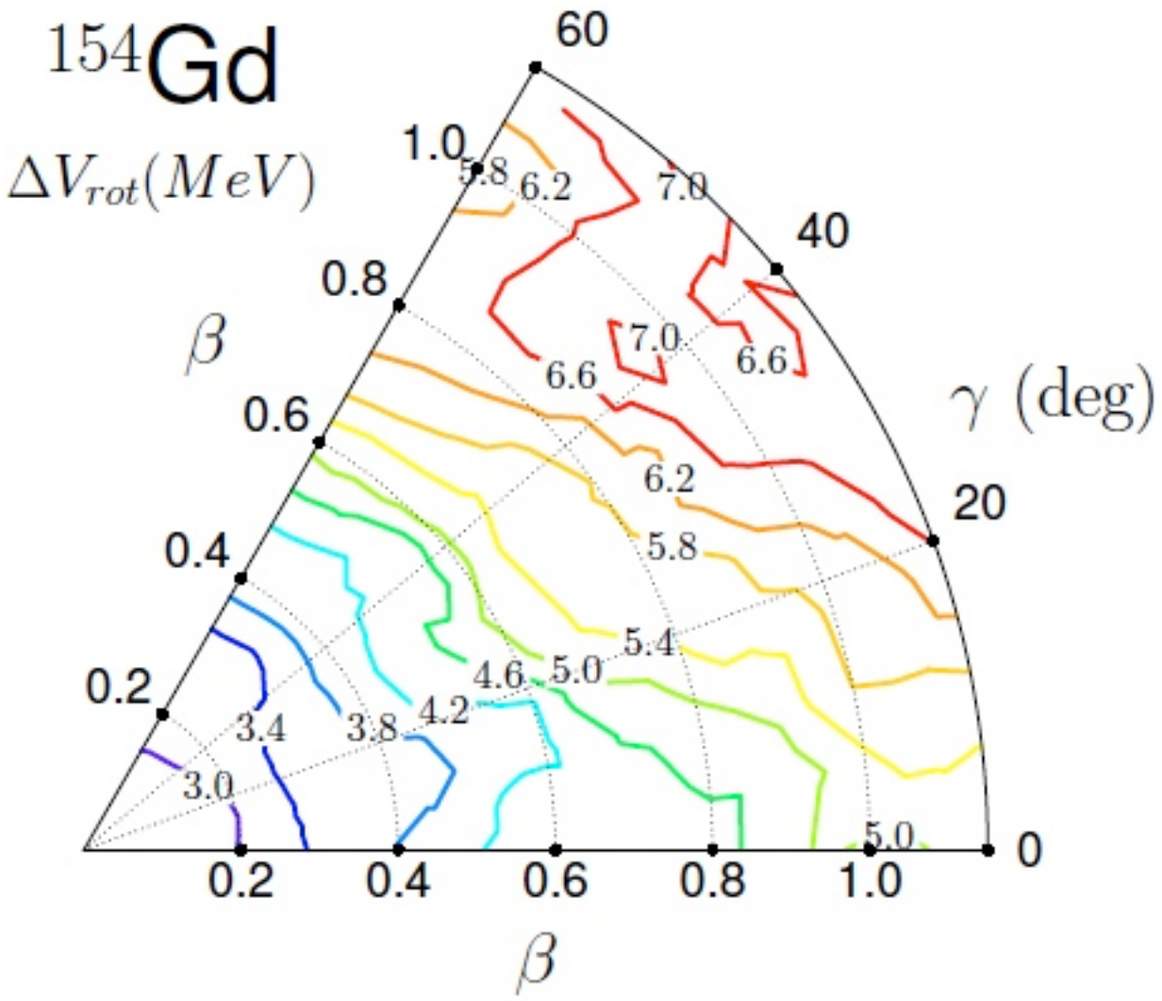


The map of the Inglis-Belyaev inertia parameter B_x

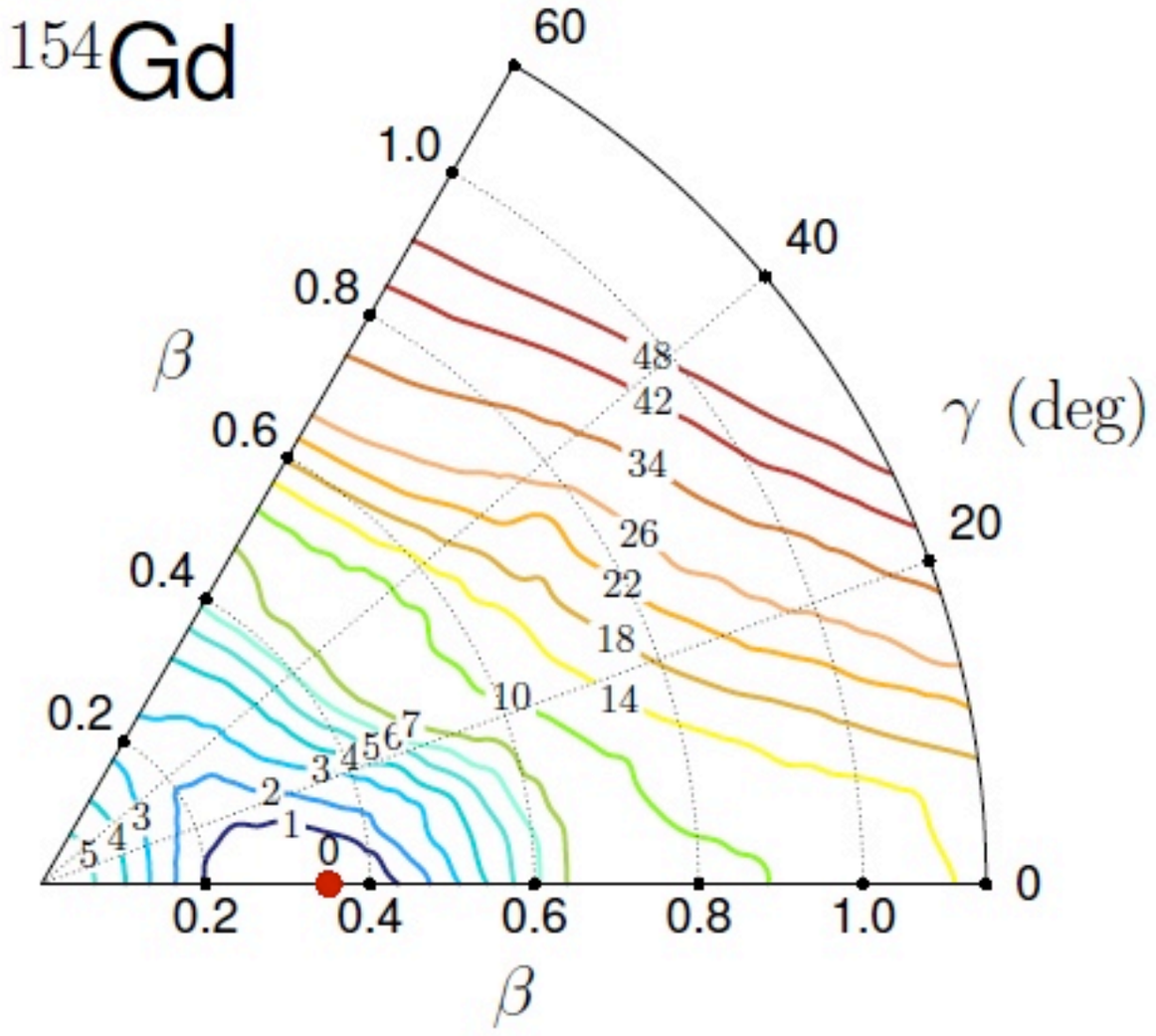


$$V_{\rm coll}(q_0, q_2) = E_{\rm tot}(q_0, q_2) - \Delta V_{\rm vib}(q_0, q_2) - \Delta V_{\rm rot}(q_0, q_2)$$

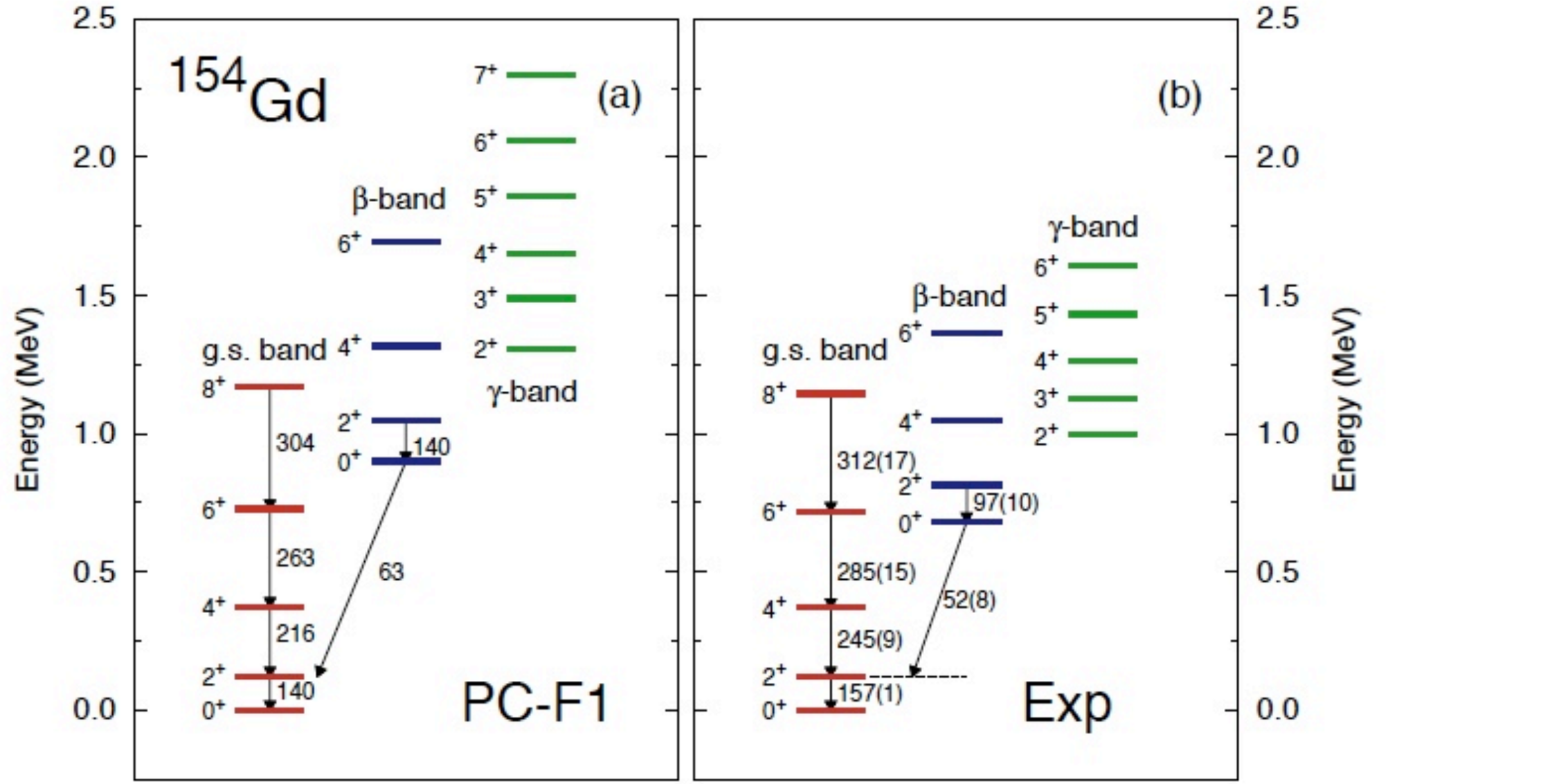
vibrational rotational
zero-point energy correction



rotational zero-point energy



collective potential



... detailed spectroscopy in the EDF framework!