Optimizing Energy Density Functionals: covariance analysis

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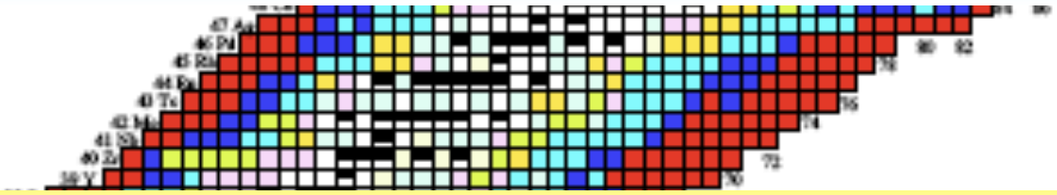
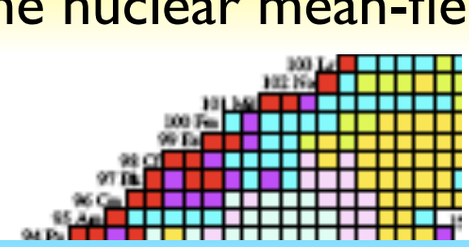
Relativistic Energy Density Functionals

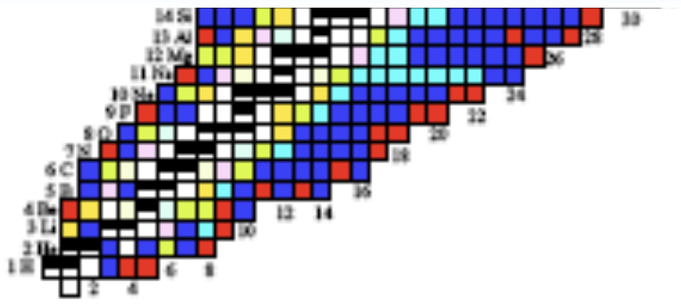
✔ natural inclusion of the *spin degree of freedom* (spin-orbit potential with empirical strength).

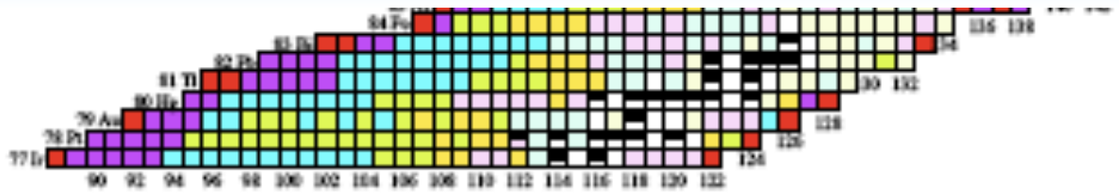


✔ unique parameterization of *time-odd components* (currents) of the nuclear mean-field.



✔ 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.

⇒ build 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:

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

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

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

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.

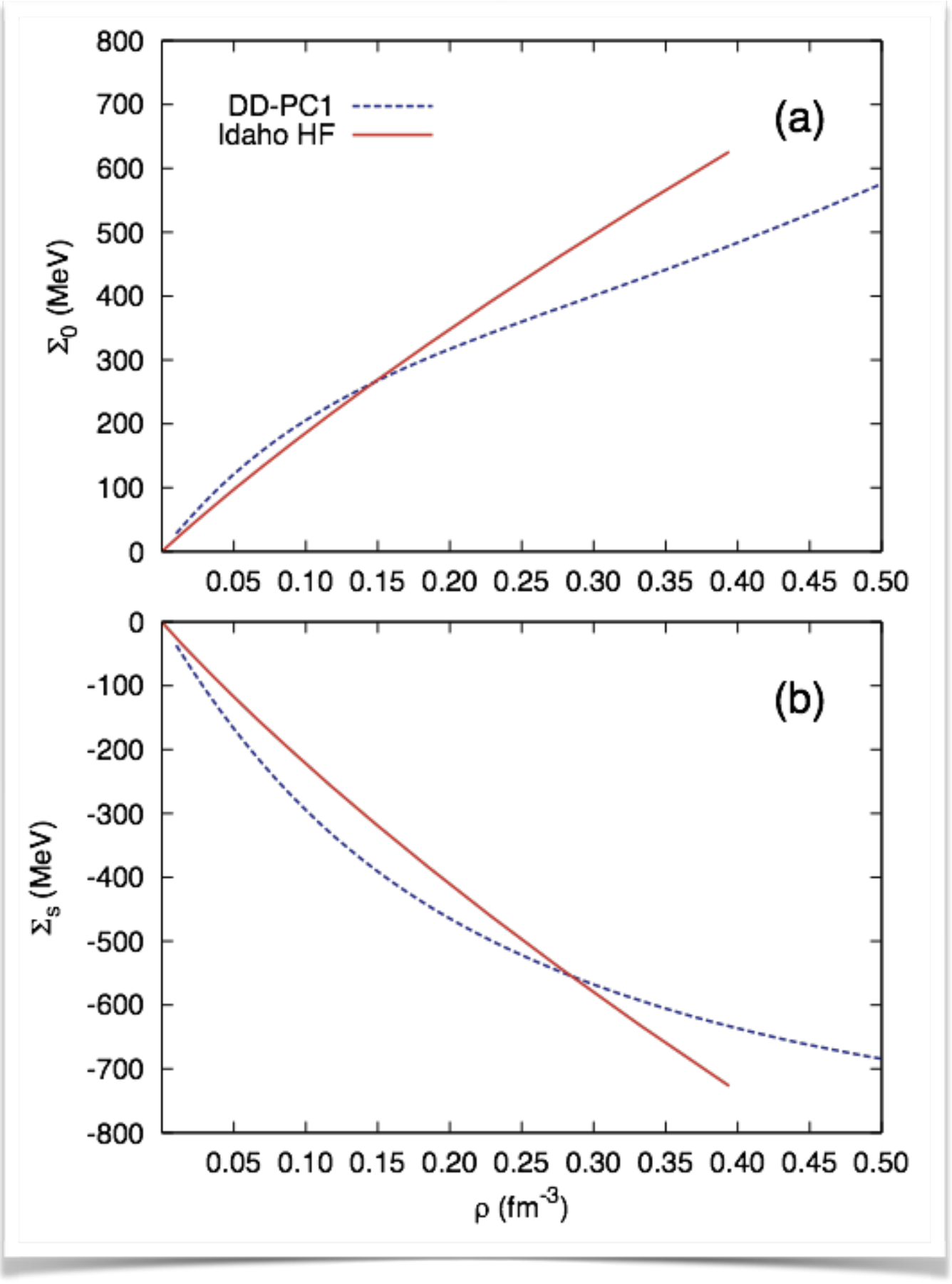
... the parameters of the functional are fine-tuned to data of finite nuclei.

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.

Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter.

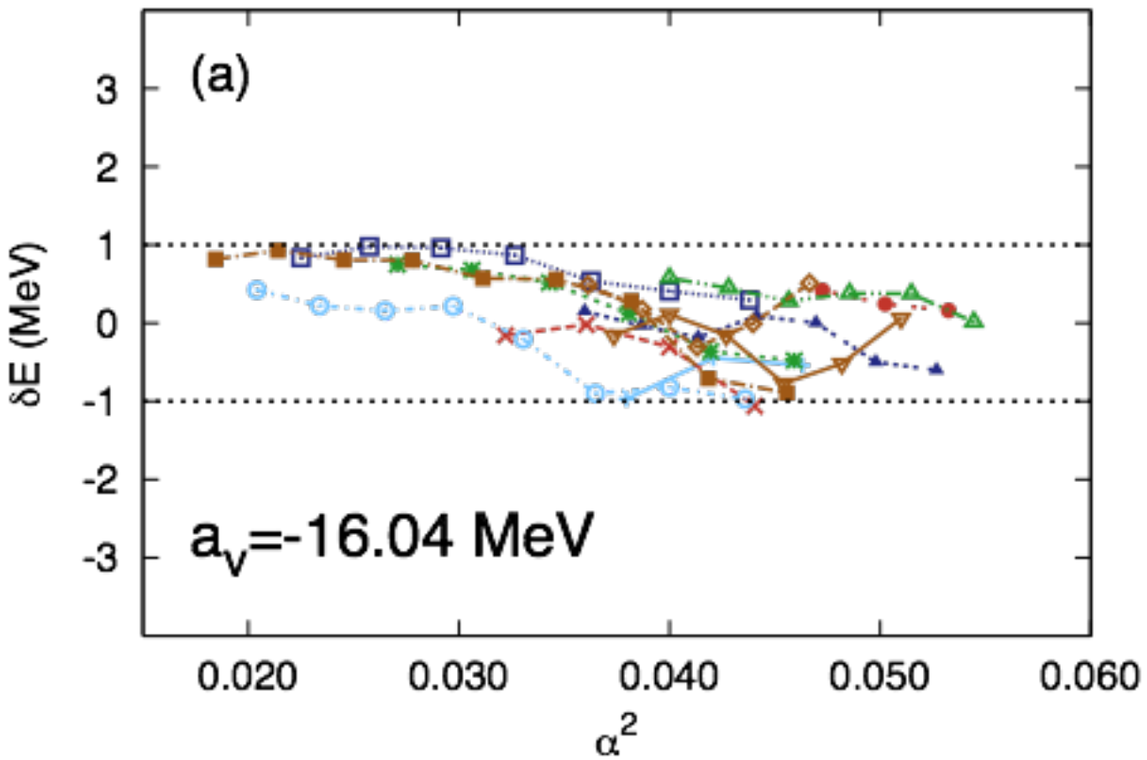


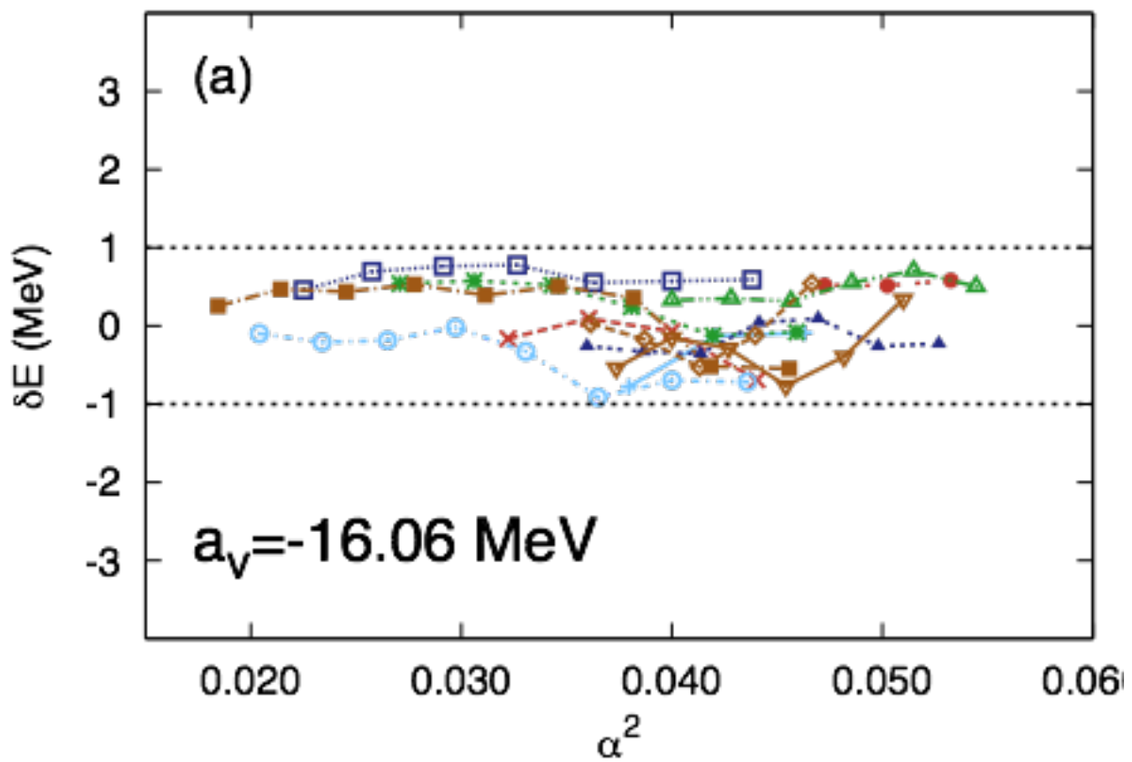
... calculated masses of finite nuclei are primarily sensitive to the three leading terms in the empirical mass formula:

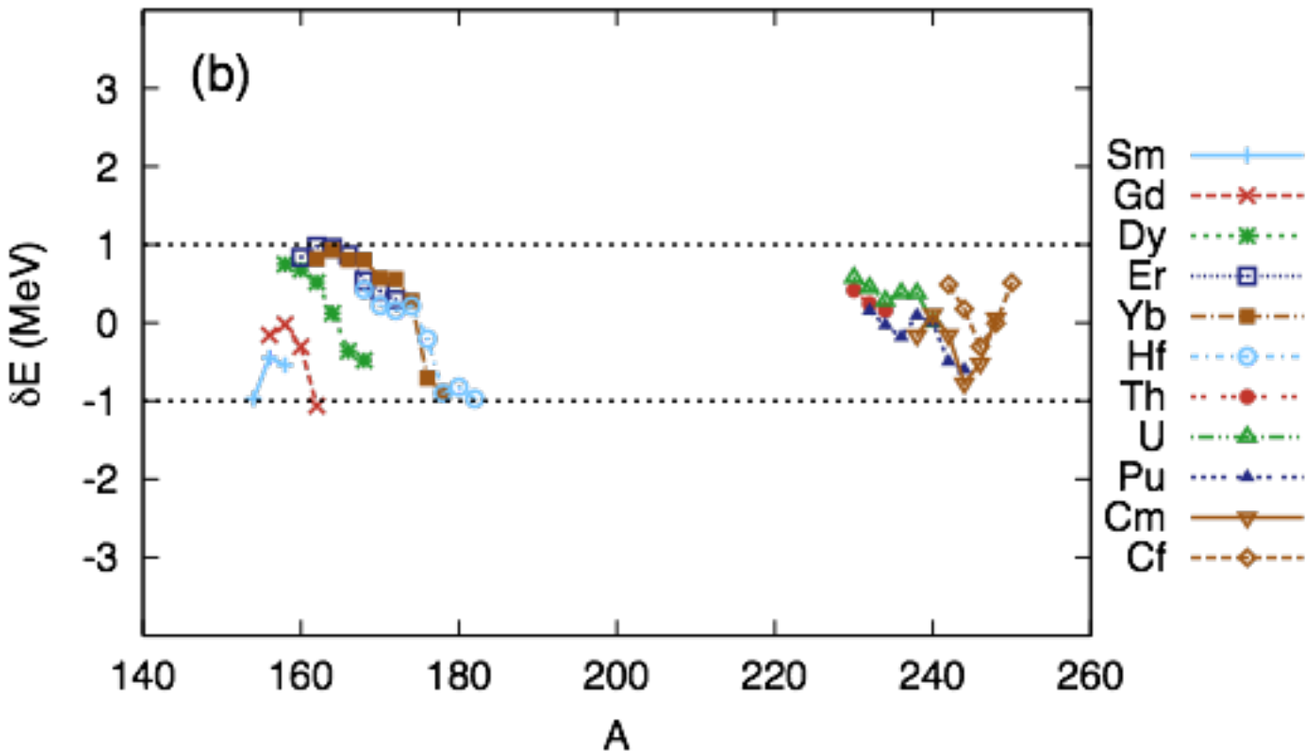
$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

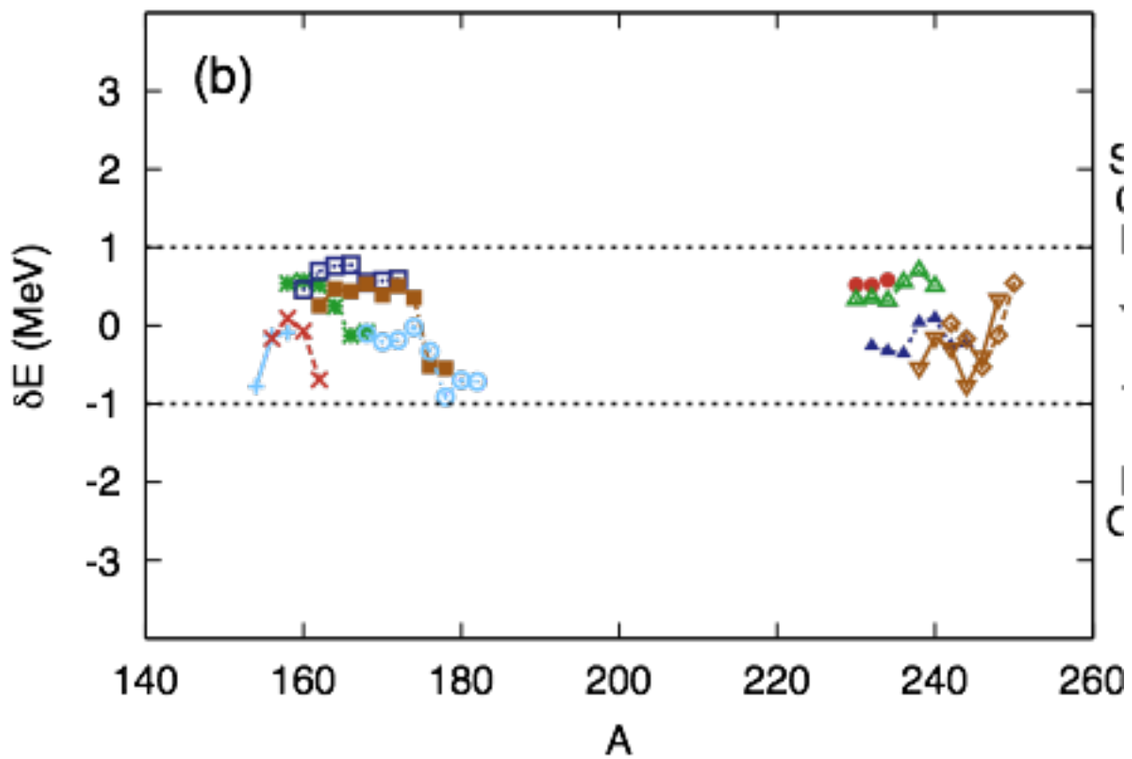
... generate families of effective interactions characterized by different values of a_v, a_s and a_4, and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

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

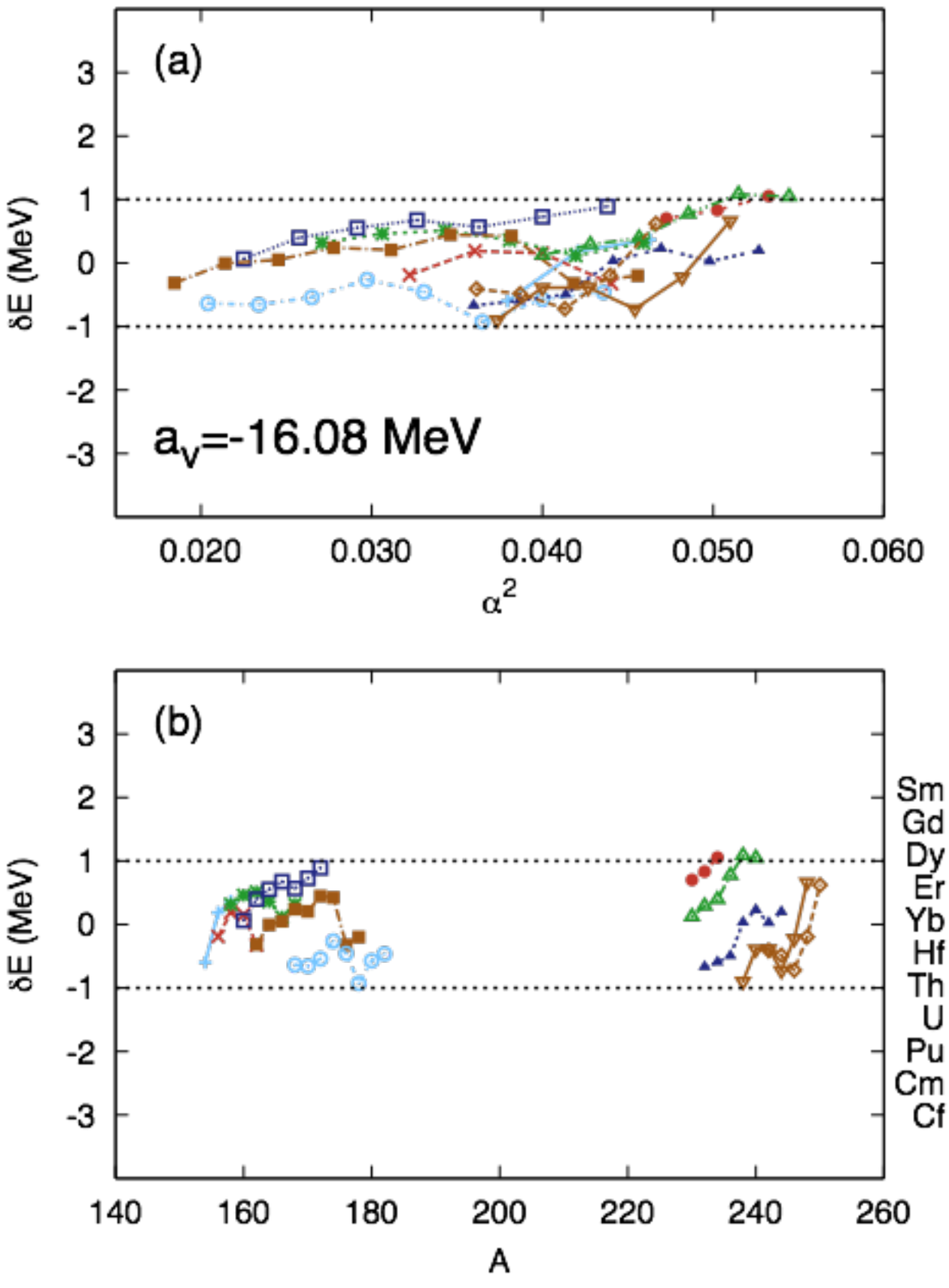


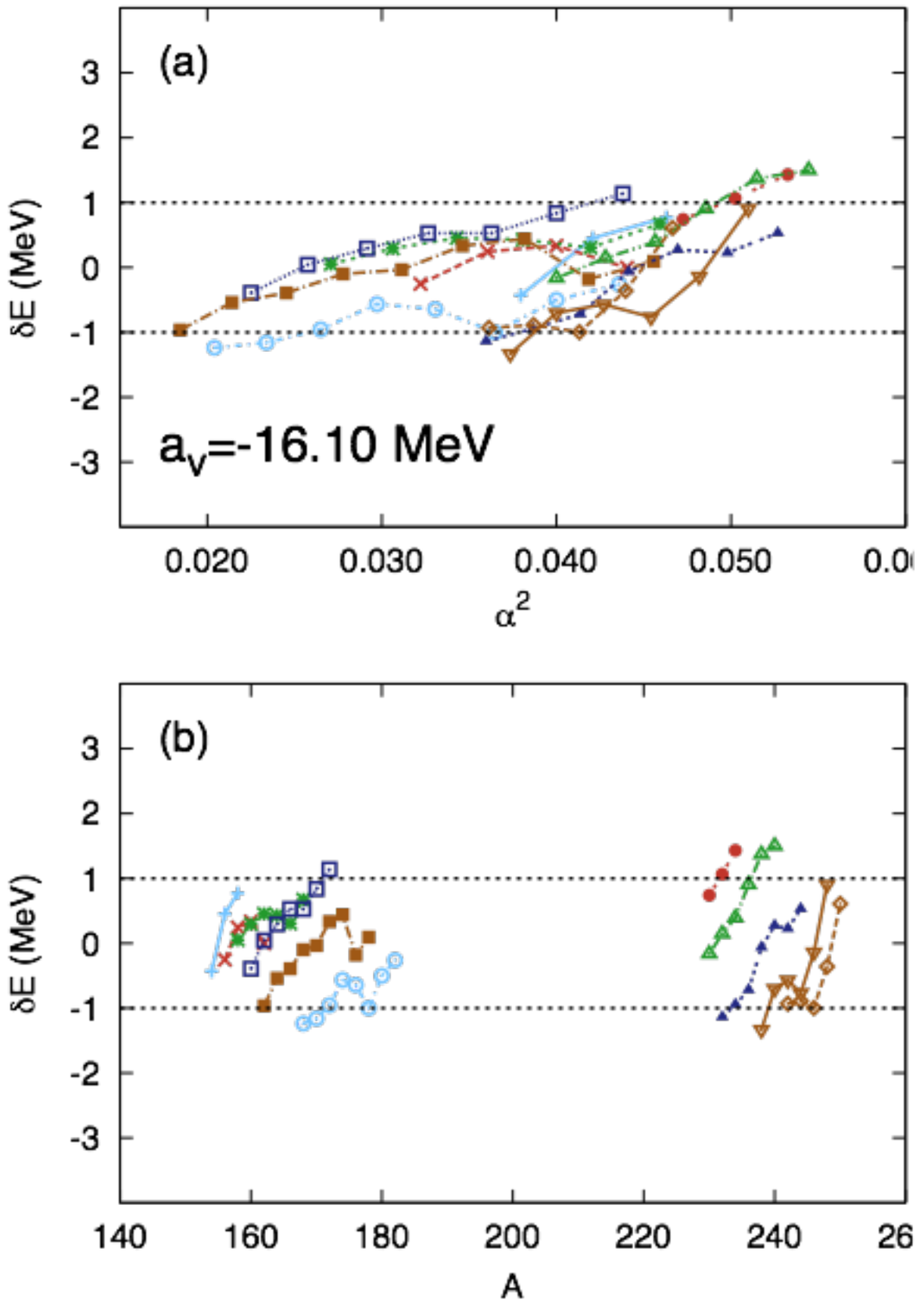






$$\alpha^2 = \frac{(N-Z)^2}{A^2}$$





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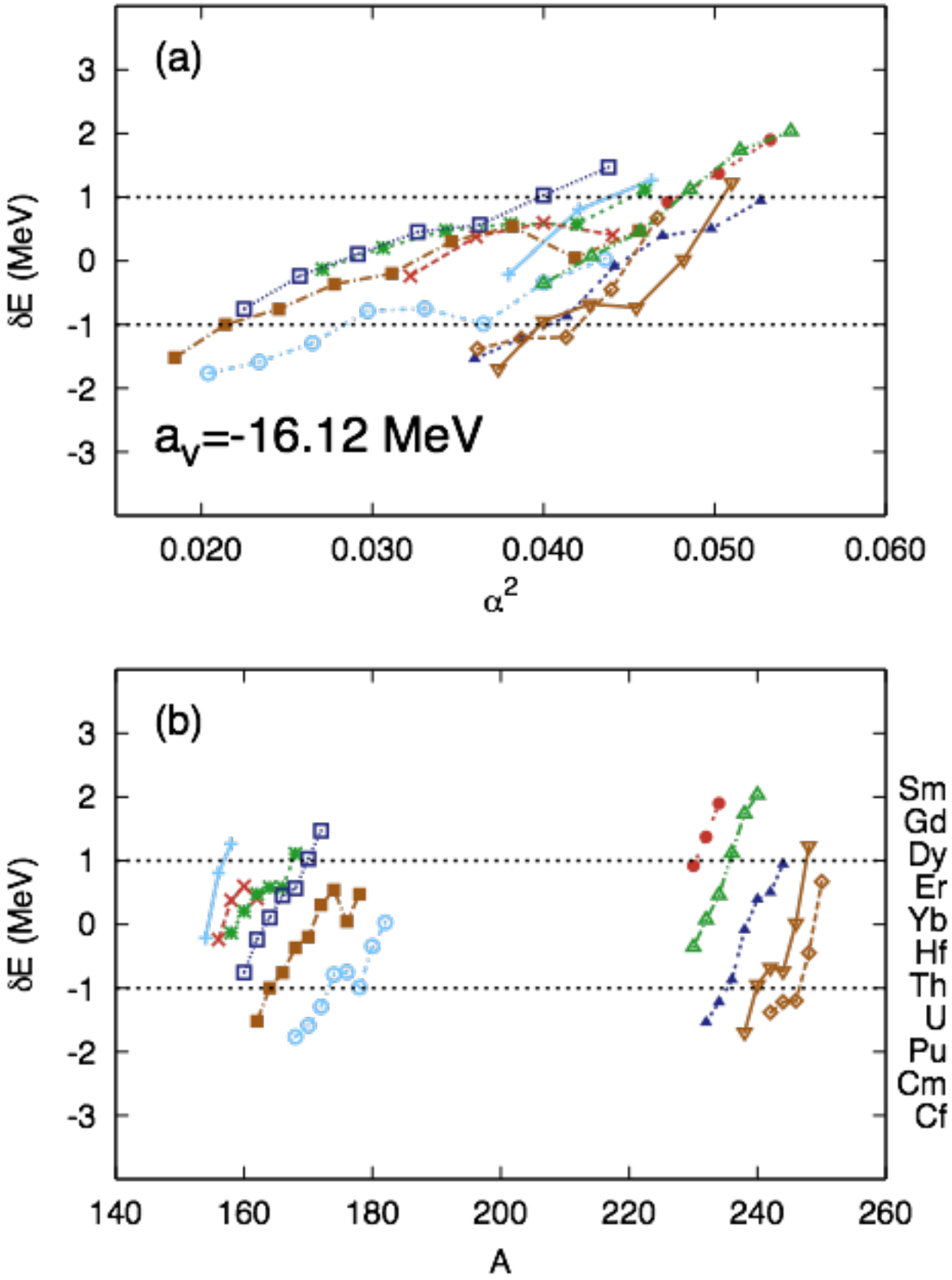
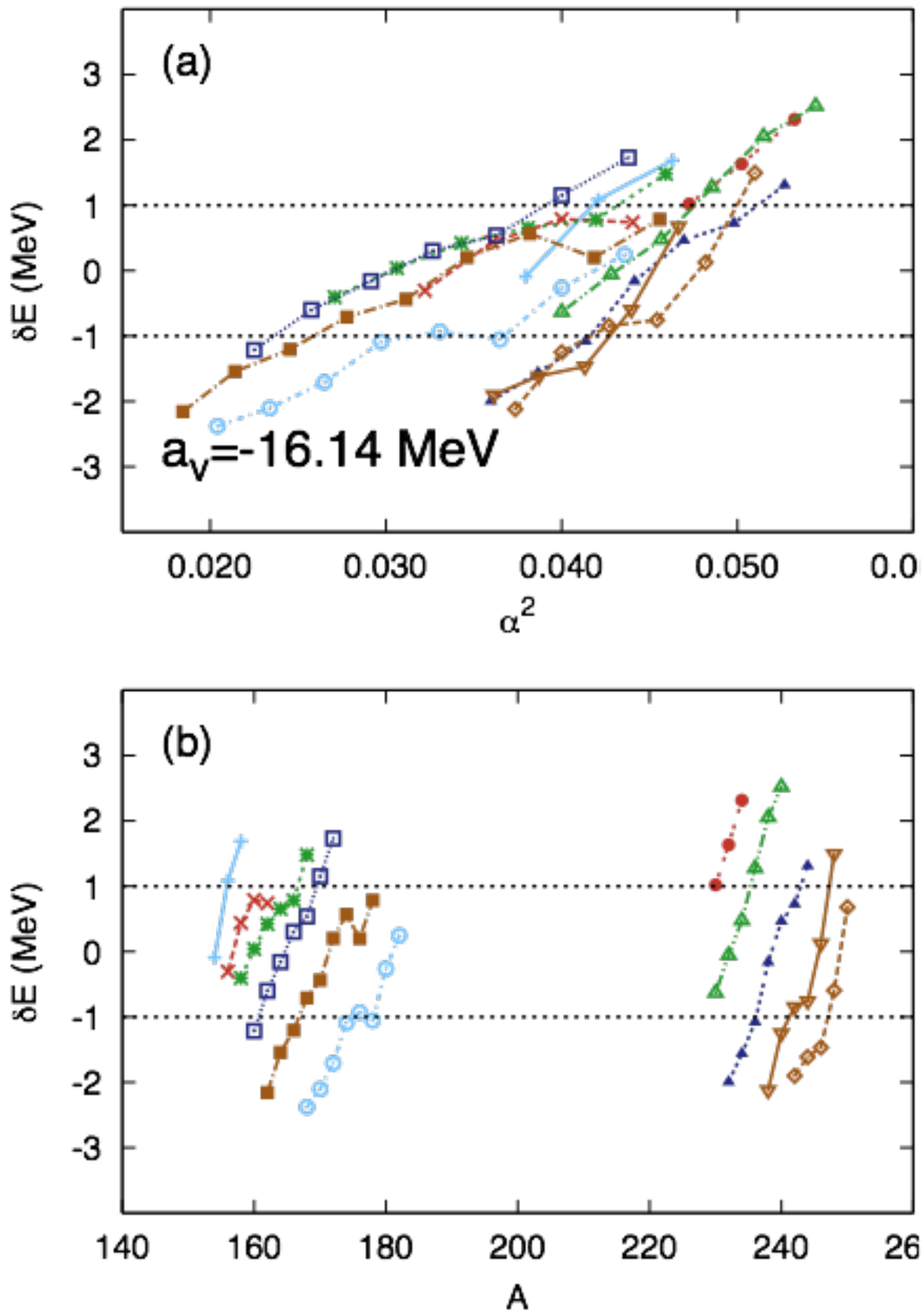
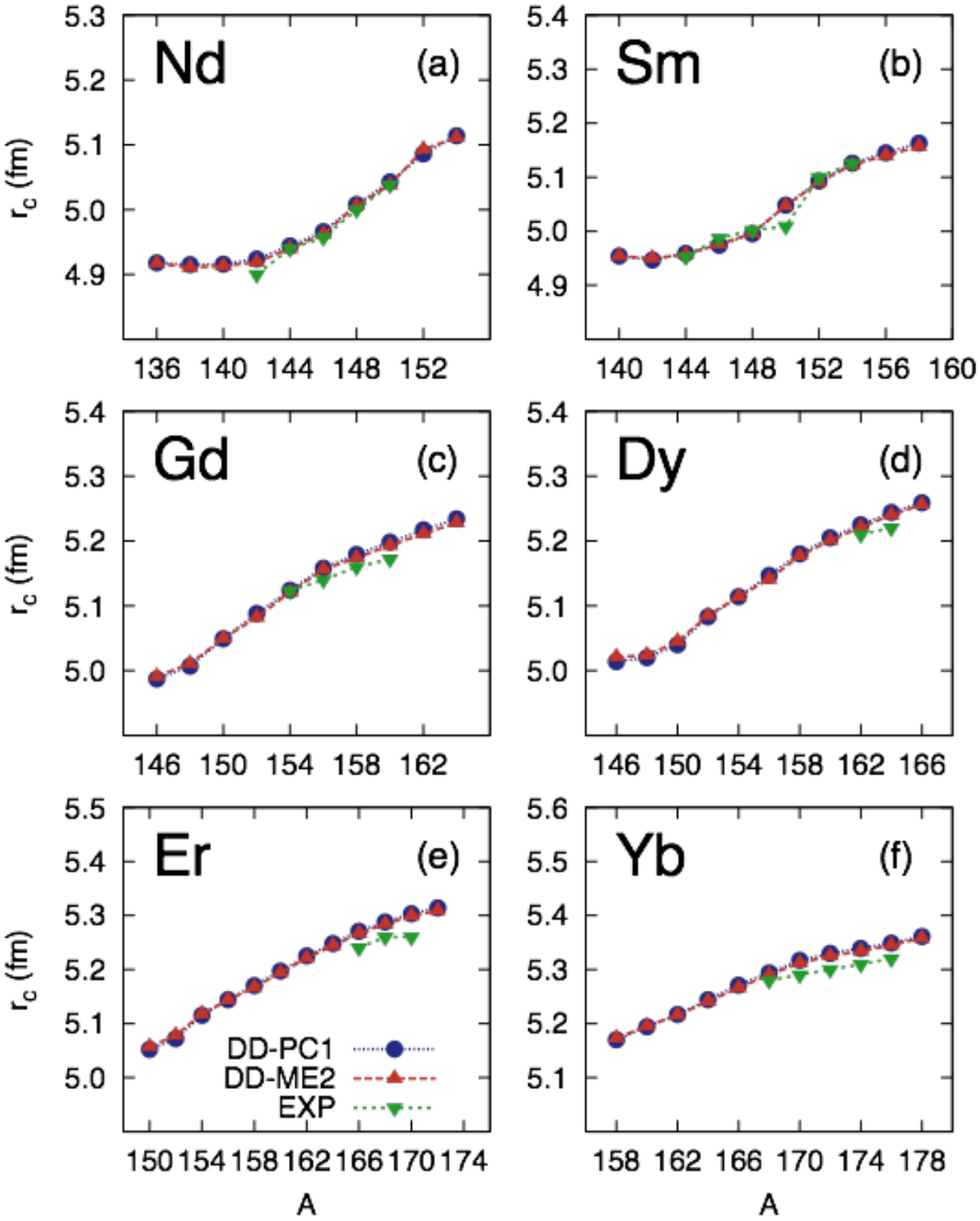




Test: calculation of observables not included in the fitting procedure

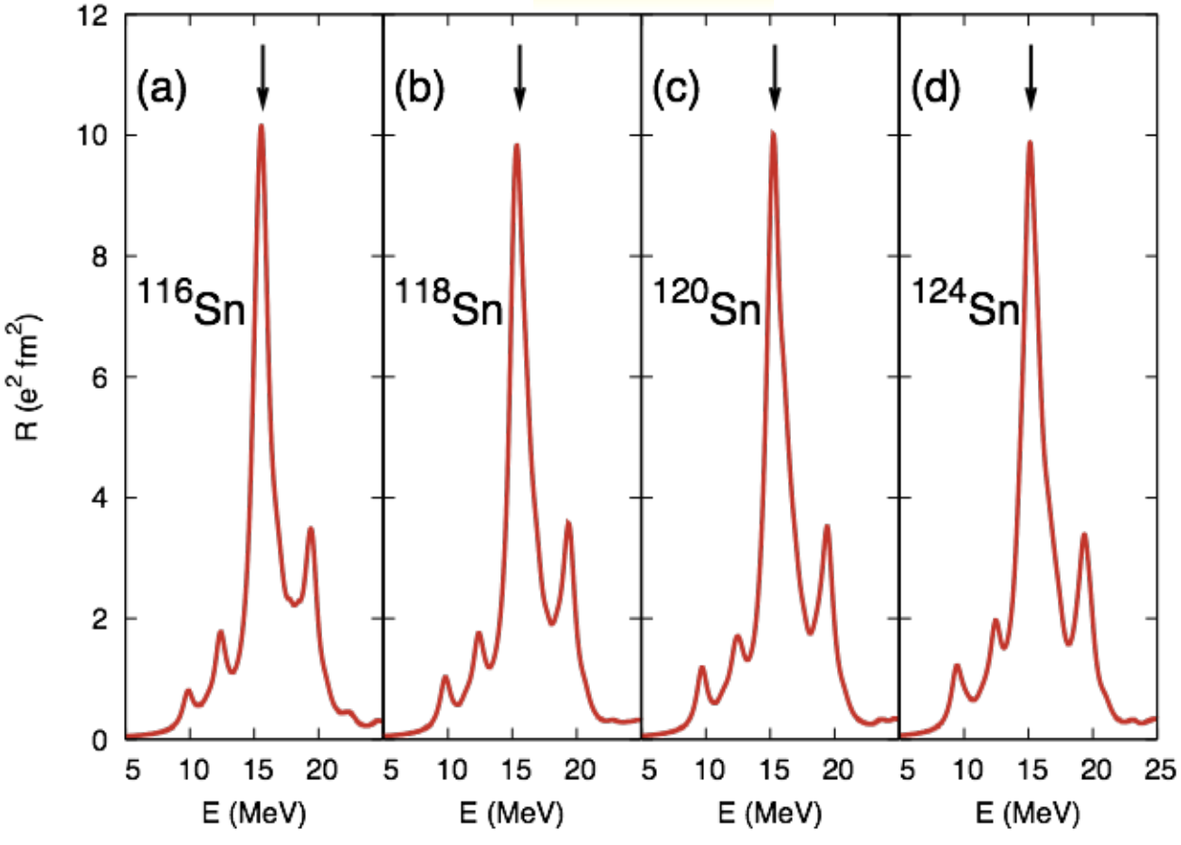
Charge radii

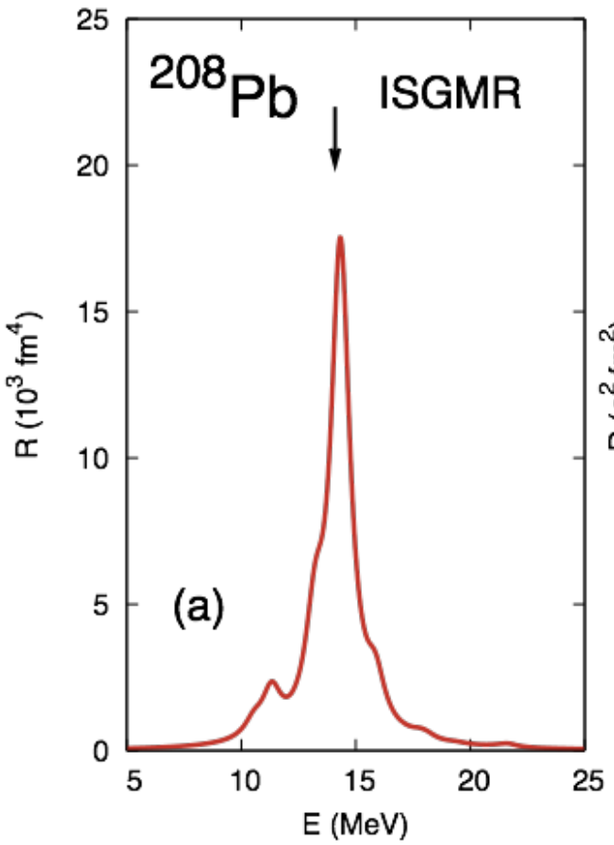
Quadrupole deformations

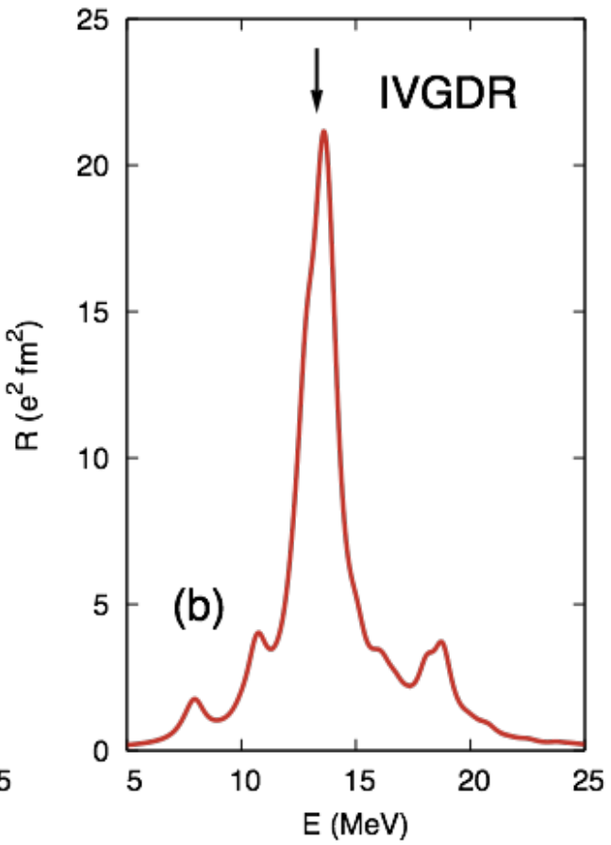


Excitation energies of collective modes:

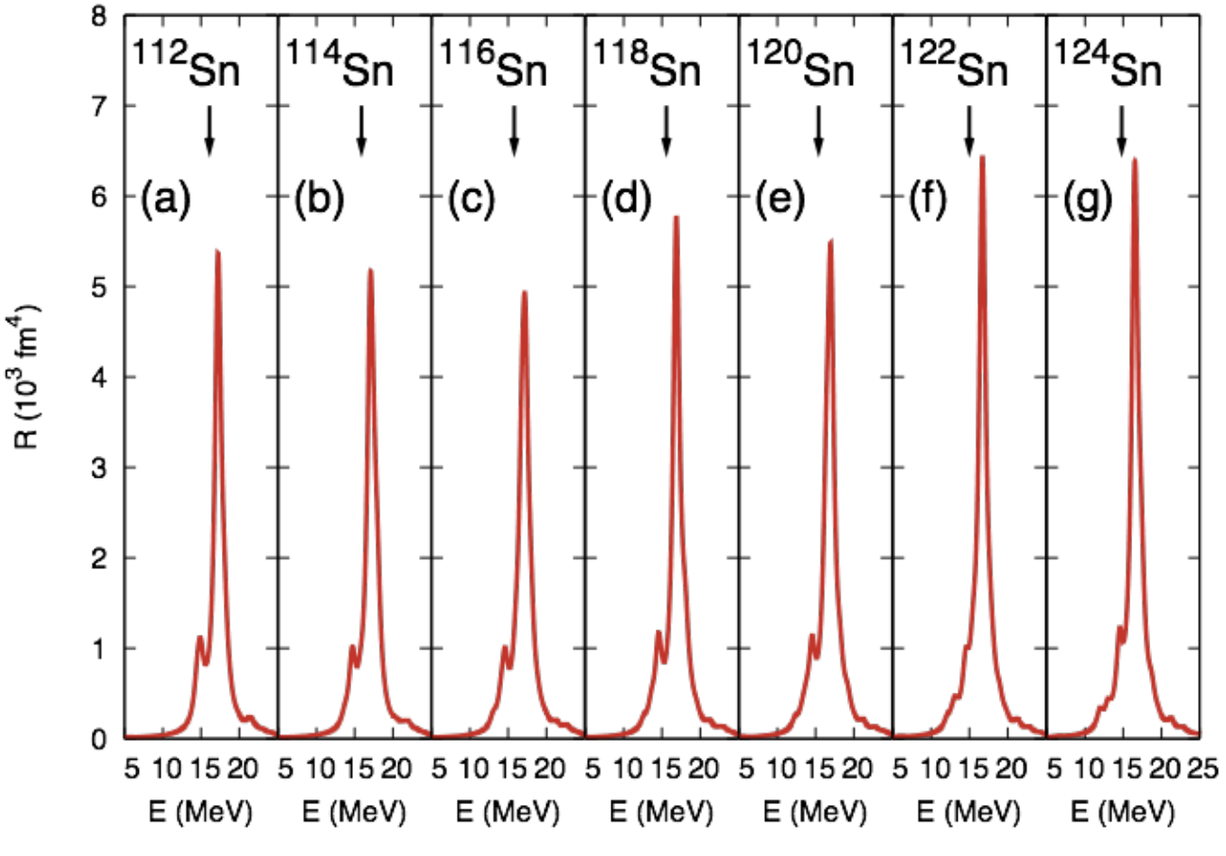
IVGDR



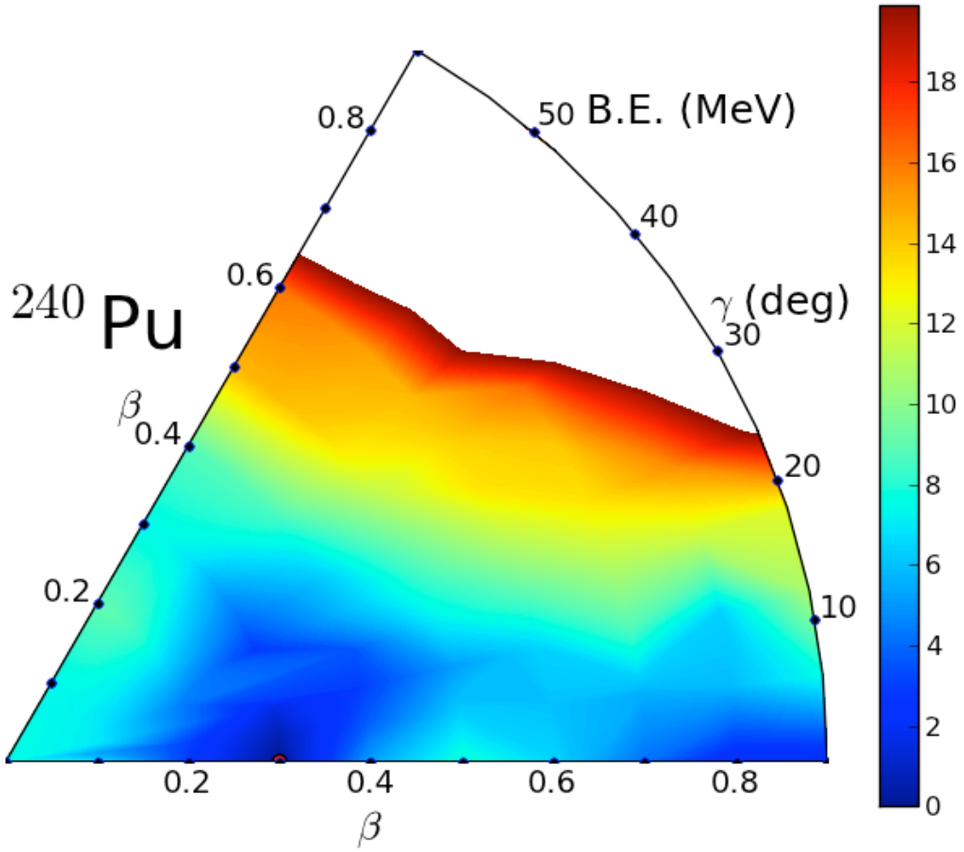


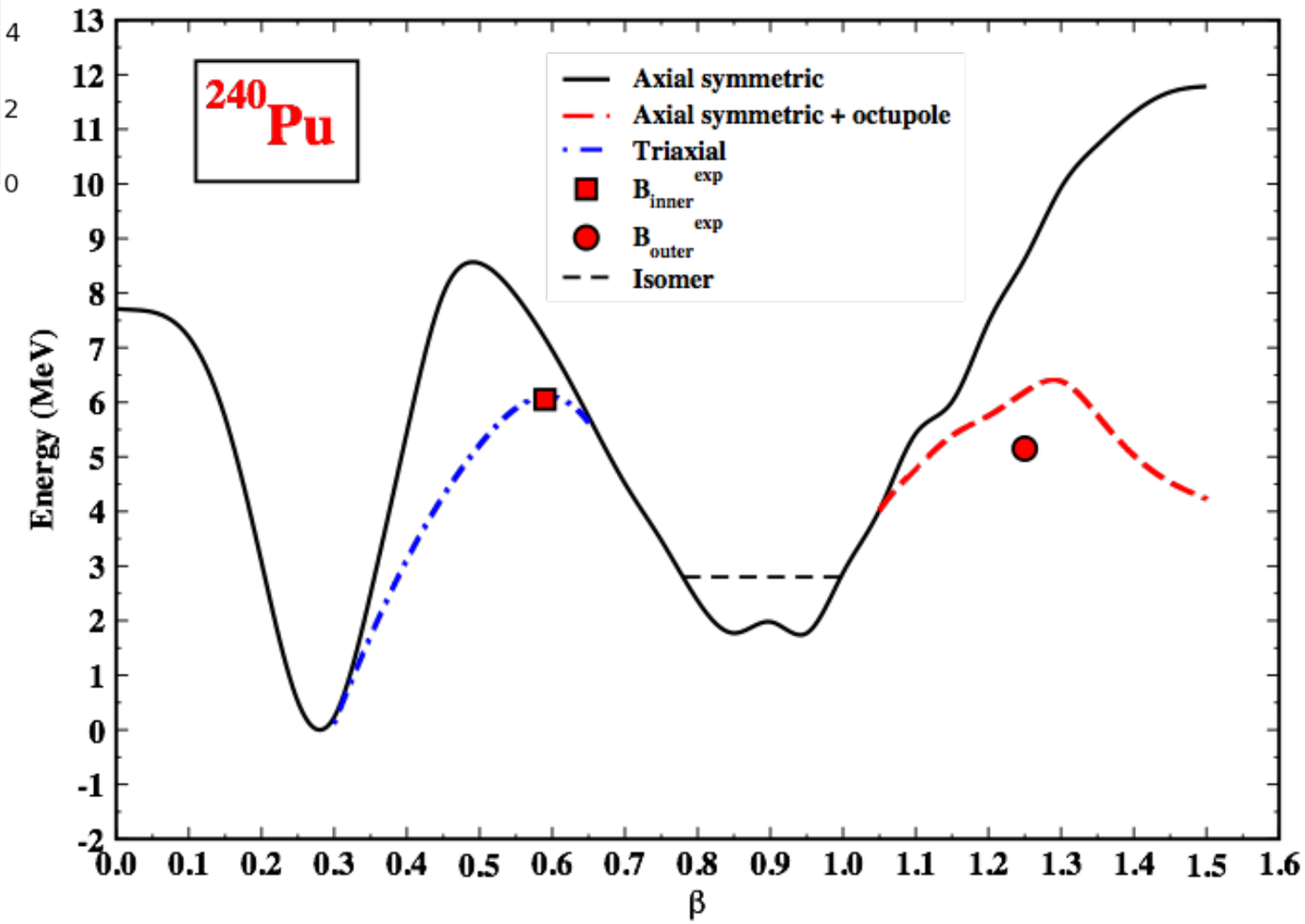


ISGMR



Test: “double-humped” fission barriers of actinides





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.

Five-dimensional collective Hamiltonian

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

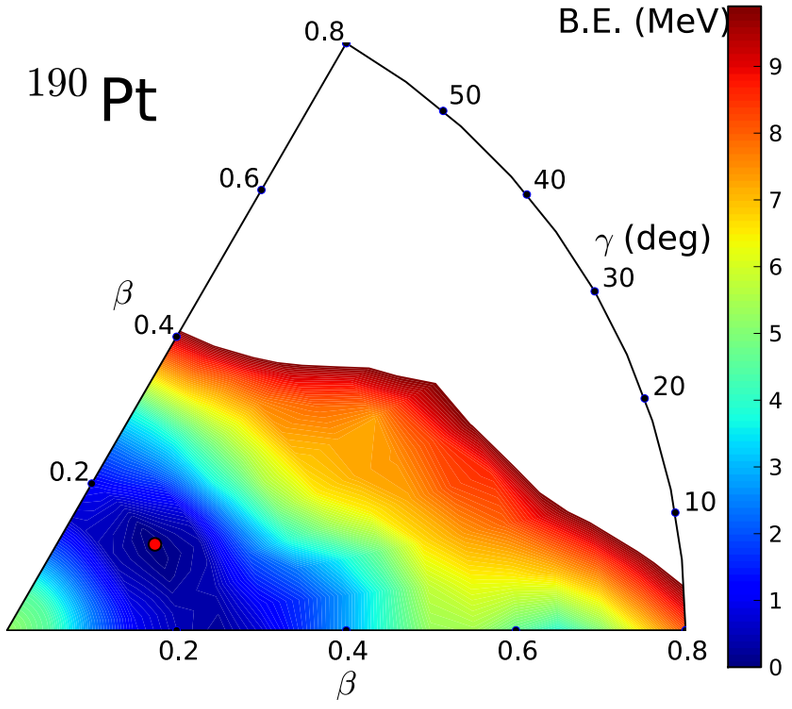
$$H_{\rm coll} = \mathcal{T}_{\rm vib}(\beta,\gamma) + \mathcal{T}_{\rm rot}(\beta,\gamma,\Omega) + \mathcal{V}_{\rm coll}(\beta,\gamma)$$

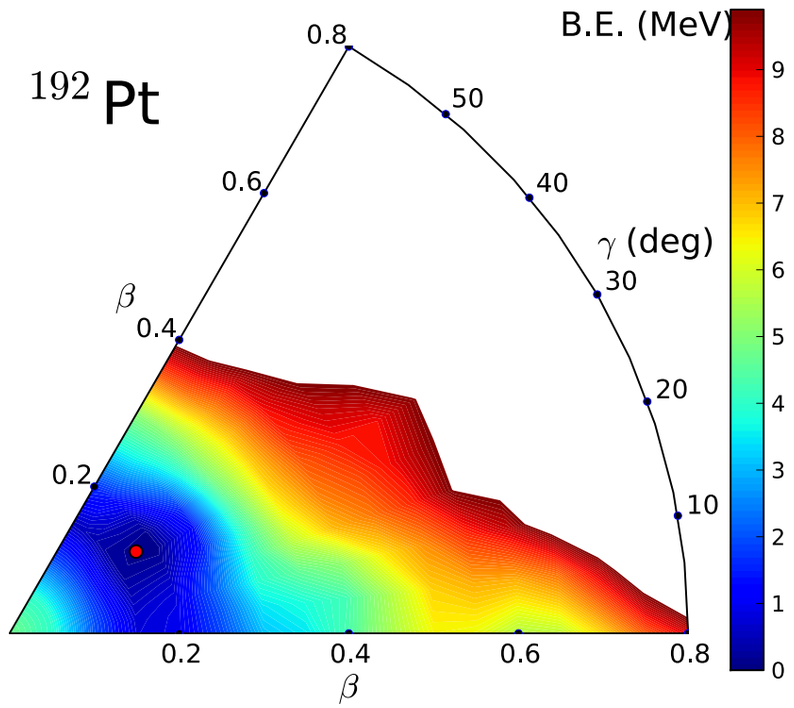
$$\mathcal{T}_{\rm vib} = \frac{1}{2}B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

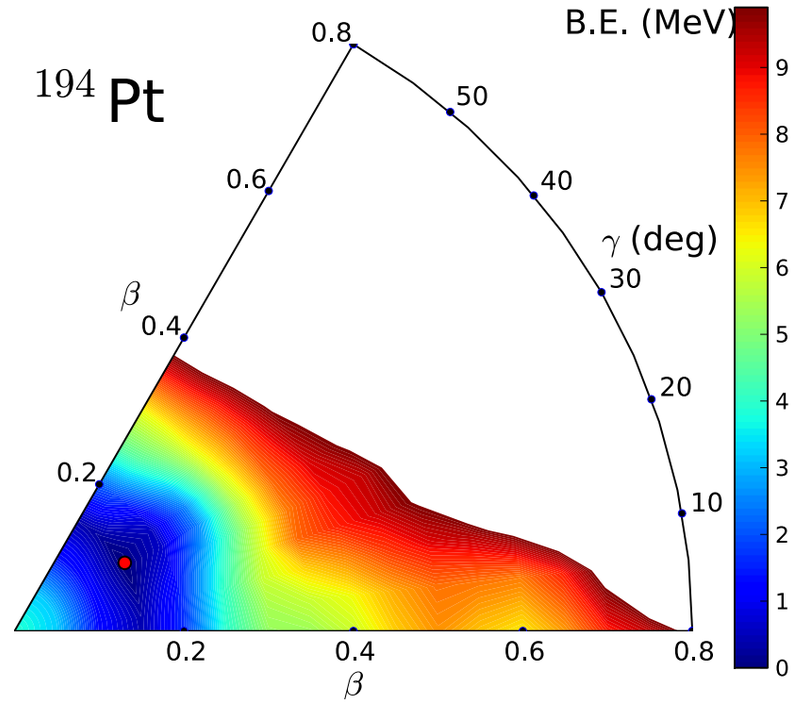
$$\mathcal{T}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

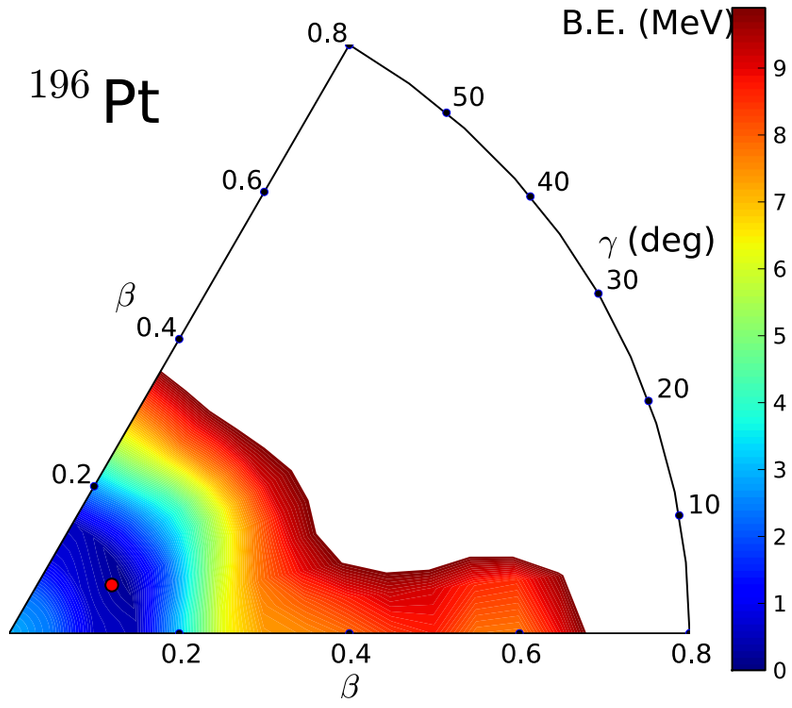
The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ: the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k.

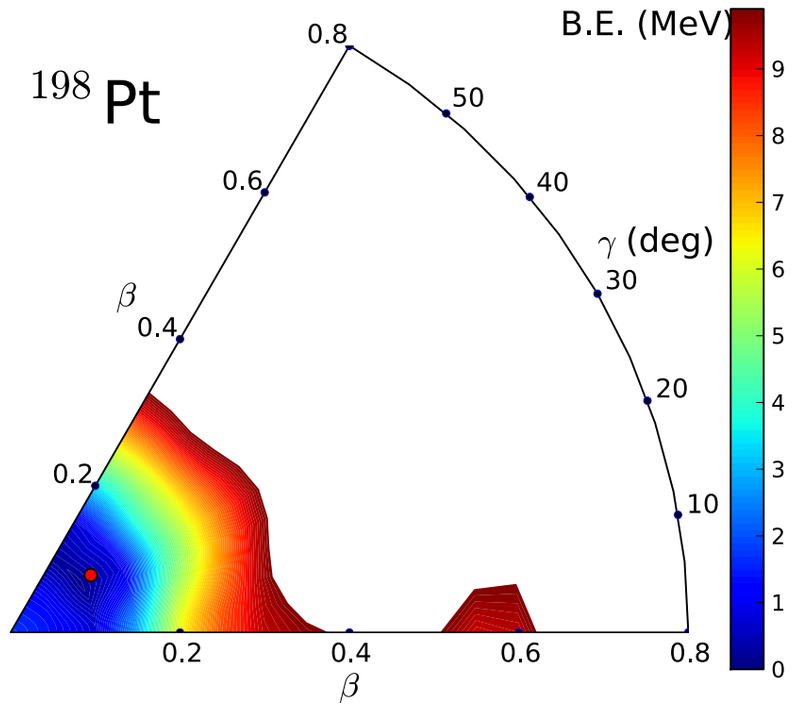
Evolution of triaxial shapes in Pt nuclei:

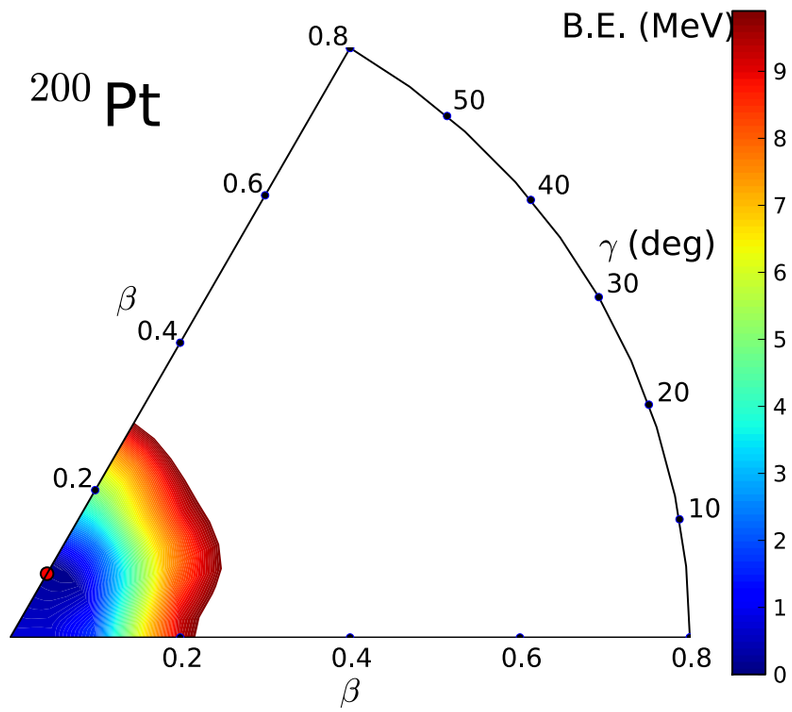


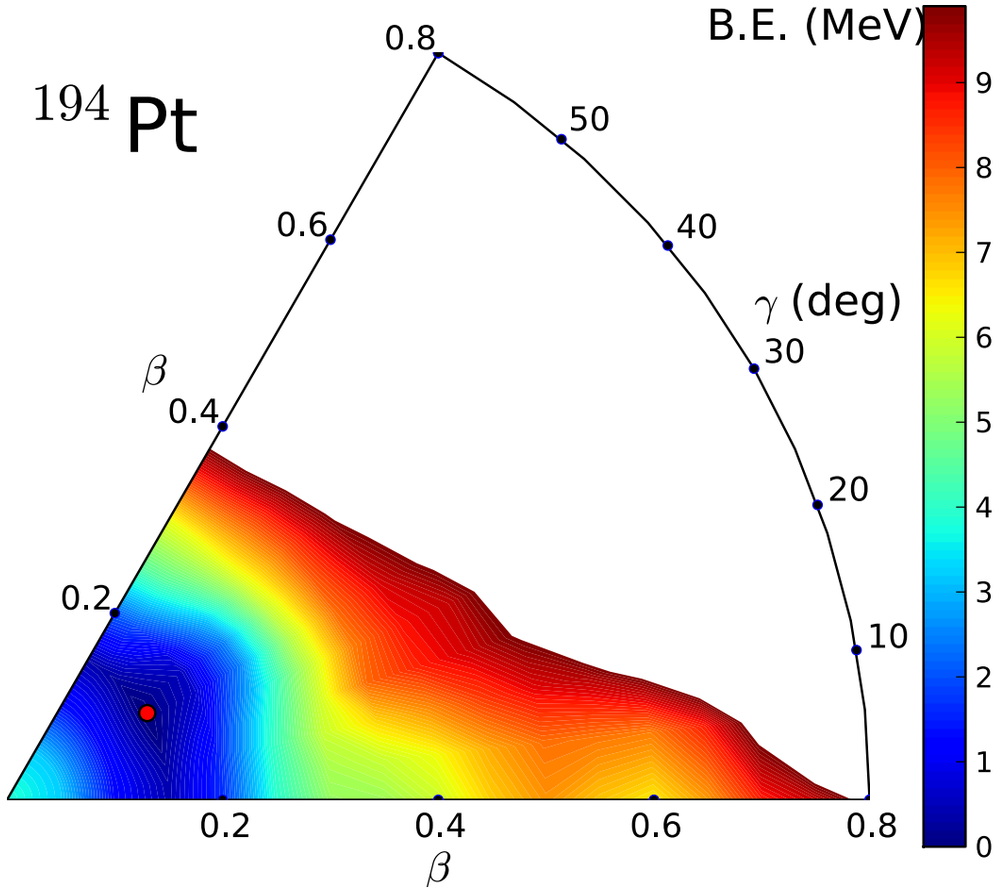






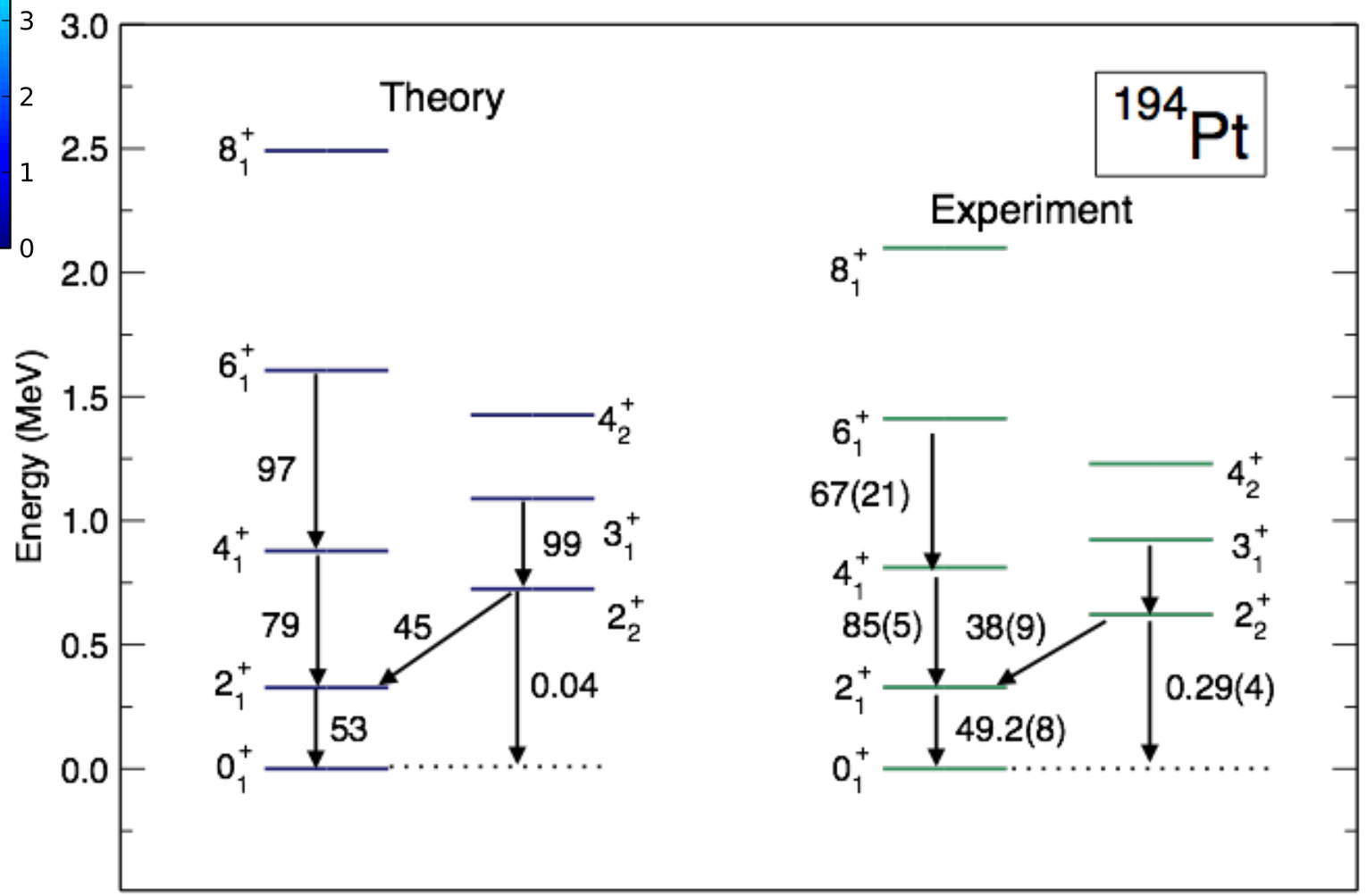


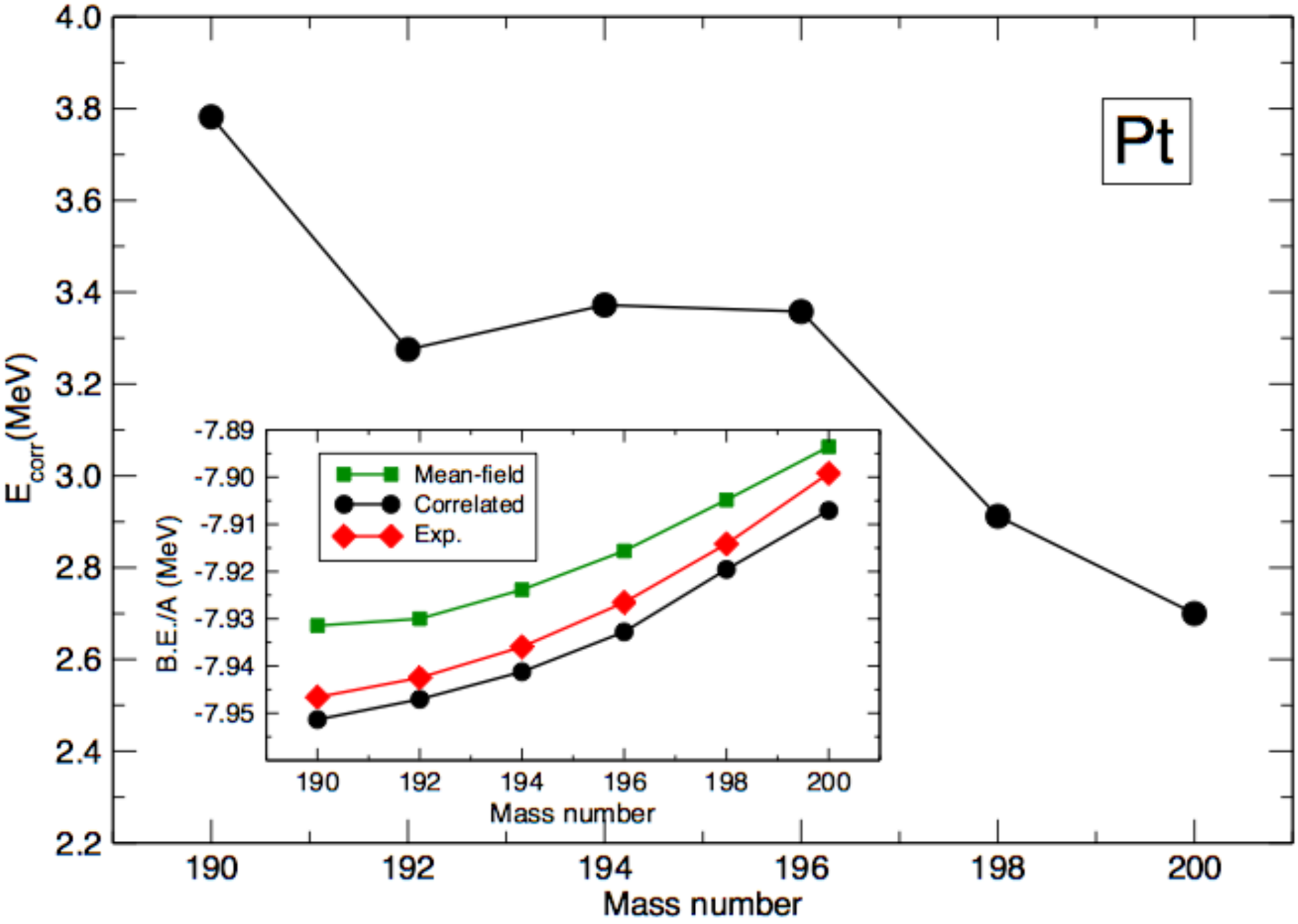




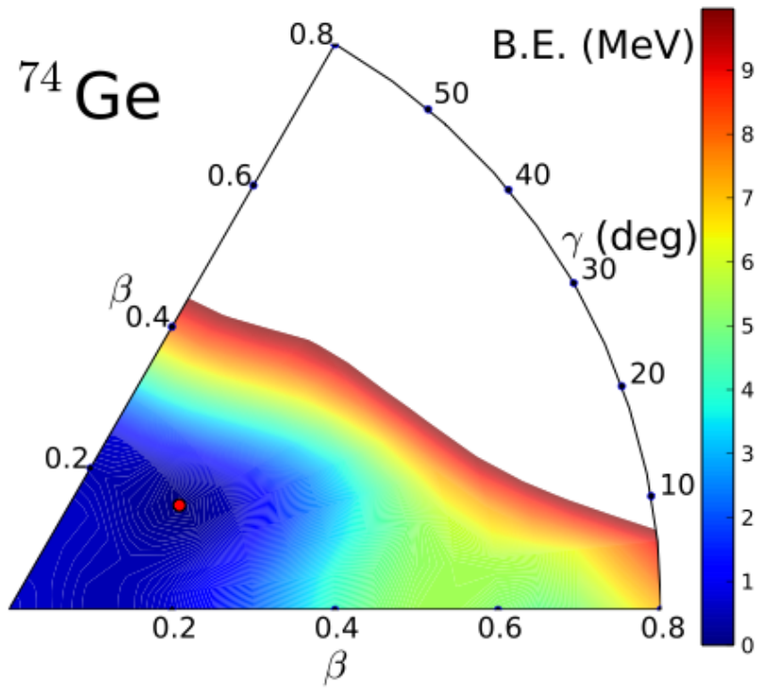
$$E^{th}_{4^+_1}/E^{th}_{2^+_1} = 2.68$$

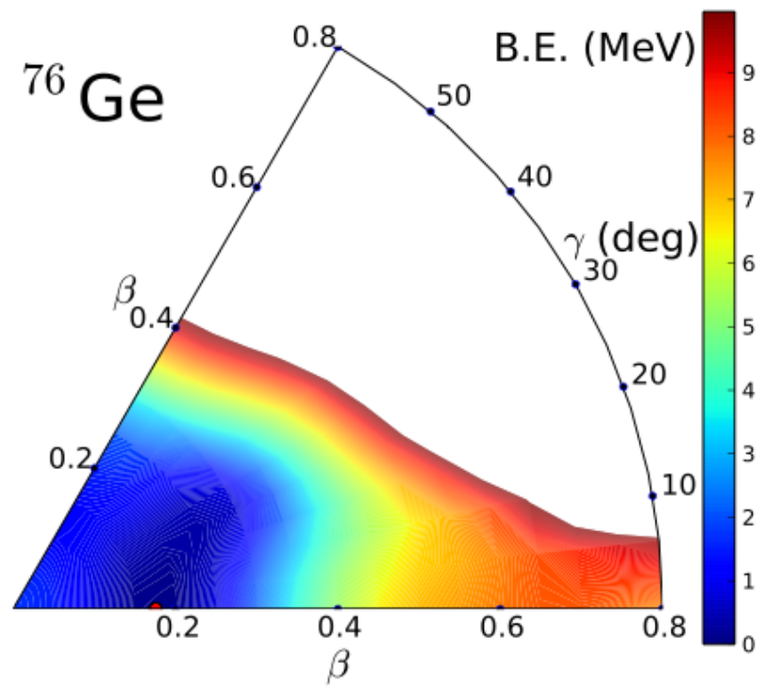
$$E^{exp}_{4^+_1}/E^{exp}_{2^+_1} = 2.47$$

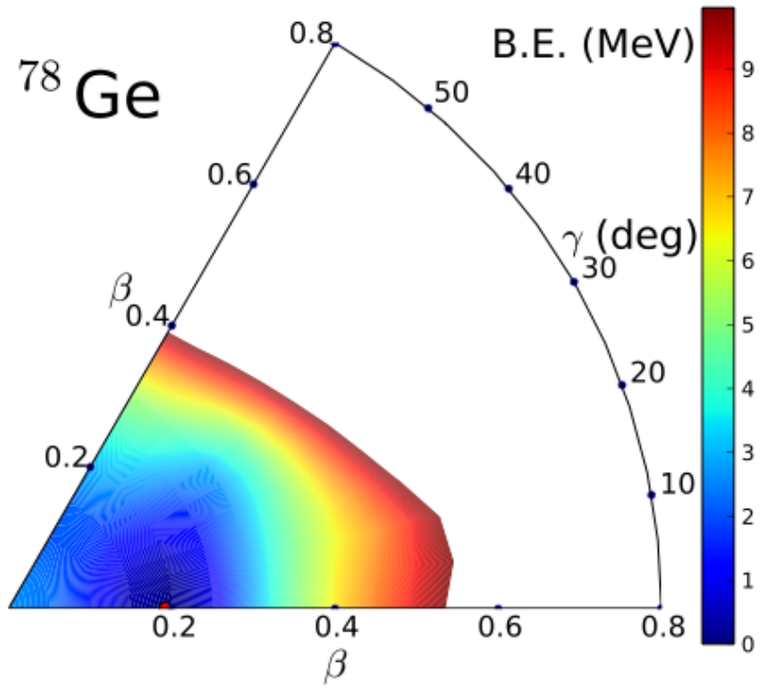


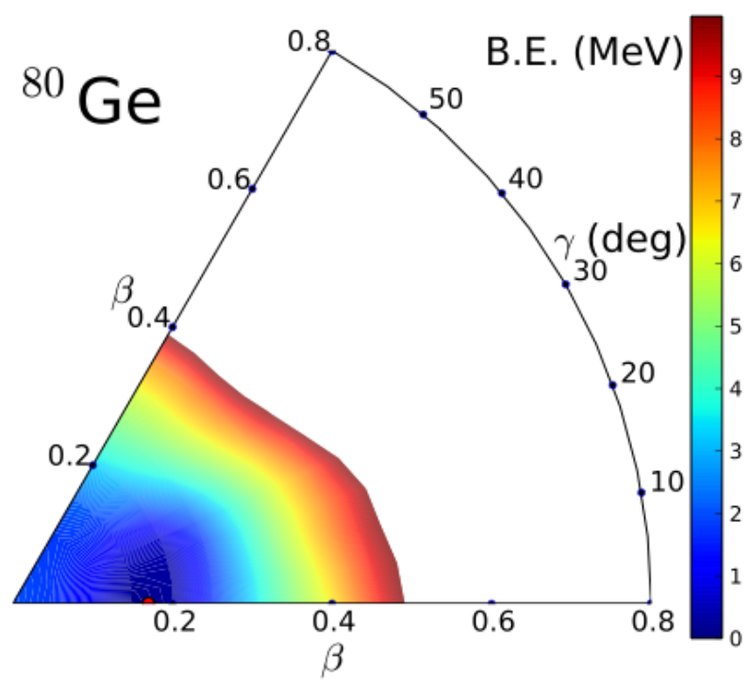

Pt
E_{corr}(MeV)
Mass number
B.E./A (MeV)
Mean-field
Correlated
Exp.

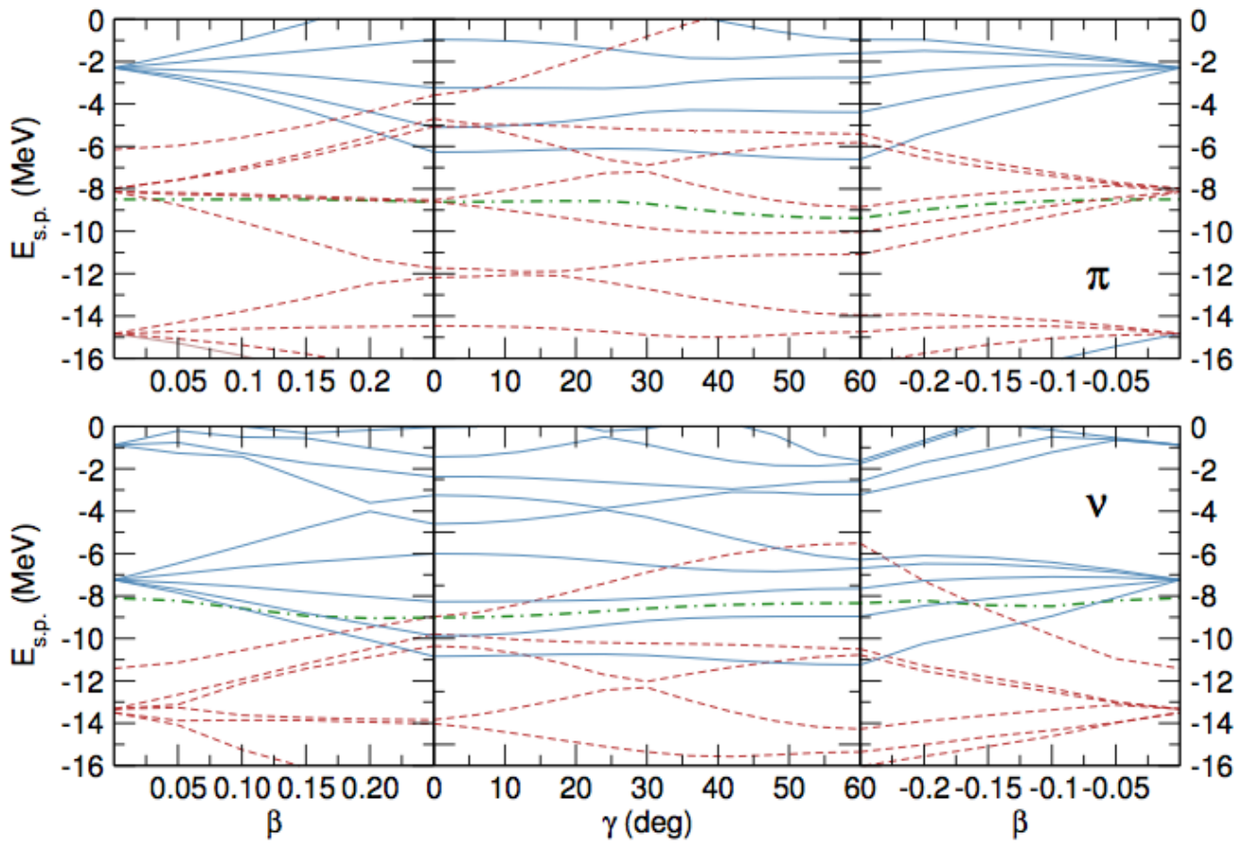
Shape evolution and triaxiality in germanium isotopes

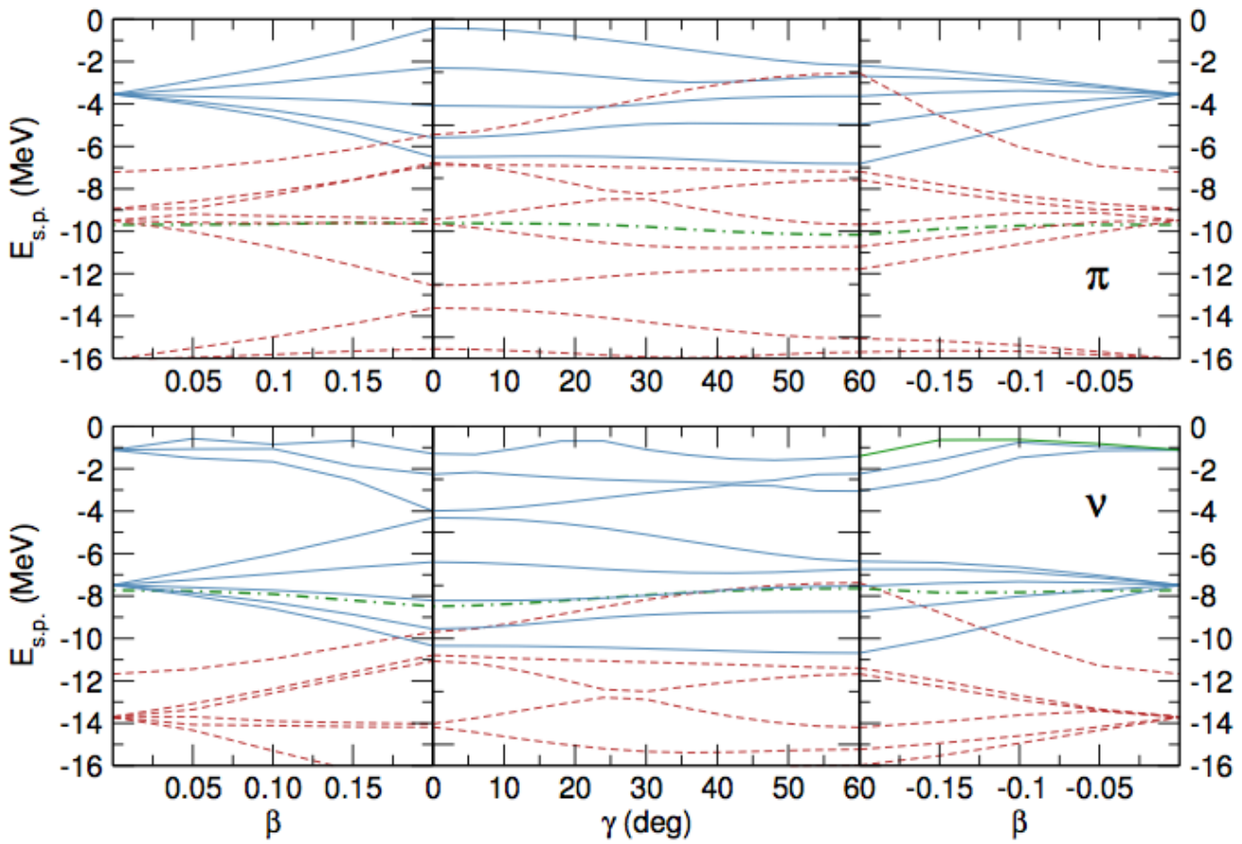


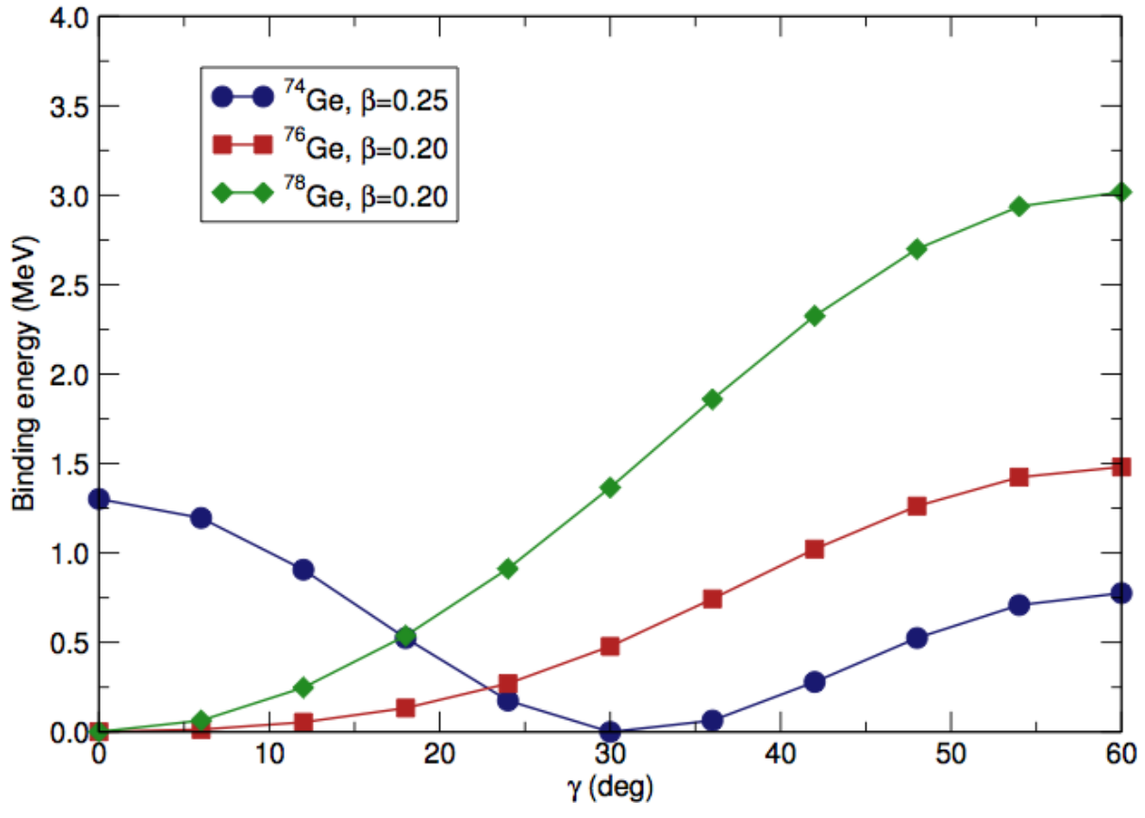




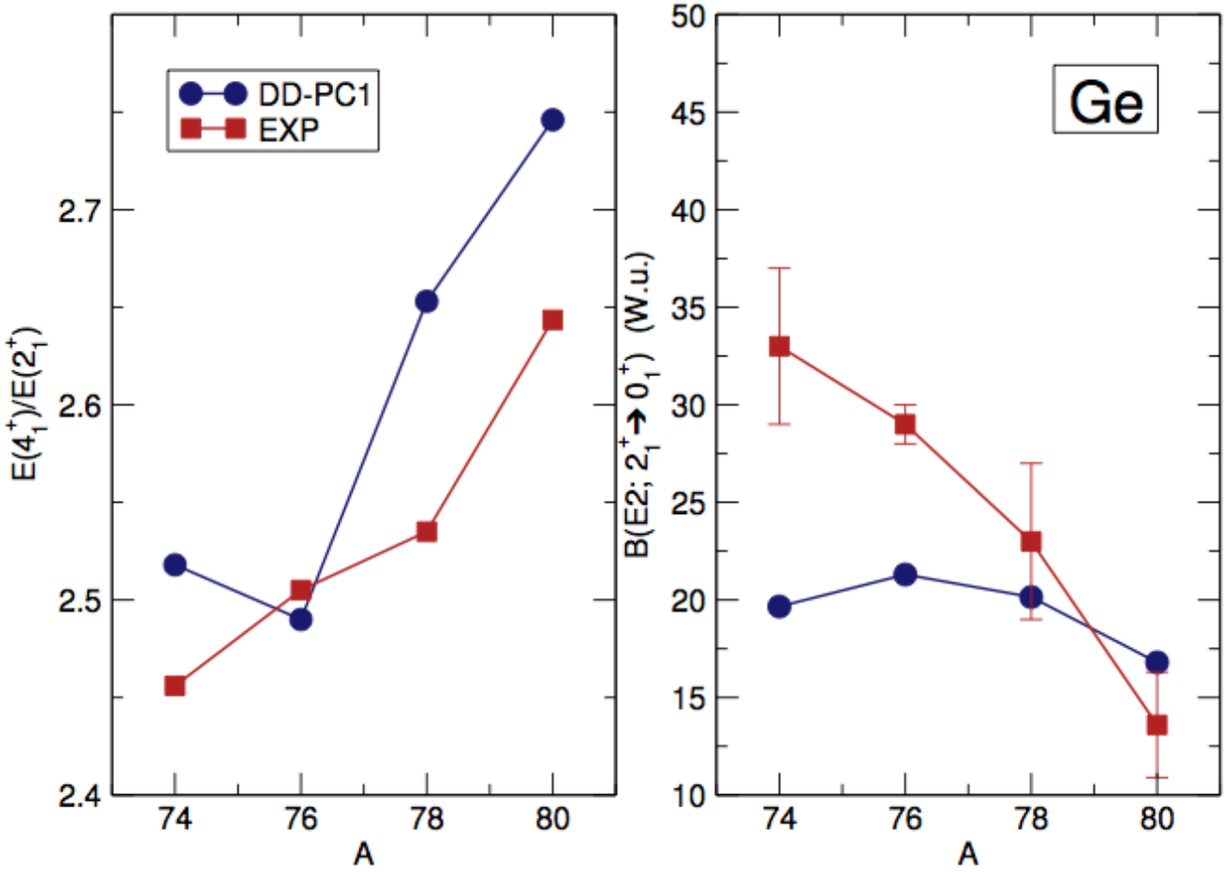


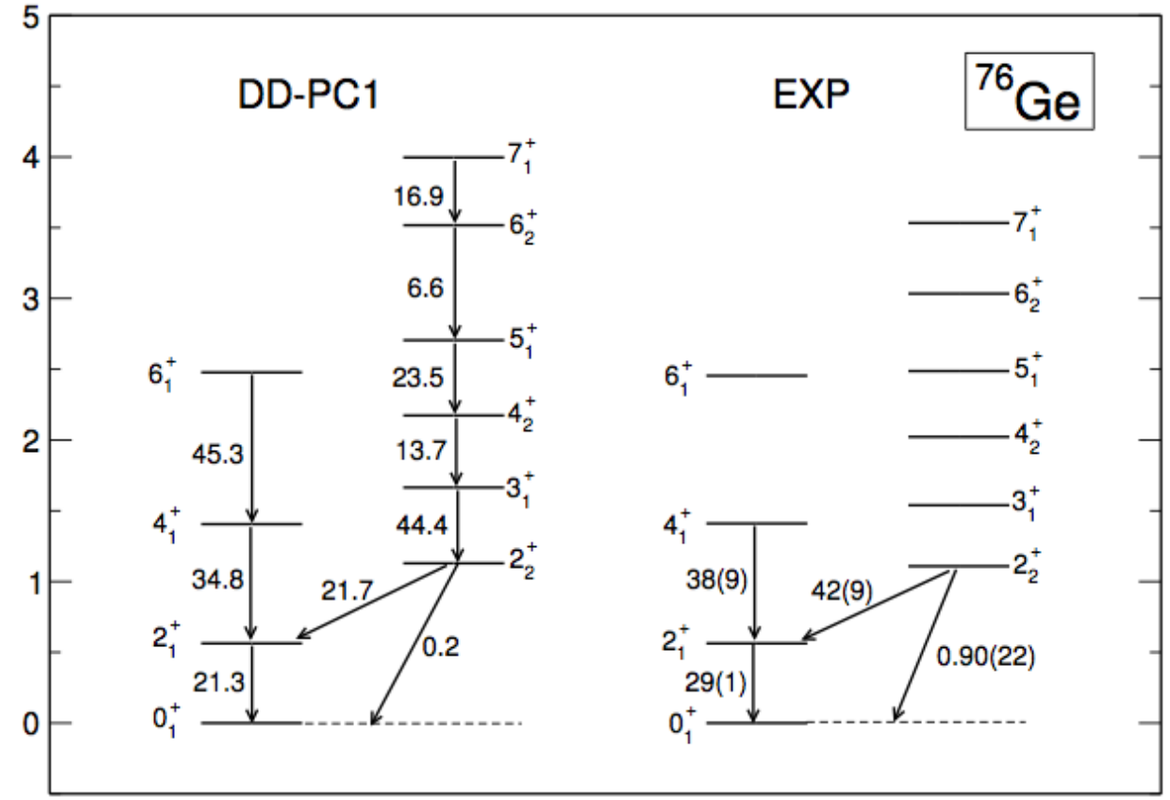

74Ge
E_s.p. (MeV)
π
ν
β
γ (deg)

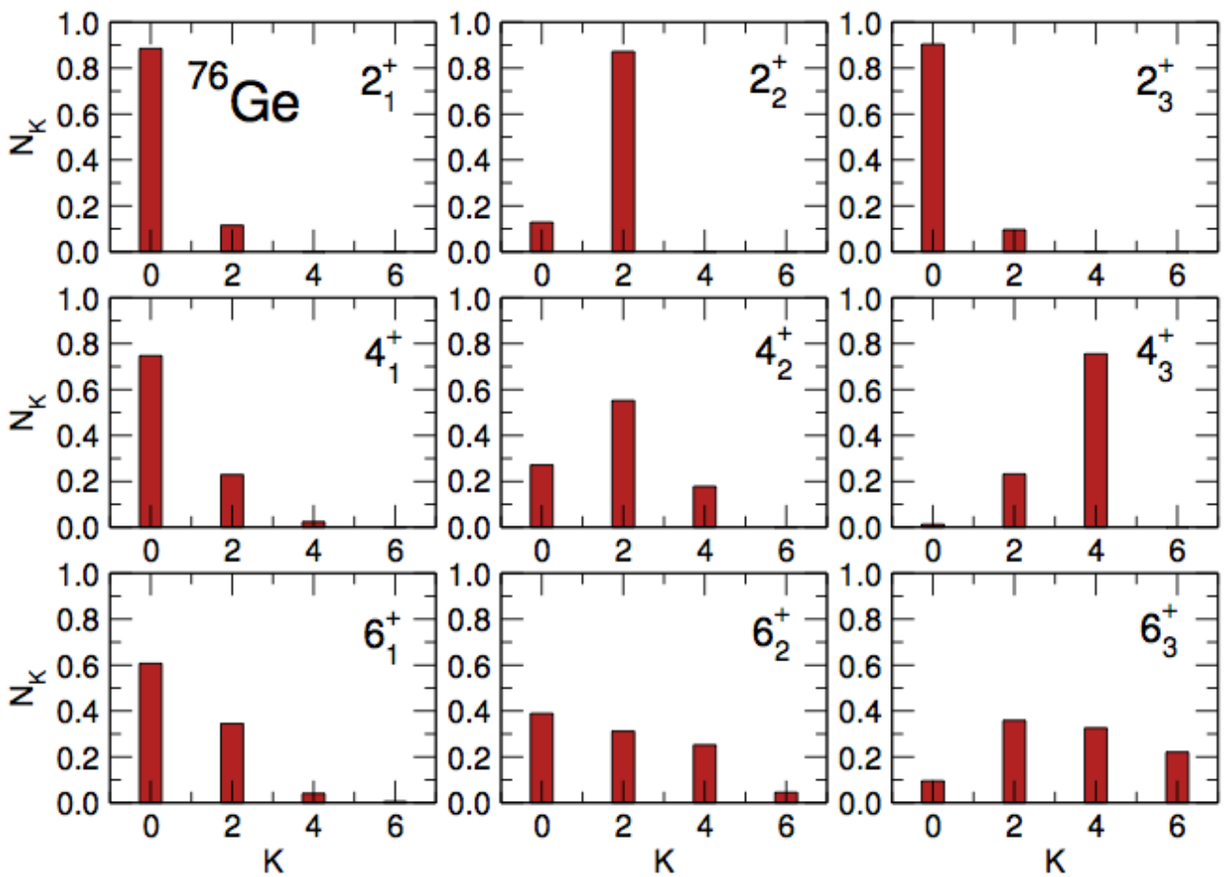

76Ge
E_s.p. (MeV)
π
ν
β
γ (deg)


74Ge, β=0.25
76Ge, β=0.20
78Ge, β=0.20
Binding energy (MeV)
γ (deg)

Quadrupole collective Hamiltonian based on the functional DD-PC1







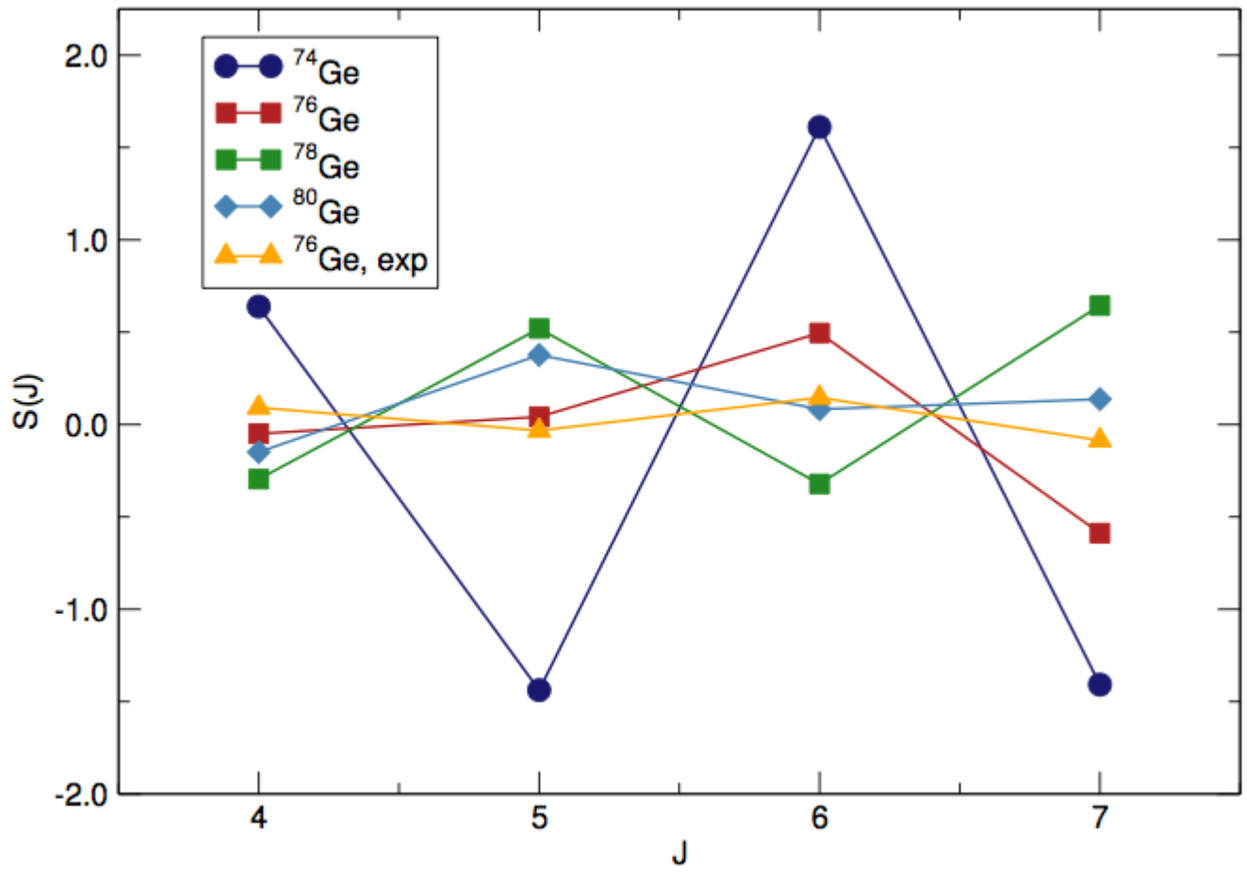
Distribution of *K* components (projection of the angular momentum on the body-fixed symmetry axis) in the collective wave functions of the nucleus ^{76}Ge.

The level of K-mixing is reflected in the staggering in energy between odd- and even-spin states in the γ band:

$$S(J) = \frac{E[J_\gamma^+] - 2E[(J-1)_\gamma^+] + E[(J-2)_\gamma^+]}{E[2_1^+]}$$

Deformed γ-soft potential ⇒ S(J) oscillates between negative values for even-spin states and positive values for odd-spin states.

γ-rigid triaxial potential ⇒ S(J) oscillates between positive values for even-spin states and negative values for odd-spin states.



The mean-field potential of ^{76}Ge is γ soft. The inclusion of collective correlations (symmetry restoration and quantum fluctuations) drives the nucleus toward triaxiality, but they are not strong enough to stabilize a $\gamma \approx 30^\circ$ triaxial shape.

Energy Density Functionals - Covariance Analysis

Quality measure:

$$\chi^2(\mathbf{p}) = \sum_{n=1}^{N} \left(\frac{\mathcal{O}_n^{(\mathrm{th})}(\mathbf{p}) - \mathcal{O}_n^{(\mathrm{exp})}}{\Delta \mathcal{O}_n} \right)^2$$

"Best model" p_0 ⇒

$$\left. \frac{\partial \chi^2(\mathbf{p})}{\partial p_i} \right|_{\mathbf{p}=\mathbf{p}_0} \equiv \partial_i \chi^2(\mathbf{p}_0) = 0 \quad (\text{for } i = 1, \ldots, F)$$

Expand the quality measure around the optimal model p_0 ⇒

$$\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}_0) + \frac{1}{2} \sum_{i,j=1}^{F} (\mathbf{p} - \mathbf{p}_0)_i (\mathbf{p} - \mathbf{p}_0)_j \partial_i \partial_j \chi^2(\mathbf{p}_0) + \ldots$$

dimensionless variables:

$$x_i \equiv \frac{(\mathbf{p} - \mathbf{p}_0)_i}{(\mathbf{p}_0)_i}$$

➔ the quadratic deviations of χ^2 from its minimum value: $\chi^2(\mathbf{p}) - \chi^2(\mathbf{p}_0) \equiv \Delta\chi^2(\mathbf{x}) = \mathbf{x}^T \hat{\mathcal{M}} \mathbf{x}$

The symmetric F×F matrix of second derivatives:

$$\mathcal{M}_{ij} = \frac{1}{2}\left(\frac{\partial \chi^2}{\partial x_i \partial x_j}\right)_{\mathbf{x}=0} = \frac{1}{2}(\mathbf{p}_0)_i (\mathbf{p}_0)_j \partial_i \partial_j \chi^2(\mathbf{p}_0)$$

Diagonalization ⇒

$$\Delta\chi^2(\mathbf{x}) = \mathbf{x}^T\left(\hat{\mathcal{A}}\hat{\mathcal{D}}\hat{\mathcal{A}}^T\right)\mathbf{x} = \xi^T\hat{\mathcal{D}}\xi = \sum_{i=1}^{F}\lambda_i\xi_i^2$$

The deviations of the χ^2 from its minimum value are parameterized in terms of F uncoupled harmonic oscillators → the eigenvalues play the role of the spring constants.

Soft direction ⟹ small eigenvalue λ, little deterioration in χ^2. The corresponding eigenvector ξ involves a particular linear combination of model parameters that is not constrained by the observables included in the fit.

Stiff direction ⟹ large eigenvalue λ, χ^2 rapidly worsens away from minimum, the fit provides a stringent constraint on this particular linear combination of parameters.

… covariance between two observables A and B:

$$\mathrm{cov}(A,B) = \frac{1}{M}\sum_{m=1}^{M}\left[\left(A^{(m)} - \langle A\rangle\right)\left(B^{(m)} - \langle B\rangle\right)\right] = \langle AB\rangle \ - \langle A\rangle\langle B\rangle$$

Pearson product-moment correlation coefficient:

$$\rho(A,B) = \frac{\mathrm{cov}(A,B)}{\sqrt{\mathrm{var}(A)\mathrm{var}(B)}}$$

$$\mathrm{cov}(A,B) = \sum_{i,j=1}^{F}\frac{\partial A}{\partial x_i}\left[\frac{1}{M}\sum_{m=1}^{M}x_i^{(m)}x_j^{(m)}\right]\frac{\partial B}{\partial x_j} \equiv \sum_{i,j=1}^{F}\frac{\partial A}{\partial x_i}C_{ij}\frac{\partial B}{\partial x_j}$$

$$\mathrm{cov}(A,B) = \sum_{i,j=1}^{F}\frac{\partial A}{\partial x_i}(\hat{\mathcal{M}}^{-1})_{ij}\frac{\partial B}{\partial x_j} = \sum_{i=1}^{F}\frac{\partial A}{\partial \xi_i}\lambda_i^{-1}\frac{\partial B}{\partial \xi_i}$$

… relativistic energy density functional DD-PC1 ⇒ is it "predictive" ? Agreement with experiment?
⇒ is it "unique"? A model is unique if all the eigenvalues λ_i of $\mathscr{M}$ are large.

$$\alpha_s(\rho) = a_s + (b_s + c_s x)e^{-d_s x}$$
$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$
$$\alpha_{tv}(\rho) = b_{tv} e^{-d_{tv} x}$$

PARAMETER	
a_s (fm^2)	-10.0462
b_s (fm^2)	-9.1504
c_s (fm^2)	-6.4273
d_s	1.3724
a_v (fm^2)	5.9195
b_v (fm^2)	8.8637
d_v	0.6584
b_{tv} (fm^2)	1.8360
d_{tv}	0.6403
δ_s (fm^4)	-0.8149

Correlations between the lowest-order terms in a Taylor expansion of the density-dependent coupling functions around the saturation point:

$$c_s = -\frac{\rho_{\rm sat}}{d_s} e^{d_s} \left[d_s \alpha_s'(\rho_{\rm sat}) + \rho_{\rm sat} \alpha_s''(\rho_{\rm sat}) \right],$$

$$b_s = c_s \left(\frac{1}{d_s} - 1 \right) - \alpha_s'(\rho_{\rm sat}) \rho_{\rm sat} \frac{e^{d_s}}{d_s},$$

$$a_s = \alpha_s(\rho_{\rm sat}) - (b_s + c_s) e^{-d_s}$$

$$d_v = -\frac{\alpha_v''(\rho_{\rm sat})}{\alpha_v'(\rho_{\rm sat})} \rho_{\rm sat},$$

$$b_v = -\alpha_v'(\rho_{\rm sat}) \frac{e^{d_v}}{d_v},$$

$$a_v = \alpha_v(\rho_{\rm sat}) - b_v e^{-d_v}$$

$$d_{tv} = -\rho_{\rm sat} \frac{\alpha_{tv}'(\rho_{\rm sub})}{\alpha_{tv}(\rho_{\rm sub})},$$

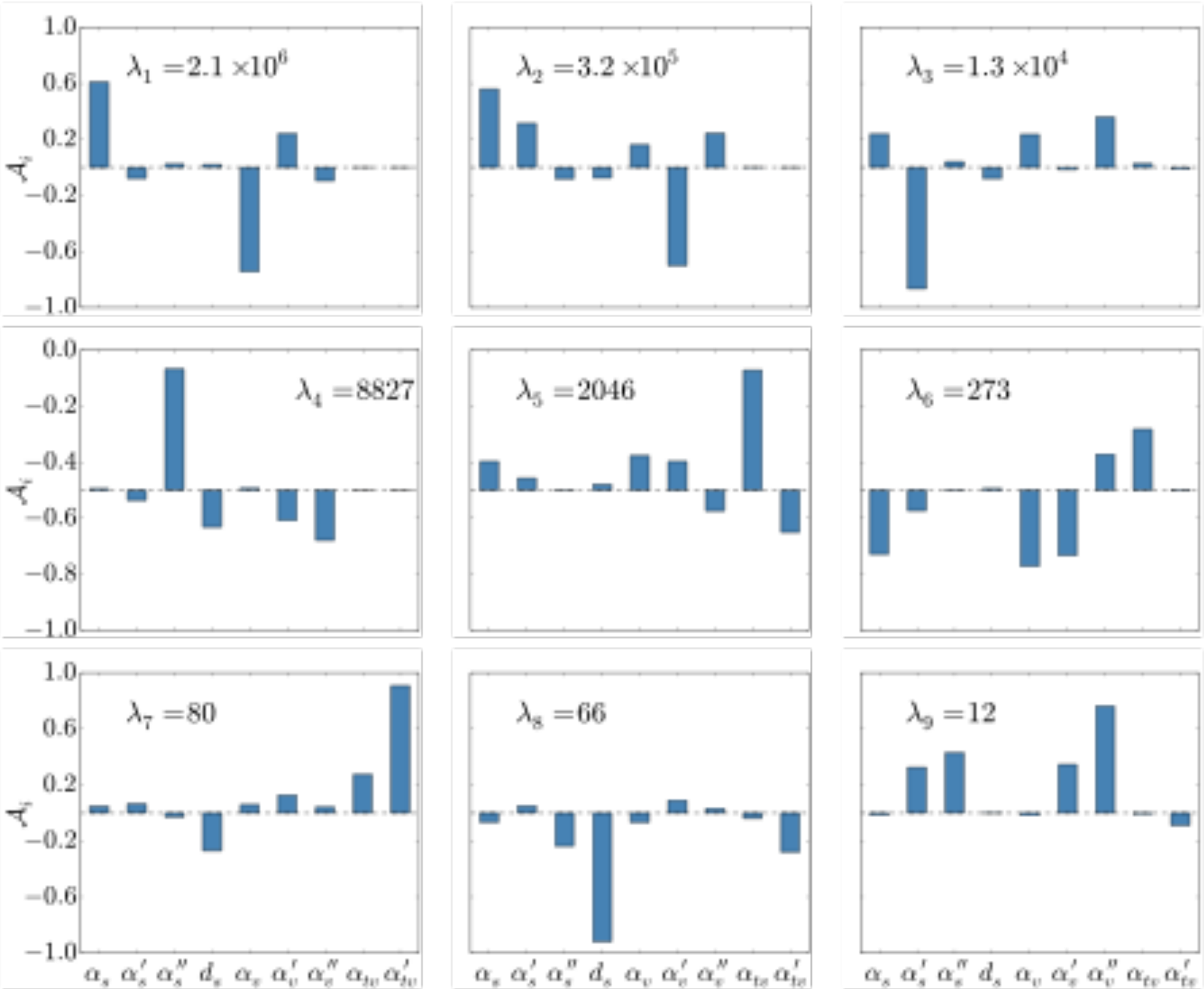
$$b_{tv} = \alpha_{tv}(\rho_{\rm sub}) e^{d_{tv}(\rho_{\rm sub}/\rho_{\rm sat})}$$

$$\rho_{\rm sub} = 0.12 \text{ fm}^{-3}$$

Nuclear matter pseudo-observables

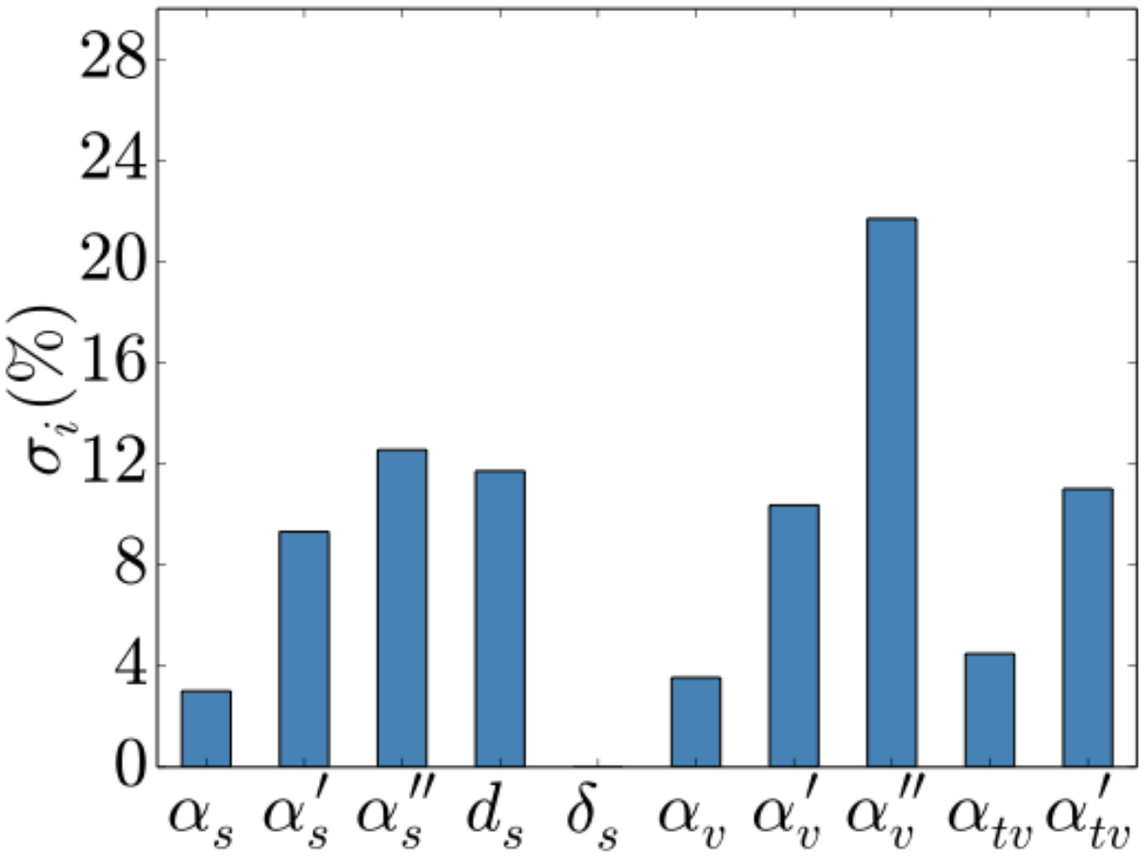
OBSERVABLE	DD-PC1
ρ_0	0.152 fm^{-3}
$\epsilon(\rho_0)$	-16.06 MeV
$\epsilon(\rho_{low})$	-6.48 MeV
$\epsilon(\rho_{high})$	34.38 MeV
K_0	230 MeV
m_D	0.58
m^*	0.66
$S_2(\rho_{\rm sub})$	27.8 MeV
$L(\rho_{\rm sub})$	57.2 MeV
a_4	33 MeV

Eigenvalues and eigenvectors of the 9 × 9 matrix of second derivatives *M* of $\chi^2(p)$ for the functional DD-PC1

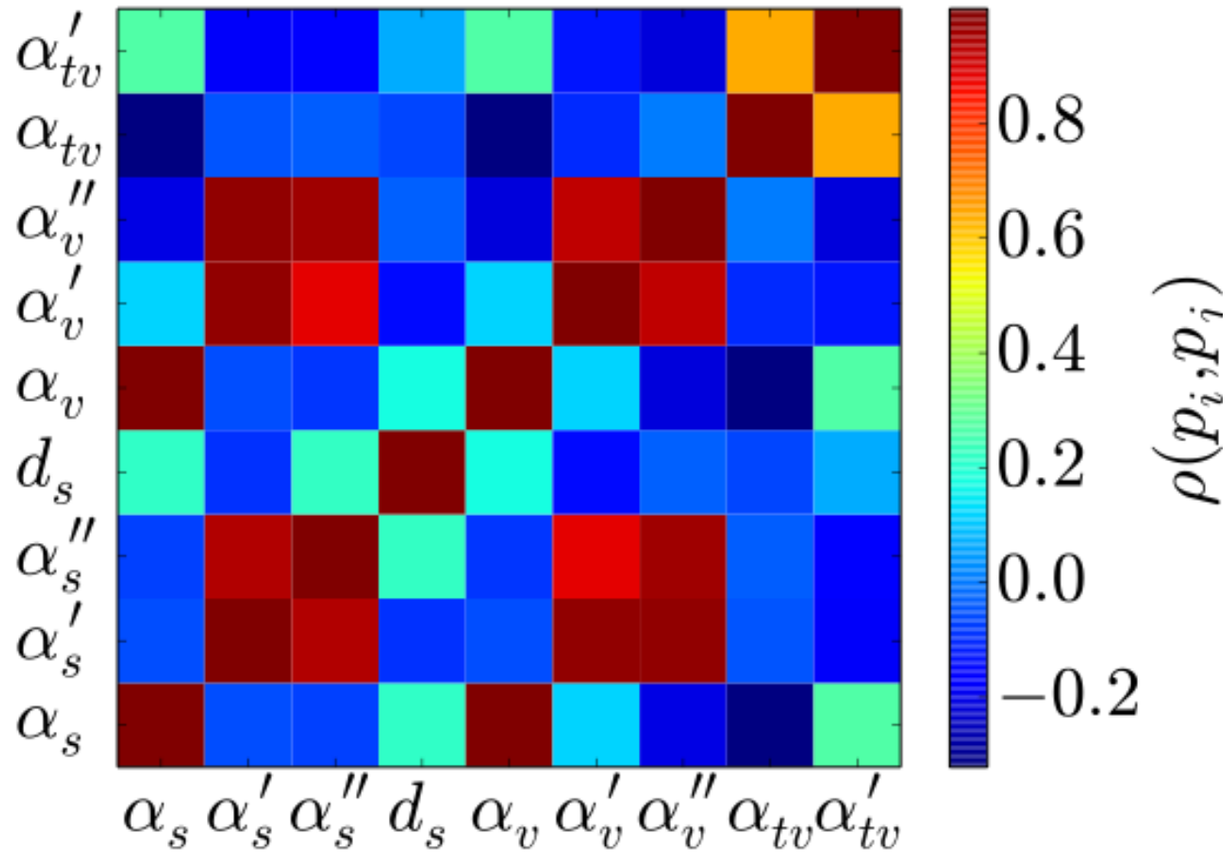


$$\sigma_i^2 = \left(\mathcal{M}^{-1}\right)_{ii} = \left(\mathcal{A}\mathcal{D}^{-1}\mathcal{A}^T\right)_{ii}$$

$$\rho(p_i, p_j) = \frac{\mathcal{M}^{-1}_{ij}}{\sqrt{\mathcal{M}^{-1}_{ii}\mathcal{M}^{-1}_{jj}}}$$



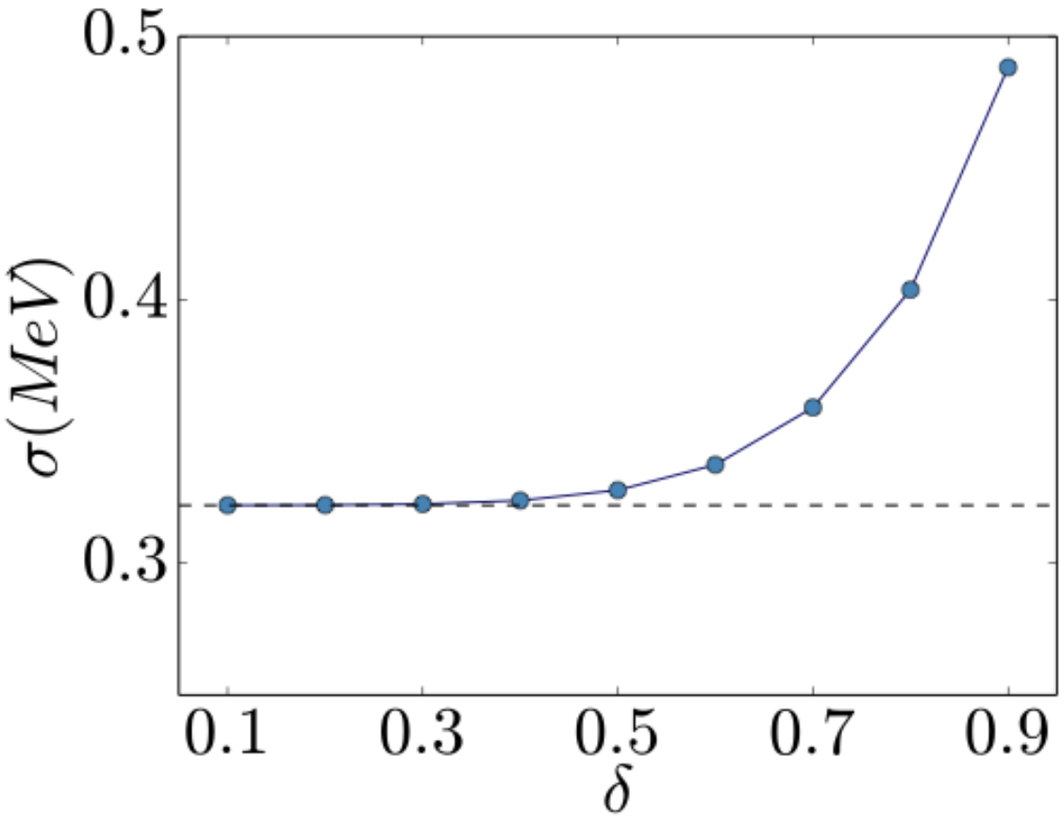
Uncertainties σ_i of model parameters for the functional DD-PC1.

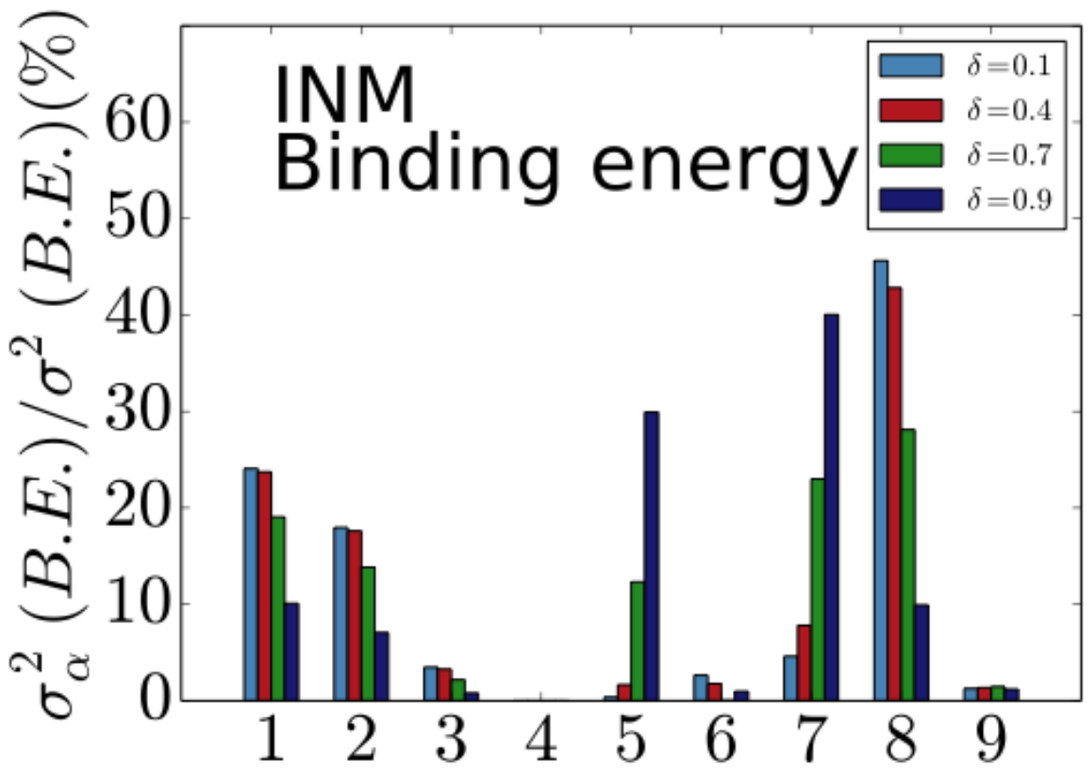


36 independent correlation coefficients between 9 model parameters that contribute to infinite nuclear matter calculations .

$$\sigma(\epsilon(\rho_0)) = \sqrt{\mathrm{var}(\epsilon(\rho_0))}$$

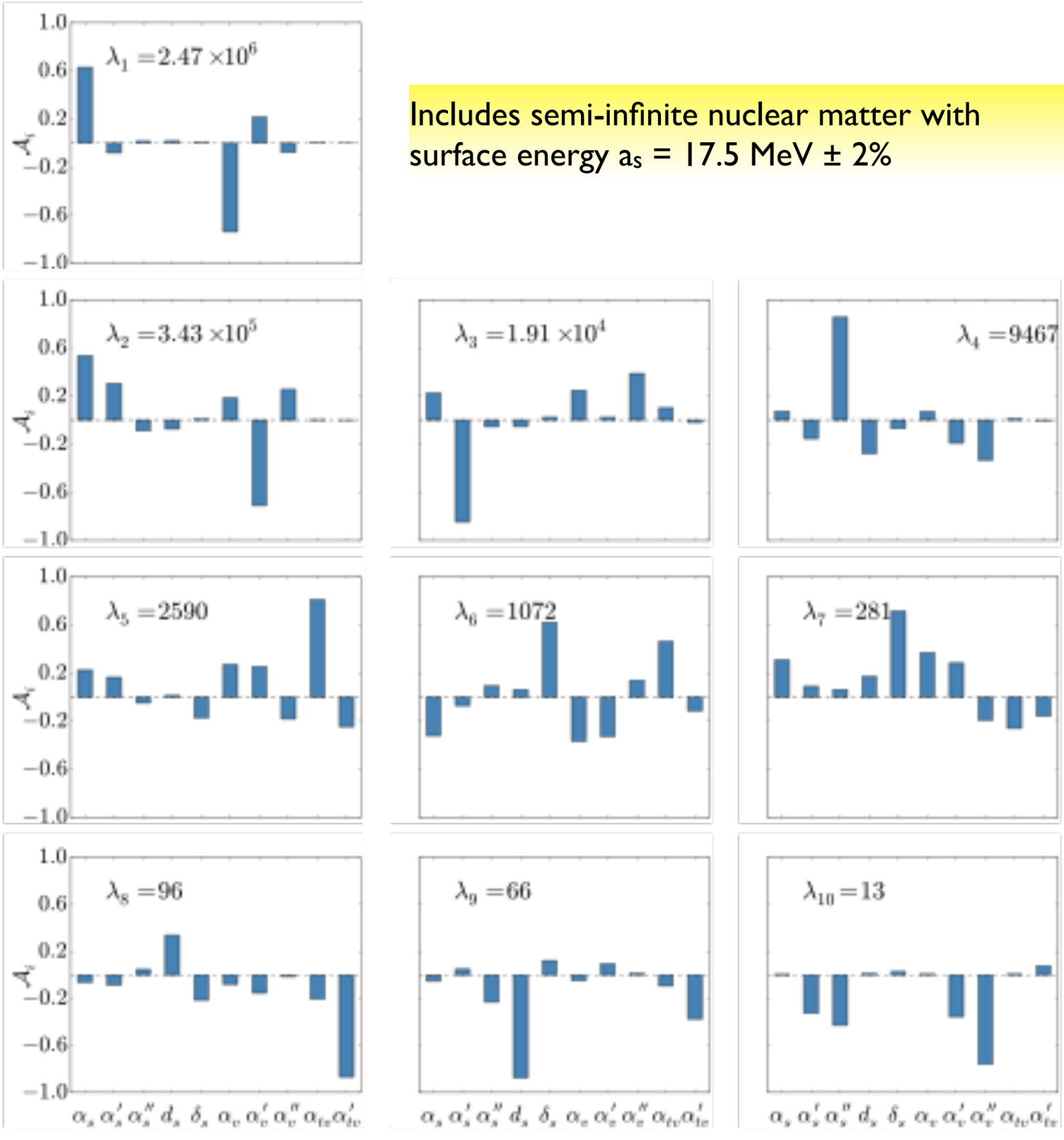
$$\frac{\sigma_\alpha^2(\mathrm{B})}{\sigma^2(\mathrm{B})} = \frac{(\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}{\sum_{\alpha=1}^{F} (\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}$$





Left: calculated uncertainty of the binding energy of asymmetric nuclear matter at the saturation density $\rho_0 = 0.152$ fm^{-3}, as a function of the asymmetry parameter.

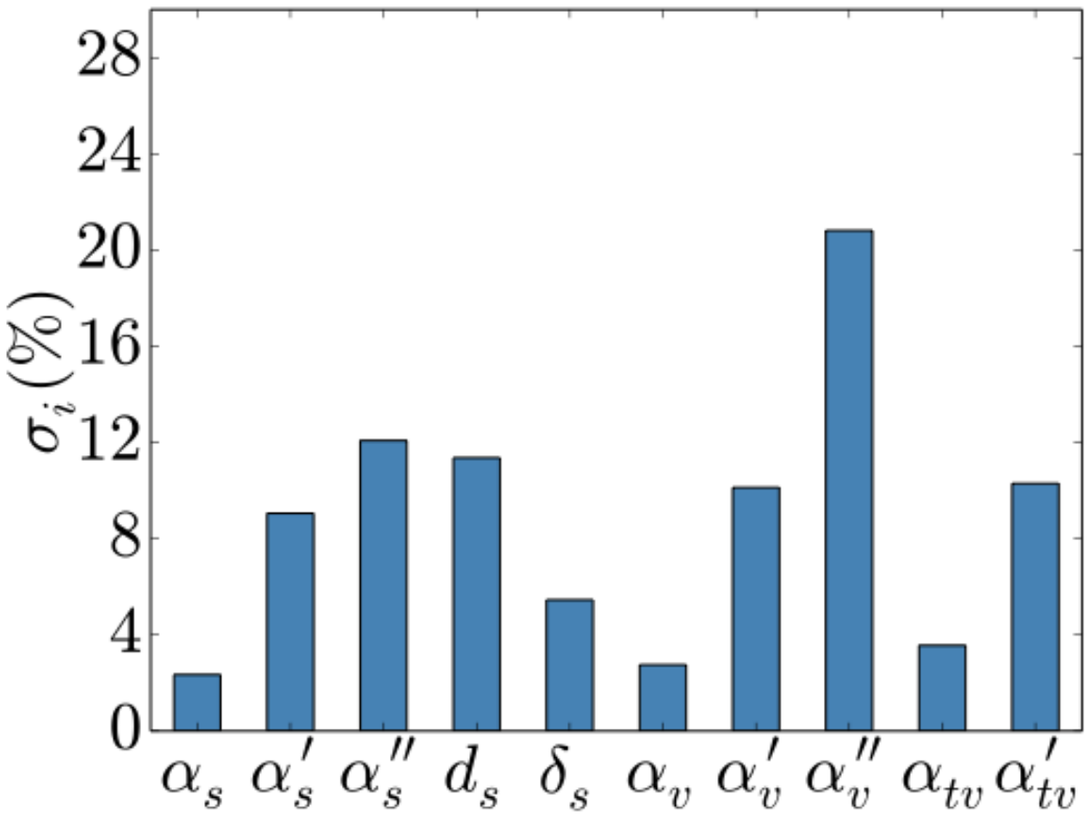
Right: relative contributions in percentage of the nine linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives *M* to the variance of the binding energy of asymmetric nuclear matter.



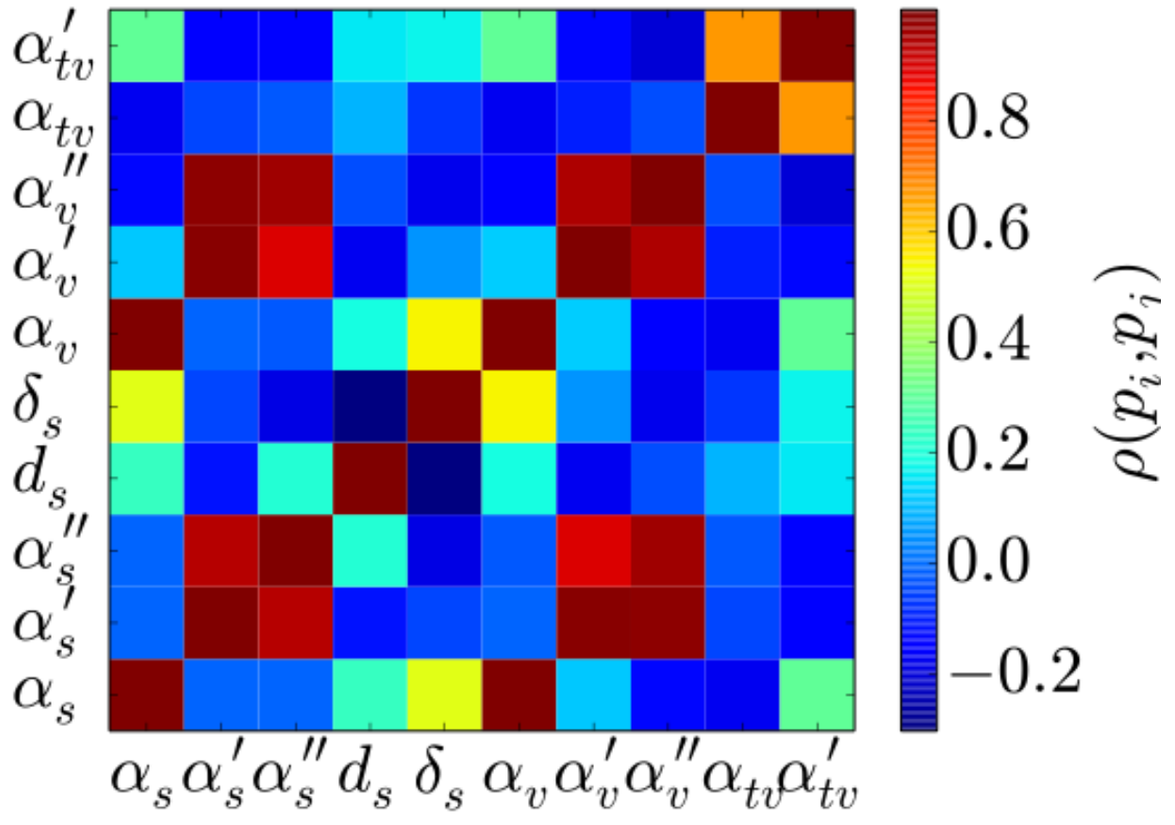
Includes semi-infinite nuclear matter with surface energy a_s = 17.5 MeV ± 2%

$$\sigma_i^2 = (\mathcal{M}^{-1})_{ii} = (AD^{-1}A^T)_{ii}$$

$$\rho(p_i, p_j) = \frac{\mathcal{M}^{-1}_{ij}}{\sqrt{\mathcal{M}^{-1}_{ii}\mathcal{M}^{-1}_{jj}}}$$



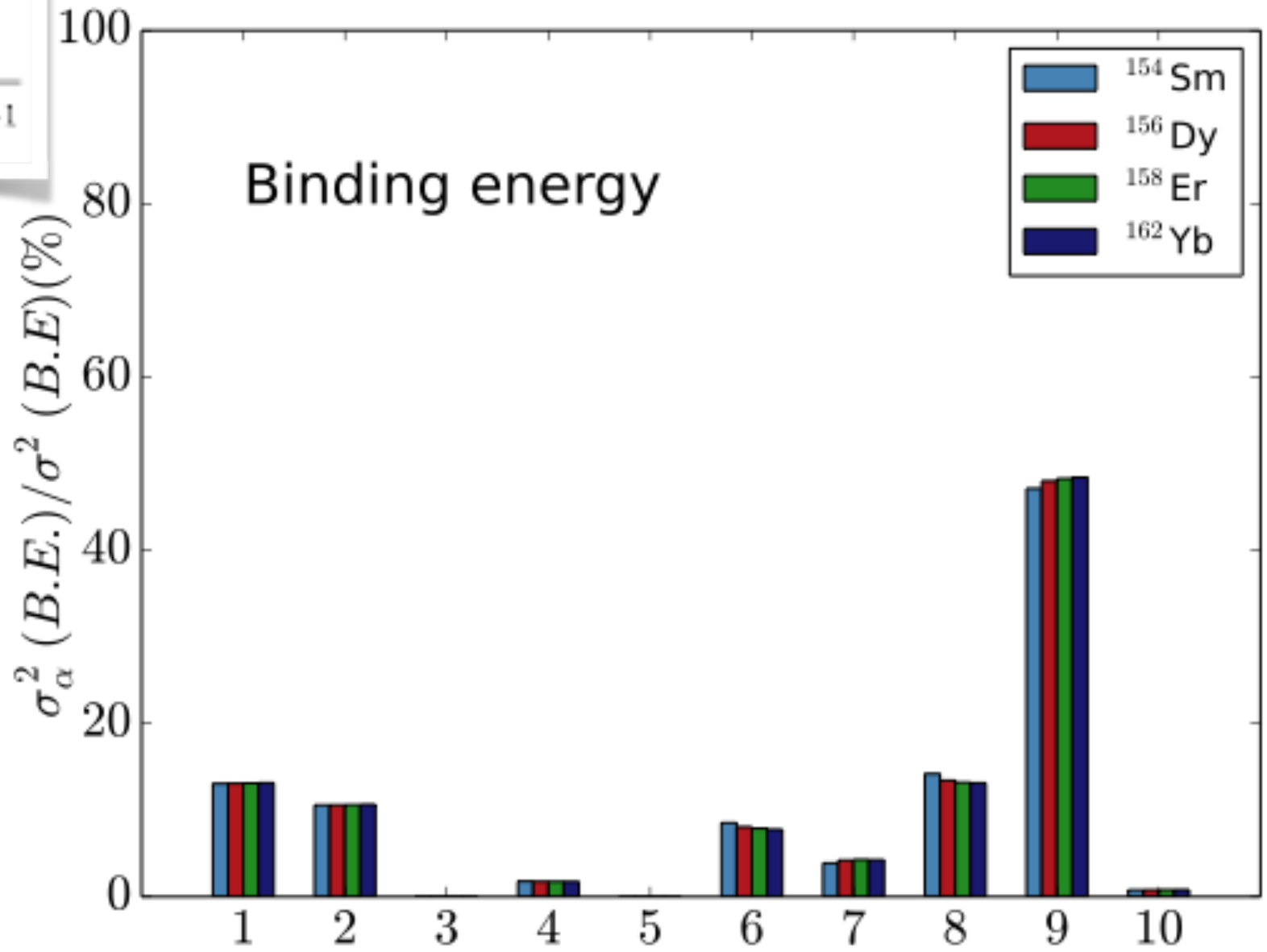
Uncertainties σ_i of model parameters for the functional DD-PC1.



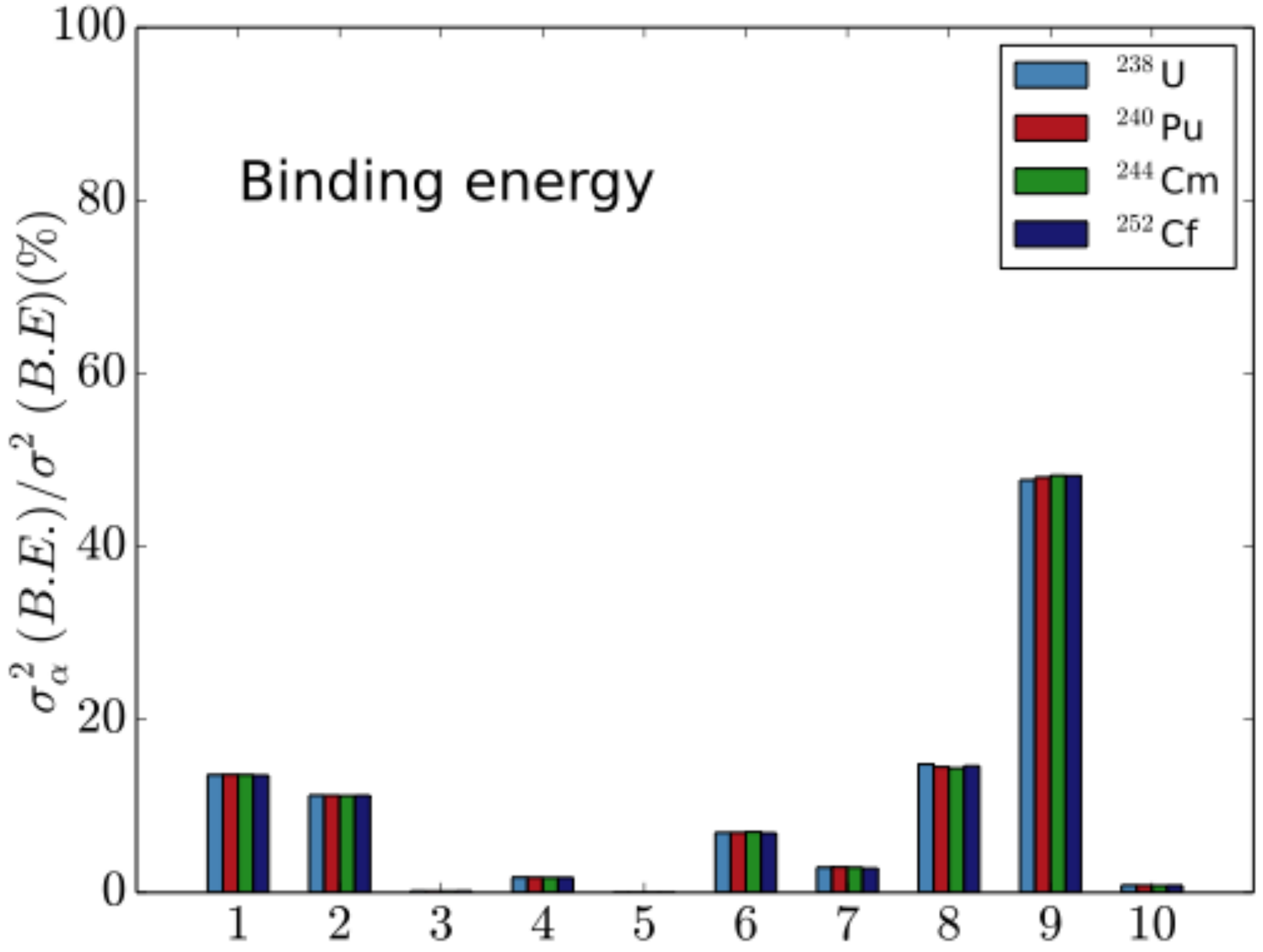
45 independent correlation coefficients between 10 model parameters that contribute to semi-infinite nuclear matter calculations .

Finite nuclei

$$\frac{\sigma_\alpha^2(\mathrm{B})}{\sigma^2(\mathrm{B})} = \frac{(\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}{\sum_{\alpha=1}^{F} (\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}$$

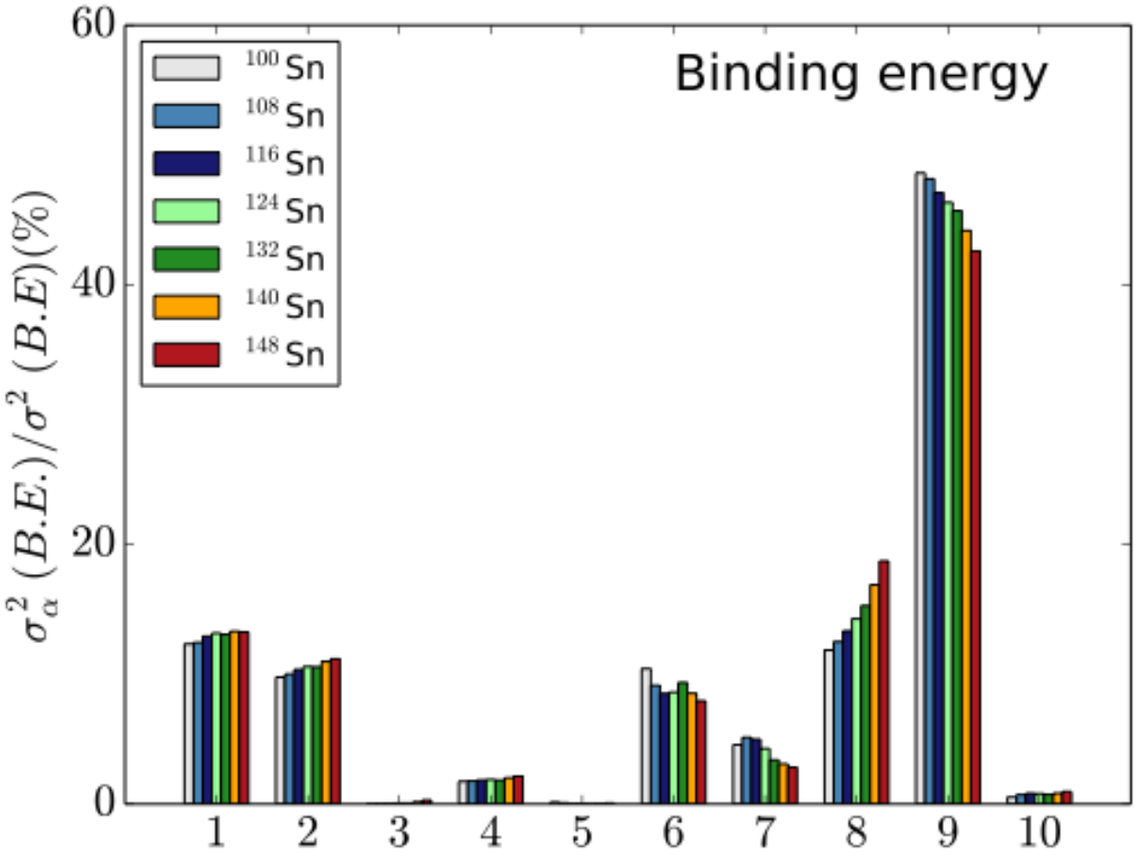


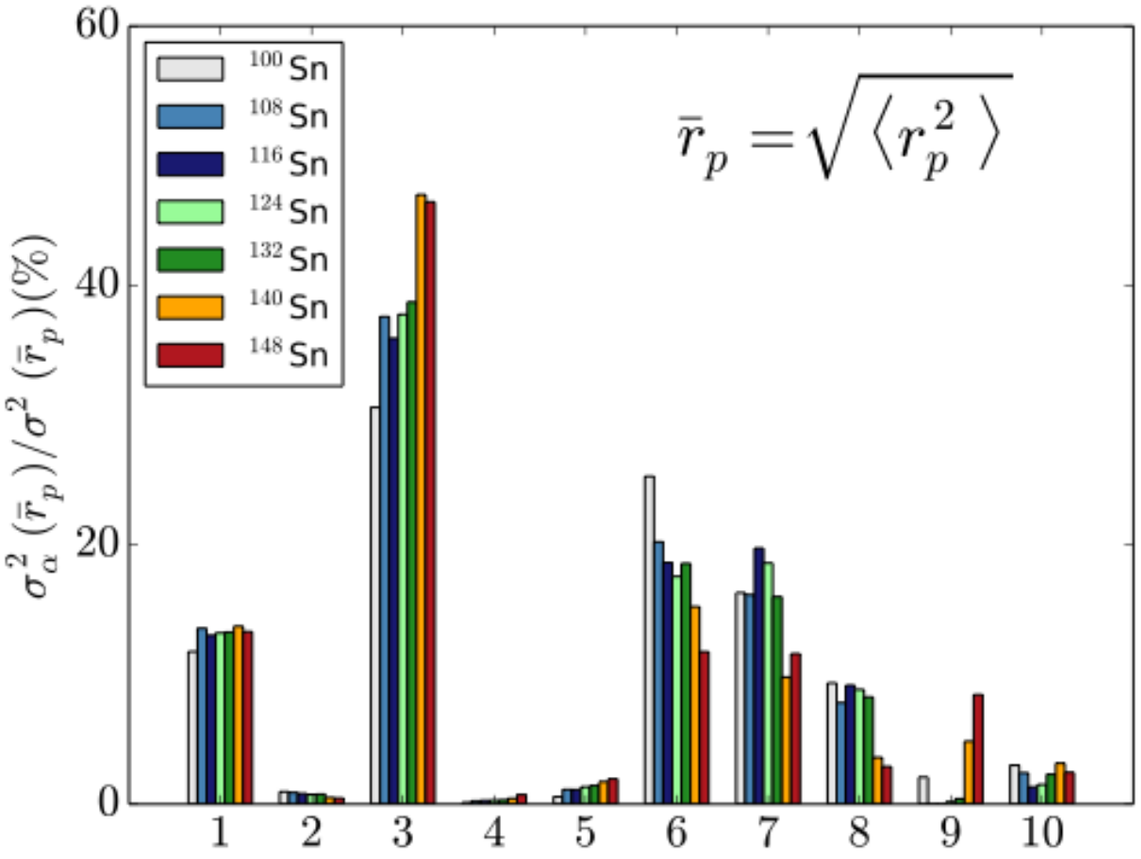
Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives $\mathscr{M}$ to the variances of the binding energy of rare-earth nuclei.



Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives $\mathscr{M}$ to the variances of the binding energy of actinide nuclei.

$$\frac{\sigma_\alpha^2(\mathrm{B})}{\sigma^2(\mathrm{B})} = \frac{(\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}{\sum_{\alpha=1}^{F} (\frac{\partial \mathrm{B}}{\partial \xi_\alpha})^2 \lambda_\alpha^{-1}}$$





Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives $\mathscr{M}$ to the variances of the binding energy and radius of the proton distribution of tin isotopes.

A simple analysis of the quality measure χ^2 around the minimum in nuclear matter can be used as a starting point in the determination of the functional density dependence of a nuclear EDF, and in the selection of the type of data that can constrain the values of model parameters.

How do uncertainties and correlations between parameters of a nuclear EDF propagate into models of nuclear structure (RPA, collective Hamiltonian etc) that are used to compute spectroscopic properties.