

Nuclear Energy Density Functionals

From Stable to Weakly-Bound Nuclei

Elements of Density Functional Theory

DFT is the most popular method for electronic structure calculations of many-electron systems. No other method achieves comparable accuracy at the same computational cost.

A. The Hohenberg-Kohn Theorem

In ground-state DFT one is interested in systems of N interacting electrons described by the Hamiltonian:

$$\begin{aligned} H &= T + V + V_{ee} \\ &= - \sum_{i=1}^N \frac{\nabla_i^2}{2} + \sum_{i=1}^N v(\mathbf{r}_i) + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \end{aligned}$$

The Hohenberg-Kohn theorem:

1. The ground state density $n(\mathbf{r})$ of a bound system of interacting electrons uniquely determines the external potential $v(\mathbf{r})$ in which the electrons move and thus all physical properties of the system.
2. The ground-state energy E_0 and the ground-state density $n_0(\mathbf{r})$ of a system characterized by the potential $v_0(\mathbf{r})$ can be obtained from a variational principle which involves only the density:

$$E_0 = E_{v_0}[n_0] < E_{v_0}[n]$$

→ the energy can be written as a functional of the density, $E_{v_0}[n]$, which gives the ground-state energy E_0 if and only if the true ground-state density $n_0(\mathbf{r})$ is inserted.

3. There exists a functional $F[n]$ such that the energy functional can be written as:

$$E_{v_0}[n] = F[n] + \int d^3r v_0(\mathbf{r})n(\mathbf{r})$$

The functional $F[n]$ is **universal** in the sense that, for a given particle-particle interaction (the Coulomb interaction in this case), it is independent of the potential $v_0(\mathbf{r})$ of the particular system under consideration, i.e., it has the same functional form for all systems.

→ formal definition of the Hohenberg-Kohn functional $F[n]$:

$$F[n] = T[n] + V_{ee}[n] = \langle \Psi[n] | T | \Psi[n] \rangle + \langle \Psi[n] | V_{ee} | \Psi[n] \rangle$$

However, the explicit density dependence of $F[n]$ remains unknown!

B. Kohn-Sham DFT

Consider an auxiliary system of N **non-interacting** particles described by the Hamiltonian:

$$H_s = T + V_s$$

HK theorem \Rightarrow there exists a unique energy functional:

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

for which the variational equation yields the exact ground-state density $n_s(\mathbf{r})$ that corresponds to H_s . $T_s[n]$ - universal kinetic energy functional of non-interacting particles.

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

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

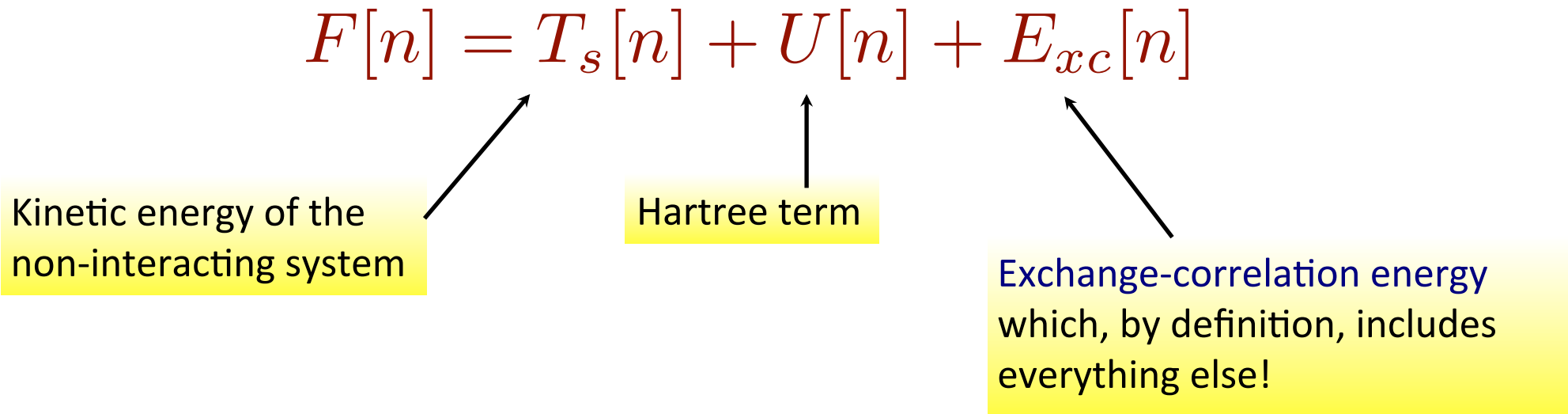
The single-particle orbitals are solutions of the Kohn-Sham equations:

$$\left[-\nabla^2/2 + v_s(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

The Hohenberg-Kohn functional is partitioned in the following way:

$$F[n] = T_s[n] + U[n] + E_{xc}[n]$$

Kinetic energy of the
non-interacting system



Hartree term

Exchange-correlation energy
which, by definition, includes
everything else!

$$U[n] = \frac{1}{2} \int d^3r \int d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

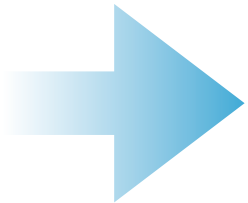
→ classical electrostatic energy of the charge distribution $n(\mathbf{r})$.

The Kohn-Sham potential:

$$v_s[n(\mathbf{r})] = v(\mathbf{r}) + \int d^3r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[n(\mathbf{r})]$$

where the **exchange-correlation potential** is defined by:

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



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

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

C. Approximations for E_{xc}

The true E_{xc} is a universal functional of the density, i.e. it has the same functional form for all systems.

(i) local density approximation (LDA):

$$E_{xc}^{LDA}[n] = \int d^3r \, n(\mathbf{r}) e_{xc}^{unif}(n(\mathbf{r}))$$

where $e_{xc}^{unif}(n)$ is the exchange-correlation energy per particle of the homogeneous electron gas with spatially uniform density n .

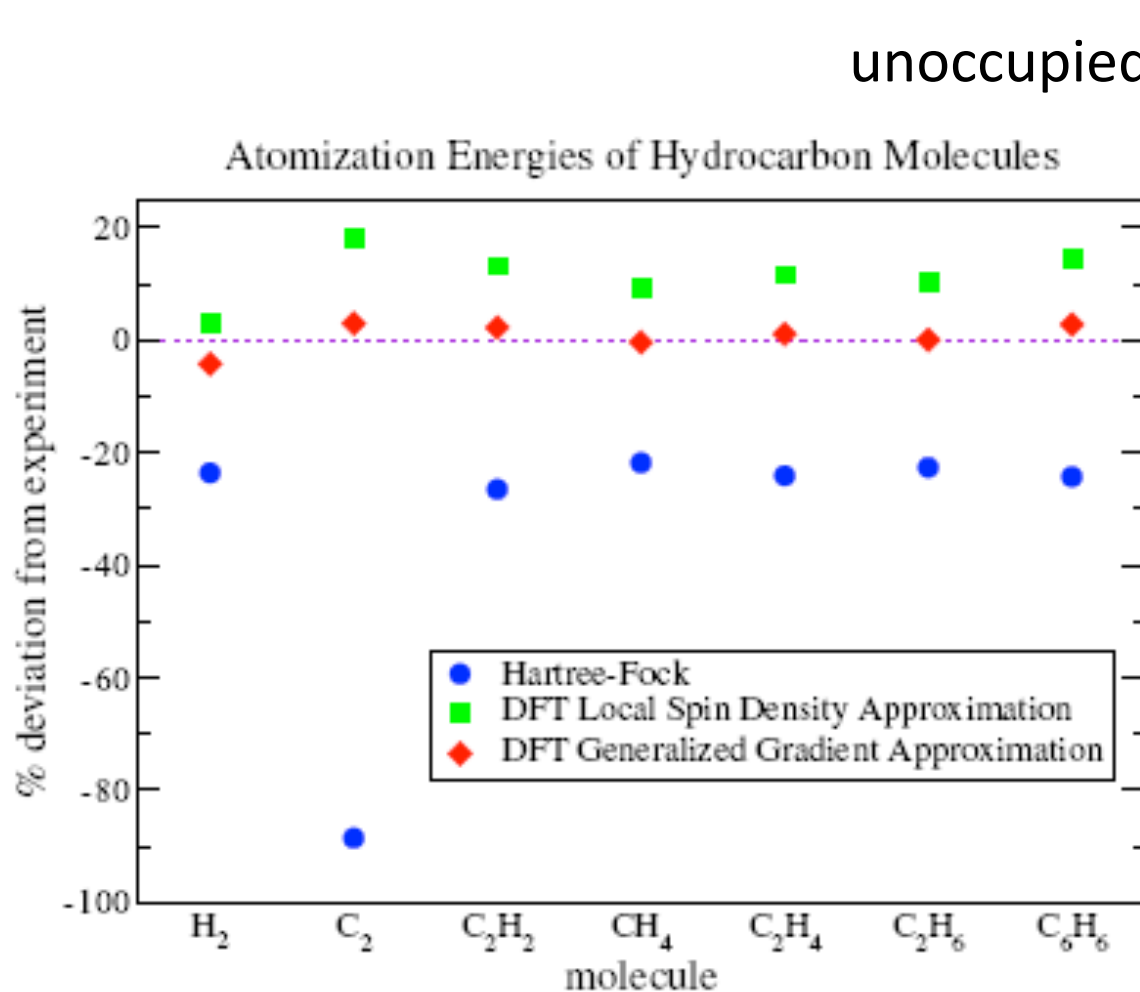
(ii) generalized gradient approximations (GGAs):

$$E_{xc}^{GGA}[n] = \int d^3r \, f(n(\mathbf{r}), \nabla n(\mathbf{r}))$$

→ the function f in GGA is not unique and many different forms have been considered.

Exchange-correlation functional:

Heaven of chemical accuracy



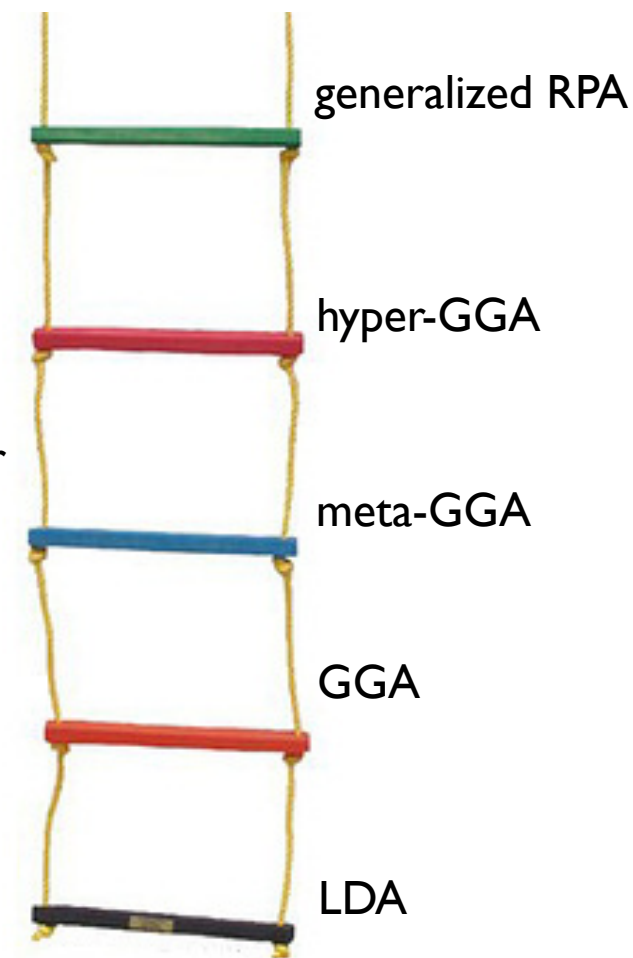
unoccupied $\{\Psi_i\}$

ϵ_x

τ and/or
 $\nabla^2 \rho$

$\nabla \rho$

ρ



Hartree world

Jacob's ladder of DFT approximations for E_{xc}

Nuclear Energy Density Functionals

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

The ***self-consistent mean-field*** approach to nuclear many-body problem is analogous to ***Kohn-Sham DFT***, and provides a unified microscopic description of the structure of stable nuclei and systems far from stability.

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

Local densities and currents

The full density matrix can be decomposed into four separate spin-isospin terms:

$$\begin{aligned} \rho(\mathbf{r}\sigma\tau, \mathbf{r}'\sigma'\tau') \\ = \frac{1}{4} \left\{ \left[\rho_{00}(\mathbf{r}, \mathbf{r}') \delta_{\sigma\sigma'} + \mathbf{s}_{00}(\mathbf{r}, \mathbf{r}') \cdot \boldsymbol{\sigma}_{\sigma'\sigma} \right] \delta_{\tau\tau'} \right. \\ \left. + \sum_{\alpha=-1}^{+1} \left[\rho_{1\alpha}(\mathbf{r}, \mathbf{r}') \delta_{\sigma\sigma'} + \mathbf{s}_{1\alpha}(\mathbf{r}, \mathbf{r}') \cdot \boldsymbol{\sigma}_{\sigma'\sigma} \right] (\tau_{\tau'\tau})_{\alpha} \right\} \end{aligned}$$

where: $\boldsymbol{\sigma}_{\sigma'\sigma} = (\sigma' | \hat{\boldsymbol{\sigma}} | \sigma)$, $\boldsymbol{\tau}_{\tau'\tau} = (\tau' | \hat{\boldsymbol{\tau}} | \tau)$

For pure proton and neutron states only the $\alpha = 0$ components of the isovector densities contribute.

There are six local densities and currents that can be derived from the full density matrix. We omit the second index in the densities, and with T=0 or 1:

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:

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

Spin-current tensor:

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

Kinetic density:

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

Kinetic spin-density:

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

The Skyrme energy density functional

In the Skyrme KS approach, the total binding energy is given by the sum of the kinetic energy, the Skyrme energy functional that models the effective interaction between nucleons, the Coulomb energy, the pair energy, and corrections for spurious motions:

$$E = E_{\text{kin}} + \int d^3r \mathcal{E}_{\text{Sk}} + E_{\text{Coul}} + E_{\text{pair}} - E_{\text{corr}}$$

The Skyrme energy functional:

$$\mathcal{E}_{\text{Sk}} = \sum_{T=0,1} \left(\mathcal{E}_T^{\text{even}} + \mathcal{E}_T^{\text{odd}} \right)$$

Density-dependent coefficients

Contains only time-even dens.

Dependence on time-odd currents

$$\mathcal{E}_T^{\text{even}} = C_T^\rho \rho_T^2 + C_T^{\Delta\rho} \rho_T \Delta\rho_T + C_T^\tau \rho_T \tau_T + C_T^J \mathcal{J}_T^2 + C_T^{\nabla J} \rho_T \nabla \cdot \mathbf{J}_T$$

$$\begin{aligned} \mathcal{E}_T^{\text{odd}} = & C_T^s \mathbf{s}_T^2 + C_T^{\Delta s} \mathbf{s}_T \cdot \Delta \mathbf{s}_T + C_T^{sT} \mathbf{s}_T \cdot \mathbf{T}_T \\ & + C_T^{\nabla s} (\nabla \cdot \mathbf{s}_T)^2 + C_T^j \mathbf{j}_T^2 + C_T^{\nabla j} \mathbf{s}_T \cdot \nabla \times \mathbf{j}_T \end{aligned}$$

does not contribute for even-even nuclei!

Single-particle hamiltonian:

The contribution from the Skyrme interaction to the single-particle Hamiltonian:

$$\hat{h}_q = U_q - \nabla \cdot B_q \nabla - \frac{i}{2} \{ \mathcal{W}_q, \nabla \sigma \} + \mathbf{S}_q \cdot \hat{\boldsymbol{\sigma}} - \nabla \cdot (\hat{\boldsymbol{\sigma}} \cdot \mathbf{C}_q) \nabla - \frac{i}{2} \{ \mathbf{A}_q, \nabla \}$$

where:
$$\{ \mathcal{W}_q, \nabla \sigma \} = \sum_{ij} \{ W_{ij}, \nabla_i \hat{\sigma}_j \} \quad (q = p, n)$$

→ the local potentials are calculated from:

time-even:
$$U_q = \frac{\delta E}{\delta \rho_q}, \quad B_q = \frac{\delta E}{\delta \tau_q}, \quad \mathcal{W}_q = \frac{\delta E}{\delta \mathcal{J}_q}$$

time-odd:
$$\mathbf{A}_q = \frac{\delta E}{\delta \mathbf{j}_q}, \quad \mathbf{S}_q = \frac{\delta E}{\delta \mathbf{s}_q}, \quad \mathbf{C}_q = \frac{\delta E}{\delta \mathbf{T}_q}$$

The time-odd fields A, C, and S contribute to the single-particle Hamiltonian only in situations where the intrinsic time-reversal symmetry is broken and the Kramers degeneracy of single-particle levels is removed.

Gogny interaction: sum of two Gaussians with space, spin and isospin exchange mixtures. In addition, a density-dependent interaction plus a spin-orbit term.

$$\begin{aligned}\hat{v}_{\text{Gogny}}(\mathbf{r}_{12}) = & \sum_{j=1}^2 e^{-(\mathbf{r}_{12}/\mu_j)^2} (W_j + B_j \hat{P}_\sigma - H_j \hat{P}_\tau - M_j \hat{P}_\sigma \hat{P}_\tau) \\ & + t_3 \left(1 + x_0 \hat{P}_\sigma\right) \delta(\mathbf{r}_{12}) \rho^\alpha \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right) \\ & + i W_{ls} (\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2) \cdot \hat{\mathbf{k}}^\dagger \times \delta(\mathbf{r}_{12}) \hat{\mathbf{k}}\end{aligned}$$

Exchange operators:

$$\begin{aligned}\hat{P}_\sigma &= \frac{1}{2}(1 + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2) & \hat{P}_\tau &= \frac{1}{2}(1 + \hat{\tau}_1 \cdot \hat{\tau}_2) \\ \mathbf{r}_{12} &= \mathbf{r}_1 - \mathbf{r}_2 & \hat{\mathbf{k}} &= -\frac{i}{2}(\nabla_1 - \nabla_2)\end{aligned}$$

The Gogny interaction is used both in the mean-field and pairing channels.

PAIRING CORRELATIONS

The pairing-energy functional:
$$E_{\text{pair}} = \sum_{q=p,n} \frac{V_q}{4} \int d^3r \left[1 - \left(\frac{\rho(\mathbf{r})}{\rho_c} \right)^\beta \right] \tilde{\rho}_q^2(\mathbf{r})$$

corresponds to the density-dependent two-body zero-range local pairing force:

$$v_{\text{pair}} = \frac{V_0}{2} (1 - \hat{P}_\sigma) \left[1 - \left(\frac{\rho(\mathbf{r}_1)}{\rho_c} \right)^\beta \right] \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

Volume pairing
 $\rho_c \rightarrow \infty$

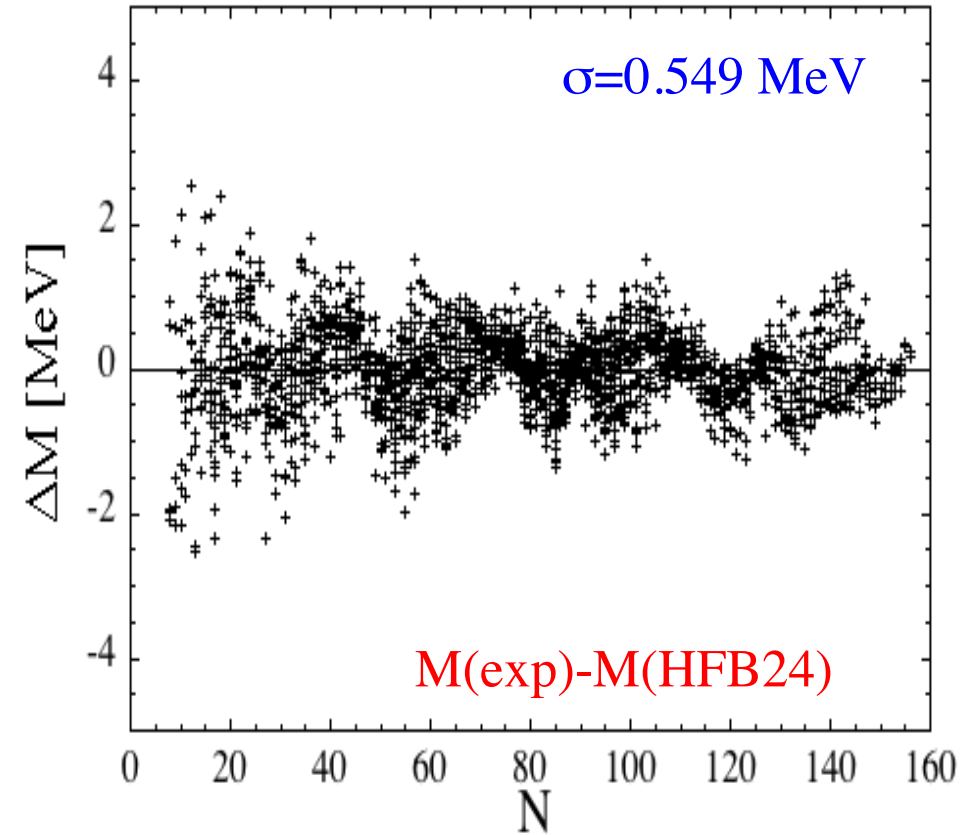
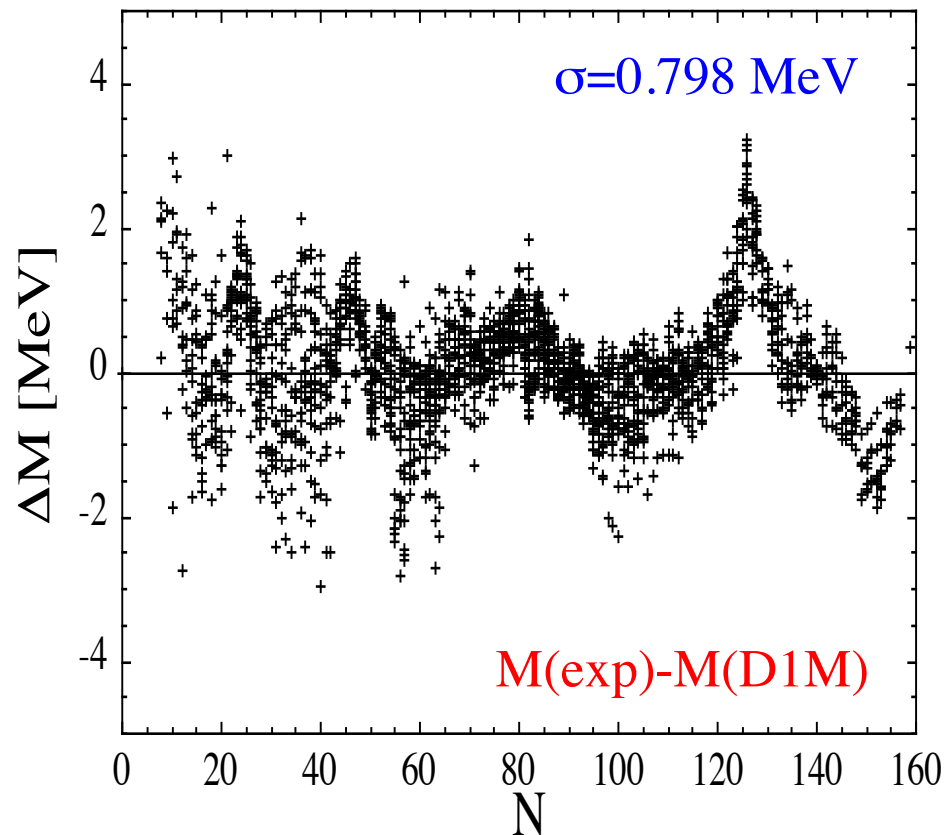
Surface pairing
 $\rho_c \approx \rho_{\text{nm}}$

The pairing strengths $V_{p,n}$ are adjusted phenomenologically to reproduce the **odd-even staggering** of energies in selected chains of nuclei.

Applications: ground-state properties

Binding Energies

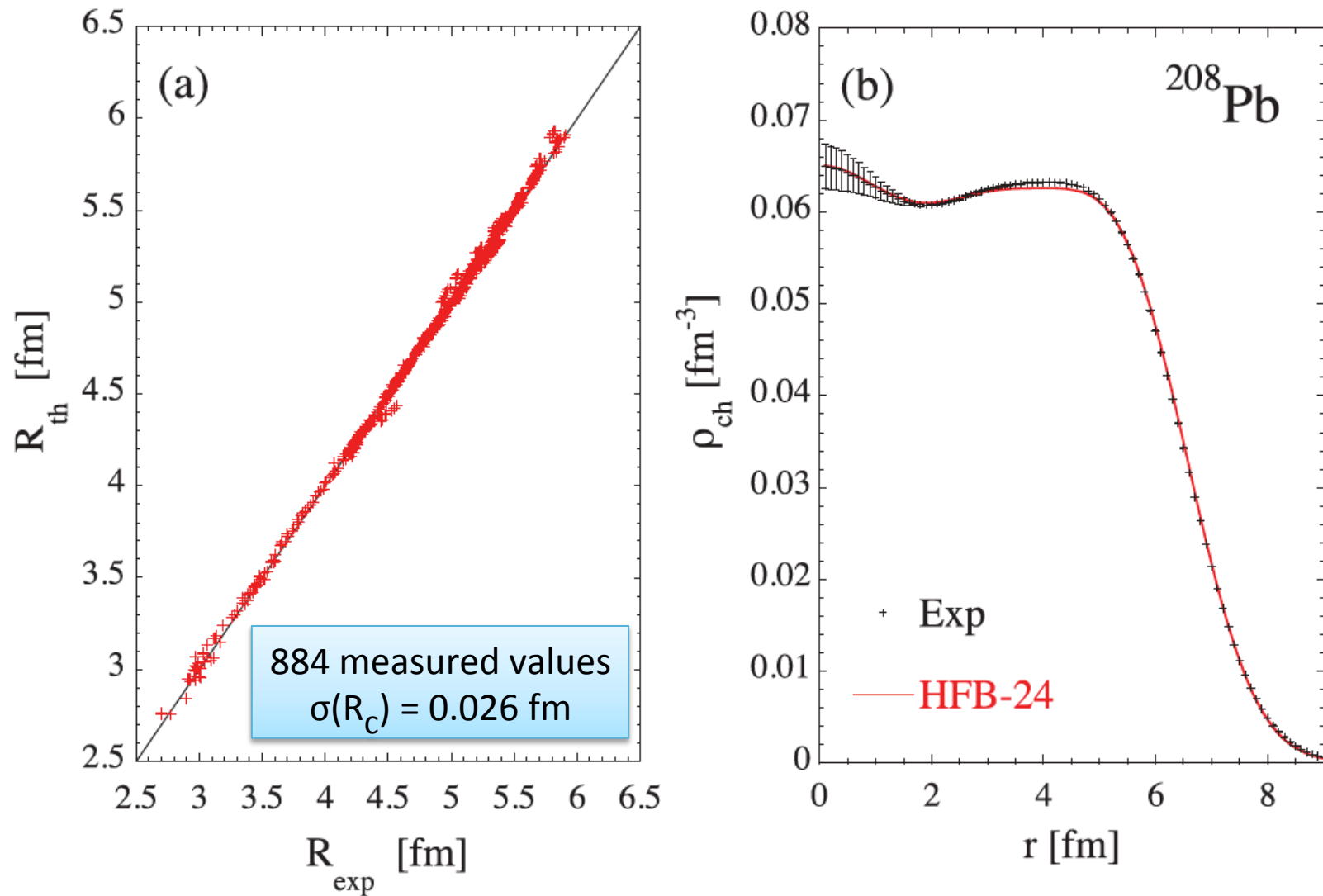
Microscopic Gogny and Skyrme Hartree-Fock-Bogoliubov mass tables:



Differences between experimental and calculated masses as a function of neutron number.

Root Mean Square Deviation with respect to the 2149 measured masses of nuclei with N and $Z \geq 8$. S. Goriely et al., Phys. Rev. C 88, 024308 (2013); C 88, 061302 (2013).

Observables of the Density Distribution



HFB-24 charge radii versus experimental values. Comparison of the measured charge density with the HFB-24 estimate for ^{208}Pb .

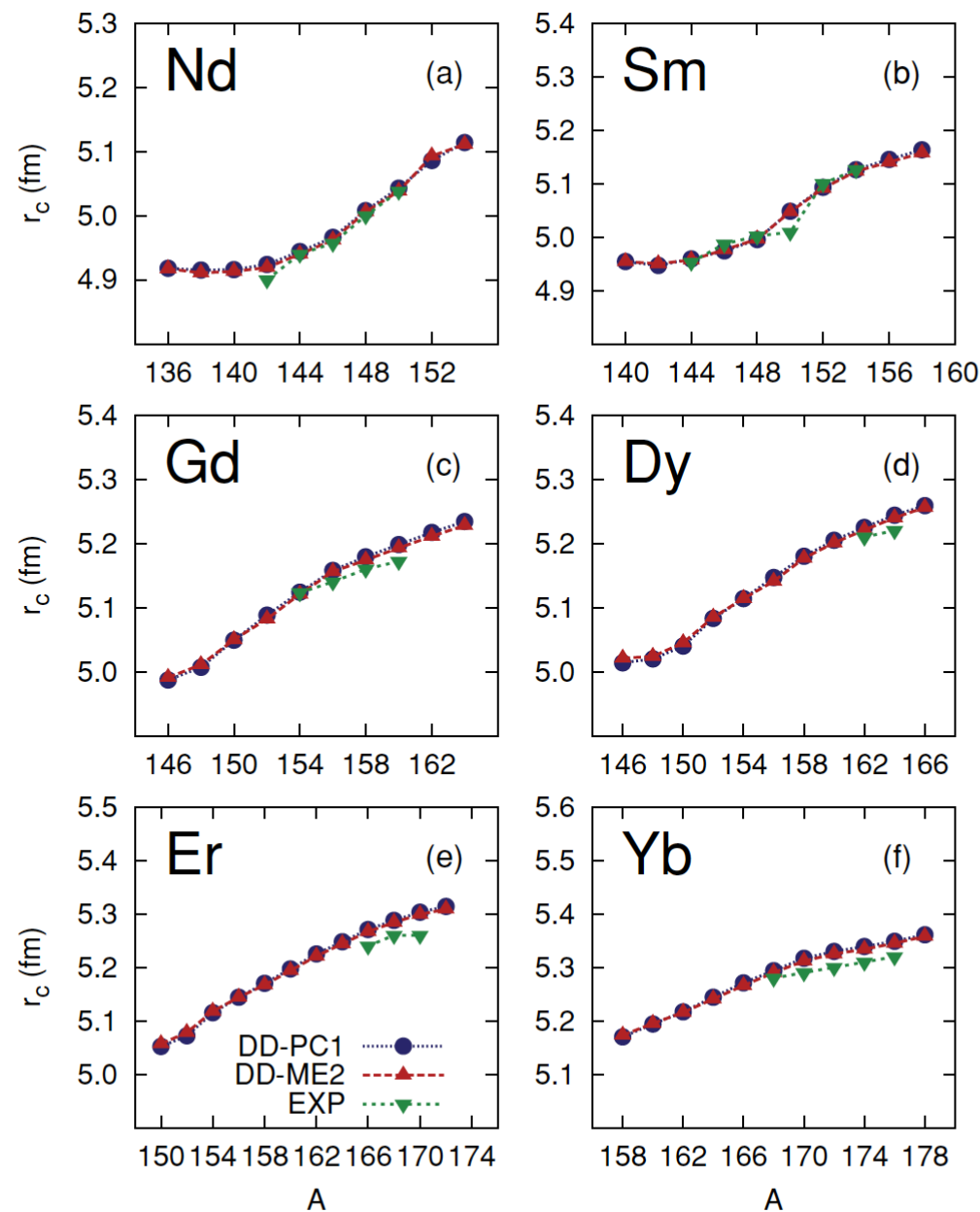


FIG. 14. (Color online) Charge radii of Nd, Sm, Gd, Dy, Er, and Yb isotopic chains. The results of the RMF + BCS calculation with the DD-PC1 and DD-ME2 interactions are compared with data [46].

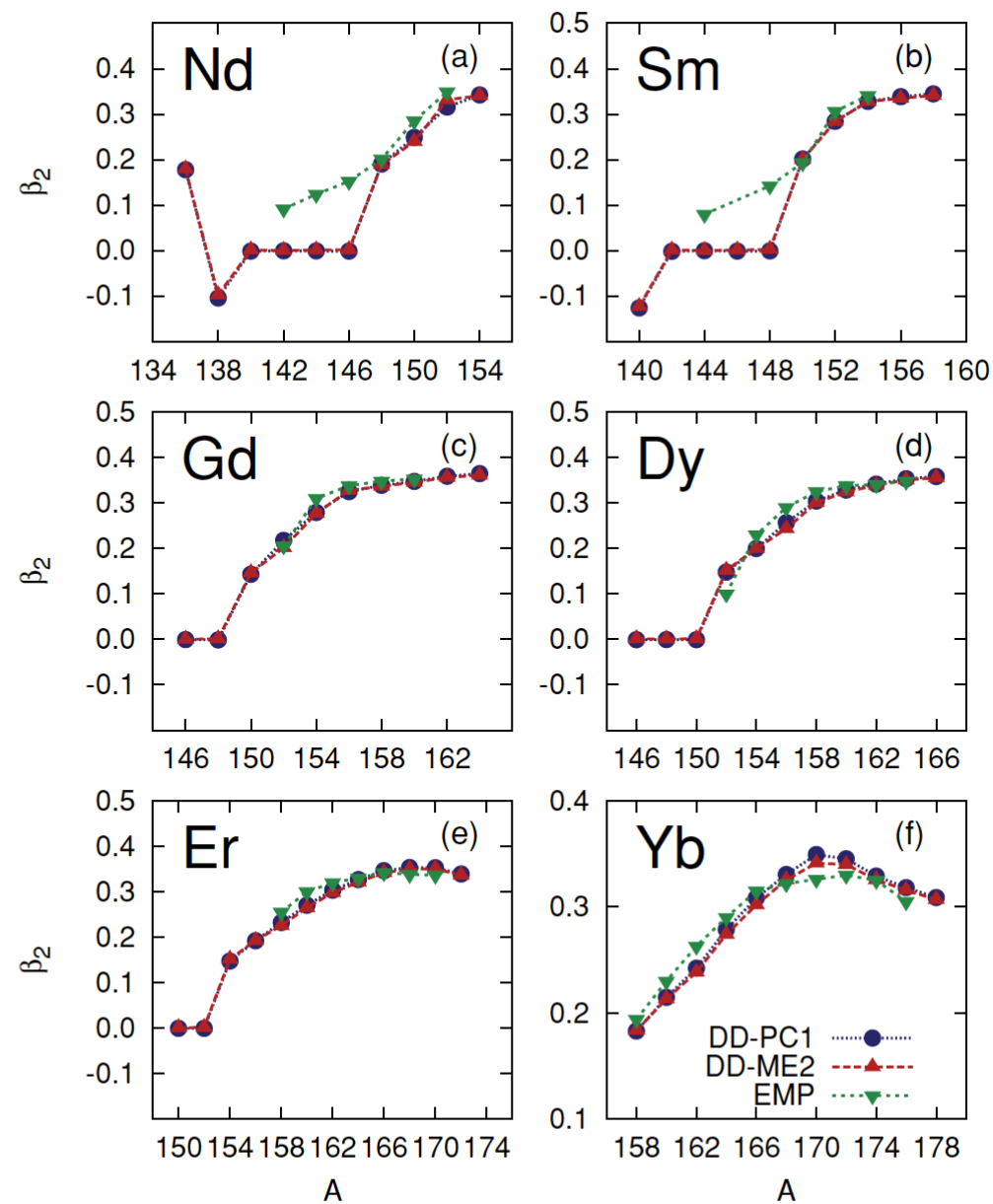
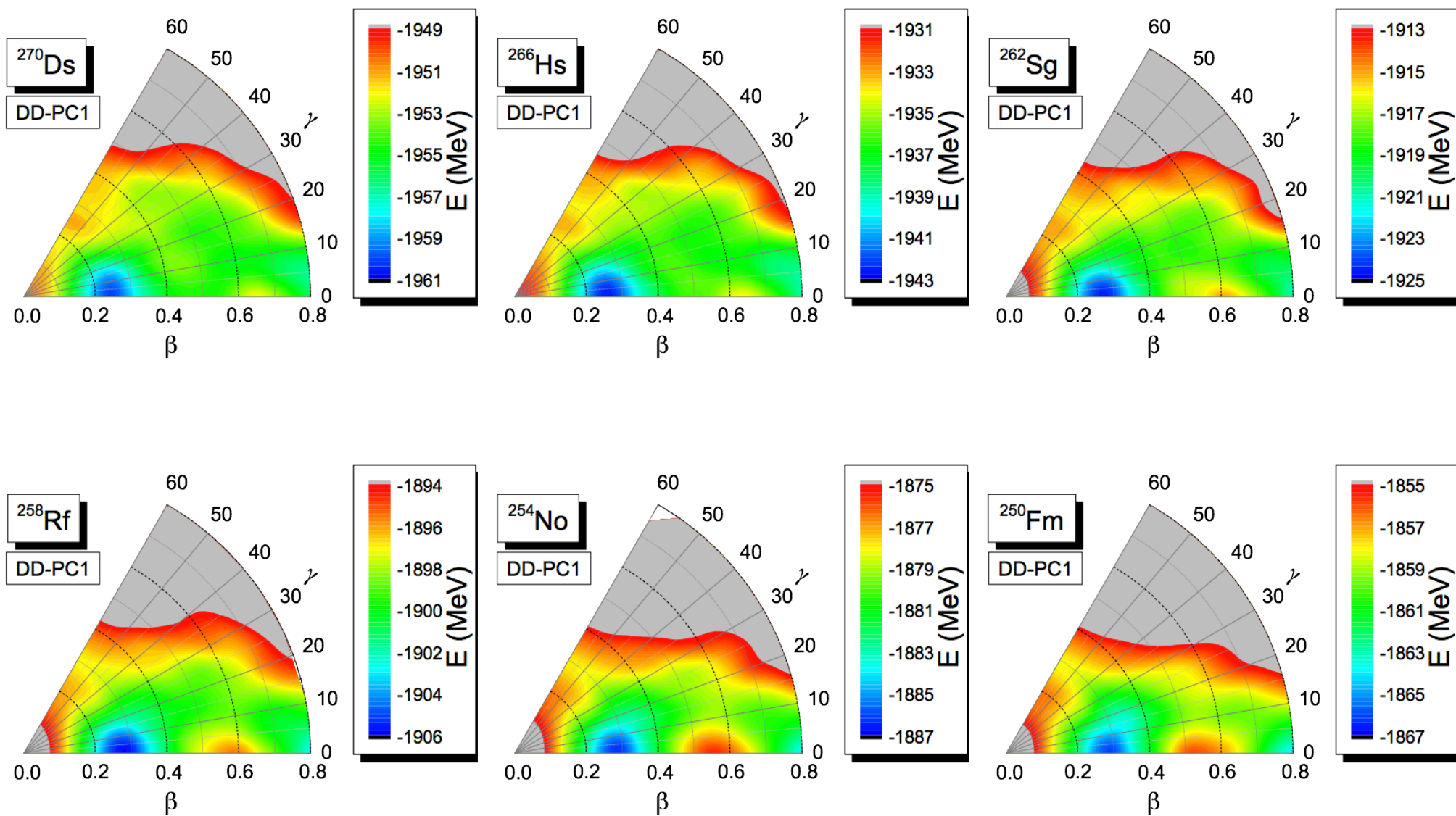
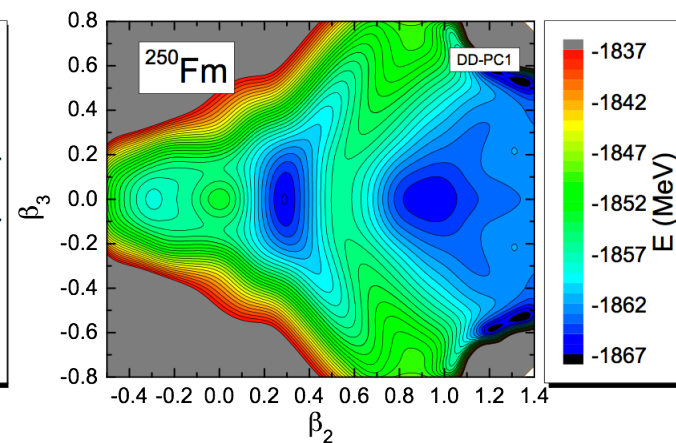
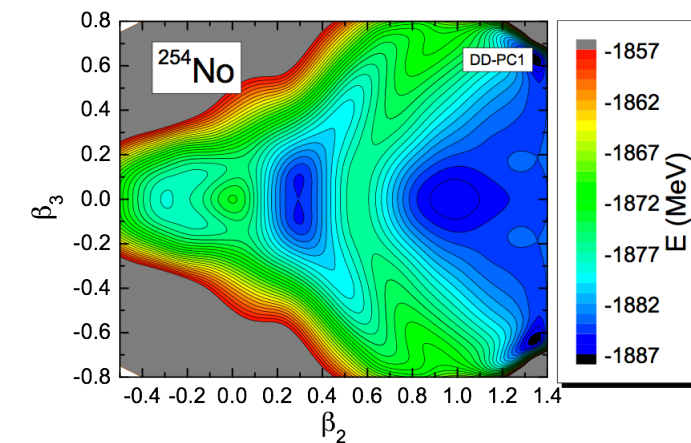
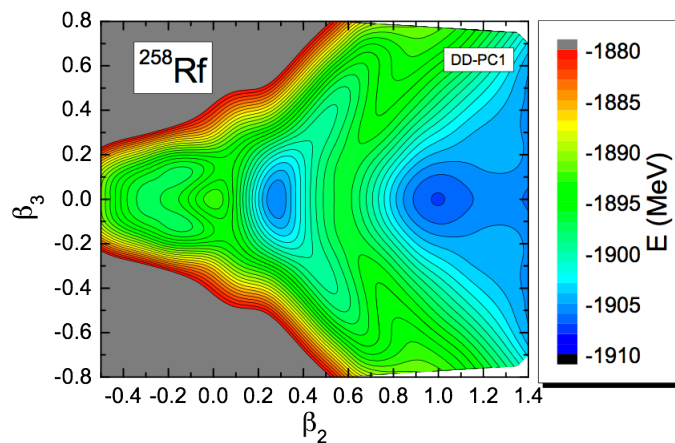
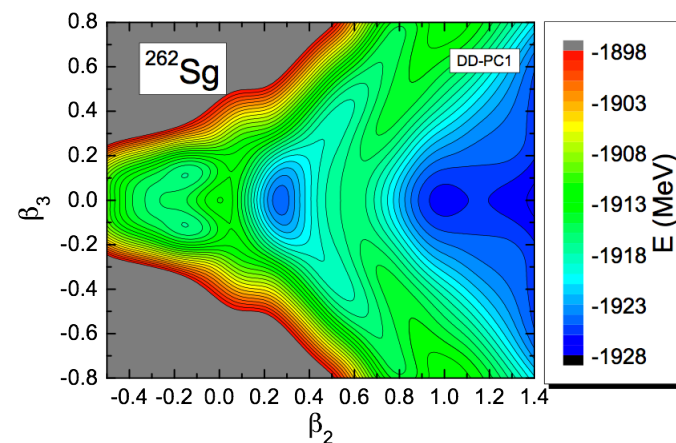
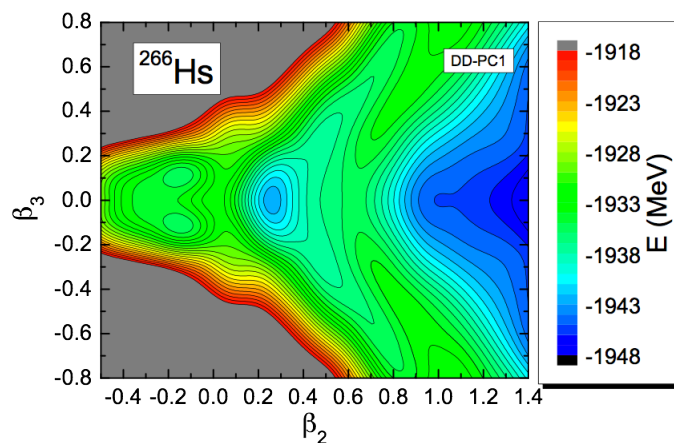
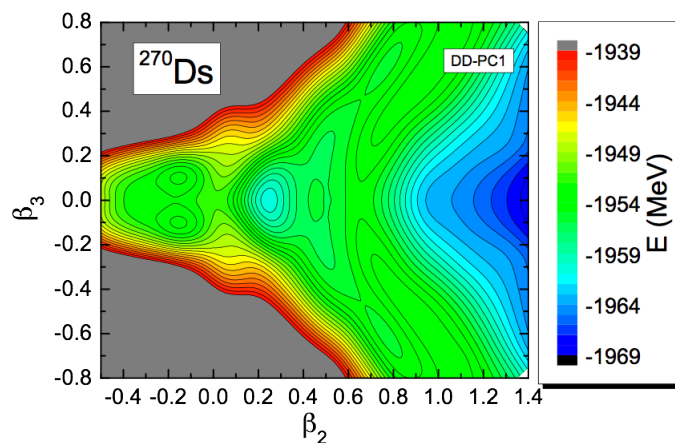


FIG. 15. (Color online) DD-PC1 and DD-ME2 predictions for the ground-state quadrupole deformations β_2 of the Nd, Sm, Gd, Dy, Er, and Yb isotopes, in comparison with empirical values [48].

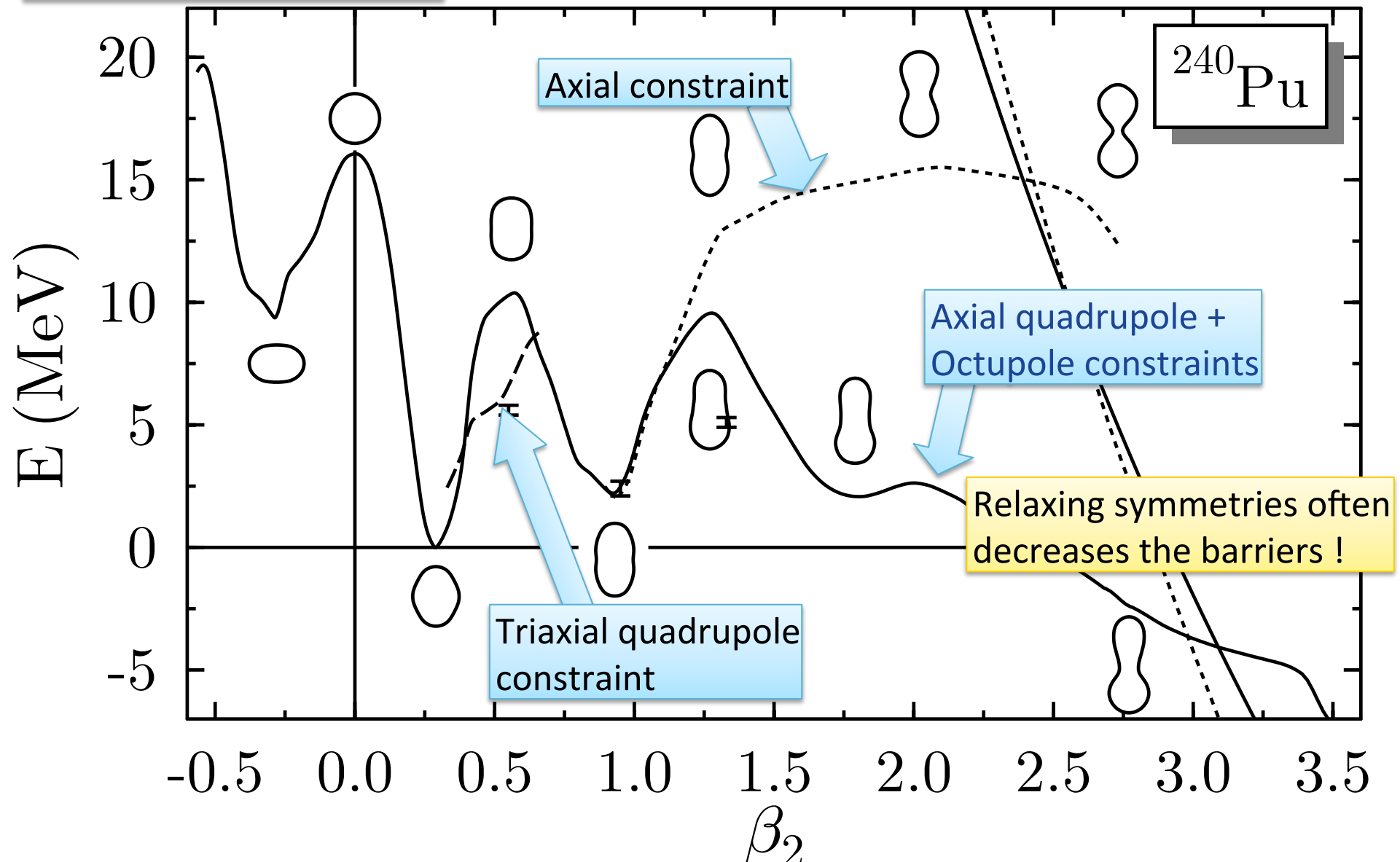
^{270}Ds α -decay chain



^{270}Ds α -decay chain



Fission barriers



Paths in the deformation energy surface of ^{240}Pu calculated with the SkI4 force. The solid line corresponds to axial quadrupole and octupole (reflection asymmetric) constraints, the dashed line to triaxial quadrupole constraints, the dotted line to axial quadrupole constraint only.

Self-consistent mean-field models

Strong points:

- (i) an intuitive interpretation of mean-field results in terms of **intrinsic shapes** and shells with **single-particle states**.
- (ii) the **full model space** of occupied states can be used; no distinction between core and valence particles, and **no need for effective charges**.
- (iii) the use of **universal effective interactions**; universal in the sense that they can be applied to all nuclei throughout the periodic chart.

Problems:

- (i) an independent particle-description establishes a **body-fixed intrinsic frame** of the nucleus. The relation of mean-field results to spectroscopic observables in the laboratory frame depends on additional assumptions.
- (ii) by construction, **a mean-field state breaks** necessarily several **symmetries** of the nuclear Hamiltonian (translational, rotational).
- (iii) the mean-field approach becomes **ill-defined** when the binding energy changes slowly with a collective degree of freedom (transitional nuclei).