TECHNISCHE UNIVERSITÄT DARMSTADT

Energy density functionals with local chiral interactions

Lars Zurek

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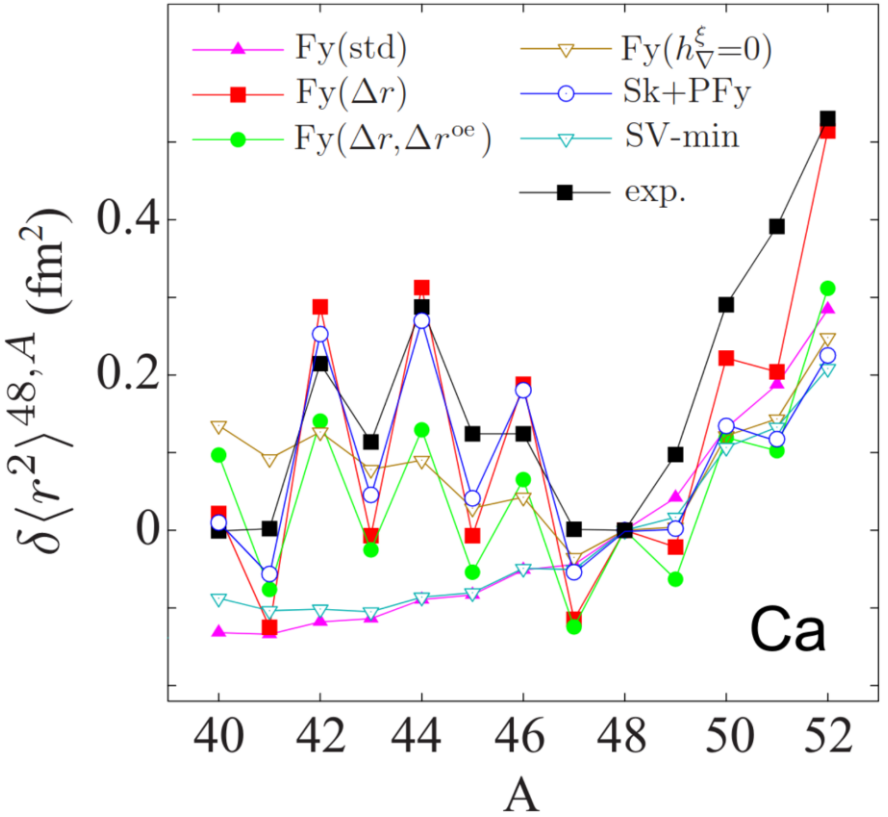
Bundesministerium für Bildung und Forschung

Energy density functionals

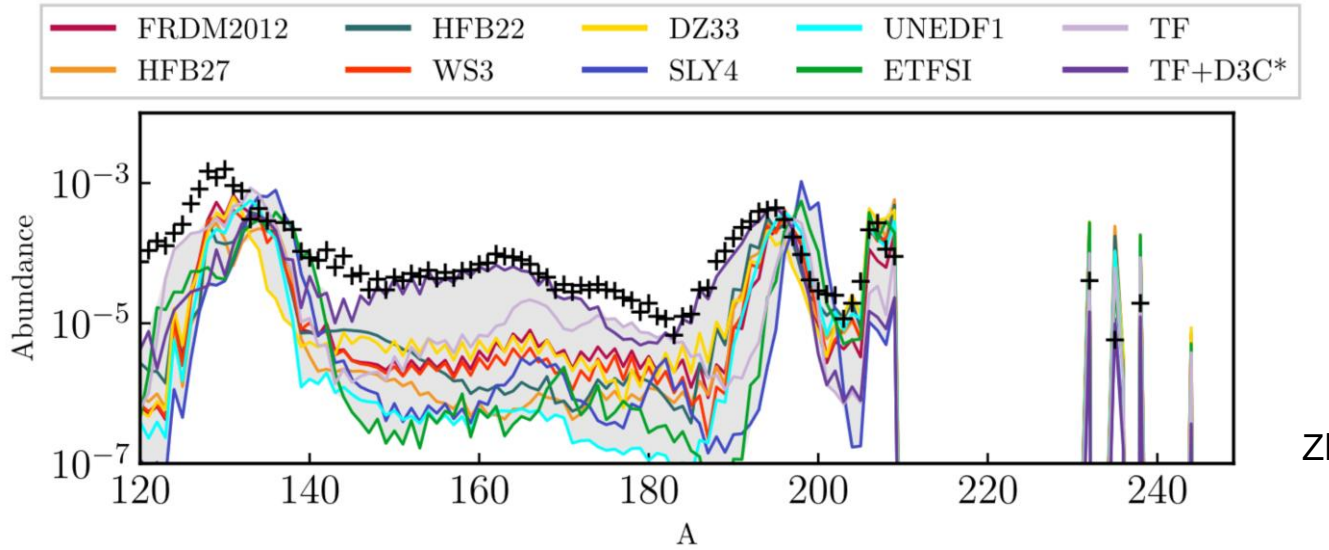
- Successful reproduction of experimental results
  - Even-even binding energy rms deviation for UNEDF2: 1.95 MeV
  - Charge radius differences in Ca with Fayans EDFs



Reinhard, Nazarewicz, PRC **95** (2017)

Energy density functionals

- Successful reproduction of experimental results
  - Even-even binding energy rms deviation for UNEDF2: 1.95 MeV
  - Charge radius differences in Ca with Fayans EDFs
- Phenomenological construction
  - Extrapolation outside fitting region uncontrolled



Zhu et al., ApJ **906** (2021)

Energy density functionals

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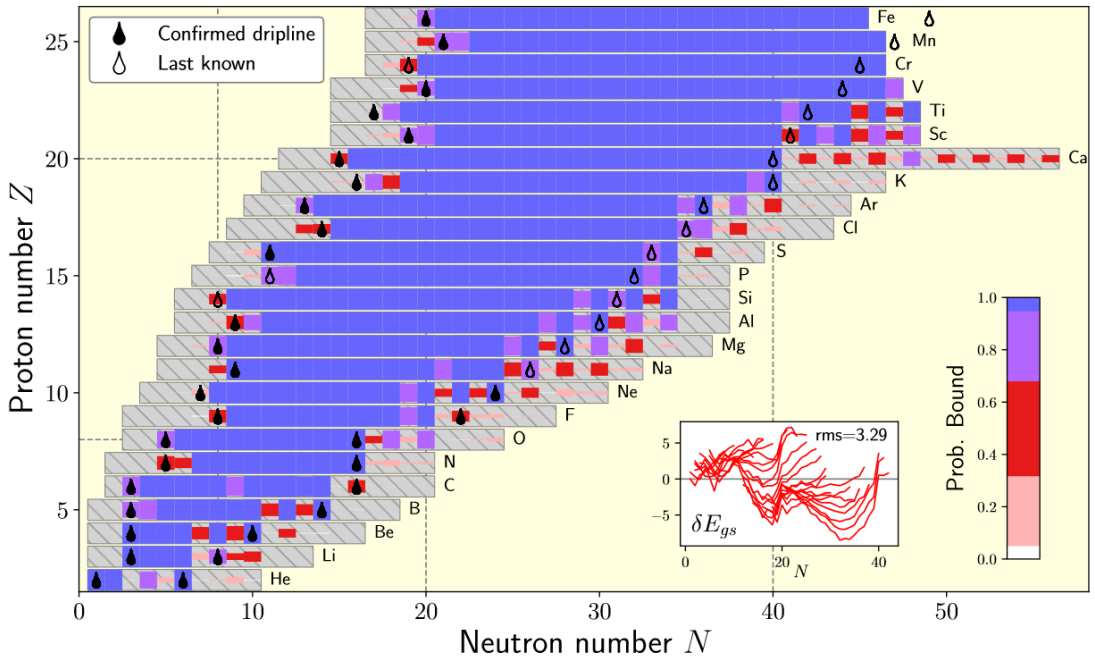
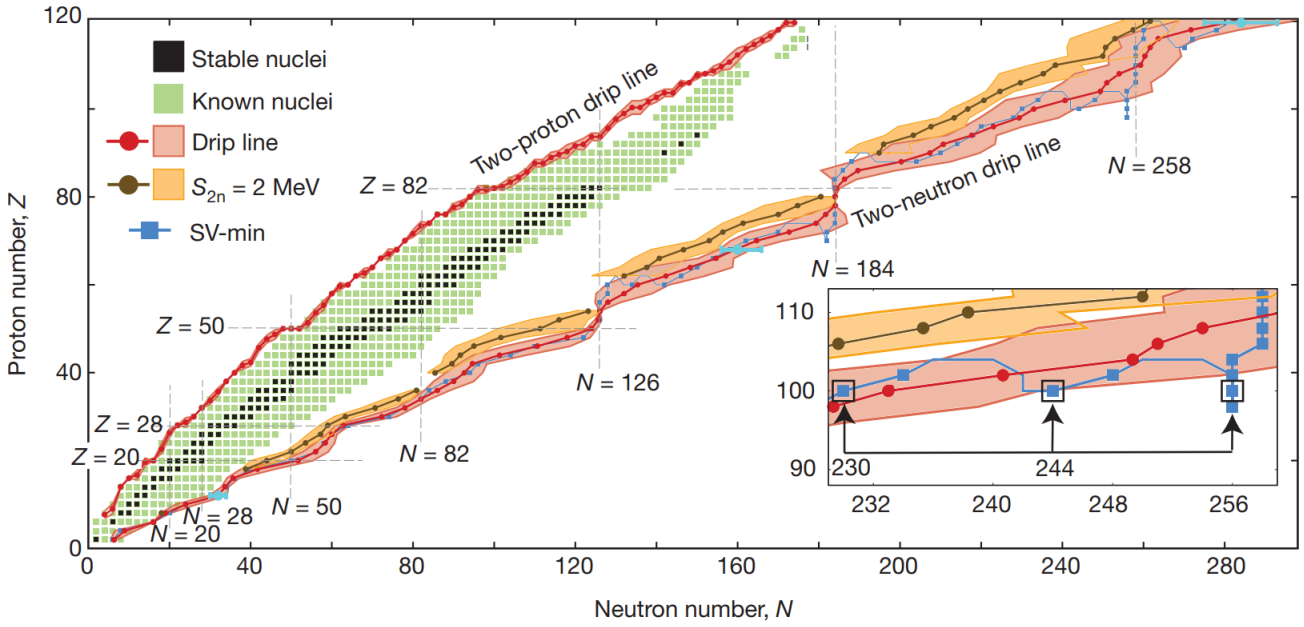
- Successful reproduction of experimental results
  - Even-even binding energy rms deviation for UNEDF2: 1.95 MeV
  - Charge radius differences in Ca with Fayans EDFs
- Phenomenological construction
  - Extrapolation outside fitting region uncontrolled
- Have standard EDFs reached their accuracy limit? McDonnell et al., PRL **114** (2015)

Ab initio calculations with chiral EFT

- At present reproduction of experimental results with larger deviations
- Computationally more expensive



Stroberg et al., PRL **126** (2021)



Erler et al., Nature **486** (2012)

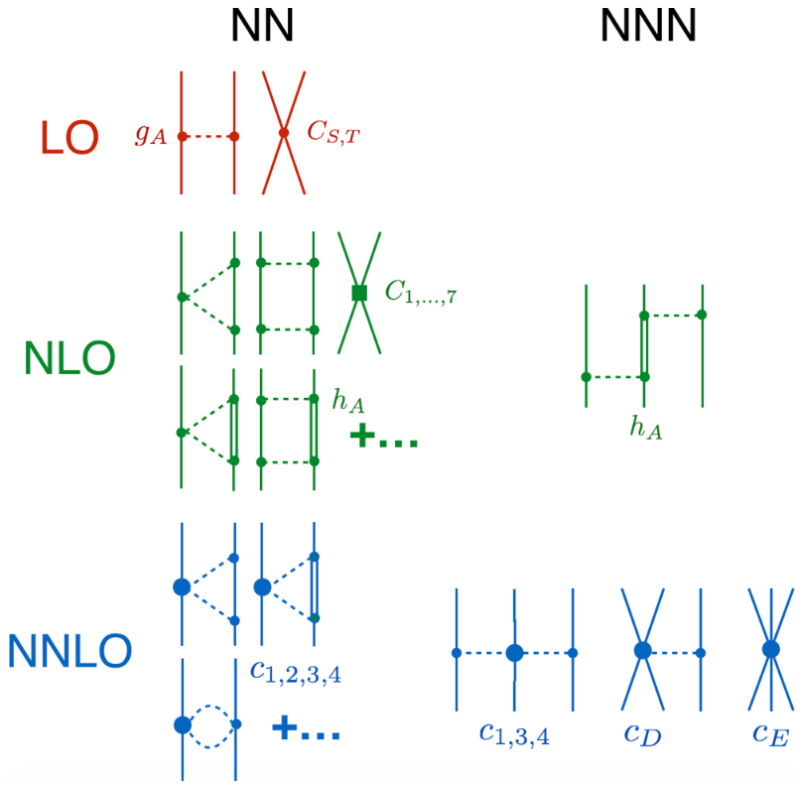
Ab initio calculations with chiral EFT

- At present reproduction of experimental results with larger deviations
- Computationally more expensive

- Systematically improvable
  - Uncertainty estimates “built-in”

→ (How) can EDFs profit from the ab initio approach?

Salvioni et al., JPG **47** (2020)
Furnstahl, EPJA **56** (2020)
Marino et al., PRC **104** (2021)
Duguet et al., 2209.03424 (2022)



Ekström et al., PRC **97** (2018)

Semi-phenomenological hybrid EDFs

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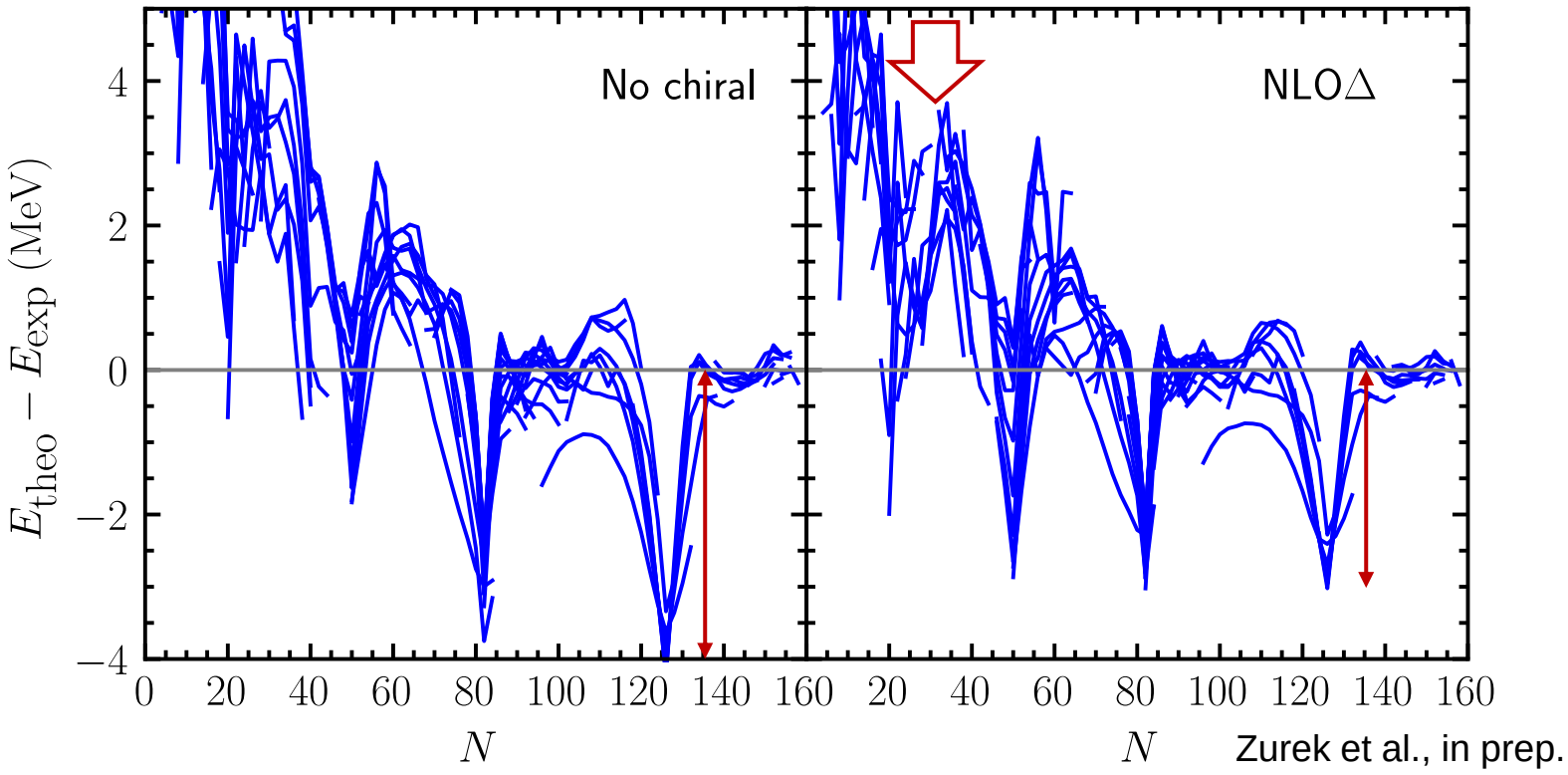
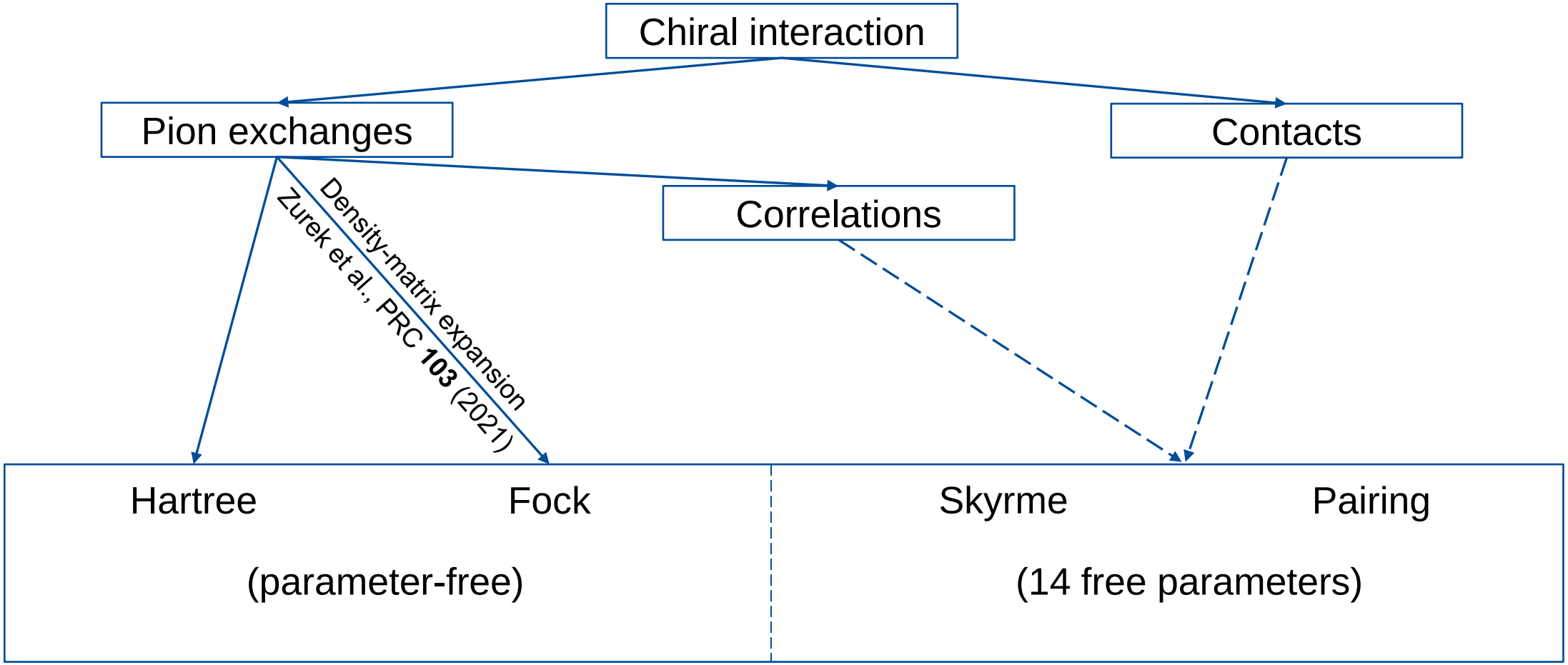
- Enhance EDFs with chiral EFT



Zurek et al., in prep.

Semi-phenomenological hybrid EDFs

Stoitsov et al., PRC **82** (2010); Navarro Pérez et al., PRC **97** (2018)



Semi-phenomenological hybrid EDFs

Navarro Pérez et al., PRC **97** (2018)

$$E_{\mathrm{H}} \propto \sum_{t=0,1} \int d\mathbf{x}_1 d\mathbf{x}_2 \, V_C(|\mathbf{x}_1 - \mathbf{x}_2|) \rho_t(\mathbf{x}_1) \rho_t(\mathbf{x}_2)$$

Density-matrix expansion

Zurek et al., PRC **103** (2021)

$$E_{\mathrm{F}} = \sum_{t=0,1} \int d\mathbf{R} \left[g_t^{\rho\rho}\big(\rho_0(\mathbf{R})\big) \rho_t^2(\mathbf{R}) + g_t^{\rho\tau}\big(\rho_0(\mathbf{R})\big) \rho_t(\mathbf{R}) \tau_t(\mathbf{R}) + \ldots \right]$$

$$E_{\mathrm{Sk}} = \sum_{t=0,1} \int d\mathbf{R} \left[\big(C_t^{\rho\rho} + C_{tD}^{\rho\rho} \rho_0^{\gamma}(\mathbf{R})\big) \rho_t^2(\mathbf{R}) + C_t^{\rho\tau} \rho_t(\mathbf{R}) \tau_t(\mathbf{R}) + \ldots \right]$$

Hartree	Fock	Skyrme	Pairing
(parameter-free)		(14 free parameters)	

Semi-phenomenological hybrid EDFs

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- Skyrme + HF long-range pions
  - At different chiral orders up to N^2LO, with and without Δs and 3N forces

  → Fit Skyrme parameters

- Strategy employed in Navarro Pérez et al., PRC **97** (2018)
  - Chiral systematics not understood

- Here: Revisit and improve all parts of EDF construction

  to allow for cleaner comparison of different functionals

Optimization of Skyrme parameters

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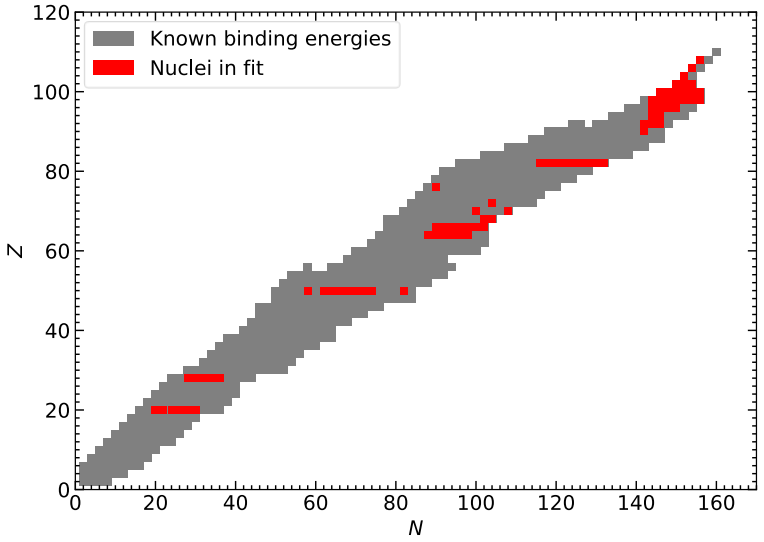
- Minimize $\chi^2(\mathbf{C}) \propto \sum_{i=1}^{n_d} \left(\frac{p_i(\mathbf{C}) - d_i}{w_i} \right)^2$
  - EDF predictions p_i from parameters $\mathbf{C}$
  - Experimental data d_i (binding energies, charge radii, odd-even mass staggerings, fission isomer energies)
  - Weights w_i (measuring importance / expected error)



- Previously: assumptions for weights as in UNEDF2 Kortelainen et al., PRC **89** (2014)
- Now: weights from Bayesian posterior estimate for UNEDF1 Schunck et al., JPG **47** (2020)

Results: parametrizations

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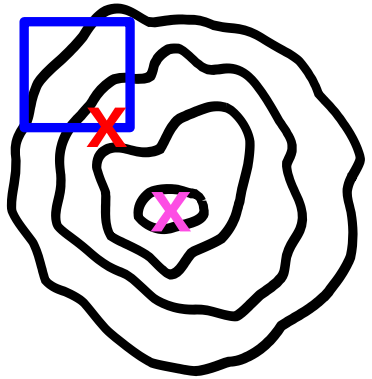
- Functionals at different chiral orders can be grouped into two classes

Class		LO & NLO	Beyond NLO
Example functional	**No chiral**	**LO**	**NLOΔ**
χ^2 at minimum	122.4	144.9	86.2
Incompressibility (MeV)	260	260	241



- Terms beyond NLO move global minima “closer” towards region allowed by parameter bounds

Results: global comparison to experiment

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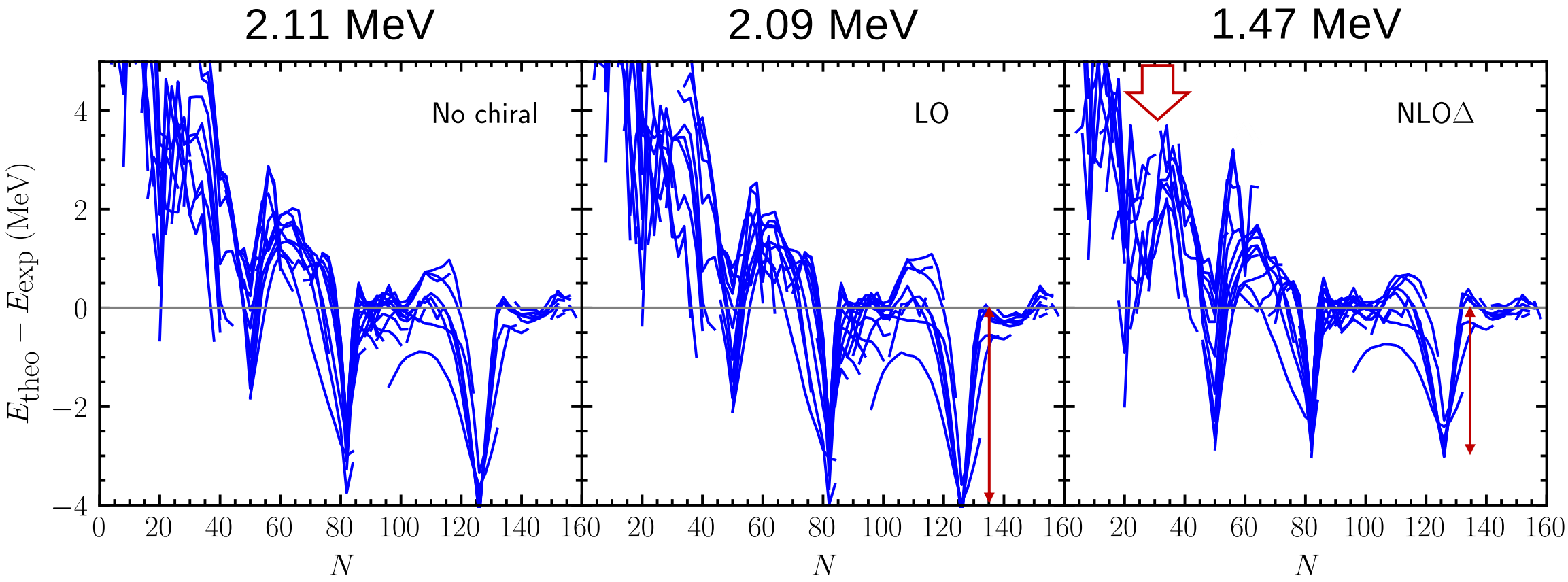
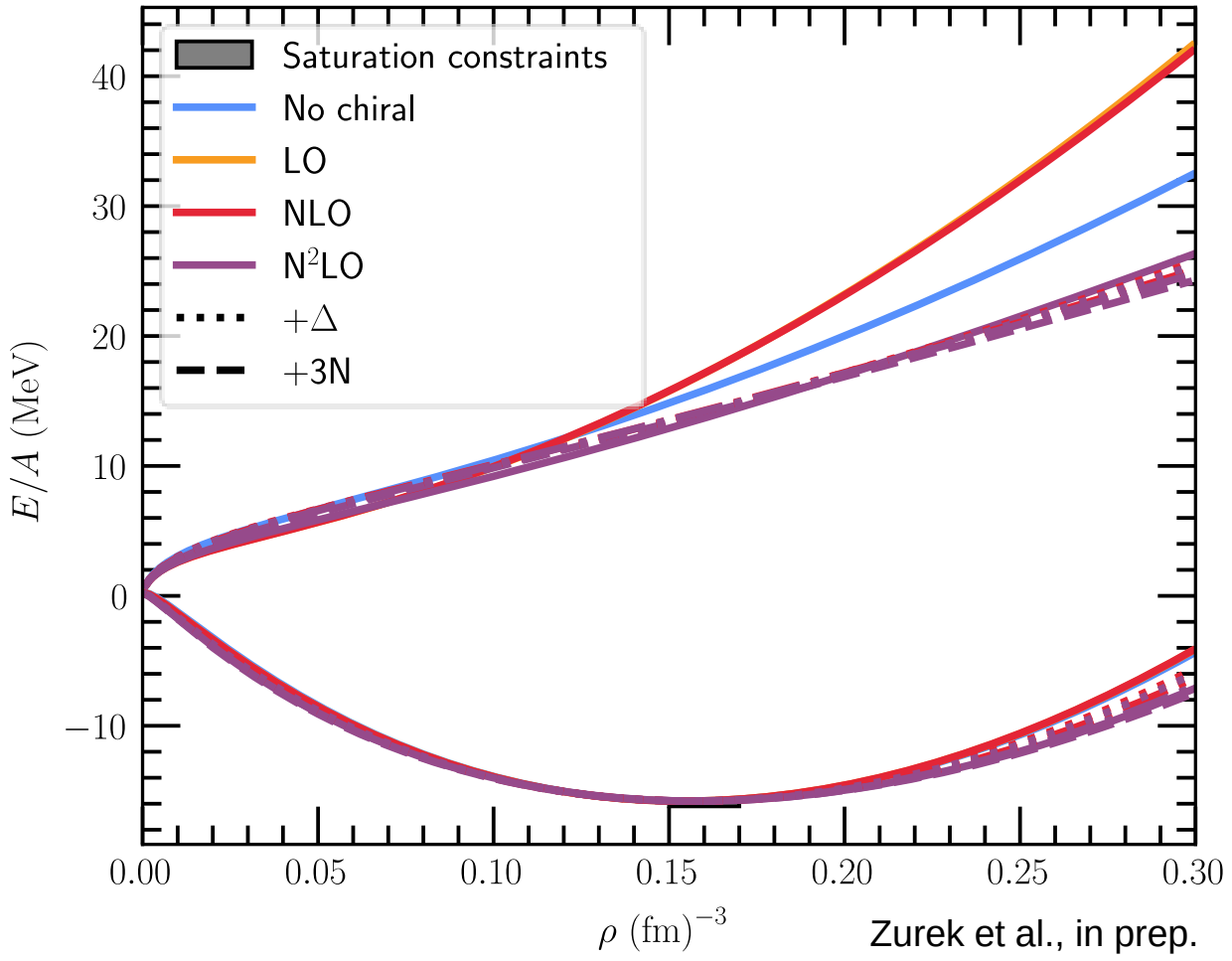
- Root-mean square deviations to experiment for even-even nuclei with Z>7:



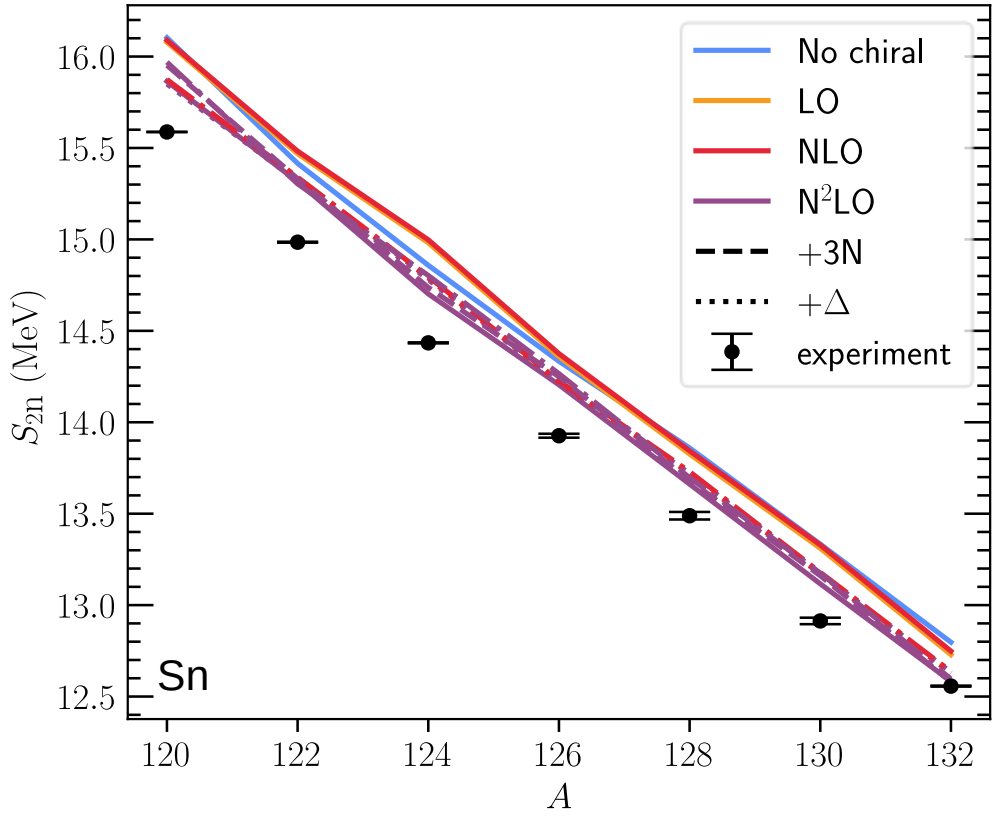
Zurek et al., in prep.

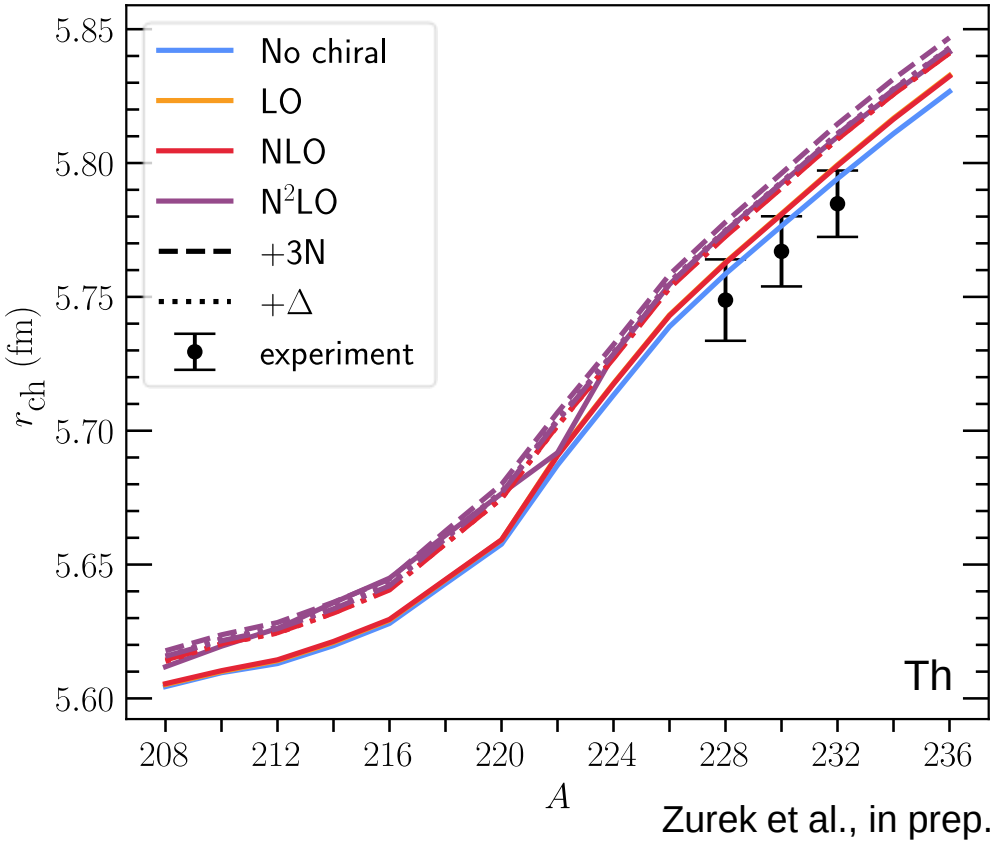
Results: infinite nuclear matter



Zurek et al., in prep.

Results: isotope chains





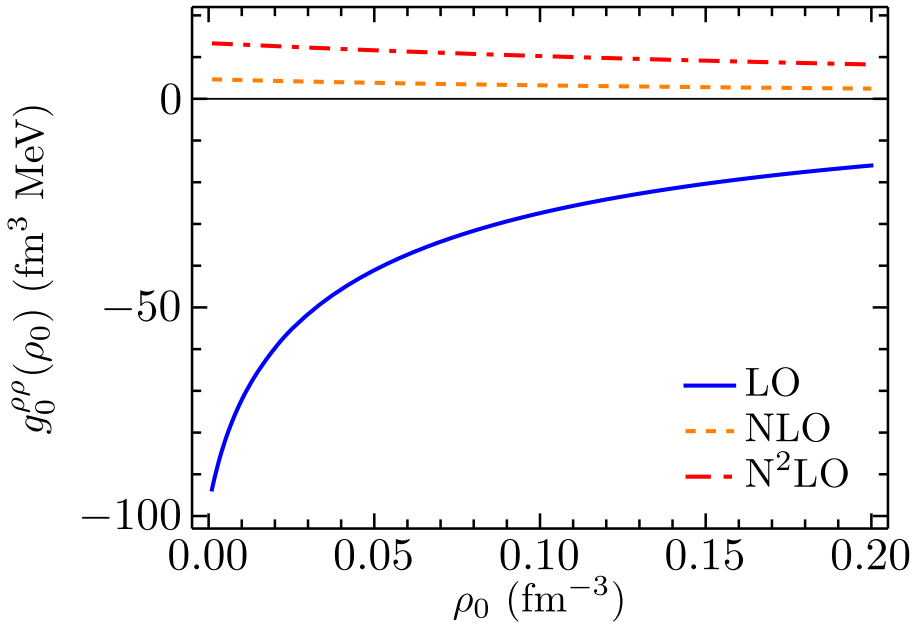
Zurek et al., in prep.

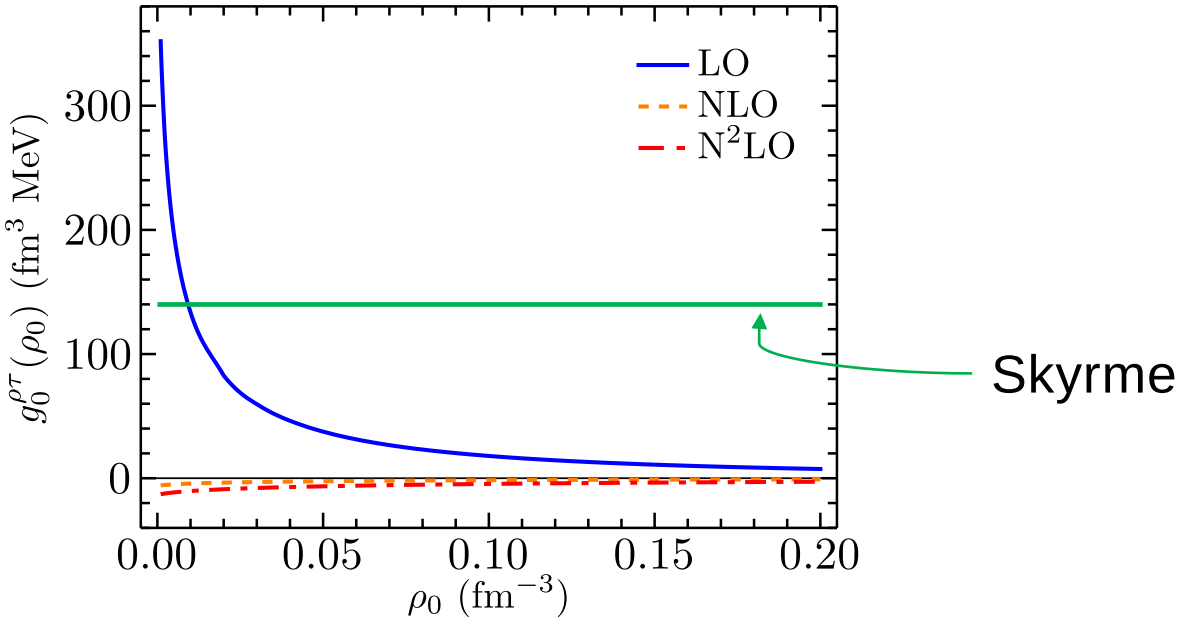
- Main effect beyond NLO
- 3N forces have basically no effect

Which terms are driving the improvements?

- Add only certain terms to Skyrme functional and optimize parameters

	χ^2
N²LO	89
N²LO Hartree, LO Fock	84





- LO Fock has strong density dependence

Summary

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- Skyrme EDF improved by adding parameter-free pion exchanges
  - Main improvement beyond NLO
  - Binding energy rms deviation decreased by 30%
  - LO Fock and N²LO Hartree seem responsible for improvement

  → Add to your functional!

Summary & outlook

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  - Main improvement beyond NLO
  - Binding energy rms deviation decreased by 30%
  - LO Fock and N²LO Hartree seem responsible for improvement

  → Add to your functional!

- Why do 3N forces seem to do nothing?

- Constrain isovector parts of EDFs by fitting to ab initio pseudodata (neutron drops)

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Thanks for your attention

and to my collaborators
Scott Bogner, Dick Furnstahl, Rodrigo Navarro Pérez,
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