# Nuclear DFT Calculations With DME Energy Density Functional

*M. Stoitsov*

*University of Tennessee Knoxville,TN & Oak Ridge National Laboratory, Oak Ridge, TN*

PEOPLE

UTK/ORNL
Markus Kortelainen
Thomas Lesinski
Nicolas Schunck
M.S.

NSCL/MSU
Scott Bogner
Biruk Gebremariam

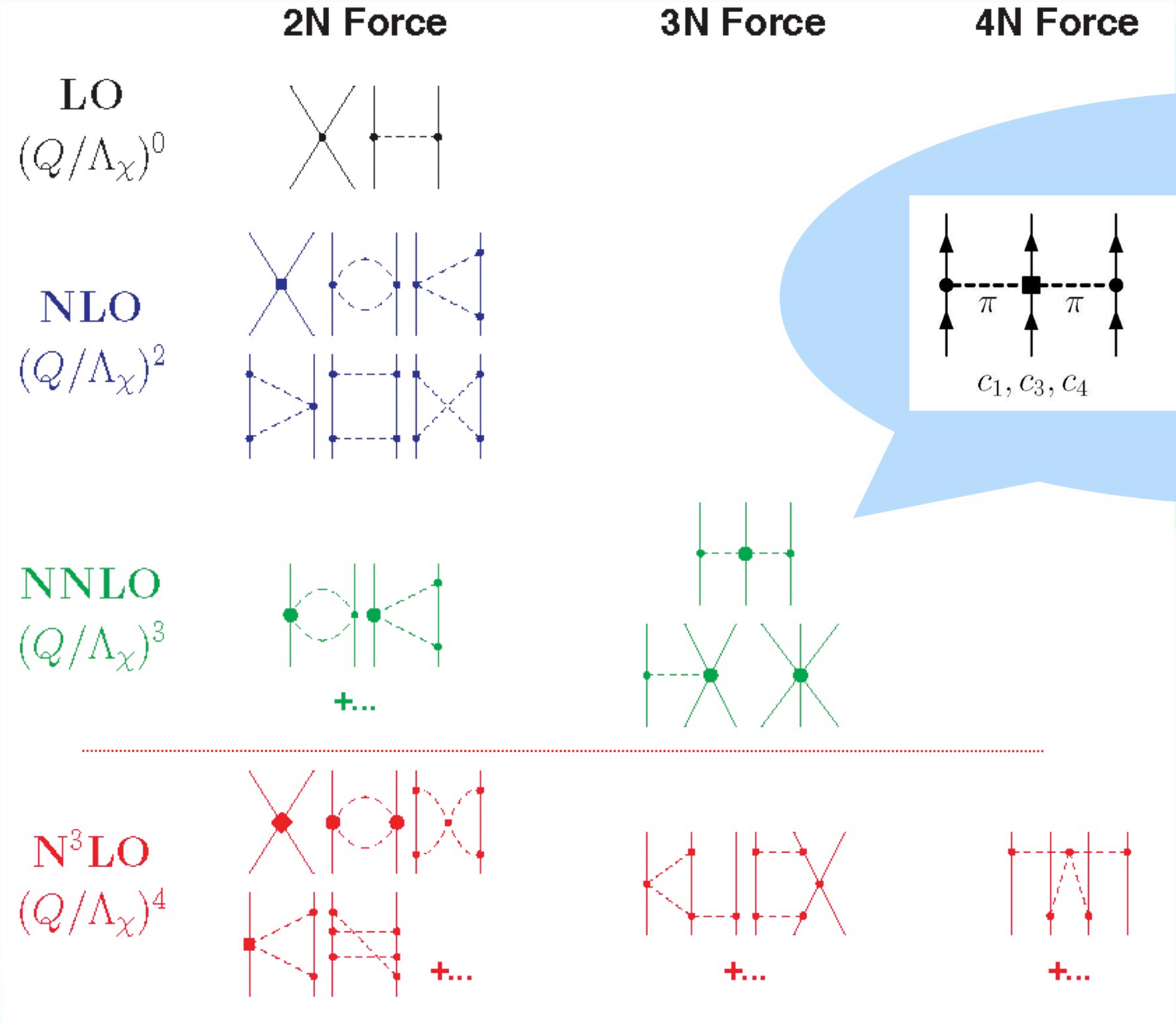
Ohio State University
Dick Furnstahl

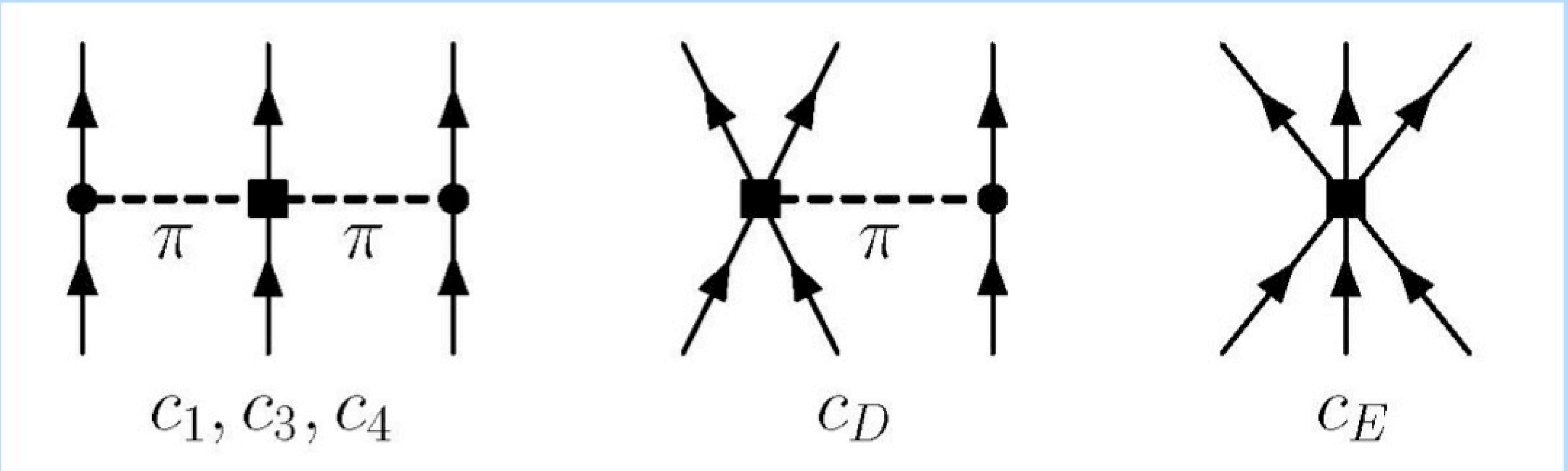
CEA
Thomas Duguet

- Ab Initio Approach
- DME Functional
- INM with DME functional
- INM constraints
- FINITE NUCLEI
- SVD Pre-Optimization
- DME results for finite nuclei
- Conclusions


# Ab Initio Approach
## Based on Chiral EFT NN and NNN Interaction

E. Epelbaum, W. Gloekle, Ulf-G. Meissner




**Interaction parameters**

| | Set A | Set B |
|---|---|---|
| $\hbar_c^{-1}$ | 197.3 | 197.327 |
| $g_A$ | 1.29 | 1.29 |
| $f_\pi$ | 92.4 $\hbar_c$ | 92.4 $\hbar_c$ |
| $m_\pi$ | 138.03 $\hbar_c$ | 138.03 $\hbar_c$ |
| $c_1$ | $-0.00081$ $\hbar_c$ | $-0.00076$ $\hbar_c$ |
| $c_3$ | $-0.0034$ $\hbar_c$ | $-0.00478$ $\hbar_c$ |
| $c_4$ | 0.0034 $\hbar_c$ | 0.00396 $\hbar_c$ |
| $c_d$ | $-2.062$ | $-2.062$ |
| $c_e$ | $-0.625$ | $-0.625$ |
| $\Lambda_x$ | 700 $\hbar_c$ | 700 $\hbar_c$ |

# Ab Initio Approach
## Based on Chiral EFT NN and NNN Interaction

$$E = \langle\Psi|T|\Psi\rangle + \langle\Psi|V|\Psi\rangle \qquad V = V^{\mathrm{NN}} + V^{\mathrm{NNN}} + \ldots$$

$$V^{\mathrm{NN}}_{EFT} = V^{\mathrm{NN}}_{ct} + V^{\mathrm{NN}}_{\pi} \qquad V^{\mathrm{NNN}}_{EFT} = V^{\mathrm{NNN}}_{ct} + V^{\mathrm{NNN}}_{\pi}$$

Contact Term Contributions

$$E_{ct} = \langle\Psi|T + V^{\mathrm{NN}}_{ct} + V^{\mathrm{NNN}}_{ct}|\Psi\rangle$$

Long-Range Pion Contributions

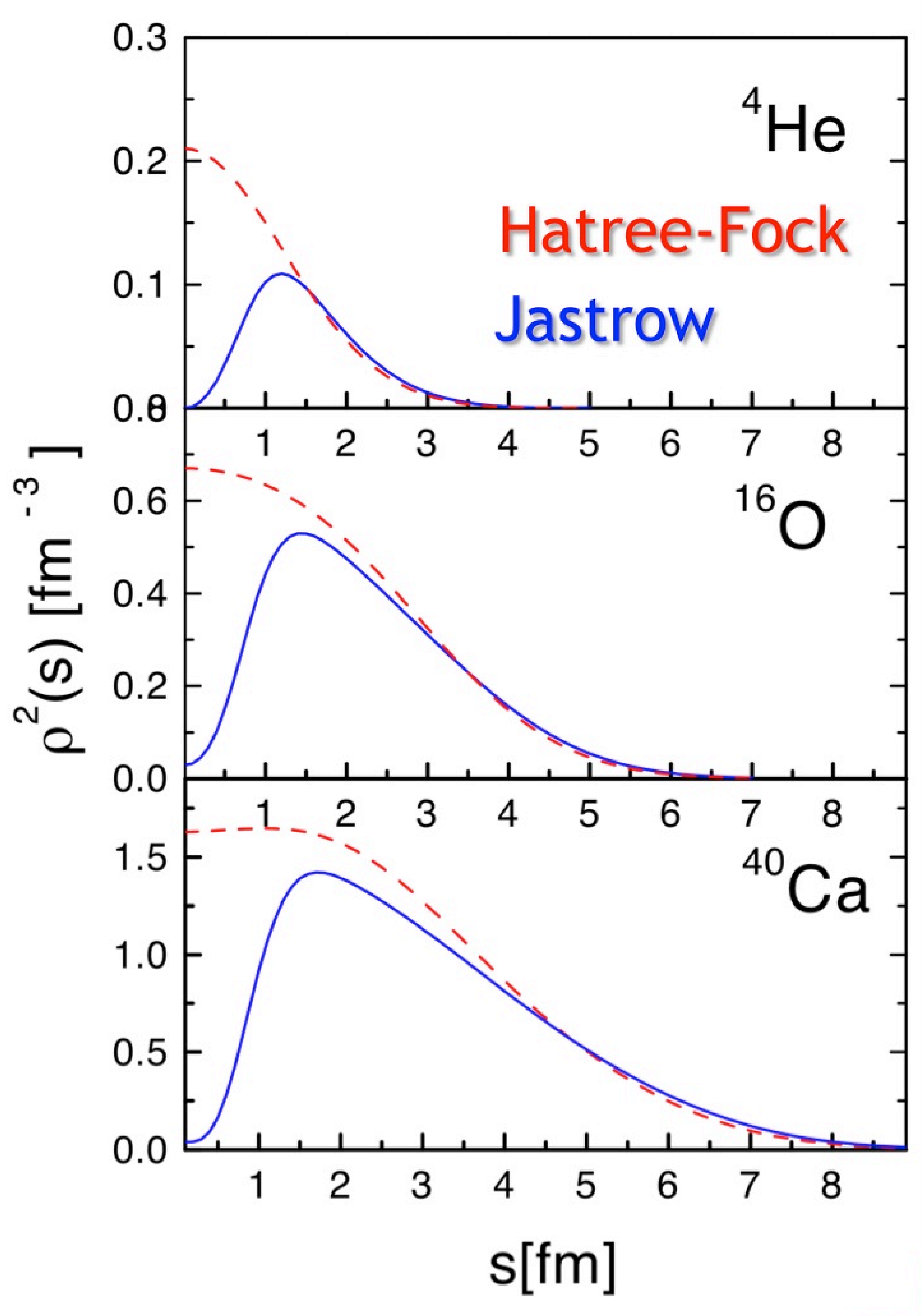
$$E_{\pi} = \langle\Psi|V^{\mathrm{NN}}_{\pi} + V^{\mathrm{NNN}}_{\pi}|\Psi\rangle$$

Total Energy

$$E = E_{ct} + E_{\pi}$$

$$\begin{aligned}
V^{\mathrm{NN}}_{\pi} &= V_C + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\, W_C \\
&+ [V_S + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\, W_S]\, \vec{\boldsymbol{\sigma}}_1\cdot\vec{\boldsymbol{\sigma}}_2 \\
&+ [V_T + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\, W_T]\, \vec{\boldsymbol{\sigma}}_1\cdot\vec{\boldsymbol{q}}\;\; \vec{\boldsymbol{\sigma}}_2\cdot\vec{\boldsymbol{q}} \\
&+ [V_{LS} + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\, W_{LS}]\, i(\vec{\boldsymbol{\sigma}}_1+\vec{\boldsymbol{\sigma}}_2)\cdot(\vec{\boldsymbol{q}}\times\vec{\boldsymbol{k}}) \\
&+ [V_{\sigma L} + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\, W_{\sigma L}]\, \vec{\boldsymbol{\sigma}}_1\cdot(\vec{\boldsymbol{q}}\times\vec{\boldsymbol{k}})\vec{\boldsymbol{\sigma}}_2\cdot(\vec{\boldsymbol{q}}\times\vec{\boldsymbol{k}}).
\end{aligned}$$

# Towards Ab Initio Nuclear Energy Density Functional
## Underlining Philosophy




Exact Two-Body Density Matrix

$$\rho^{(2)}(x_1, x_2; x_1', x_2') = \langle\Psi|a^+(x_1)\, a^+(x_2)\, a(x_1')\, a(x_2')|\Psi\rangle$$

$$\rho^{(2)}(\mathbf{s}) = \int \rho^{(2)}(\mathbf{R}+\mathbf{s}/2, \mathbf{R}-\mathbf{s}/2)d\mathbf{R}$$

Two-Body Density Matrix in Hartree-Fock Approximation

$$\rho^{(2)}_{HF}(x_1, x_2; x_1', x_2') = \langle\Phi|a^+(x_1)\, a^+(x_2)\, a(x_1')\, a(x_2')|\Phi\rangle$$

$$\rho^{(2)}_{HF}(\mathbf{s}) = \int \rho^{(2)}_{HF}(\mathbf{R}+\mathbf{s}/2, \mathbf{R}-\mathbf{s}/2)d\mathbf{R}$$

Contact part as it is but optimized

DME expansion in HF approximation

$$E = E_{ct} + E_\pi \quad \Longrightarrow \quad E[\rho] = E_{ct}[\rho] + E_\pi[\rho]$$

Exact Energy

DME Functional

# Time-Even DME Functional
## General Structure

$$E[\rho] = \int \mathcal{H}(\mathbf{r})\mathbf{dr} \qquad \mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \sum_{tt'} \mathcal{H}_{tt'}(\mathbf{r})$$

$$\mathcal{H}_{tt'}(\mathbf{r}) = U^{\rho^2}_{tt'}\rho_t\rho_{t'} + U^{\rho\tau}_{tt'}\rho_t\tau_{t'} + U^{J^2}_{tt'}\mathbf{J_t J_{t'}} + \mathbf{U}^{\rho\boldsymbol{\Delta}\rho}_{\mathbf{tt'}}\rho_\mathbf{t}\boldsymbol{\Delta}\rho_{\mathbf{t'}} + \mathbf{U}^{\rho\nabla\mathbf{J}}_{\mathbf{tt'}}\rho_\mathbf{t}\nabla\mathbf{J_{t'}}$$

Looks like Skyrme functional with density dependent coupling constants and non-diagonal terms due to NNN in N2LO (isospin invariant)

Notations

$$U^m_{tt'} = U^m_{tt'}\left(\rho_t, \tau_t, \mathbf{J_t}, \ldots\right) \qquad m = \{\rho^2, \rho\tau, \rho\Delta\rho, \rho\nabla J, J^2\}, \quad t = \{0, 1\}$$

$$\mathbf{J_t J_{t'}} = \sum_{\mathbf{ij}} \mathbf{J^t_{ij} J^{t'}_{ij}}, \quad \rho_\mathbf{t}\nabla\mathbf{J_{t'}} = \sum_{\mathbf{ijk}} \varepsilon_{\mathbf{ijk}}\ \rho_\mathbf{t}\nabla_\mathbf{k}\mathbf{J^{t'}_{ij}},$$

# DME Functional
## Explicit Form

$$U^m_{tt'} = \left(C^m_t + g^m_t(u) + \rho_0\ h^m_t(u)\right)\delta_{t,t'} + \rho_1\ h^m_{tt'}(u)\left(1-\delta_{t,t'}\right)$$

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\mathbf{r}) + \mathcal{H}_\mathbf{1}(\mathbf{r}) + \mathcal{H}_\mathbf{2}(\mathbf{r})$$

$$\begin{aligned}
\mathcal{H}_t(\mathbf{r}) = & \left(C^{\rho^2}_{t0} + C^{\rho^2}_{tD}\rho_0^\gamma + g^{\rho^2}_t(u) + \rho_0 h^{\rho^2}_t\right)\rho_t^2 \\
& + \left(C^{\rho\tau}_t + g^{\rho\tau}_t(u) + \rho_0 h^{\rho\tau}_t(u)\right)\rho_t\tau_t \\
& + \left(C^{\rho\Delta\rho}_t + g^{\rho\Delta\rho}_t(u) + \rho_0 h^{\rho\Delta\rho}_t(u)\right)\rho_t\Delta\rho_t \\
& + \left(C^{\rho\nabla J}_t + g^{\rho\nabla J}_t(u) + \rho_0 h^{\rho\nabla J}_t(u)\right)\rho_t\nabla J_t, \\
& + \left(C^{J^2}_t + g^{J^2}_t(u) + \rho_0 h^{J^2}_t(u)\right)J_t^2
\end{aligned}$$

$$\begin{aligned}
\mathcal{H}_2(\mathbf{r}) = & \ \rho_1 h^{\rho\tau}_{10}(u)\rho_1\tau_0 + \rho_1 h^{\rho\Delta\rho}_{10}(u)\rho_1\Delta\rho_0 \\
& + \rho_1 h^{J^2}_{10}(u)J_1J_0 + \rho_1 h^{\rho\nabla J}_{10}(u)\rho_1\nabla J_0
\end{aligned}$$

DME amplitudes

$$g^m_t(u), \quad h^m_{tt'}(u)$$

$$\left(h^m_t = \delta_{tt'}h^m_{tt'}\right)$$

Local Density Approximation (LDA)

$$u = \frac{k_F(\mathbf{r})}{m_\pi}$$

Slater LDA Prescription

$$k_F(\mathbf{r}) = \left(\frac{3\pi^2}{2}\rho_0(\mathbf{r})\right)^{1/3}$$

Campy and Boyssys LDA Prescripton

$$k_F(\mathbf{r}) = \sqrt{\frac{5}{3}\frac{\tau_0(\mathbf{r}) - \frac{1}{4}\Delta\rho_0(\mathbf{r})}{\rho_0(\mathbf{r})}}$$

$$E[\rho] = E_{ct}[\rho] + E_\pi[\rho]$$

# DME Functional
## Contact Part

$$E[\rho] = \boxed{E_{ct}[\rho]} + E_\pi[\rho]$$

$$\mathcal{H}_{ct}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0^{ct}(\mathbf{r}) + \mathcal{H}_1^{ct}(\mathbf{r})$$

$$\mathcal{H}_t^{ct}(\mathbf{r}) = \left(C_{t0}^{\rho^2} + C_{tD}^{\rho^2}\rho_0^\gamma\right)\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\nabla J}\rho_t\nabla J_t + C_t^{J^2}J_t^2$$

Coincides with the Skyrme functional with coupling constants generally defined in terms of the parameters of the EFT interaction

Depends on 13 parameters which could be released for optimization

$$\{C_{t0}^{\rho^2}, C_{tD}^{\rho^2}, C_t^{\rho\Delta\rho}, C_t^{\rho\tau}, C_t^{J^2}, C_t^{\rho\nabla J}, \gamma\}$$

# DME Functional
## Long Range Part

$$E[\rho] = E_{ct}[\rho] + E_{\pi}[\rho]$$

$$\mathcal{H}_{\pi}(\mathbf{r}) = \mathcal{H}_0^{\pi}(\mathbf{r}) + \mathcal{H}_1^{\pi}(\mathbf{r}) + \mathcal{H}_2^{\pi}(\mathbf{r})$$

$$\begin{aligned} \mathcal{H}_t^{\pi}(\mathbf{r}) &= \left(g_t^{\rho^2}(u) + \rho_0 h_t^{\rho^2}\right)\rho_t^2 + \left(g_t^{\rho\tau}(u) + \rho_0 h_t^{\rho\tau}(u)\right)\rho_t\tau_t + \left(g_t^{\rho\Delta\rho}(u) + \rho_0 h_t^{\rho\Delta\rho}(u)\right)\rho_t\Delta\rho_t \\ &+ \left(g_t^{J^2}(u) + \rho_0 h_t^{J^2}(u)\right)J_t^2 + \left(g_t^{\rho\nabla J}(u) + \rho_0 h_t^{\rho\nabla J}(u)\right)\rho_t\nabla J_t \end{aligned}$$

$$\mathcal{H}_2^{\pi}(\mathbf{r}) = \rho_1 h_{10}^{\rho\tau}(u)\rho_1\tau_0 + \rho_1 h_{10}^{\rho\Delta\rho}(u)\rho_1\Delta\rho_0 + \rho_1 h_{10}^{J^2}(u)J_1 J_0 + \rho_1 h_{10}^{\rho\nabla J}(u)\rho_1\nabla J_0$$

New complicated density dependence due to the DME amplitudes but no additional parameters except the parameters of the EFT interaction

$$u = \frac{k_F(\mathbf{r})}{m_\pi}$$

$g_A, f_\pi, m_\pi$
$c_1, c_3, c_4$
$c_d, c_e, \Lambda_x$

# DME Functional
## NN and NNN amplitudes

### ❖ NN

$$g_t^m(u) = g_t^m(u)|_{LO} + g_t^m(u)|_{NLO} + g_t^m(u)|_{N^2LO}$$

$$\begin{aligned} g(u)|_{LO} &= \alpha_0^g + \beta_0^g \log\left(1+4u^2\right) + \gamma_0^g \arctan(2u) \\ g(u)|_{NLO} &= \alpha_1^g + \beta_1^g \left(\log\left(1+2u^2+2u\sqrt{1+u^2}\right)\right)^2 \\ &+ \gamma_1^g \sqrt{1+u^2} \log\left(1+2u^2+2u\sqrt{1+u^2}\right) \\ g(u)|_{N^2LO} &= \alpha_2^g + \beta_2^g \log\left(1+u^2\right) + \gamma_2 \arctan(u) \end{aligned}$$

### ❖ NNN

$$\begin{aligned} h_{tt'}^m(u) &= \alpha_0^h + \beta_0^h \log\left(1+4u^2\right) + \beta_1^h \left(\log\left(1+4u^2\right)\right)^2 \\ &+ \gamma_0^h \arctan(u) + \gamma_1^h \left(\arctan(2u)\right)^2 \\ &+ \gamma_2^h \log\left(1+4u^2\right) \arctan(2u) \end{aligned}$$

$\alpha_k = \alpha_k(u),\ \beta_k = \beta_k(u),\ \gamma_k = \gamma_k(u)$

rational polynomials of $u$

$$u = \frac{k_F(\mathbf{r})}{m_\pi}$$

## ➢ Mathematica Notebooks

Complete analytical expressions in Mathematica
*.nb format

*B. Gebremariam, T. Duguet and S.K. Bogner (submitted)*

*(see the talk by S. Bogner)*

## ➢ FORTRAN 90 module

Can be ported to any DFT solver
Already working with HFBRAD and HFBTHO

*M. Kortelainen and M. Stoitsov (in preparation)*

*(see the talk by M. Kortelinen)*

# DME Functional
## Volume Parameters in Terms of INM Quantities

### INM EOS With DME Functional

$$W(I,\rho) = \frac{\hbar^2}{2m}\tau_0 + \left(C_{00}^{\rho^2} + C_{0D}^{\rho^2}\rho^\gamma + g_0^{\rho^2}(\tilde{k}_F) + \rho h_0^{\rho^2}(\tilde{k}_F)\right)\rho + \left(C_{10}^{\rho^2} + C_{1D}^{\rho^2}\rho^\gamma + g_1^{\rho^2}(\tilde{k}_F) + \rho h_1^{\rho^2}(\tilde{k}_F)\right) I^2\rho + \left(C_0^{\rho\tau} + g_0^{\rho\tau}(\tilde{k}_F) + \rho h_0^{\rho\tau}(\tilde{k}_F) + I^2 \rho h_{10}^{\rho\tau}(\tilde{k}_F)\right)\tau_0 + \left(C_1^{\rho\tau} + g_1^{\rho\tau}(\tilde{k}_F) + \rho h_1^{\rho\tau}(\tilde{k}_F)\right) I\tau_1$$

### INM Equilibrium Characteristics

$$W(\rho, I) = W(\rho) + S_2(\rho)I^2 + S_4(\rho)I^4$$

$$W(\rho) = \frac{E^{NM}}{A} + \frac{P^{NM}}{\rho_c^2}(\rho-\rho_c) + \frac{K^{NM}}{18\rho_c^2}(\rho-\rho_c)^2$$

$$S_2(\rho) = a_{sym}^{NM} + \frac{L^{NM}}{3\rho_c}(\rho-\rho_c) + \frac{\Delta K^{NM}}{18\rho_c^2}(\rho-\rho_c)^2$$

### Symmetric INM

$C_{00}^{\rho^2}, C_{0D}^{\rho^2}, C_0^{\rho\tau}$ ⟷ $\frac{E^{NM}}{A}, \rho_c, M_s^{*NM}$

$$C_{00}^{\rho^2} = \frac{3(\gamma+1)\frac{E^{NM}}{A} - \frac{\hbar^2}{2m}\left(3-(2-3\gamma)M_s^*\right)\tau_c + A_{00}(u)}{3\gamma\rho_c}$$

$$C_{0D}^{\rho^2} = \frac{-3\frac{E^{NM}}{A} - \frac{\hbar^2}{2m}(2M_s^*-3)\tau_c + A_{0D}(u)}{3\gamma\rho_c^{\gamma+1}}$$

$$C_0^{\rho\tau} = \frac{\hbar^2}{2m}(M_s^*-1)\frac{1}{\rho_c} - g_0^{\rho\tau}(u) - h_0^{\rho\tau}(u)\rho_c$$

$$\gamma = \frac{-K^{\rm NM} - 9\frac{E^{NM}}{A} + \frac{\hbar^2}{2m}(4M_s^*-3)\tau_c + A_\gamma(u)}{9\frac{E^{NM}}{A} + 3\frac{\hbar^2}{2m}(2M_s^*-3)\tau_c + B_\gamma(u)}$$

### Asymmetric INM

$C_{10}^{\rho^2}, C_{1D}^{\rho^2}, C_1^{\rho\tau}$ ⟷ $a_{sym}^{NM}, L^{NM}, M_v^*$

$$C_{10}^{\rho^2} = \frac{27(\gamma+1)a_{sym}^{NM} - 9L^{NM} + 20(2-3\gamma)C_0^{\rho\tau}\rho_c\tau_c}{27\gamma\rho_c} + \frac{\frac{\hbar^2}{2m}\left((9\gamma-6)M_v^* - 12\gamma + 5\right)\tau_c + A_{10}(u)}{27\gamma\rho_c}$$

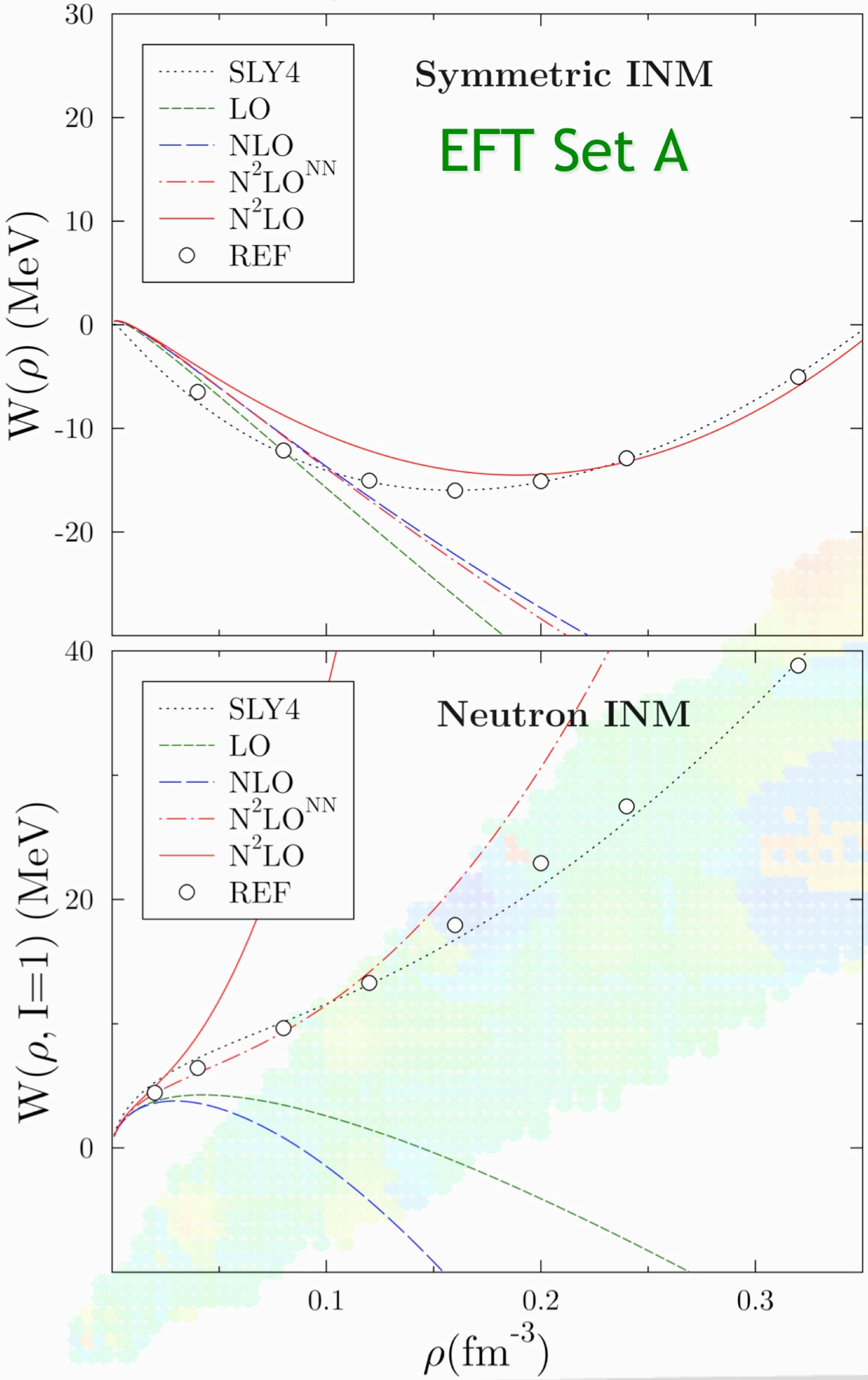
$$C_{1D}^{\rho^2} = \frac{-27a_{sym}^{NM} + 9L^{NM} - 40C_0^{\rho\tau}\rho_c\tau_c}{27\gamma\rho_c^{\gamma+1}} + \frac{\frac{\hbar^2}{2m}(30M_v^*-25)\tau_c + A_{1D}(u)}{27\gamma\rho_c^{\gamma+1}}$$

$$C_1^{\rho\tau} = \frac{\hbar^2}{2m}(M_s^*-M_v^*)\frac{1}{\rho_c} - g_1^{\rho\tau}(u) - h_1^{\rho\tau}(u)\rho_c$$

$$\rho = \rho_n + \rho_p, \quad I = \frac{\rho_n - \rho_p}{\rho} \qquad \tau = C_k\rho^{2/3}, \quad C_k = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3} \qquad u = \tilde{k}_F = \frac{k_F}{m_\pi} = \frac{1}{m_\pi}\left(\frac{3\pi^2}{2}\right)^{1/3}\rho^{1/3}$$

# DME Functional
## Infinite Nuclear Matter

### No free parameters




$E_{ct}[\rho]$ - part

constrained to:

$$\frac{E^{NM}}{A} = -15.97 \text{ MeV},$$

$$K^{NM} = 229.9 \text{ MeV},$$

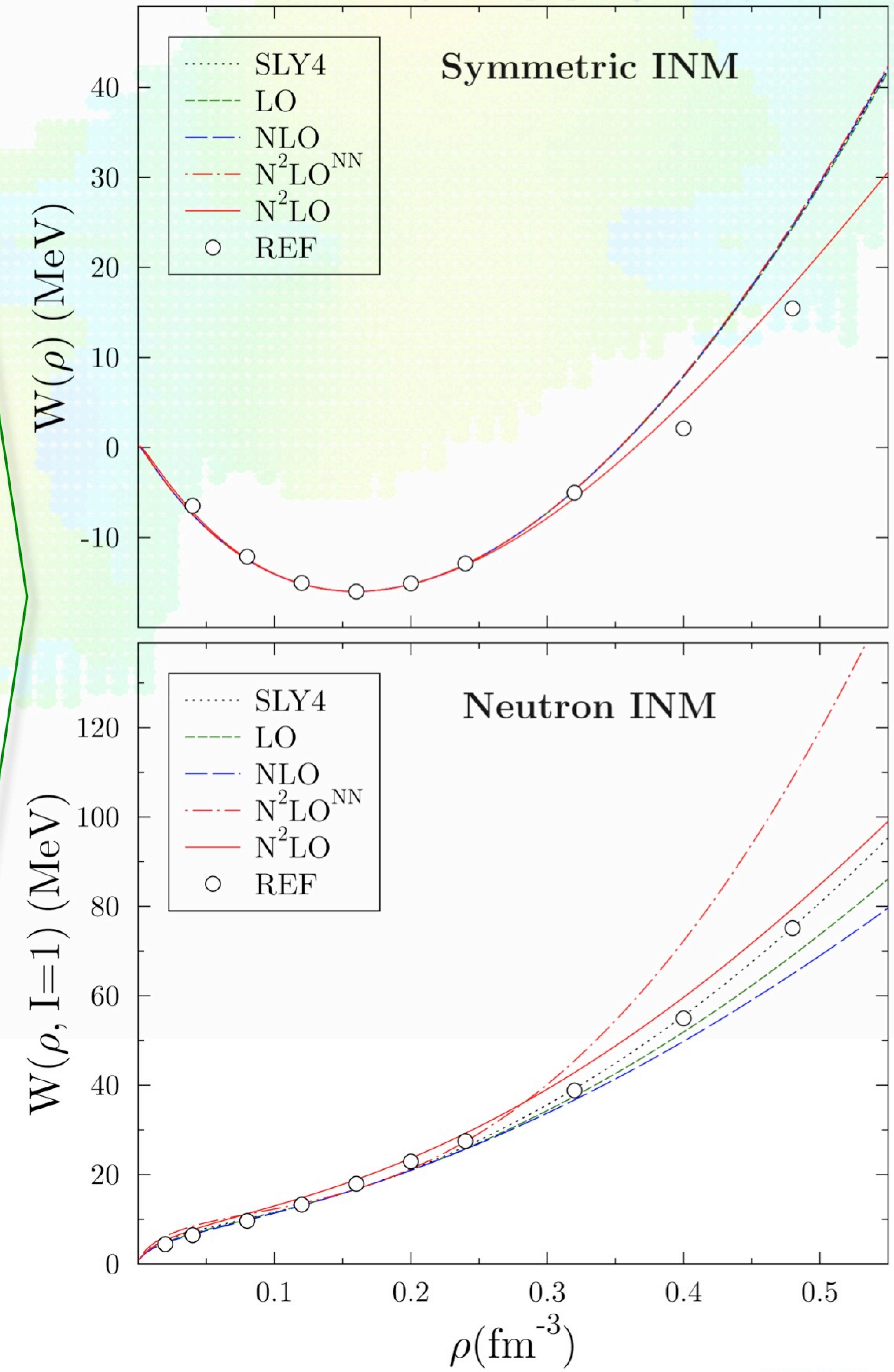
$$a_{sym}^{NM} = 32.0 \text{ MeV},$$

$$\rho_c = 0.1595 \text{ fm}^{-3},$$

$$M_{s/v}^{*-1} = 0.695/0.8,$$

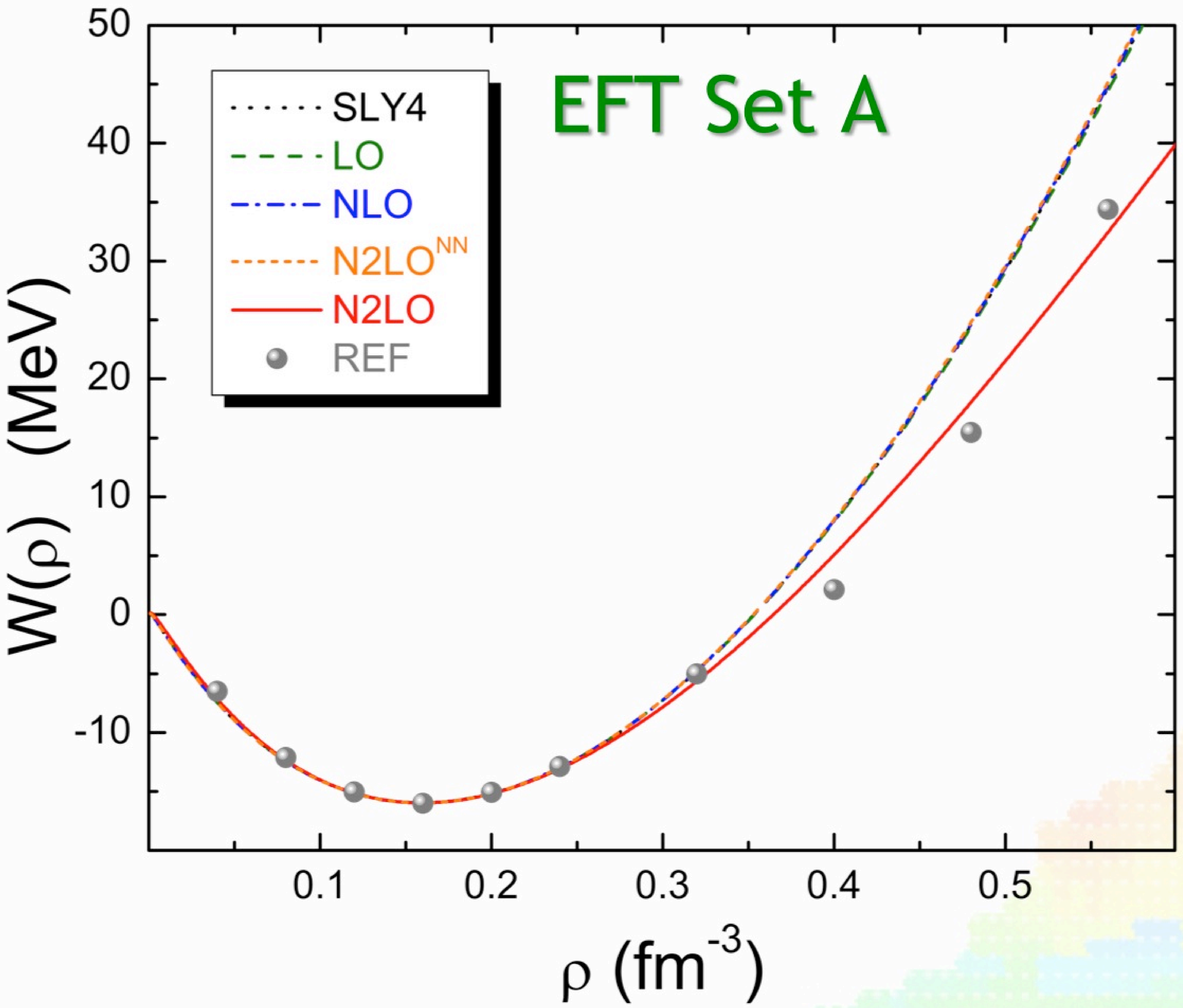
$$L^{NM} = 45.96 \text{ MeV}$$

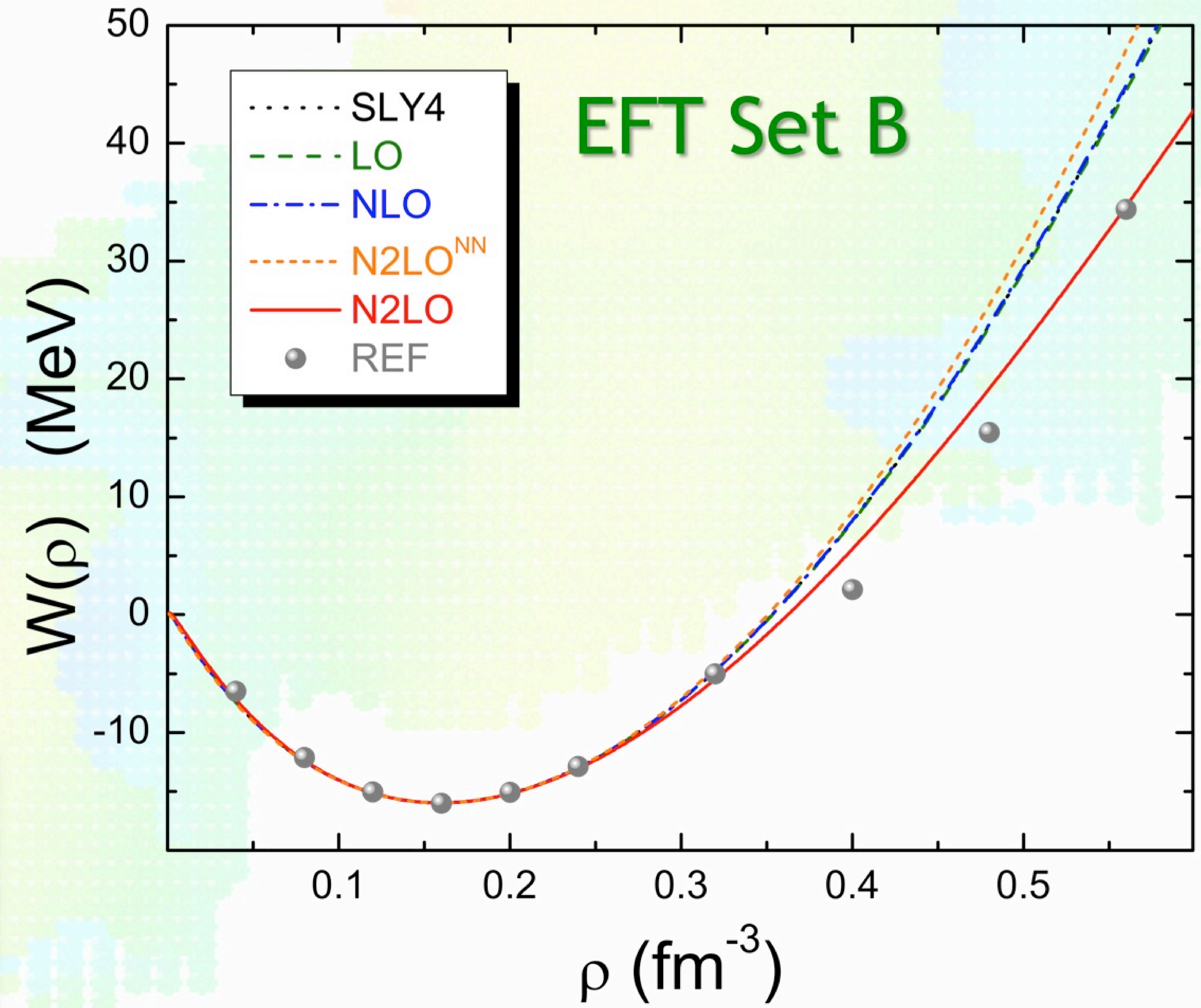
### EFT Set A ( $E_\pi[\rho]$ - part)



# DME Functional

## Influence of EFT Parameters on INM

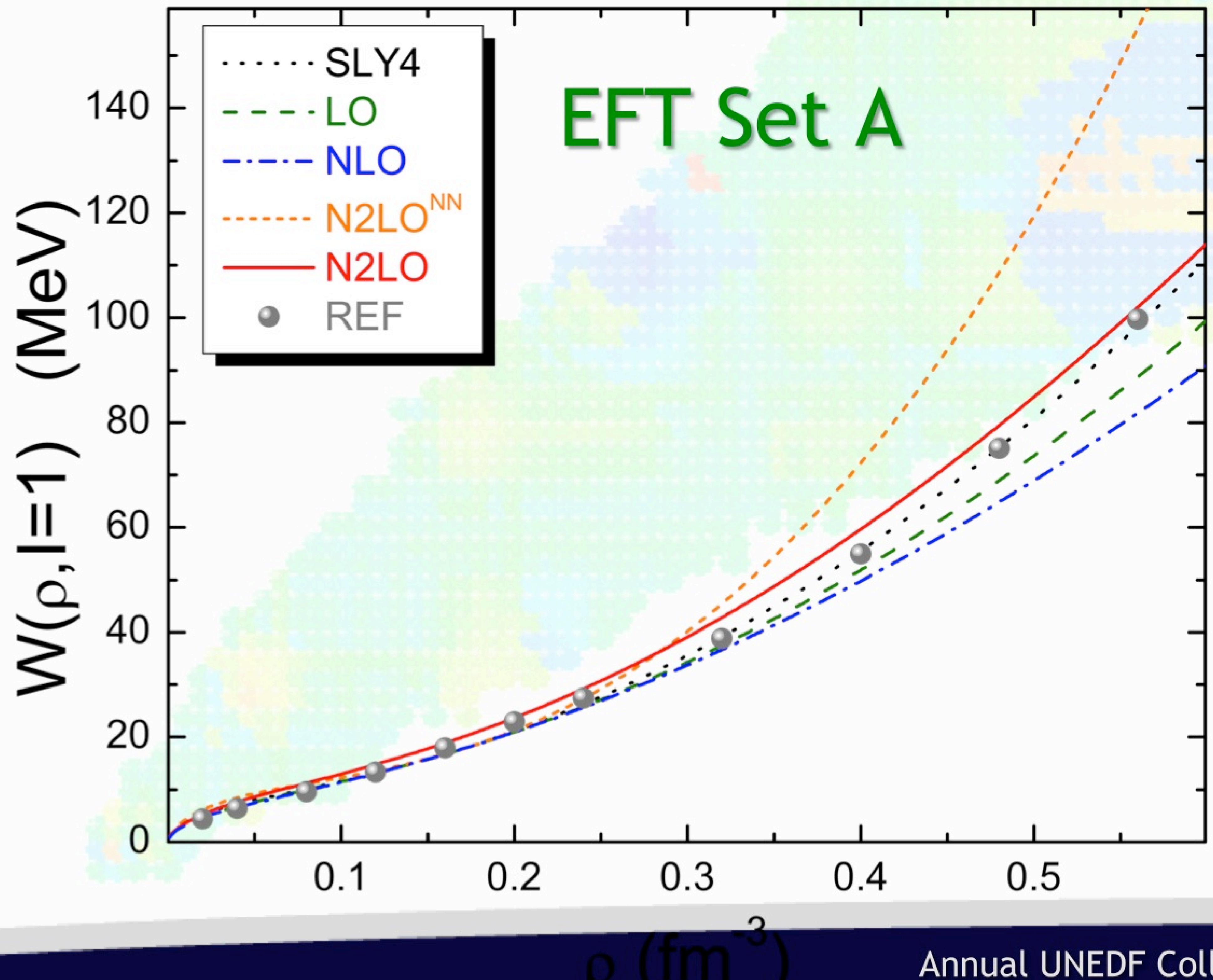


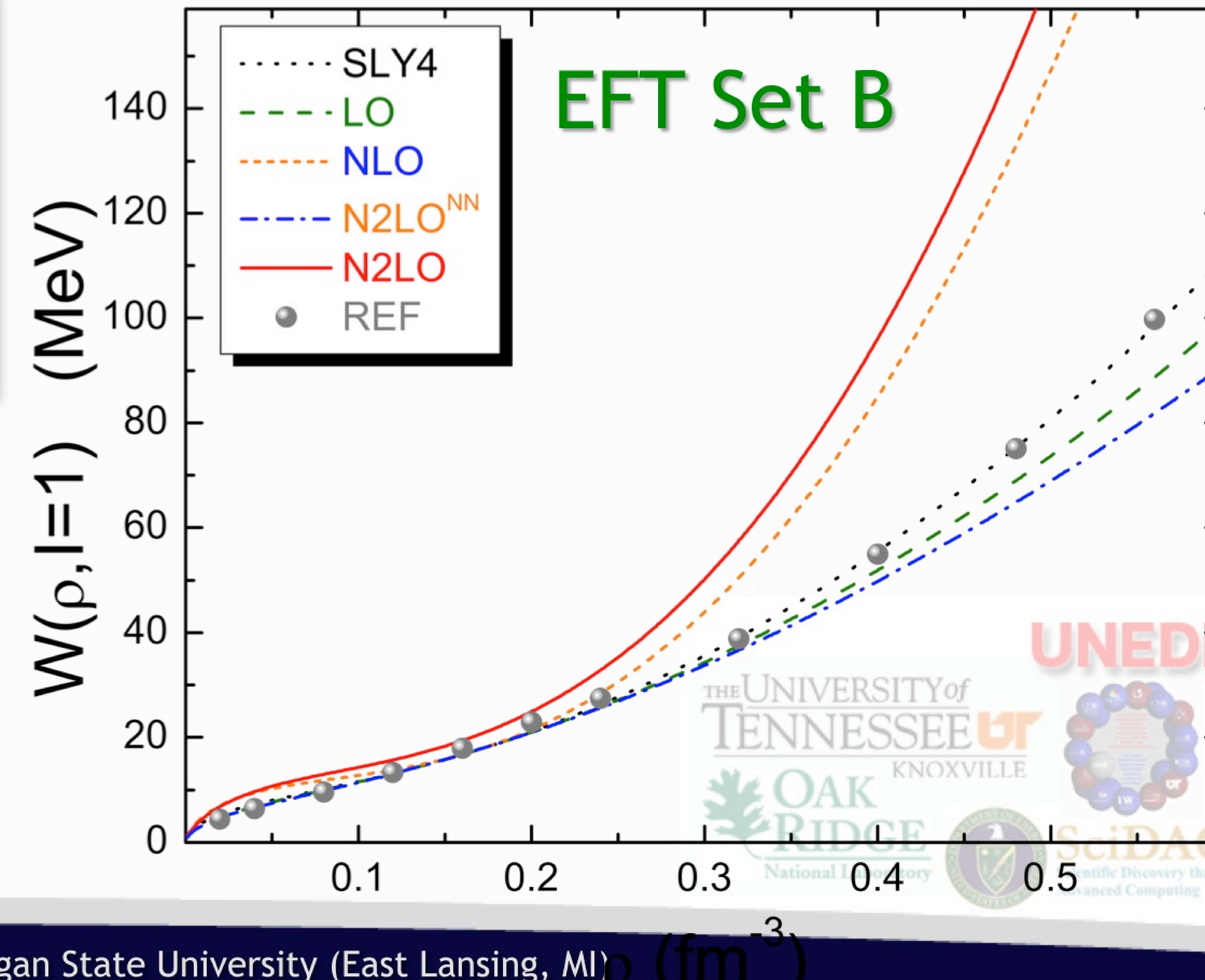




**Volume parameters from SLY4 INM**

**Interaction parameters**

| | Set A | Set B |
|---|---|---|
| $\hbar_c^{-1}$ | 197.3 | 197.327 |
| $g_A$ | 1.29 | 1.29 |
| $f_\pi$ | 92.4 $\hbar_c$ | 92.4 $\hbar_c$ |
| $m_\pi$ | 138.03 $\hbar_c$ | 138.03 $\hbar_c$ |
| $c_1$ | $-0.00081$ $\hbar_c$ | $-0.00076$ $\hbar_c$ |
| $c_3$ | $-0.0034$ $\hbar_c$ | $-0.00478$ $\hbar_c$ |
| $c_4$ | 0.0034 $\hbar_c$ | 0.00396 $\hbar_c$ |
| $c_d$ | $-2.062$ | $-2.062$ |
| $c_e$ | $-0.625$ | $-0.625$ |
| $\Lambda_x$ | 700 $\hbar_c$ | 700 $\hbar_c$ |



# DME Functional – Finite Nuclei
## SVD optimization

### SVD-optimization to the energies

Notations for N parameters (k=1,2,…,N)

$$k \mapsto \{m, t\} \quad \{C_k\} \mapsto \{C_t^m\}$$

$$m = \{\rho^2, \rho\tau, \rho\Delta\rho, \rho\nabla J, J^2\}, \quad t = \{0, 1\}$$

Energies of M nuclei (i=1,2,…,M) with mass numbers $A_i$

$$E_{A_i} = e^0_{A_i} + \sum_{k=1}^{N} C_k e^k_{A_i}$$

$$k_0 = \{\rho\tau, 0\} \mapsto C_{k_0} = C_0^{\rho\tau} \mapsto e^{k_0}_{A_i} = \int \rho_0(\mathbf{r})\tau_0(\mathbf{r})d\mathbf{r}$$

System of M x N equations using experimental energies

$$\sum_{k=1}^{N} C_k e^k_{A_i} = E^{exp}_{A_i} - e^0_{A_i}, \ (i = 1, \dots, M \geq N).$$

Its SVD solution minimizes the chi-square

$$\chi^2 = \frac{1}{M - N} \sum_{i=1}^{M} \left( \frac{E^{exp}_{A_i} - E_{A_i}}{\sigma_{A_i}} \right)^2$$

### SVD-optimization to the pairing gaps

$$E^{pp} = \frac{1}{2} \int \left(1 - \frac{\rho}{2\rho_0}\right) (V_n \tilde{\rho}_n^2 + V_p \tilde{\rho}_p^2) \, d\mathbf{r},$$

$$\Delta_q = \frac{V_q}{N_q} \int \left(1 - \frac{\rho(\mathbf{r})}{2\rho_0}\right) \rho_q(\mathbf{r}) \tilde{\rho}_q(\mathbf{r})$$

$$\Delta_q^{A_j \, exp} = \Delta_q^{A_j}, \ (j = 1, \dots, M_q)$$

### Actual optimization

$$C^{\rho^2}_{t0}, C^{\rho^2}_{tD}, C^{\rho\tau}_t$$

$$C_t^{\rho\Delta\rho}, C_t^{\rho\nabla J}, \sout{C_t^{J^2}}, V_n, V_p$$

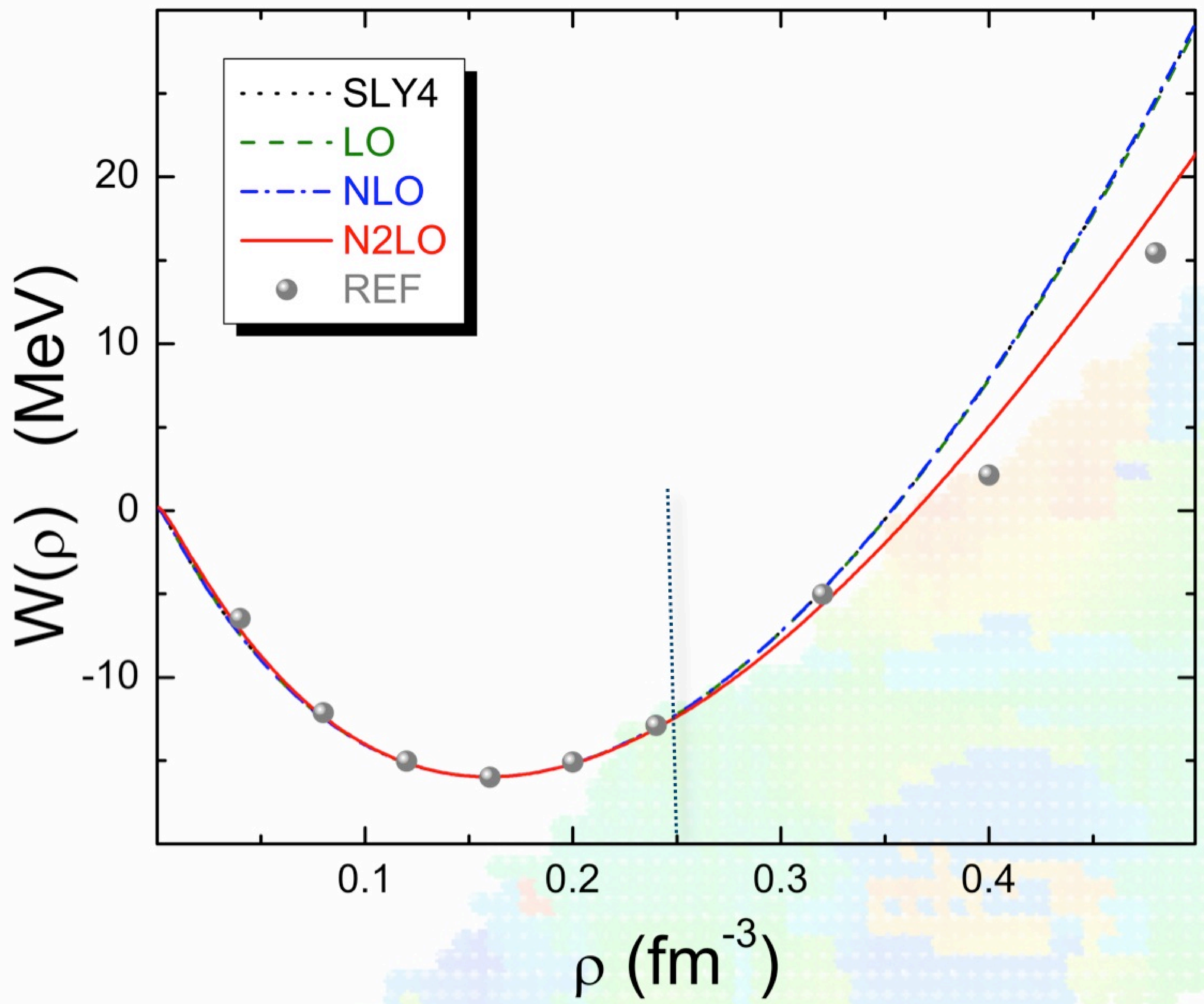
6 volume parameters fitted to INM

6 surface and pairing parameters fitted to finite nuclei

# DME Functional - Finite Nuclei
## Pre-Optimization: Volume Part

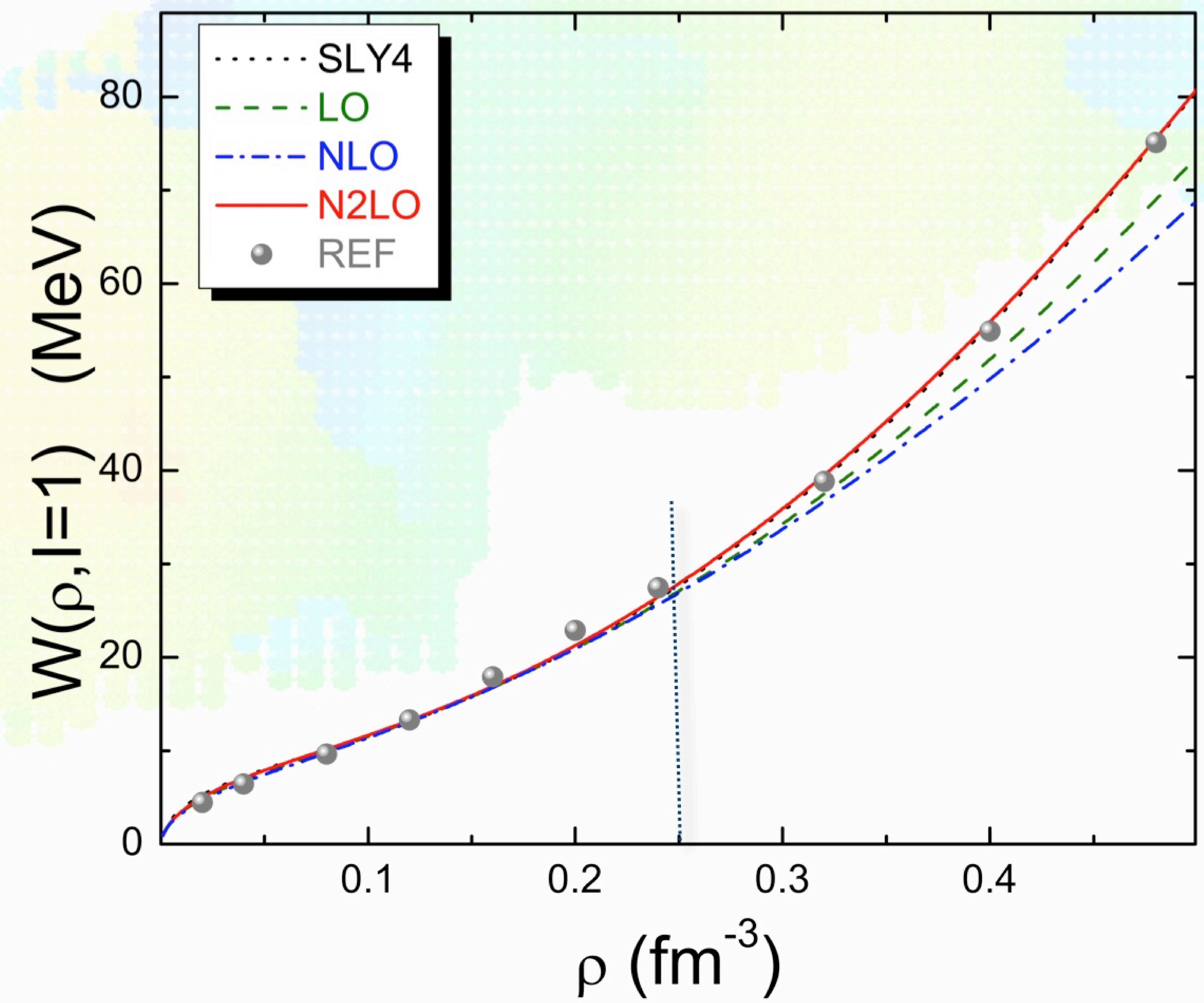
### Symmetric INM

$C_{00}^{\rho^2}, C_{0D}^{\rho^2}, C_0^{\rho\tau}$ ← $\frac{E^{NM}}{A},\ \rho_c,\ M_s^{*NM}$




### Asymmetric INM

$C_{10}^{\rho^2}, C_{1D}^{\rho^2}, C_1^{\rho\tau}$ ← $a_{sym}^{NM},\ L^{NM},\ M_v^*$




### Skyrme, LO, NLO to SLY4 values

$$\frac{E^{NM}}{A} = -15.97\ \text{MeV}, \qquad \rho_c = 0.1595\ \text{fm}^{-3},$$

$$K^{NM} = 229.9\ \text{MeV}, \qquad M_{s/v}^{*-1} = 0.695/0.8,$$

$$a_{sym}^{NM} = 32.0\ \text{MeV}, \qquad L^{NM} = 45.96\ \text{MeV}$$

**EFT Set A**

### Exception for N2LO

$$a_{sym}^{NM} = 30.0\ \text{MeV}, \quad L^{NM} = 40.96\ \text{MeV}$$

# DME Functional
## Pre-Optimization: Surface part - Results

| Parameters | SLY4 | SLY4′ | LO | NLO | N2LO |
|---|---|---|---|---|---|
| **Volume Parameters** | | | | | |
| $C_{00}^{\rho^2}$ | -933.342 | | -727.093 | -757.689 | -607.108 |
| $C_{10}^{\rho^2}$ | 830.052 | | 474.871 | 477.931 | 316.939 |
| $C_{0D}^{\rho^2}$ | 861.062 | | 612.104 | 628.504 | -1082.854 |
| $C_{1D}^{\rho^2}$ | -1064.273 | | -705.739 | -694.665 | -4369.425 |
| $C_0^{\rho\tau}$ | 57.129 | | 33.885 | 18.471 | 322.4 |
| $C_1^{\rho\tau}$ | 24.657 | | 32.405 | 92.233 | -156.901 |
| $\gamma$ | 0.16667 | | 0.30622 | 0.287419 | 1.06429 |
| **Surface Parameters** | | | | | |
| $C_0^{\rho\Delta\rho}$ | -76.287 | -76.180 | -67.437 | -63.996 | -197.132 |
| $C_1^{\rho\Delta\rho}$ | 15.951 | 24.823 | 21.551 | -9.276 | -12.503 |
| $C_0^{\rho\nabla J}$ | -92.250 | -92.959 | -95.451 | -95.463 | -193.188 |
| $C_1^{\rho\nabla J}$ | -30.75 | -82.356 | -65.906 | -60.800 | 37.790 |
| **Pairing Parameters** | | | | | |
| $V_n$ | -258.992 | -232.135 | -241.203 | -241.484 | -272.164 |
| $V_p$ | -258.992 | -244.050 | -252.818 | -252.222 | -286.965 |
| **SVD Optimization Results** | | | | | |
| $\chi^2$ | 12.5002 | 2.1235 | 1.837 | 1.7662 | 1.7884 |
| $RMSD(E)$ | 7.008 | 2.6931 | 2.5539 | 2.5143 | 2.590 |
| $RMSD(\Delta_n)$ | 0.1297 | 0.0828 | 0.0587 | 0.0554 | 0.0476 |
| $RMSD(\Delta_p)$ | 0.094 | 0.0988 | 0.0902 | 0.0866 | 0.0706 |

### EFT Set A

Volume parameters fitted to INM

SLY4, SLY4’, LO, NLO, N2LO

Surface and pairing parameters fitted to finite nuclei (SVD optimization)

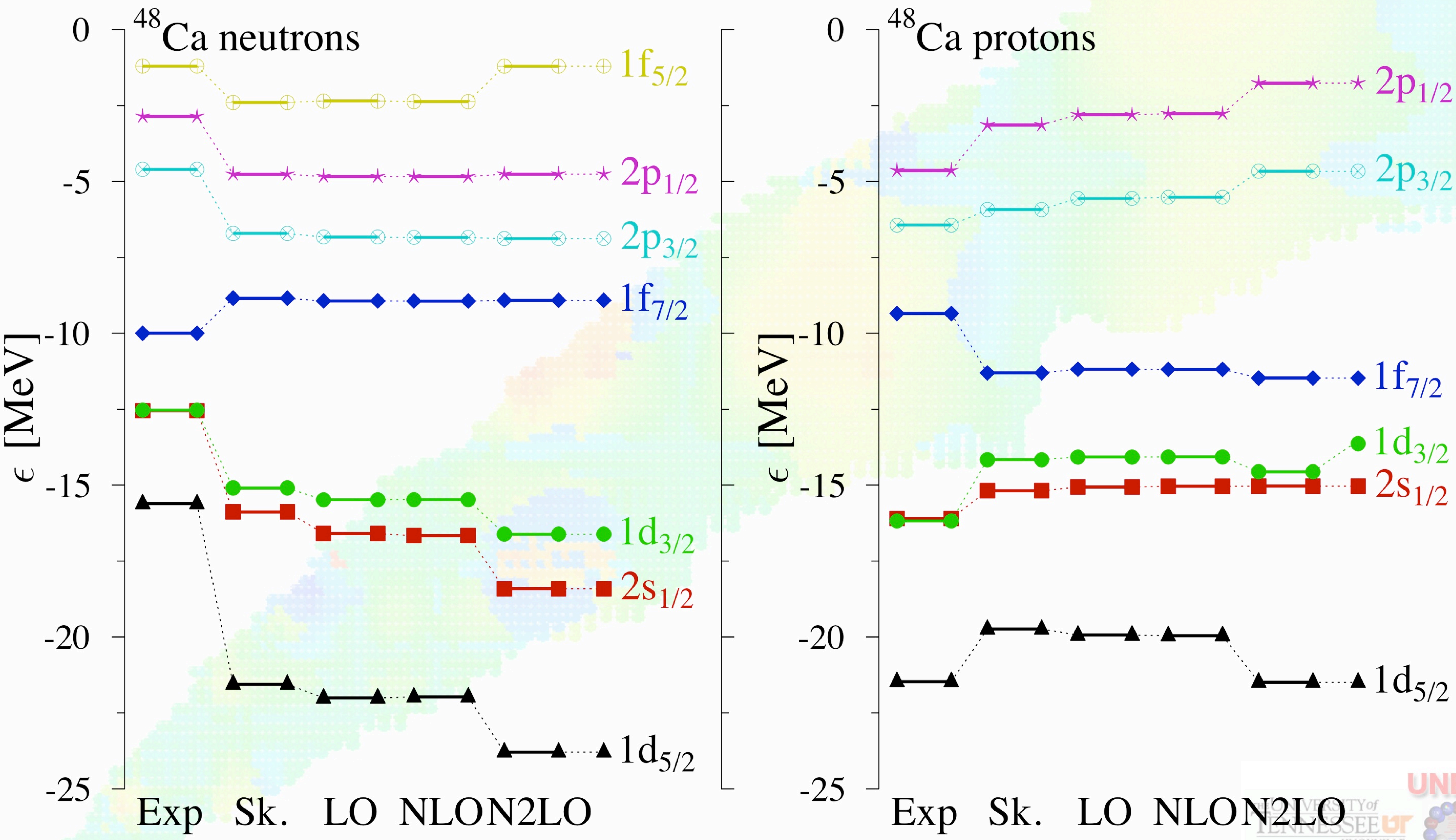
HFBTHO solver (HFB+LN)

- ✓ binding energies of 72 nuclei
- ✓ 30 spherical and 42 deformed
- ✓ 4 neutron OEM differences
- ✓ 4 proton OEM differences

The same set of data as UNDEFpre

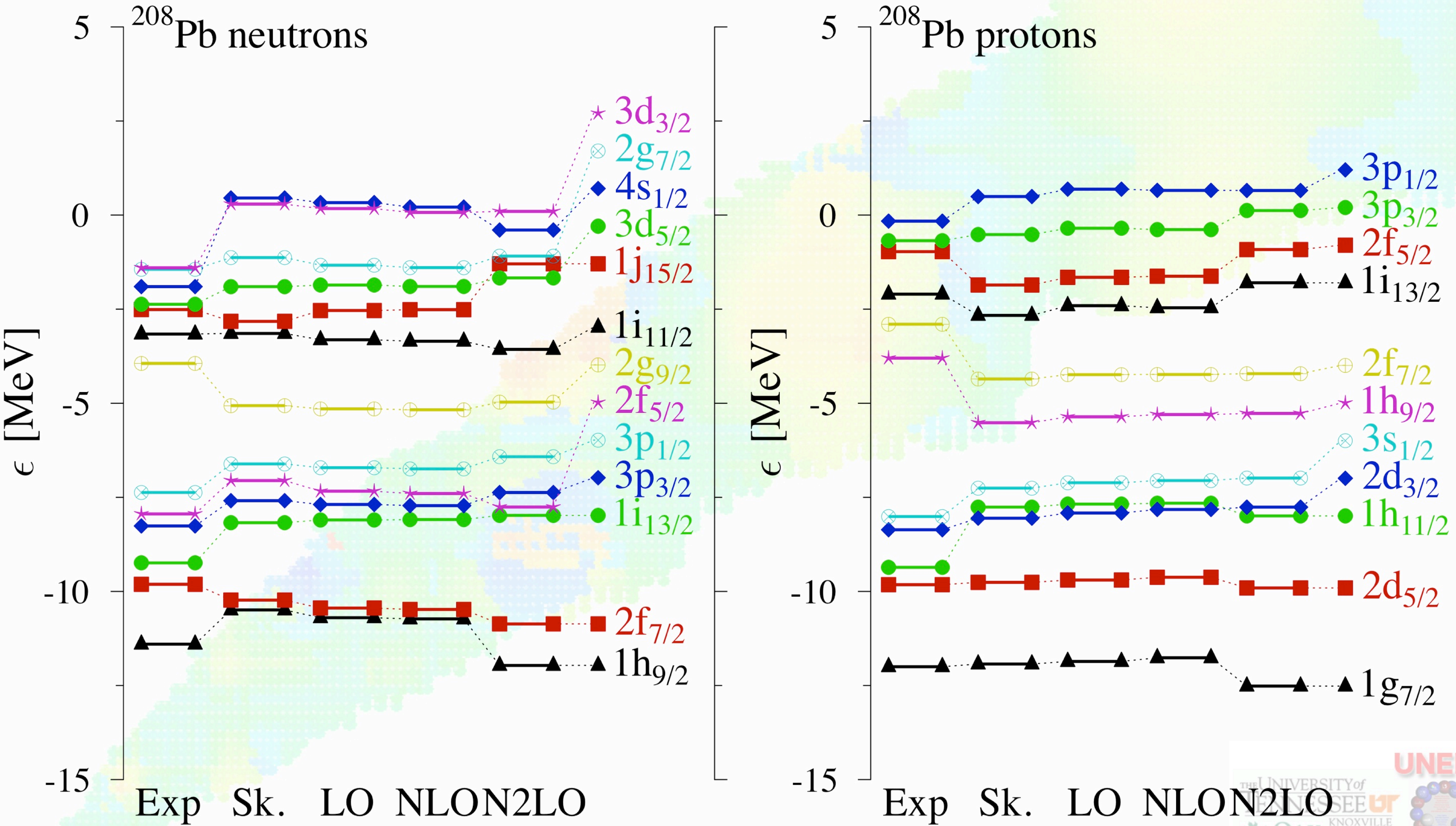
*(see the talk by N. Schunck)*

# DME Functional
## Single-Particle Energies



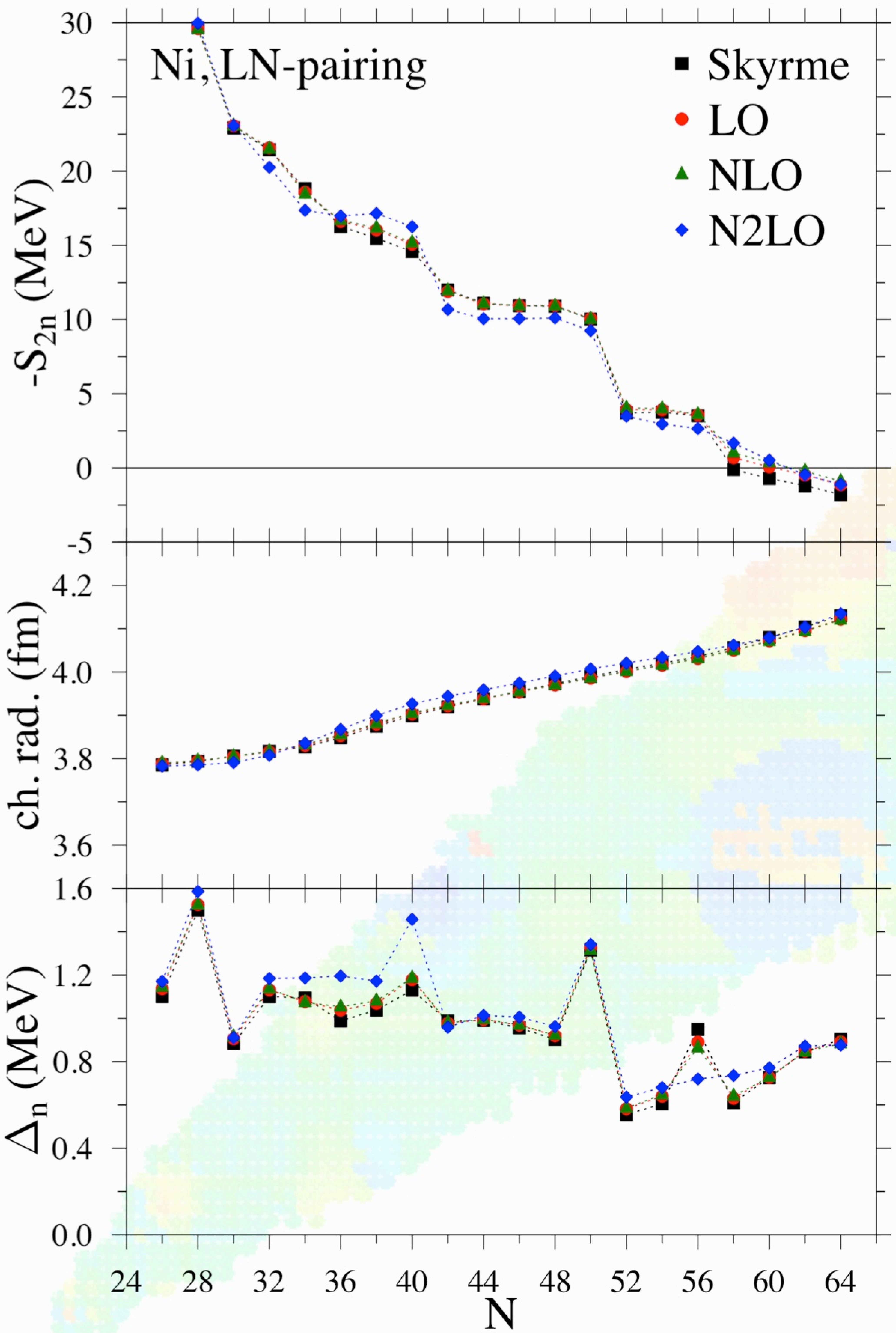
# DME Functional

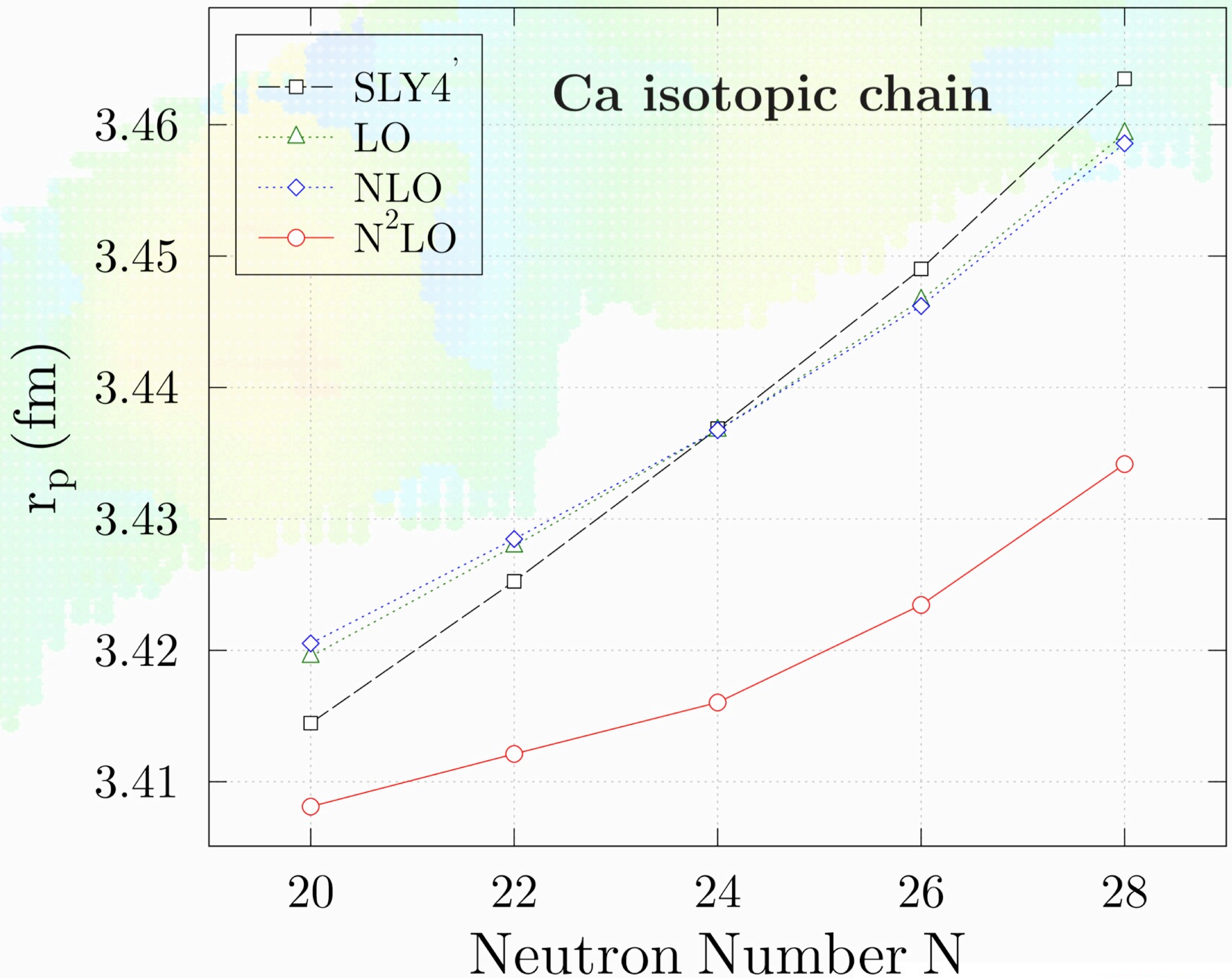
## Single-Particle Energies



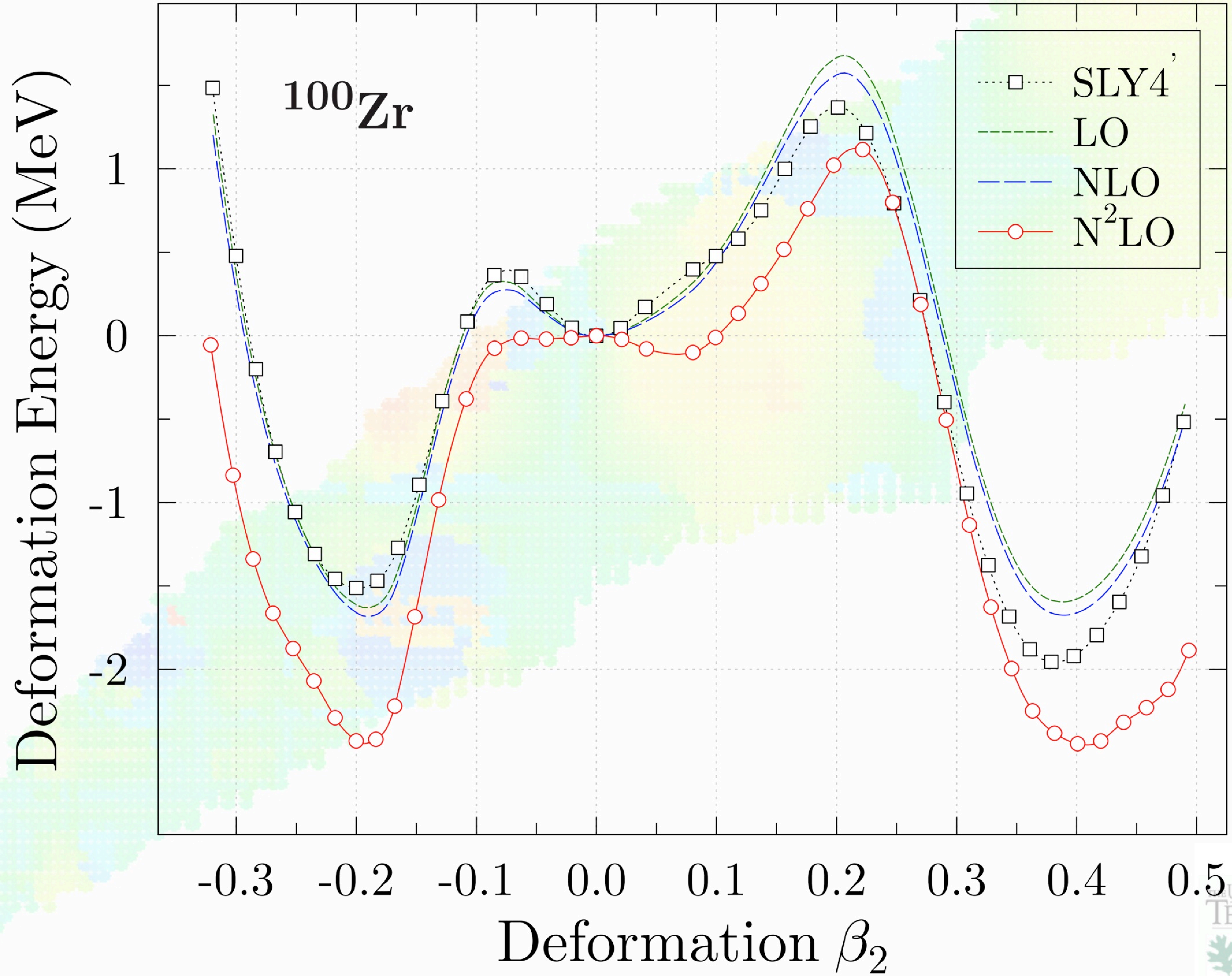
# DME Functional

## $S_{2n}$, Radii, Pairing Gaps

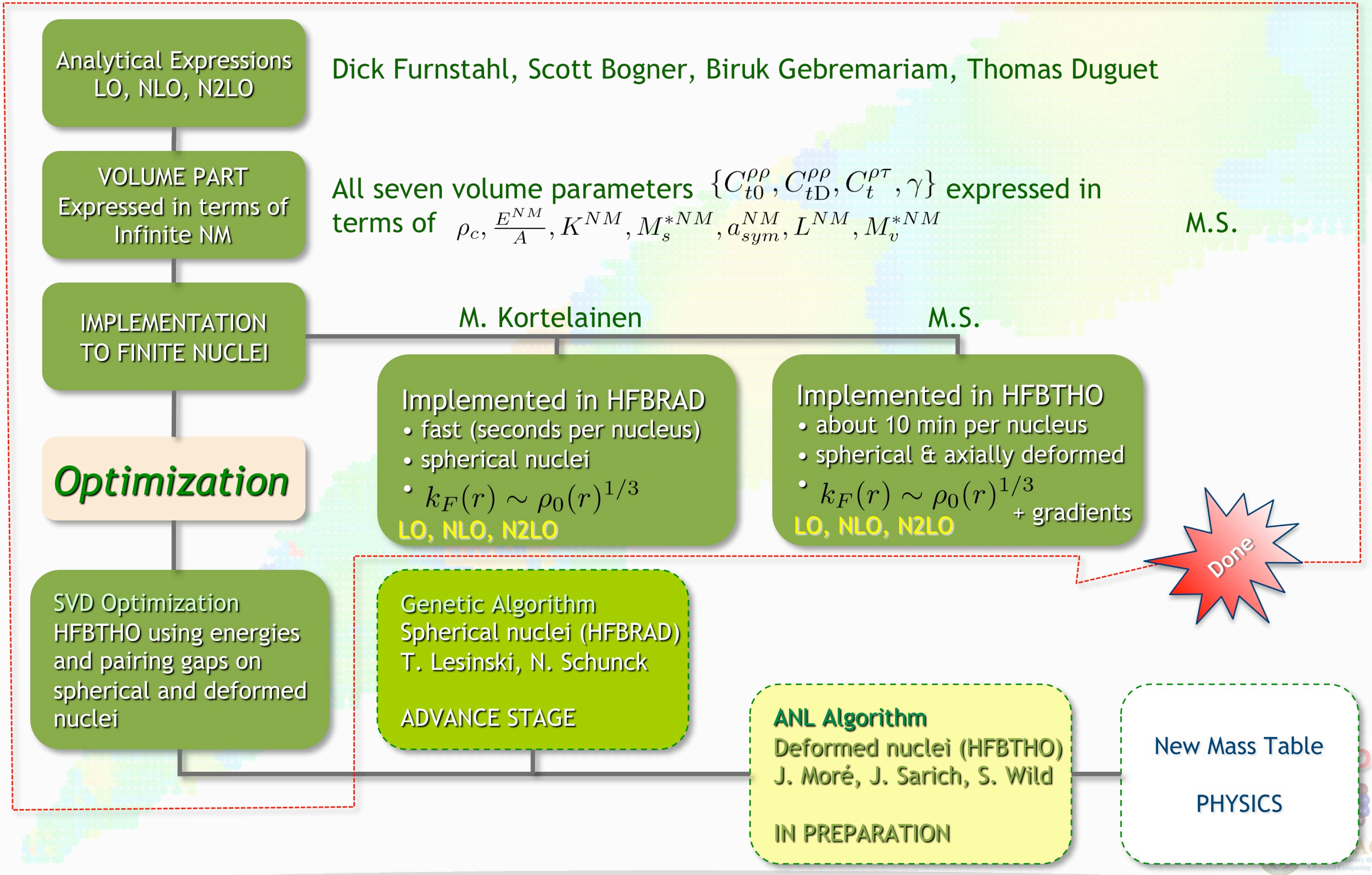


# DME Functional
## Deformability



# DME Functional
## Optimization Roadmap



# Nuclear DFT Calculations With DME Energy Density Functional
## Conclusions

✓ DME contributions modify the functional to such extent that it cannot be applied without optimization

✓ DME functional performs in almost the same way (or slightly better) as the standard Skyrme functional with respect to the optimized binding energies and OEM differences

✓ Infinite nuclear matter can have reasonable EOS, including an incompressibility $K^{NM}$ = 230 MeV, with a density dependence power  of the order of one

✓ The new, microscopically motivated, density dependence leads to some modifications of the results as, e.g., in the deformability of the functional, which are expected to further improve the ability of the functional to capture physics in the areas where the standard Skyrme functional is known that has deficiencies

## Restrictions to be removed

✧ The Hartree contribution has been treated in LDA

✧ Tensor contributions have been discarded nevertheless they naturally appear in the DME functional

## Improvements

➢ Further improvements of the DME techniques - could bring more precise fine tuning

➢ Other interactions could be an option to investigate

…, Optimization, …, Physics …