

Chiral Three-Nucleon Interactions in Nuclear Reactions and Medium-Mass Nuclei

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Workshop on "Structure of Light Nuclei"

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Outline

- Reminder — Similarity Renormalization Group
- Ab-initio Description of Nuclear Reactions Including 3N Interactions
 - The NCSM/RGM Approach
 - Treatment of 3N Interactions
 - n-⁴He, n-¹²C and n-¹⁶O scattering
- Medium-Mass Nuclei with 3N Interactions
 - The Normal-Ordering as efficient tool to treat 3N interactions
 - Ab-initio Benchmarks via IT-NCSM and CCSD
- Soft Interactions in Many-Body Perturbation Theory

Reminder: Similarity Renormalization Group

Wegner, Glazek, Wilson, Perry, Bogner, Furnstahl, Hergert, Roth, Jurgenson, Navratil,...

...yields an evolved Hamiltonian with
improved convergence properties in
many-body calculations

- **unitary transformation** of Hamiltonian driven by

$$\frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \quad \eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha]$$

- NN interaction @ N³LO [Entem, Machleidt, Phys.Rev C68, 041001(R) (2003)]
- 3N interaction @ N²LO
 - standard 3N: c_D & c_E fixed by binding energy and β -decay halflife of triton [Gazit et.al., Phys.Rev.Lett. 103, 102502 (2009)]
 - reduced cutoff $\Lambda = 400$ MeV 3N: c_D & c_E fixed by β -decay halflife of triton and ⁴He [Roth et.al., Phys. Rev. Lett 109, 052501 (2012)]

Reminder: Similarity Renormalization Group

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Different SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two- and three-body terms

Three-Nucleon Interactions in the NCSM/RGM Approach

- S. Quaglioni and P. Navrátil — Phys. Rev. Lett. 101, 092501 (2008)
P. Navrátil, R. Roth and S. Quaglioni — Phys. Rev. C 82, 034609 (2010)
S. Quaglioni, P. Navratil, G. Hupin, J. Langhammer et al. — arXiv:1210.2020
S. Quaglioni, P. Navrátil, R. Roth, W. Horiuchi — arXiv:1203.0268

In collaboration with:

Guillaume Hupin, Sofia Quaglioni, Petr Navrátil, Robert Roth

Motivation

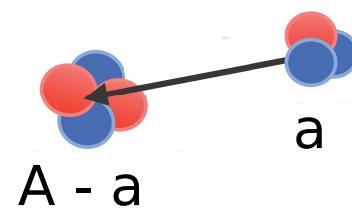
Realistic ab-initio description of light nuclei

bound states
& spectroscopy

(IT-)NCSM

ab-initio description
of nuclear clusters

(IT-)NCSM/RGM
approach



resonances
& scattering states

RGM

cluster technique that as-
sumes clustered nucleons

successfully applied with NN interaction

this talk:
inclusion of
3N interaction

General Approach of NCSM/RGM

- Represent $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **overcomplete basis**

$$|\psi^{J\pi T}\rangle = \sum_{\nu} \int dr r^2 \frac{g_{\nu}^{J\pi T}(r)}{r} \mathcal{A}_{\nu} |\phi_{\nu r}^{J\pi T}\rangle \quad g_{\nu}^{J\pi T}(r) \text{ unknown}$$

with the binary-cluster channel states

$$|\phi_{\nu r}^{J\pi T}\rangle = \left\{ |\phi^{(A-a)}\rangle |\phi^{(a)}\rangle \right\}^{J\pi T} \frac{\delta(r-r_{A-a,a})}{rr_{A-a,a}}$$

NCSM delivers
 $|\phi^{(A-a)}\rangle$ and $|\phi^{(a)}\rangle$

- Solve **generalized eigenvalue** problem

$$\sum_{\nu} \int dr r^2 [\mathcal{H}_{\nu,\nu'}^{J\pi T}(r',r) - E \mathcal{N}_{\nu,\nu'}^{J\pi T}(r',r)] \frac{g_{\nu r}^{J\pi T}}{r} = 0$$

Hamiltonian kernel

$$\langle \phi_{\nu' r'}^{J\pi T} | \mathcal{A}_{\nu'} H \mathcal{A}_{\nu} | \phi_{\nu r}^{J\pi T} \rangle$$

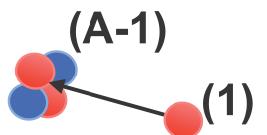
Norm kernel

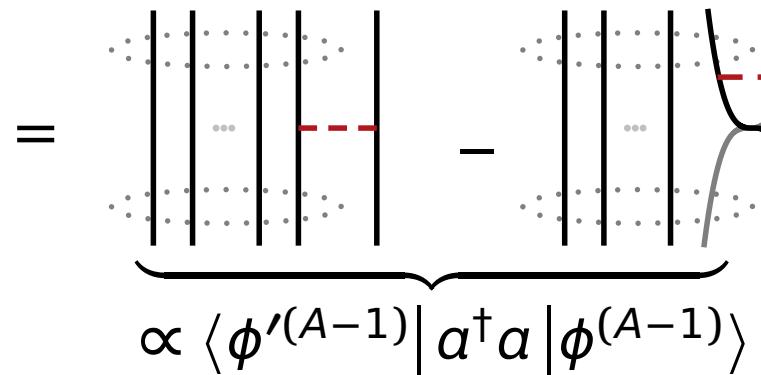
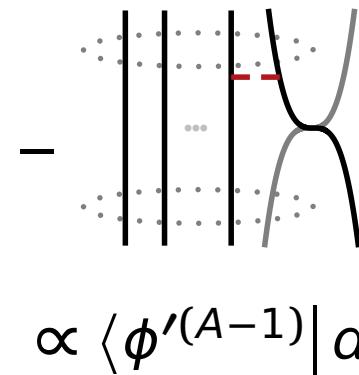
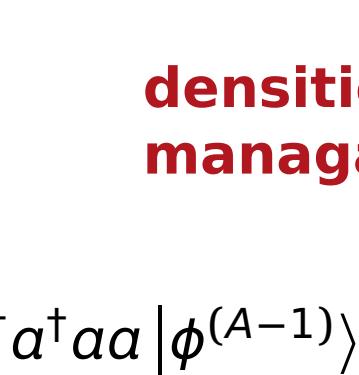
$$\langle \phi_{\nu' r'}^{J\pi T} | \mathcal{A}_{\nu'} \mathcal{A}_{\nu} | \phi_{\nu r}^{J\pi T} \rangle$$

The Hamiltonian Kernel: NN Diagrams

- Consider NN-interaction kernels with **single-nucleon projectiles**

$$\begin{aligned}
 \langle \phi_{\nu' r'}^{J\pi T} | V_{NN} A^2 | \phi_{\nu r}^{J\pi T} \rangle &= \langle \phi_{\nu' r'}^{J\pi T} | V_{NN} [1 - \sum_{i=1}^{A-1} T_{i,A}] | \phi_{\nu r}^{J\pi T} \rangle \\
 &= (A-1) \langle \phi_{\nu' r'}^{J\pi T} | V_{A-1,A} | \phi_{\nu r}^{J\pi T} \rangle \\
 &\quad - (A-1) \langle \phi_{\nu' r'}^{J\pi T} | V_{A-1,A} T_{A-1,A} | \phi_{\nu r}^{J\pi T} \rangle \\
 &\quad - (A-1)(A-2) \langle \phi_{\nu' r'}^{J\pi T} | V_{A-2,A} T_{A-1,A} | \phi_{\nu r}^{J\pi T} \rangle \quad \text{"exchange" kernel}
 \end{aligned}$$



$=$  $-$  $-$ 

**densities
managable**

Towards Inclusion of Full 3N Forces

- Derive expressions for Hamiltonian kernel with 3N interaction
 \Rightarrow 3N-interaction kernel

$$\begin{aligned}
 \langle \phi_{\nu' r'}^{J\pi T} | V_{NNN} A^2 | \phi_{\nu r}^{J\pi T} \rangle &= \langle \phi_{\nu' r'}^{J\pi T} | V_{NNN} [1 - \sum_{i=1}^{A-1} T_{i,A}] | \phi_{\nu r}^{J\pi T} \rangle \\
 &= \frac{(A-1)(A-2)}{2} \langle \phi_{\nu' r'}^{J\pi T} | V_{A-2, A-1, A} | \phi_{\nu r}^{J\pi T} \rangle \\
 &\quad - \frac{(A-1)(A-2)}{2} \langle \phi_{\nu' r'}^{J\pi T} | V_{A-2, A-1, A} T_{A-2, A} | \phi_{\nu r}^{J\pi T} \rangle \\
 &\quad - \frac{(A-1)(A-2)}{2} \langle \phi_{\nu' r'}^{J\pi T} | V_{A-1, A-2, A} T_{A-1, A} | \phi_{\nu r}^{J\pi T} \rangle \\
 &\quad - \frac{(A-1)(A-2)(A-3)}{2} \langle \phi_{\nu' r'}^{J\pi T} | V_{A-3, A-2, A} T_{A-1, A} | \phi_{\nu r}^{J\pi T} \rangle
 \end{aligned}$$

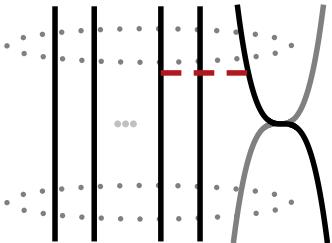
"direct" kernel

challenge:
**handling of
3-body density**

$$= \underbrace{\dots}_{\propto \langle \phi'^{(A-1)} | a^\dagger a^\dagger a a | \phi^{(A-1)} \rangle} - \underbrace{\dots}_{\propto \langle \phi'^{(A-1)} | a^\dagger a^\dagger a^\dagger a a a | \phi^{(A-1)} \rangle} - \dots$$

Two Ways of Handling the Three-Body Density

① Precomputed coupled densities



$$\sum_{\substack{j_0 j'_0 \\ K J_0}} \sum_{\substack{t_0 t'_0 \\ \tau T_0}} \sum_{\substack{n_\alpha l_\alpha j_\alpha \\ n_b l_b j_b}} \sum_{\substack{n_\alpha' l_\alpha' j_\alpha' \\ n_a' l_a' j_a'}} \frac{1}{12} \hat{\tau} \hat{K} \hat{j}_0 \hat{\tau}_0 \hat{g}' \hat{t}'_g (-1)^{j'_a + j'_b - j'_0 + j' + K + I_1 + J} (-1)^{3/2 - t'_0 + j' + \tau + T_1 + T}$$

$$\left\{ \begin{matrix} I_1 & K & I'_1 \\ j' & J & j \end{matrix} \right\} \left\{ \begin{matrix} j' & K & j \\ g' & j'_0 & J_0 \end{matrix} \right\} \left\{ \begin{matrix} T_1 & \tau & T'_1 \\ \frac{1}{2} & T & \frac{1}{2} \end{matrix} \right\} \left\{ \begin{matrix} \frac{1}{2} & \tau & \frac{1}{2} \\ t'_g & t'_0 & \tau \end{matrix} \right\}$$

3-body density
cannot be stored

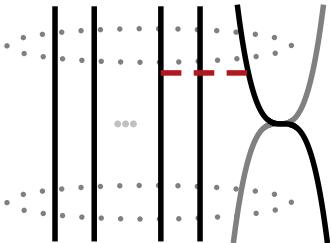
$$\langle \phi'^{(A-1)} I'_1 T'_1 \rangle \left[(a_{nlj}^\dagger (a_{n'_b l'_b j'_b}^\dagger a_{n'_a l'_a j'_a}^\dagger)^{j'_0 t'_0})^{g' t'_g} ((\tilde{a}_{n_\alpha l_\alpha j_\alpha} \tilde{a}_{n_\alpha l_\alpha j_\alpha})^{j_0 t_0} \tilde{a}_{n_b l_b j_b})^{j_0 T_0} \right]^{K \tau} \|\phi^{(A-1)} I_1 T_1 \rangle$$

$${}_a \langle ((n'_a l'_a j'_a, n'_b l'_b j'_b) j'_0 t'_0, n' l' j') J_0 T_0 | V_{3N} | ((n_\alpha l_\alpha j_\alpha, n_\alpha l_\alpha j_\alpha) j_0 t_0, n_b l_b j_b) j_0 T_0 \rangle$$

make use of JT -coupled
3N matrix elements

Two Ways of Handling the Three-Body Density

① Precomputed coupled densities



$$\sum_{\substack{j_0 j'_0 \\ J_0 T_0}} \sum_{t_0 t'_0} \sum_{\substack{n_a l_a j_a \\ n_b l_b j_b}} \sum_{\substack{n_\alpha l_\alpha j_\alpha \\ n'_a l'_a j'_a \\ g' t'_g}} \sum_{\substack{\phi'' I_\beta T_\beta \\ g' t'_g}} \frac{1}{12} \hat{J}_0 \hat{T}_0 \hat{g}' \hat{t}'_g (-1)^{j'_a + j'_b + J_0 + g' + I_\beta - I_1 + j} (-1)^{3/2 + T_0 + t'_g - T_1 + T_\beta}$$

$$\left\{ \begin{array}{c} I_\beta \ g' \ I'_1 \\ J_0 \ j'_0 \ j' \\ J_1 \ j \ J \end{array} \right\} \left\{ \begin{array}{c} T_\beta \ t'_g \ T'_1 \\ T_0 \ t'_0 \ \frac{1}{2} \\ T_1 \ \frac{1}{2} \ T \end{array} \right\}$$

applicable up to ${}^4\text{He}$ targets
coded by G. Hupin

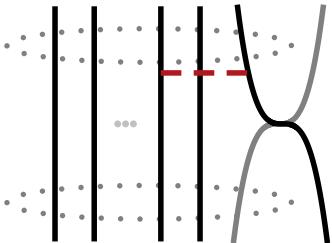
$$\langle \phi'^{(A-1)} I'_1 T'_1 \|(a_{nlj}^\dagger (a_{n'_b l'_b j'_b}^\dagger a_{n'_a l'_a j'_a}^\dagger)^{j'_0 t'_0})^{g' t'_g} \| \phi''^{(A-4)} I_\beta T_\beta \rangle$$

$$\langle \phi''^{(A-4)} I_\beta T_\beta \|\langle \tilde{a}_{n_\alpha l_\alpha j_\alpha} \tilde{a}_{n_a l_a j_a} \rangle^{j_0 t_0} \tilde{a}_{n_b l_b j_b} \rangle^{j_0 T_0} \| \phi^{(A-1)} I_1 T_1 \rangle$$

$${}_a \langle ((n'_a l'_a j'_a, n'_b l'_b j'_b) j'_0 t'_0, n' l' j') J_0 T_0 | V_{3N} | ((n_\alpha l_\alpha j_\alpha, n_a l_a j_a) j_0 t_0, n_b l_b j_b) J_0 T_0 \rangle_a$$

Two Ways of Handling the Three-Body Density

② Compute uncoupled densities on-the-fly



$$\sum_{jj'} \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \sum_{M'_1 m'_j} \sum_{M'_{T_1} m'_t} \frac{1}{12} (-1)^{I_1 + I'_1 +}$$

$$\begin{pmatrix} I_1 & j \\ M_1 & m_j \end{pmatrix} \left| \begin{array}{c} J \\ M_J \end{array} \right\rangle \begin{pmatrix} T_1 & \frac{1}{2} \\ M_{T_1} & m_t \end{pmatrix} \left| \begin{array}{c} T \\ m_t \end{array} \right\rangle$$

$$\sum_{\beta_{A-3}} \sum_{\beta_{A-2}} \sum_{\beta'_{A-3}} \sum_{\beta'_{A-2}} \sum_{\beta'_{A-1}}$$

$$\langle \phi'^{(A-1)} I'_1 M'_1 T'_1 M'_{T_1} | a^\dagger_{nljm_j \frac{1}{2} m_t} a^\dagger_{\beta_{A-2}} a^\dagger_{\beta_{A-3}} a_{\beta'_{A-3}} a_{\beta'_{A-2}} a_{\beta'_{A-1}} | \phi^{(A-1)} I_1 M_1 T_1 M_{T_1} \rangle$$

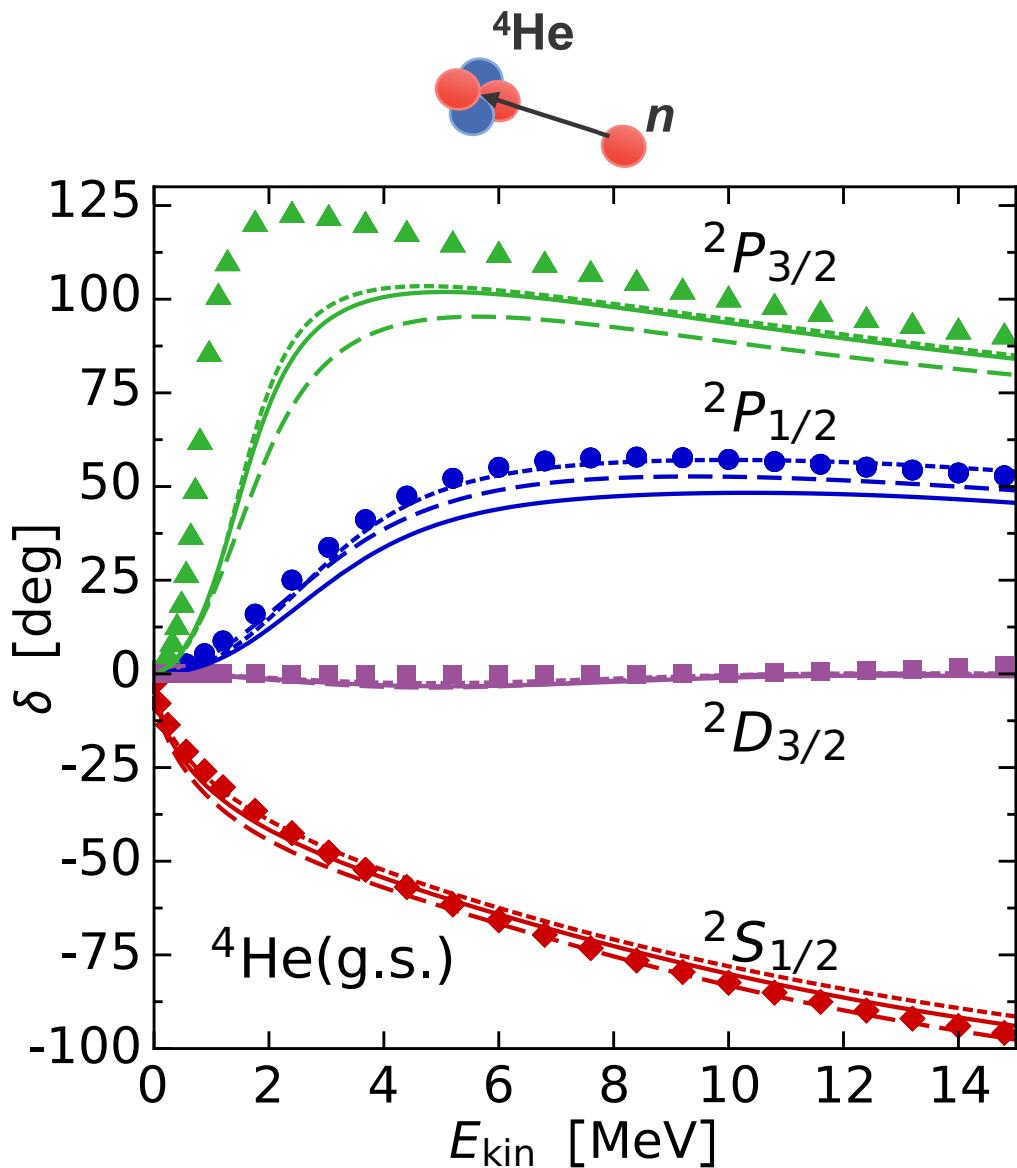
$$_a \langle \beta_{A-3} \beta_{A-2} n' l' j' m'_j \frac{1}{2} m'_t | V_{3N} | \beta'_{A-3} \beta'_{A-2} \beta'_{A-1} \rangle_a$$

- + acces to heavier targets
- + no averaged isospin
- + perfectly parallel

treatment of M_J & M_T q.n.
new computational scheme
& infrastructure

efficient
decoupling

Scattering Phase Shifts: n + ^4He



Comparison against
experiment

$$N_{\max} = 13$$

◆▲●■ experiment

..... NN-only

--- NN+3N-ind

— NN+3N-full

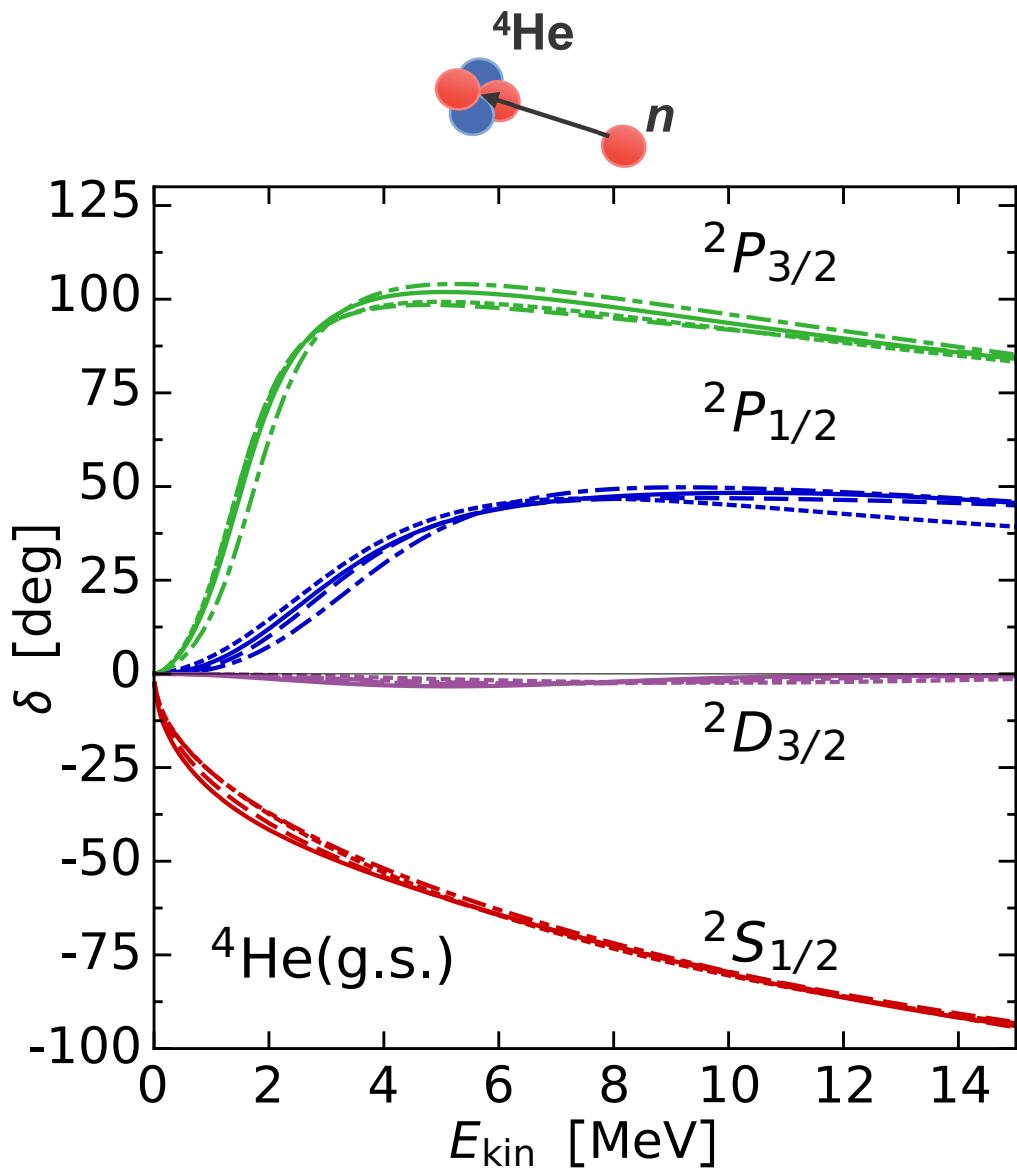
increased spin-orbit
splitting by initial 3N

$$\alpha = 0.0625 \text{ fm}^4$$

$$(\lambda = 2.0 \text{ fm}^{-1})$$

$$\hbar\Omega = 20 \text{ MeV}$$

Scattering Phase Shifts: n + ^4He



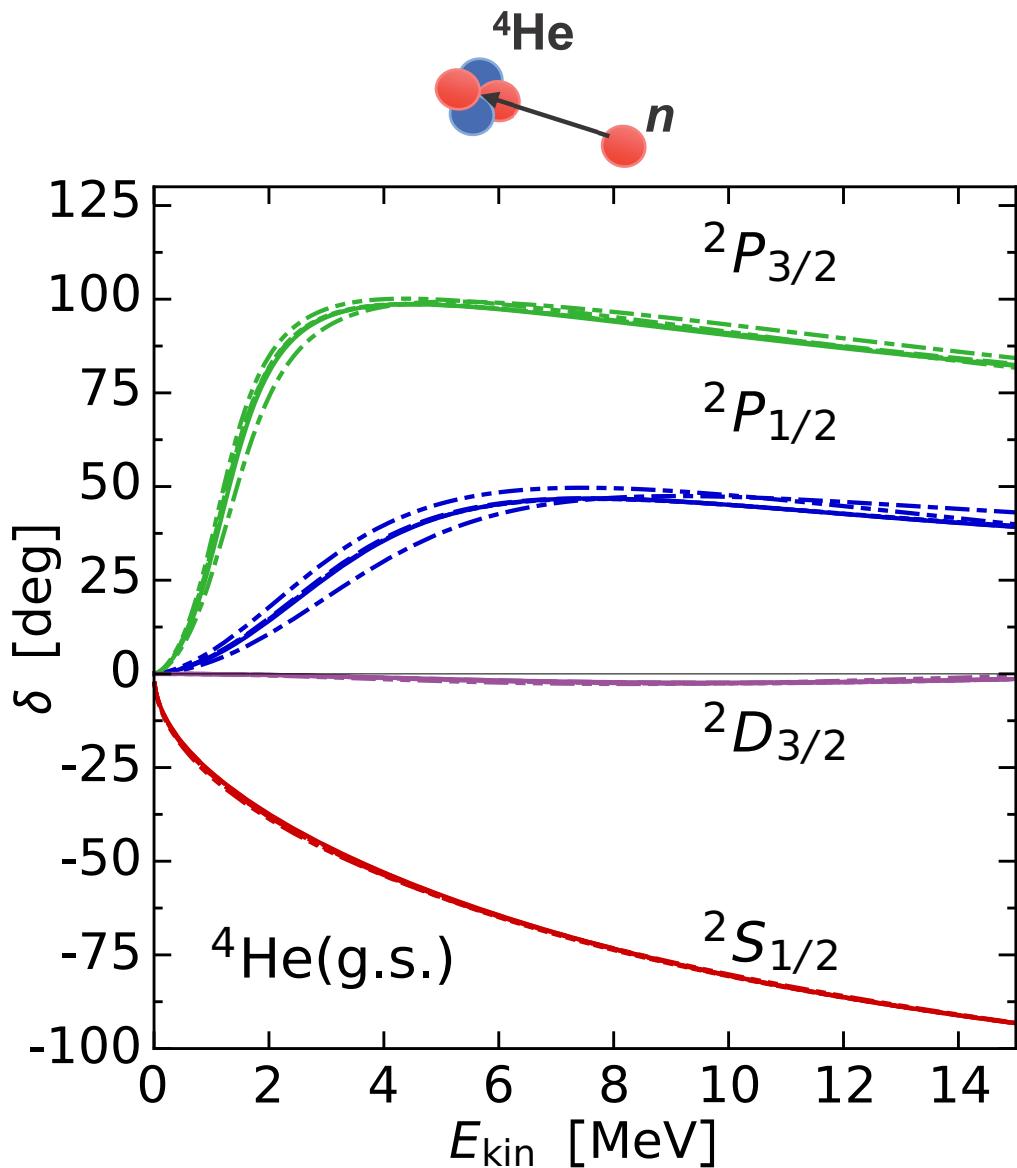
Convergence w.r.t. N_{\max}

NN+3N-full

- $N_{\max} = 7$
- - - $N_{\max} = 9$
- - - $N_{\max} = 11$
- $N_{\max} = 13$

$$\begin{aligned}\alpha &= 0.0625 \text{ fm}^4 \\ (\lambda &= 2.0 \text{ fm}^{-1}) \\ \hbar\Omega &= 20 \text{ MeV}\end{aligned}$$

Scattering Phase Shifts: n + ${}^4\text{He}$



Convergence w.r.t.
 $E_{3\max} = \max\{e_1 + e_2 + e_3\}$

NN+3N-full

$$N_{\max} = 7$$

$$E_{3\max} = 4$$

$$E_{3\max} = 6$$

$$E_{3\max} = 8$$

$$--- E_{3\max} = 10$$

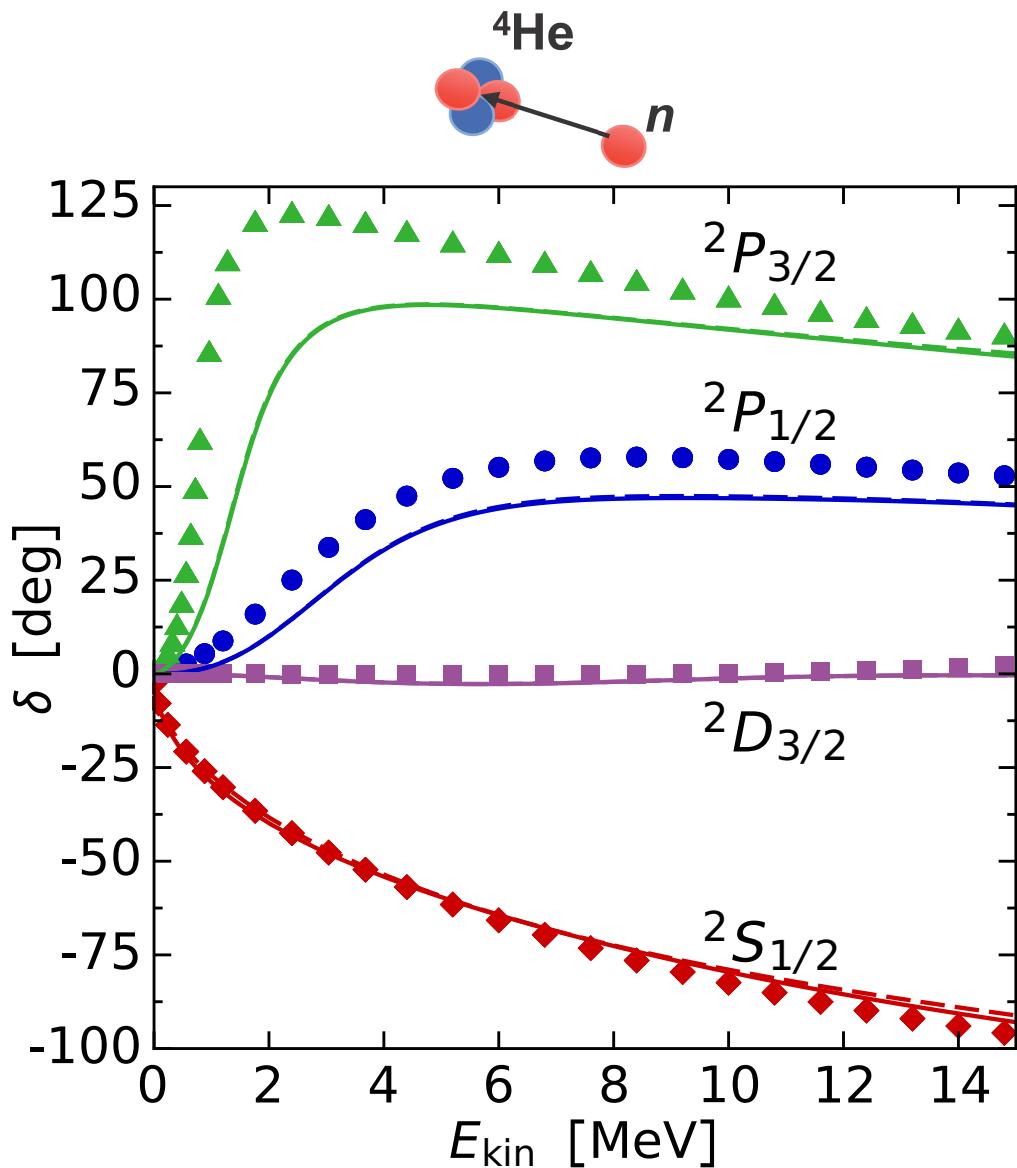
$$— E_{3\max} = 12$$

$$\alpha = 0.0625 \text{ fm}^4$$

$$(\lambda = 2.0 \text{ fm}^{-1})$$

$$\hbar\Omega = 20 \text{ MeV}$$

Scattering Phase Shifts: n+⁴He



Taking into account
excited states of ${}^4\text{He}$

NN+3N-full

$$N_{\max} = 11$$

◆▲●■ experiment

— ${}^4\text{He } 0^+(g.s.)$

--- ${}^4\text{He } 0^+(g.s.), 0^+$

$$\alpha = 0.06 \angle_\omega$$

$$(\lambda = 2.0 \text{ fm}^{-1})$$

$$\hbar\Omega = 20 \text{ MeV}$$

need more excited
states...work in
progress

Conclusions NCSM/RGM

NCSM/RGM delivers **ab-initio description of low-energy nuclear reactions**

- **strict test** of predictive power of **chiral forces**
- inclusion of 3N interactions challenging but practically completed
 - first n+⁴He results show expected **enhanced spin-orbit splitting**
 - consideration of more ⁴He eigenstates necessary
 - new computational scheme → **heavy targets accesible**
- stay tuned...

Medium Mass Nuclei with 3N Interactions

R. Roth, S. Binder, K. Vobig, et al. — Phys. Rev. Lett 109, 052501 (2012)

Normal-Ordered 3N Interaction

avoid technical challenge of
including explicit 3N interactions in
many-body calculation

- **idea:** write 3N interaction in normal-ordered form with respect to an A-body reference Slater-determinant ($0\hbar\Omega$ state)

$$\hat{V}_{3N} = \sum V_{oooooo}^{3N} \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o \hat{a}_o \hat{a}_o$$

$$= W_{oo}^{0B} + \sum W_{ooo}^{1B} \{ \hat{a}_o^\dagger \hat{a}_o \} + \sum W_{oooo}^{2B} \{ \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o \hat{a}_o \}$$

$$+ \sum W_{oooooo}^{3B} \{ \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o \hat{a}_o \hat{a}_o \}$$

$$= \hat{W}_{0B} + \hat{W}_{1B} + \hat{W}_{2B} + \hat{W}_{3B}$$

operator identity

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$$= W_{oo}^{0B} + \sum W_{ooo}^{1B} \{ \hat{a}_o^\dagger \hat{a}_o \} + \sum W_{oooo}^{2B} \{ \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o \hat{a}_o \}$$

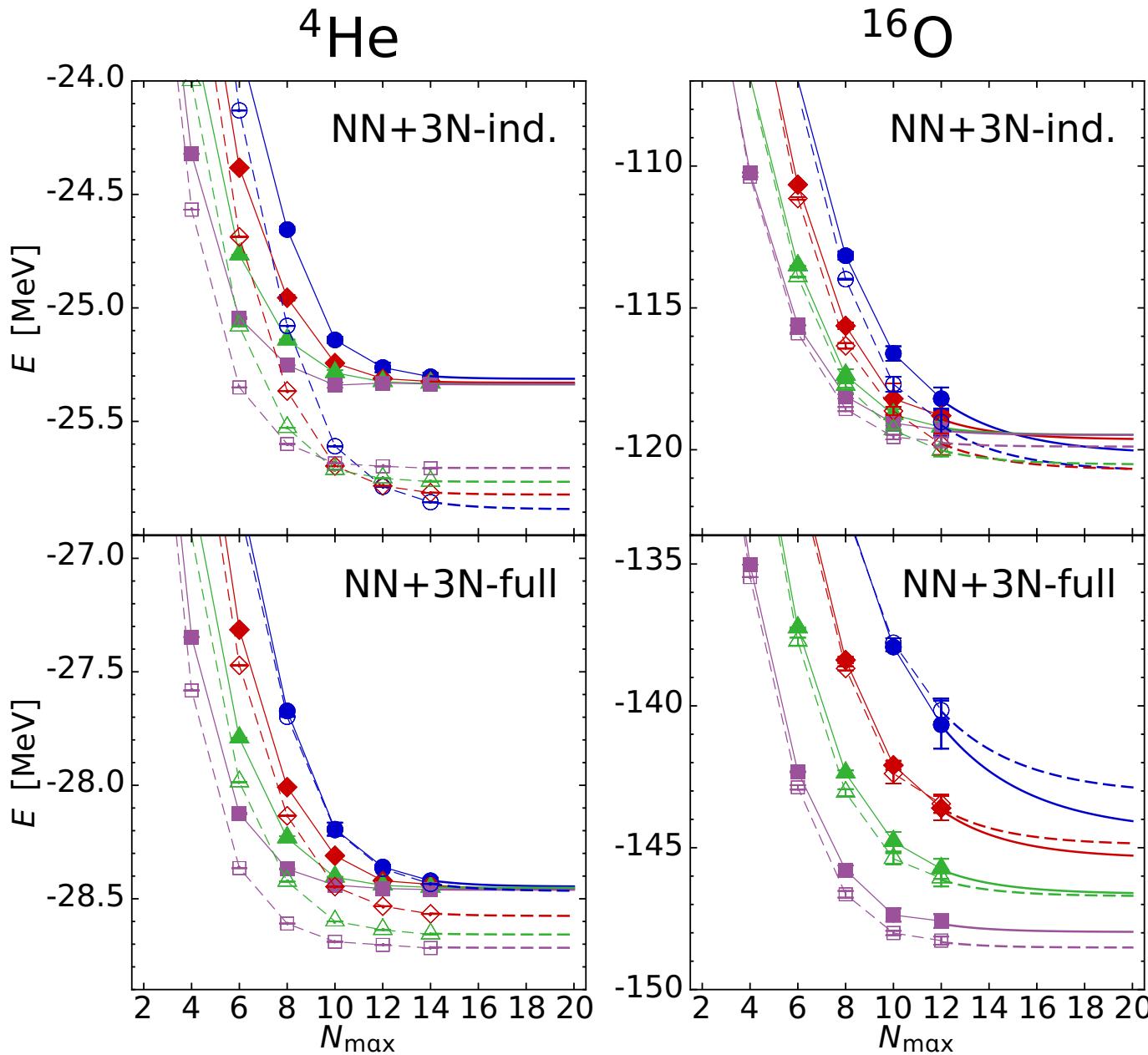
$$+ \sum W_{oooooo}^{3B} \{ \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o^\dagger \hat{a}_o \hat{a}_o \hat{a}_o \}$$

$$= \hat{W}_{0B} + \hat{W}_{1B} + \hat{W}_{2B} + \hat{W}_{3B}$$

operator identity

- **question:** if we neglect the normal-ordered \hat{W}_{3B} 3B term, how well does this approximation work?

Benchmark of Normal-Ordered 3N



- compare IT-NCSM results with **complete 3N to normal-ord. 3N** truncated at 2B level
- typical deviations up to 2% for ${}^4\text{He}$ and 1% for ${}^{16}\text{O}$

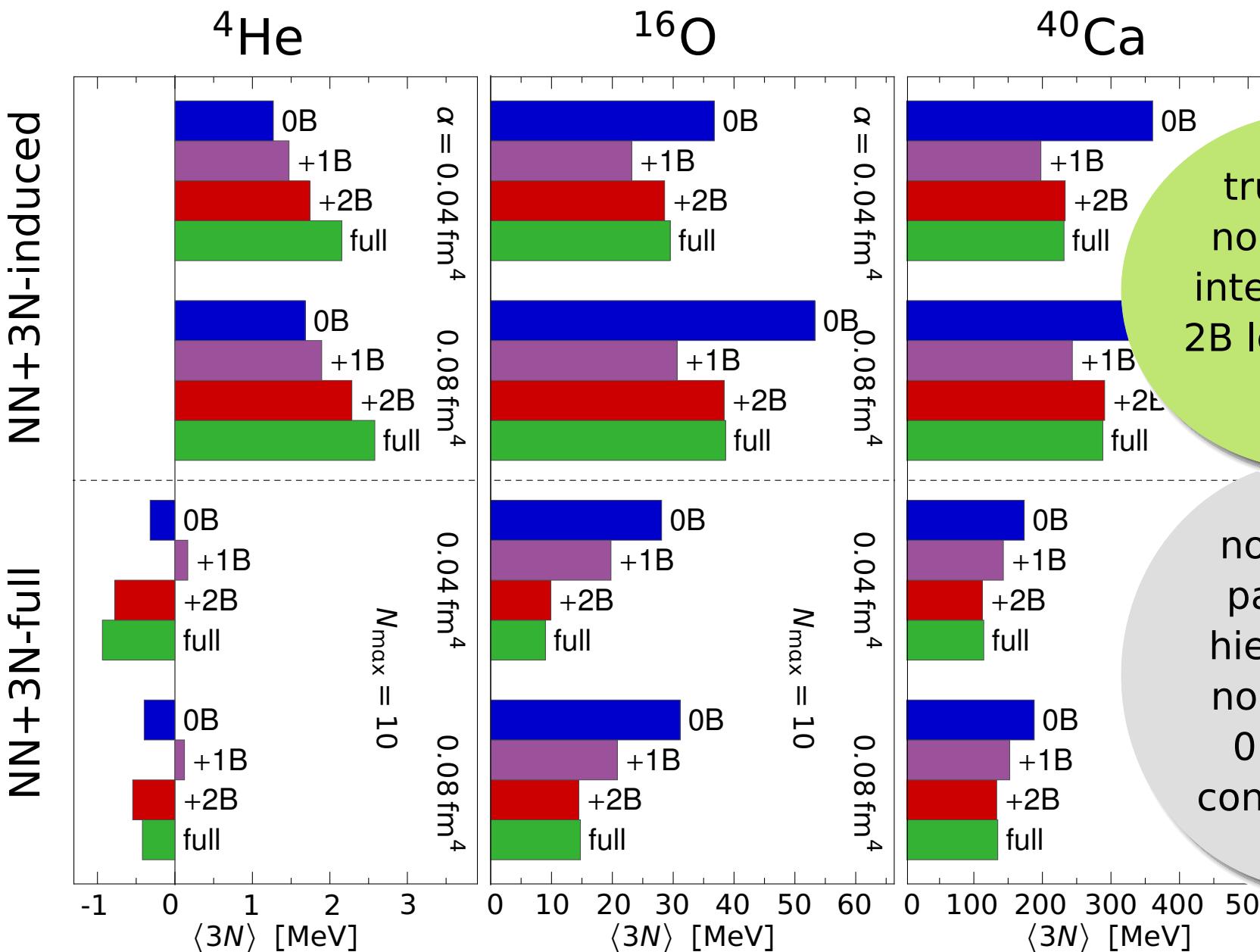
complete / NO2B

● / ○	$\alpha = 0.04 \text{ fm}^4$
◆ / ◊	$\alpha = 0.05 \text{ fm}^4$
▲ / △	$\alpha = 0.0625 \text{ fm}^4$
■ / □	$\alpha = 0.08 \text{ fm}^4$

$\hbar\Omega = 20 \text{ MeV}$

$E_{3\max}$

Anatomy of Normal-Ordered 3N



truncating
normal-ord.
interaction at
2B level works
well

no general pattern or hierarchy in normal-ord.
0B-1B-2B contributions

Coupled Cluster Method using Normal-Ordered 3N Interactions

- R. Roth, S. Binder, K. Vobig, et al. — Phys. Rev. Lett 109, 052501 (2012)
G. Hagen, T. Papenbrock, D.J. Dean, and M. Hjorth-Jensen — Phys. Rev. C 82, 034330 (2010)
G. Hagen, T. Papenbrock, D. J. Dean, et al. — Phys. Rev. C 76, 034302 (2007)
A.G. Taube and R.J. Bartlett — J. Chem. Phys. 128, 044110 (2008)
A.G. Taube and R.J. Bartlett — J. Chem. Phys. 128, 044111 (2008)

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \dots + \hat{T}_A}|\Phi_0\rangle$$

- \hat{T}_n : **nph excitation** ("cluster") operators

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\dots \\ abc\dots}} t_{ijk\dots}^{abc\dots} \{ \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i \}$$

- **similarity-transformed** Schrödinger Equation

$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle , \quad \hat{\mathcal{H}} \equiv e^{-\hat{T}} \hat{H}_{NO} e^{\hat{T}}$$

- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

Coupled Cluster - Equations

- **CCSD**: truncate \hat{T} at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$
- obtain the CCSD equations by projecting $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

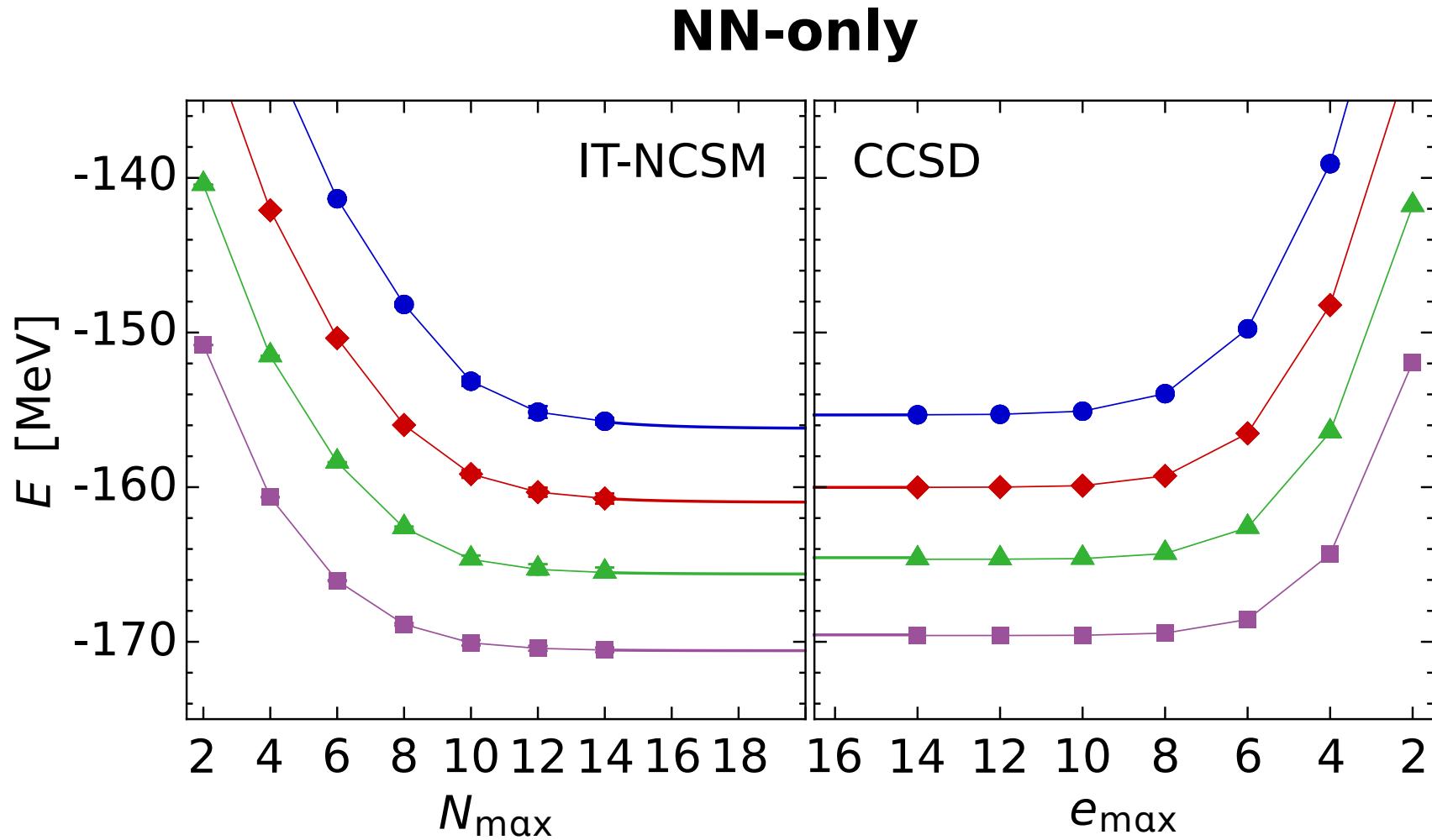
$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle \right\}$$

$$\Delta E_{CCSD}^{NN} = \langle \phi_0 | \hat{\mathcal{H}} | \phi_0 \rangle = \langle \phi_0 | \hat{H}_{NO} (\hat{T}_2 + \hat{T}_1 + \frac{1}{2} \hat{T}_1^2) | \phi_0 \rangle_C$$

$$0 = \langle \phi_i^a | \hat{\mathcal{H}} | \phi_0 \rangle = T_{1,CCSD}^{NN} = \langle \phi_i^a | \hat{H}_{NO} (1 + \hat{T}_2 + \hat{T}_1 + \hat{T}_1 \hat{T}_2 + \frac{1}{2} \hat{T}_1^2 + \frac{1}{3!} \hat{T}_1^3) | \phi_0 \rangle_C$$

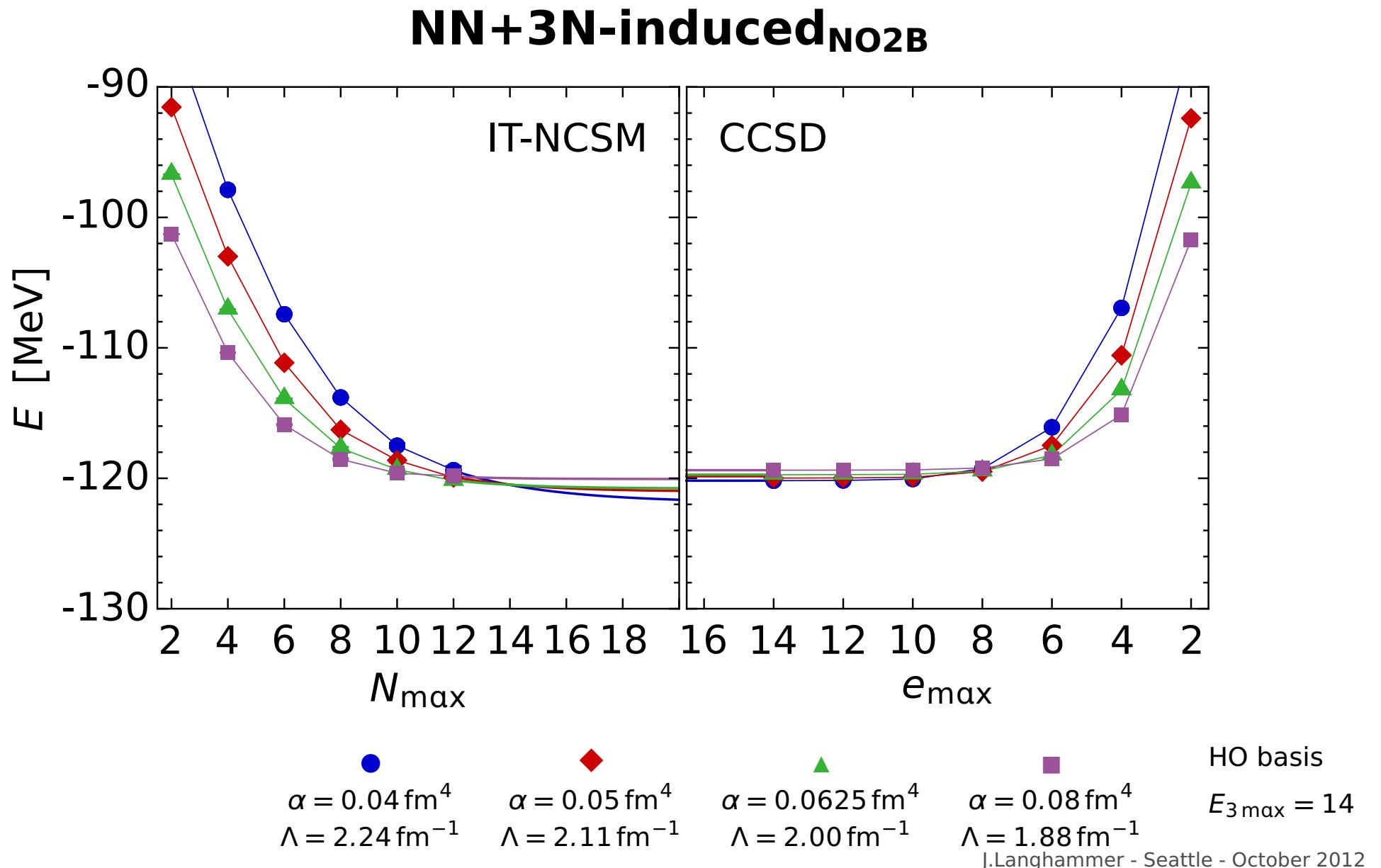
$$\begin{aligned} 0 = \langle \phi_{ij}^{ab} | \hat{\mathcal{H}} | \phi_0 \rangle = T_{2,CCSD}^{NN} = & \langle \phi_{ij}^{ab} | \hat{H}_{NO} (1 + \hat{T}_2 + \frac{1}{2} \hat{T}_2^2 + \hat{T}_1 + \hat{T}_1 \hat{T}_2 \\ & + \frac{1}{2} \hat{T}_1^2 + \frac{1}{2} \hat{T}_1^2 \hat{T}_2 + \frac{1}{3!} \hat{T}_1^3 + \frac{1}{4!} \hat{T}_1^4) | \phi_0 \rangle_C \end{aligned}$$

^{16}O : IT-NCSM vs. Coupled-Cluster

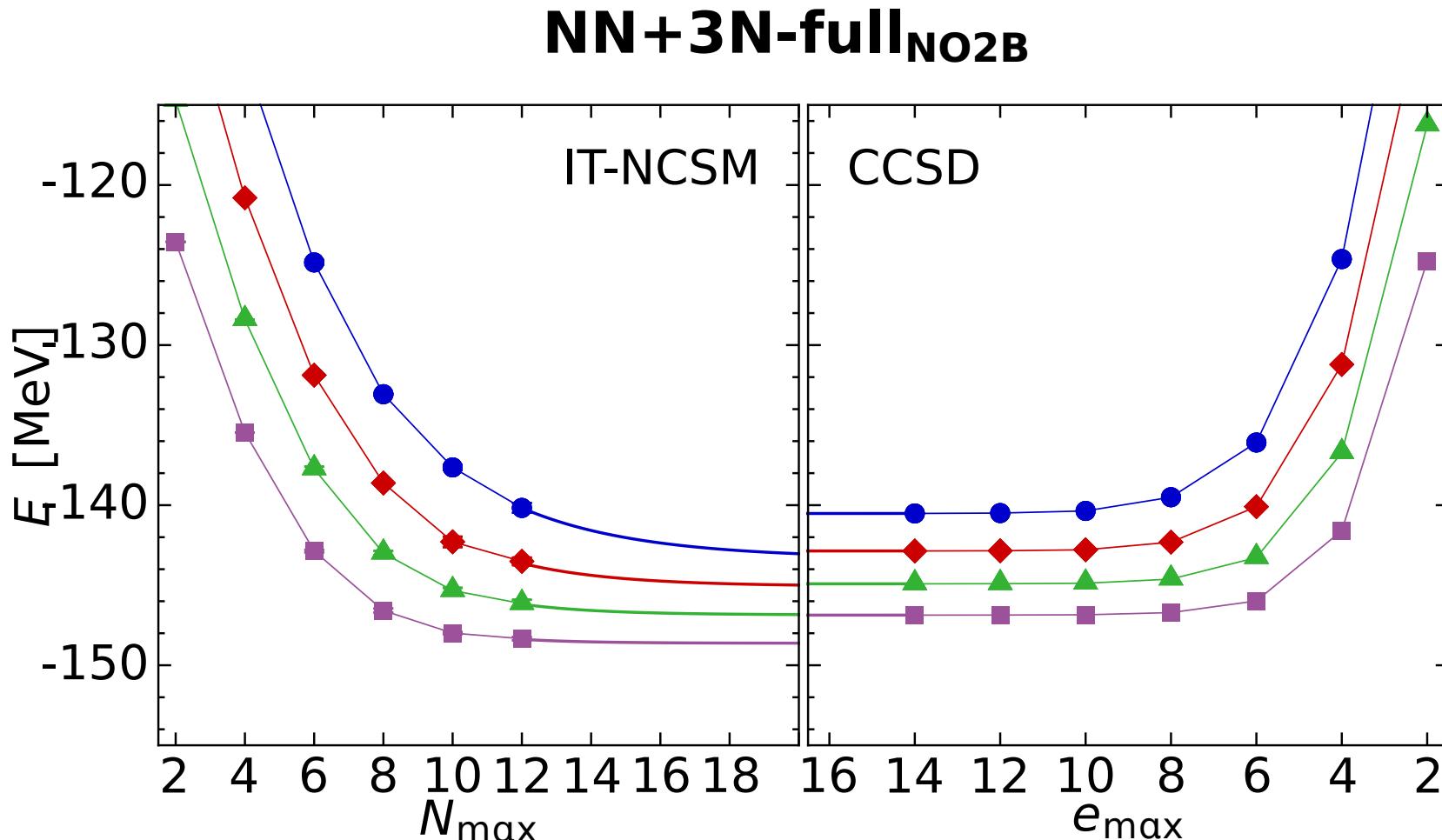


\bullet $\alpha = 0.04 \text{ fm}^4$ $\Lambda = 2.24 \text{ fm}^{-1}$	\diamond $\alpha = 0.05 \text{ fm}^4$ $\Lambda = 2.11 \text{ fm}^{-1}$	\blacktriangle $\alpha = 0.0625 \text{ fm}^4$ $\Lambda = 2.00 \text{ fm}^{-1}$	\blacksquare $\alpha = 0.08 \text{ fm}^4$ $\Lambda = 1.88 \text{ fm}^{-1}$	HO basis $E_{3\max} = 14$
-------------------------------------------------------------------------------	--------------------------------------------------------------------------------	----------------------------------------------------------------------------------------	------------------------------------------------------------------------------------	------------------------------

^{16}O : IT-NCSM vs. Coupled-Cluster

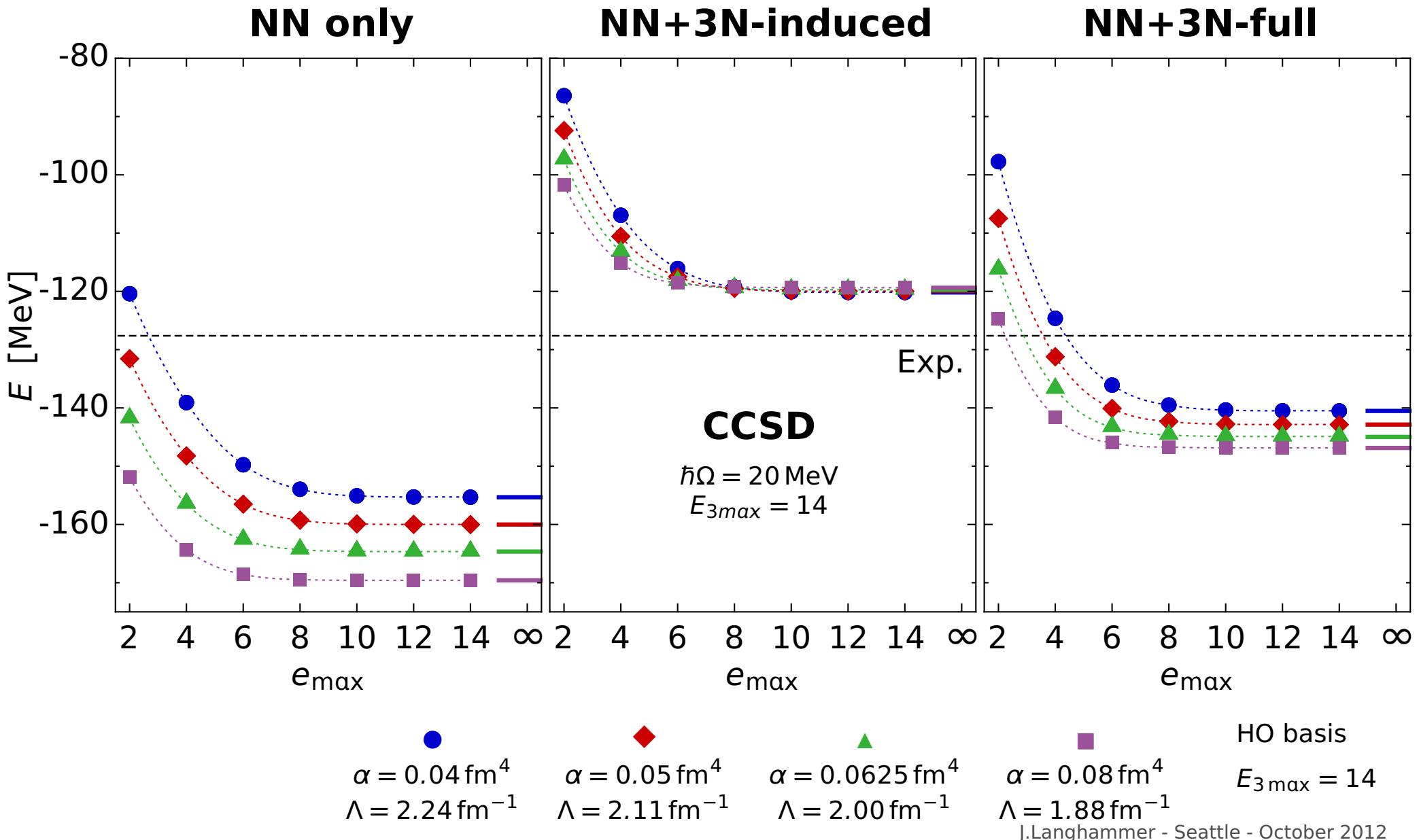


^{16}O : IT-NCSM vs. Coupled-Cluster

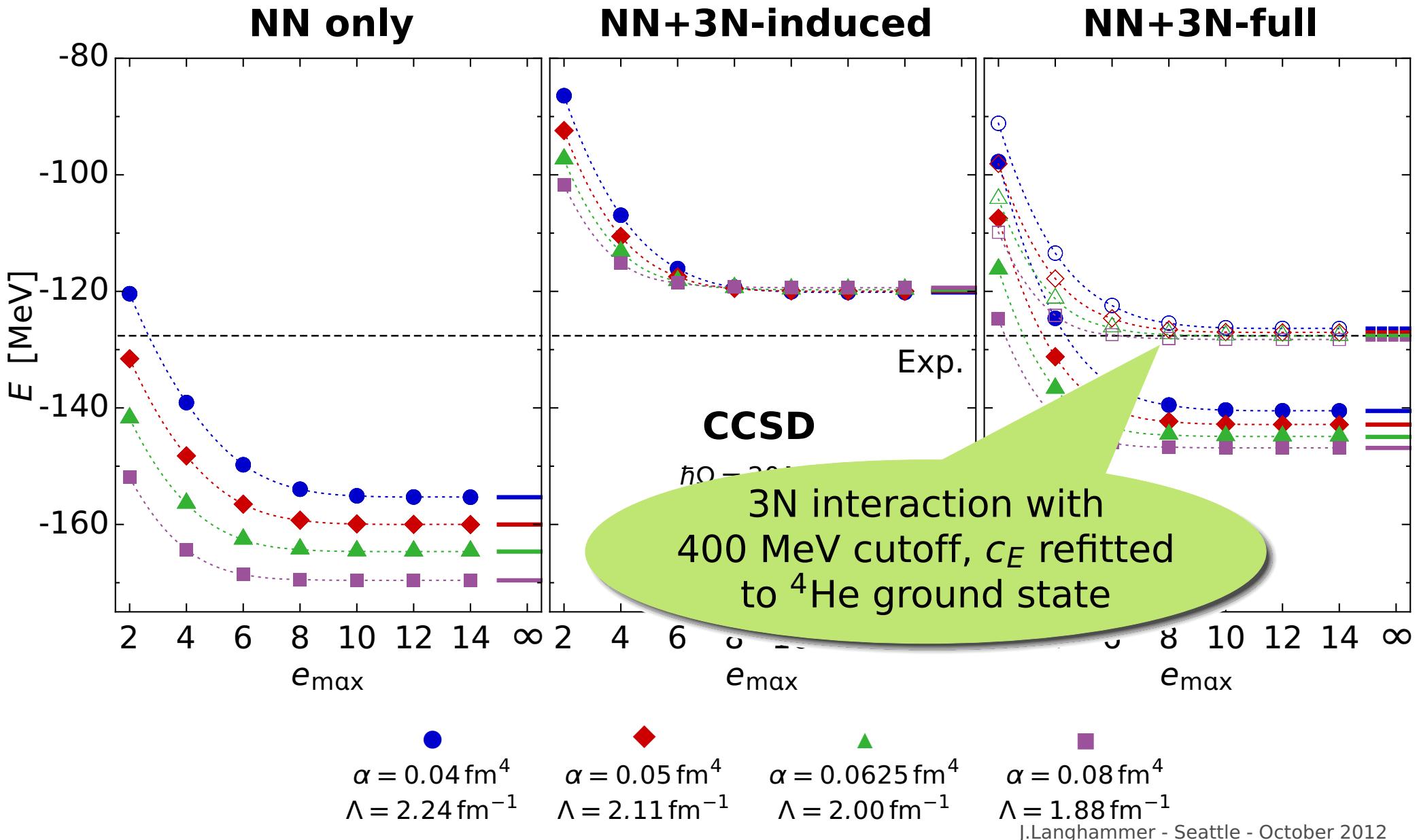


\bullet $\alpha = 0.04 \text{ fm}^4$ $\Lambda = 2.24 \text{ fm}^{-1}$	\diamond $\alpha = 0.05 \text{ fm}^4$ $\Lambda = 2.11 \text{ fm}^{-1}$	\blacktriangle $\alpha = 0.0625 \text{ fm}^4$ $\Lambda = 2.00 \text{ fm}^{-1}$	\blacksquare $\alpha = 0.08 \text{ fm}^4$ $\Lambda = 1.88 \text{ fm}^{-1}$	HO basis $E_{3\max} = 14$
-------------------------------------------------------------------------------	--------------------------------------------------------------------------------	----------------------------------------------------------------------------------------	------------------------------------------------------------------------------------	------------------------------

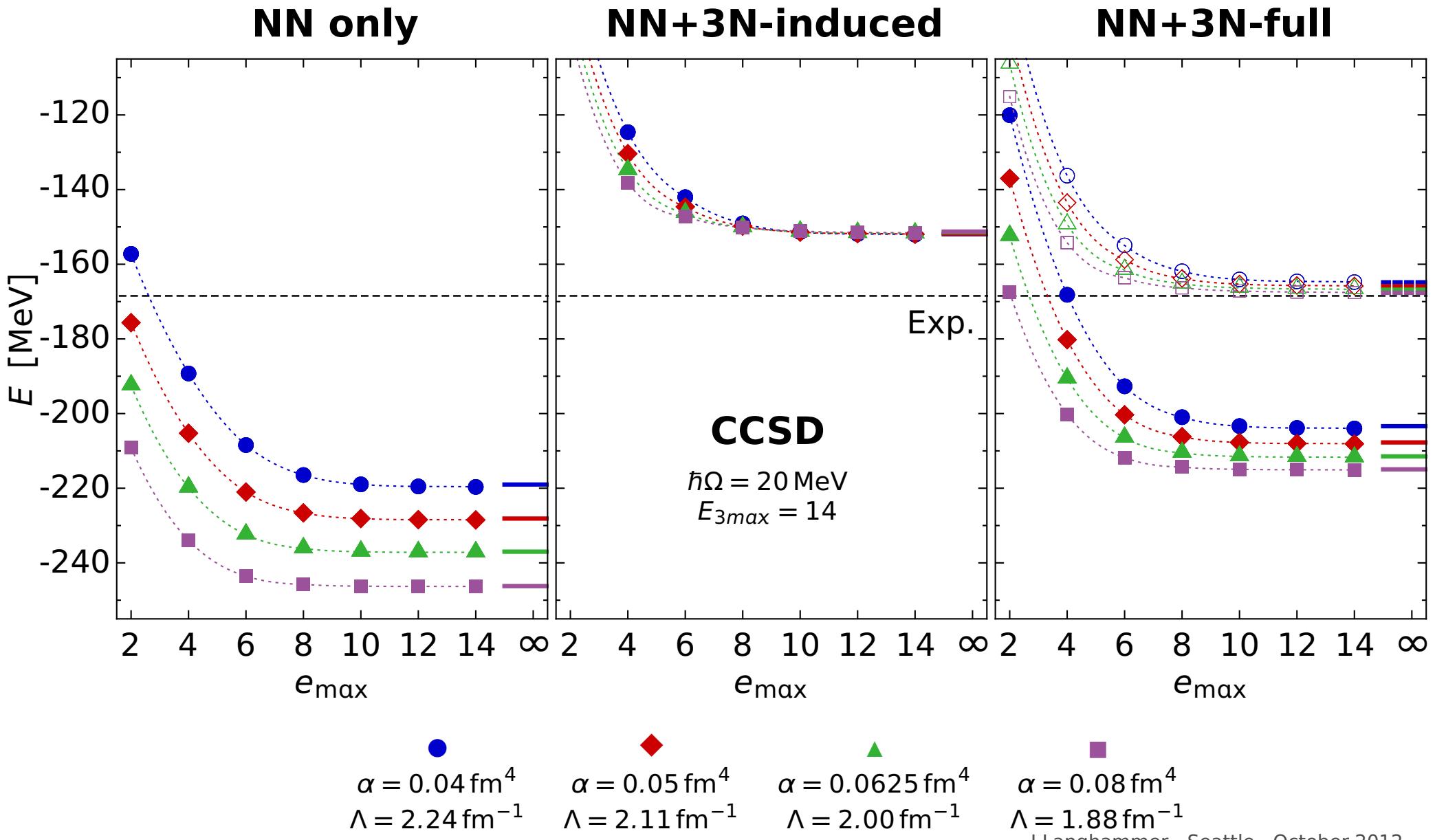
^{16}O : Coupled-Cluster with 3N_{NO2B}



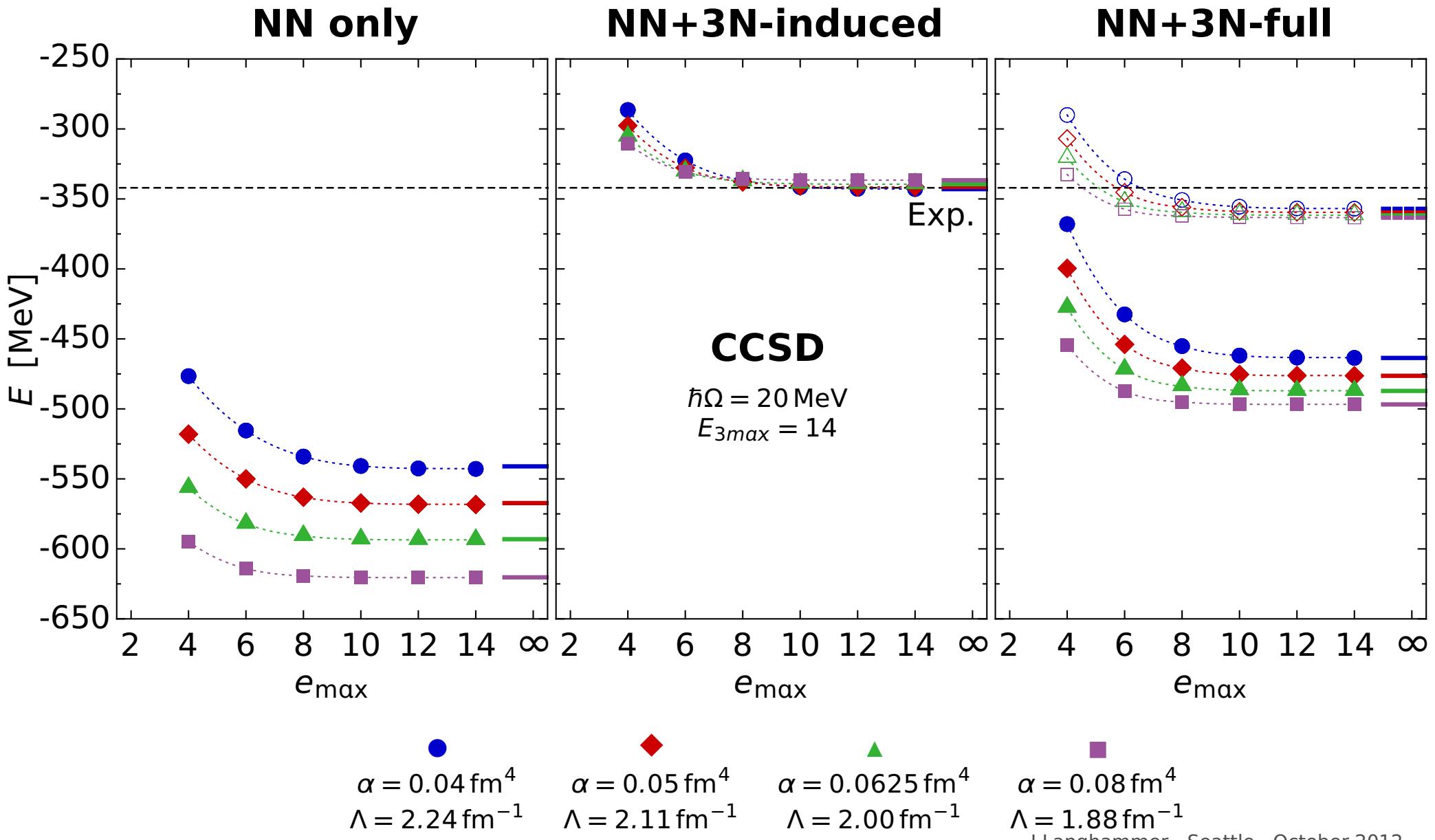
^{16}O : Coupled-Cluster with 3N_{NO2B}



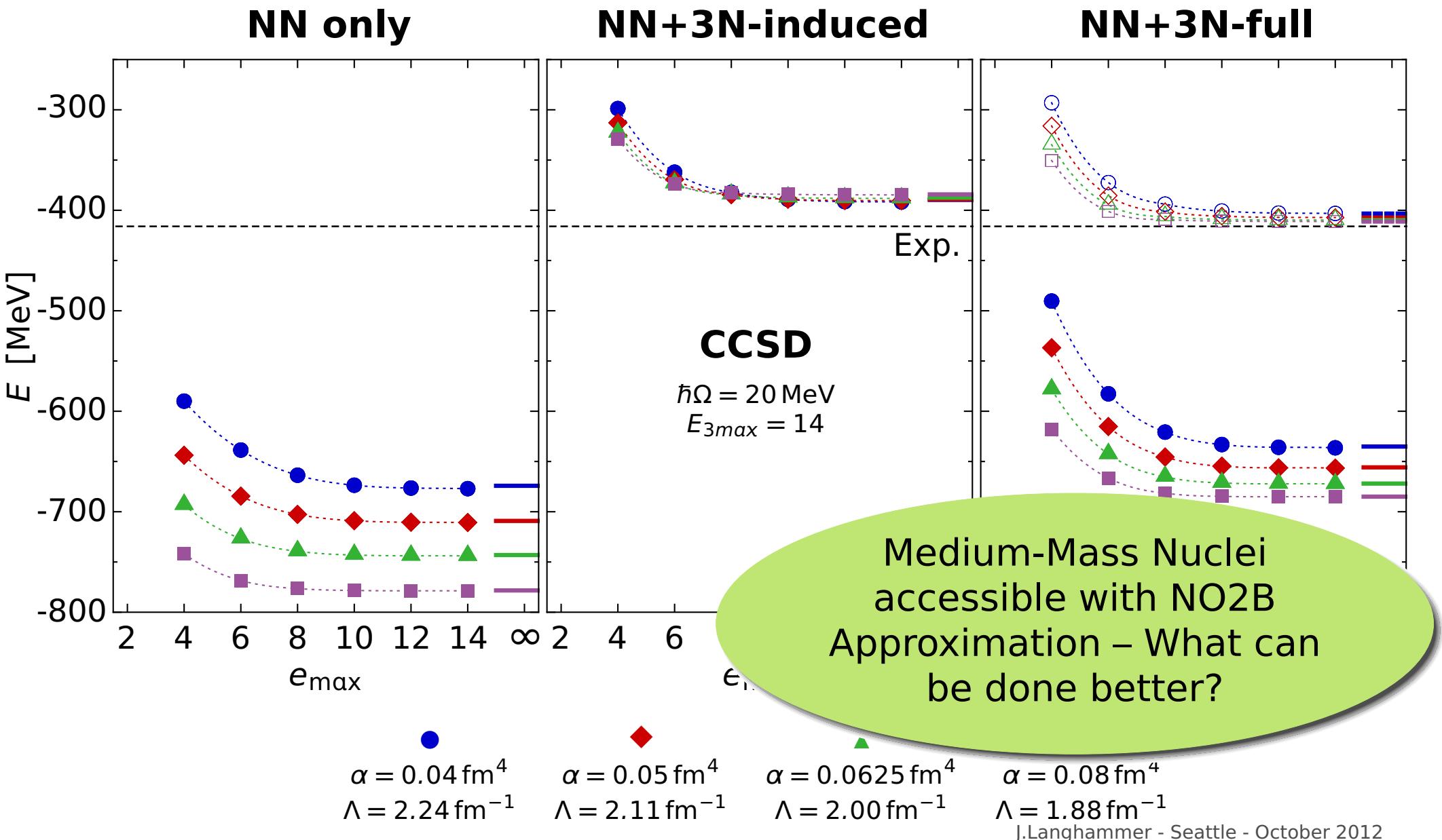
^{24}O : Coupled-Cluster with 3N_{NO2B}



^{40}Ca : Coupled-Cluster with 3N_{NO2B}



^{48}Ca : Coupled-Cluster with 3N_{NO2B}



Coupled Cluster Method with Complete 3N Interactions

Binder, Langhammer, Calci, Roth — in prep.

most of the work
done by **Sven
Binder**

The CCSD3B Equations

- the CCSD equations with complete 3N read

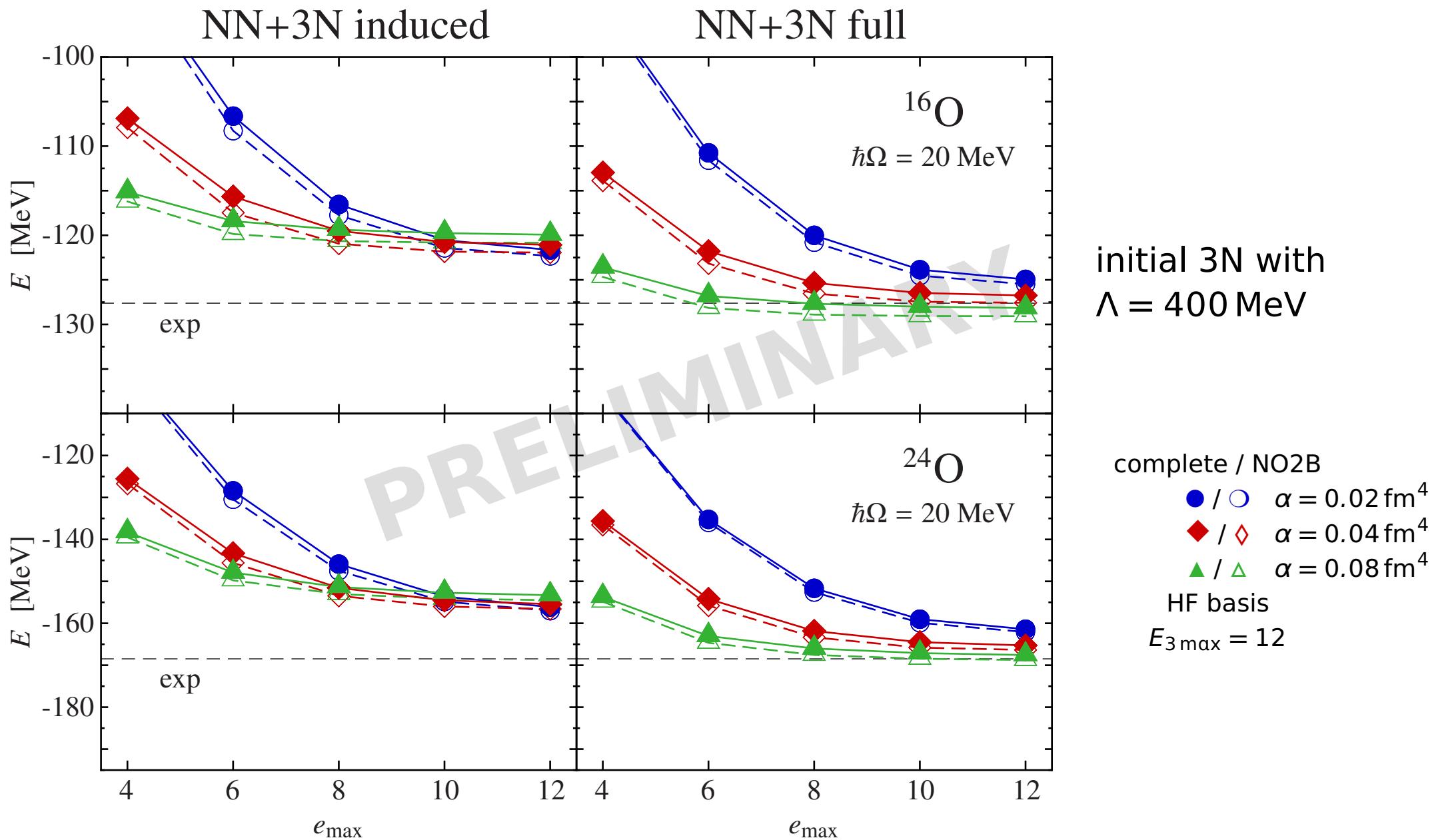
$$\Delta E_{\text{CCSD}}^{3N} = \Delta E_{\text{CCSD}}^{NN} + \langle \Phi_0 | \hat{W}_{3B} (\hat{T}_1 \hat{T}_2 + \frac{1}{3!} \hat{T}_1^3) | \Phi_0 \rangle_C$$

$$0 = T_{1,\text{CCSD}}^{NN} + \langle \Phi_i^a | \hat{W}_{3B} (\hat{T}_2 + \frac{1}{2} \hat{T}_1^2 + \hat{T}_1 \hat{T}_2 + \frac{1}{2} \hat{T}_2^2 + \frac{1}{3!} \hat{T}_1^3 + \frac{1}{2} \hat{T}_1^2 \hat{T}_2 + \frac{1}{4!} \hat{T}_1^4) | \Phi_0 \rangle_C$$

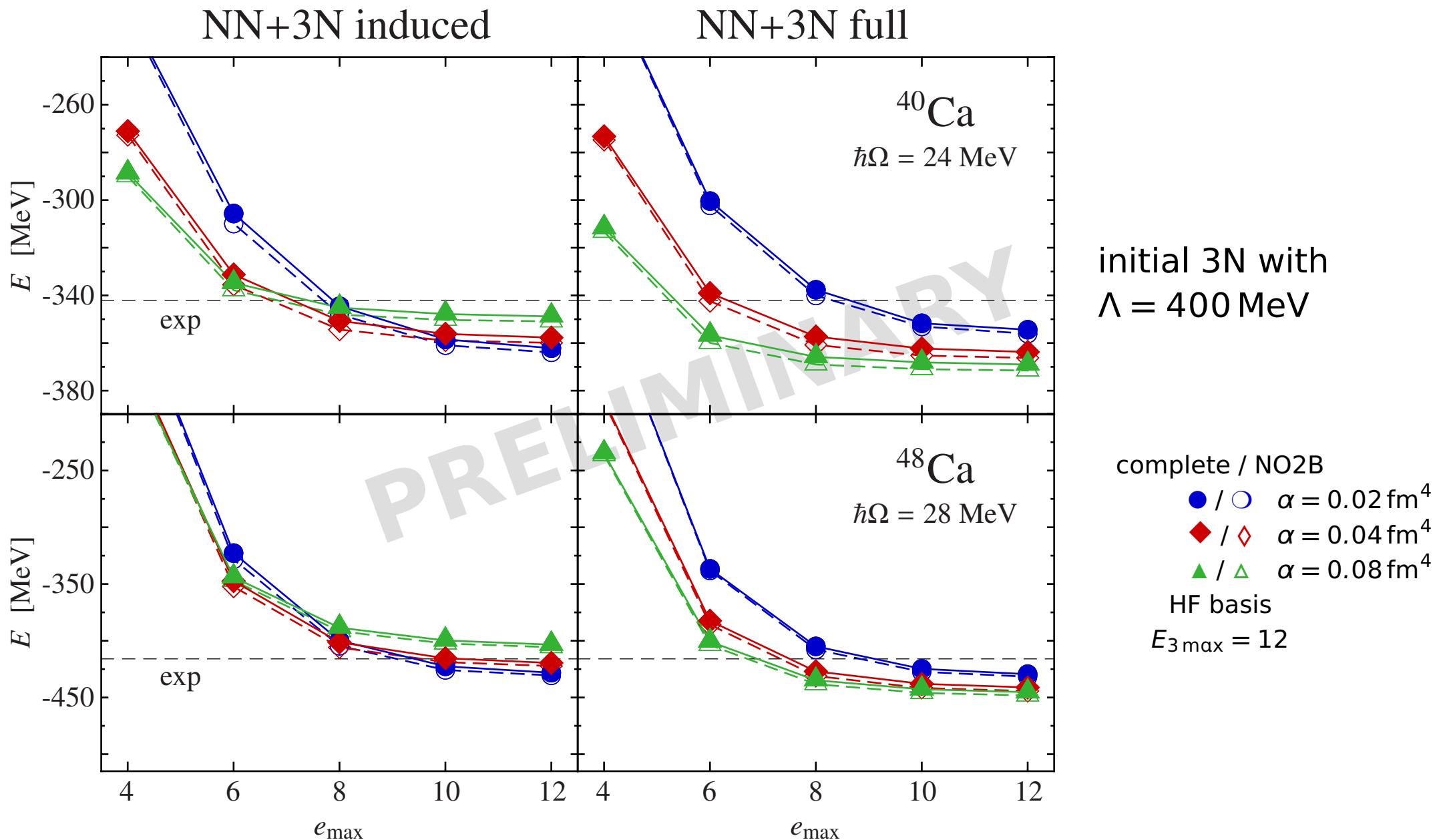
$$0 = T_{2,\text{CCSD}}^{NN} + \langle \Phi_{ij}^{ab} | \hat{W}_{3B} (\hat{T}_1 + \hat{T}_2 + \frac{1}{2} \hat{T}_1^2 + \hat{T}_1 \hat{T}_2 + \frac{1}{2} \hat{T}_2^2 + \frac{1}{3!} \hat{T}_1^3 + \frac{1}{2} \hat{T}_1^2 \hat{T}_2 + \frac{1}{2} \hat{T}_1 \hat{T}_2^2 + \frac{1}{4!} \hat{T}_1^4 + \frac{1}{5!} \hat{T}_1^5) | \Phi_0 \rangle_C$$

- all new contributions stem from \hat{W}_{3B}
- we developed an efficient code to solve the CCSD3B equations in the **spherical scheme**
- calculations use a **Hartree-Fock** single-particle basis and reference state

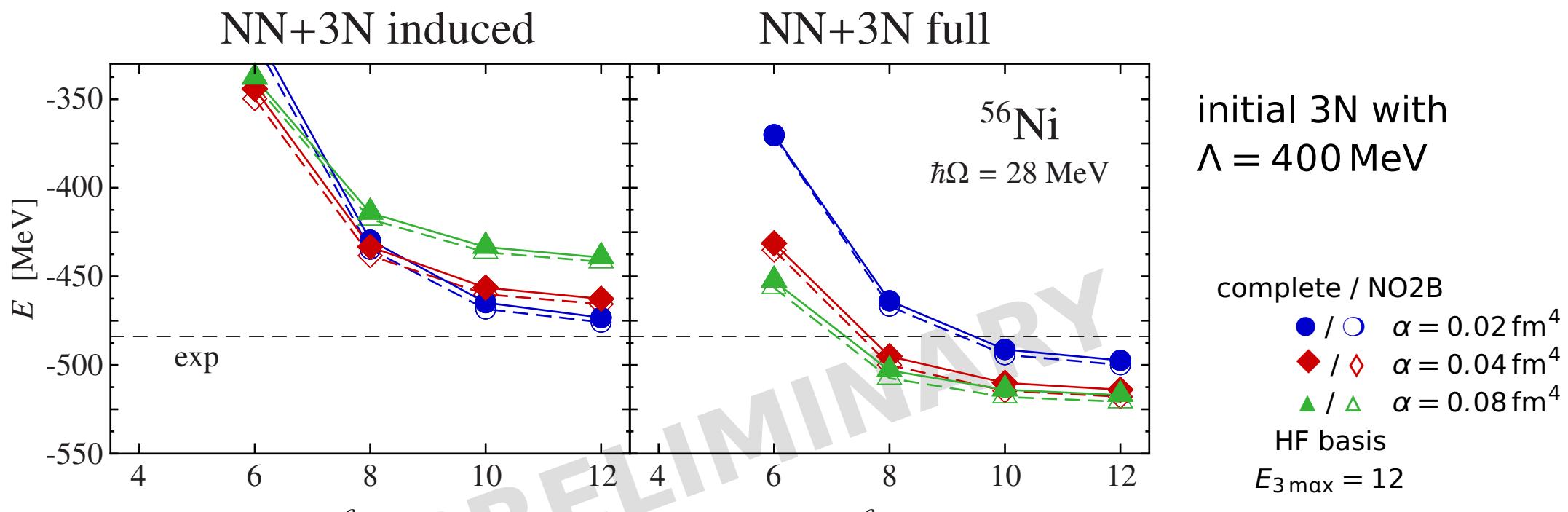
CCSD with Complete 3N Interaction



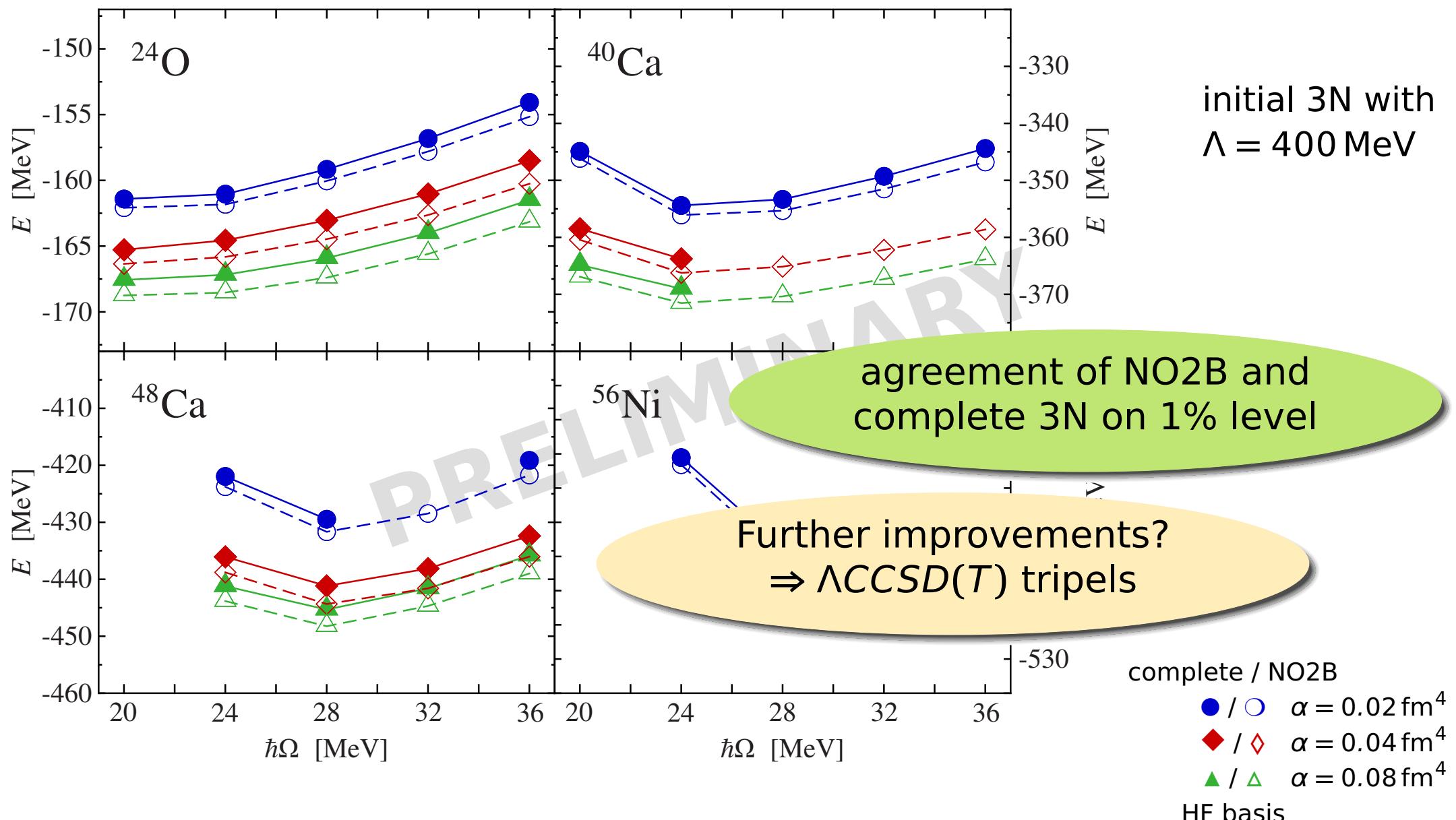
CCSD with Complete 3N Interaction



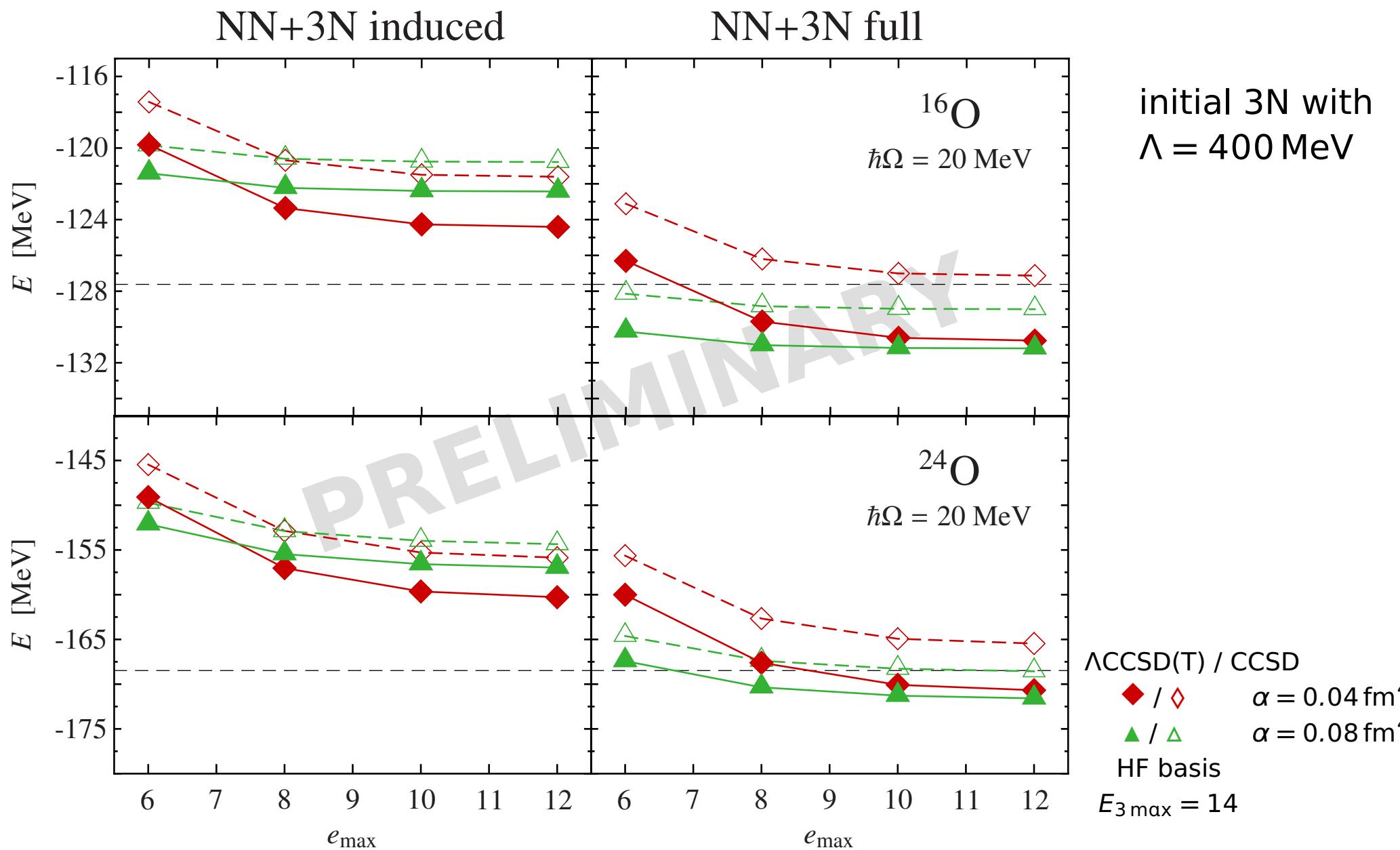
CCSD with Complete 3N Interaction



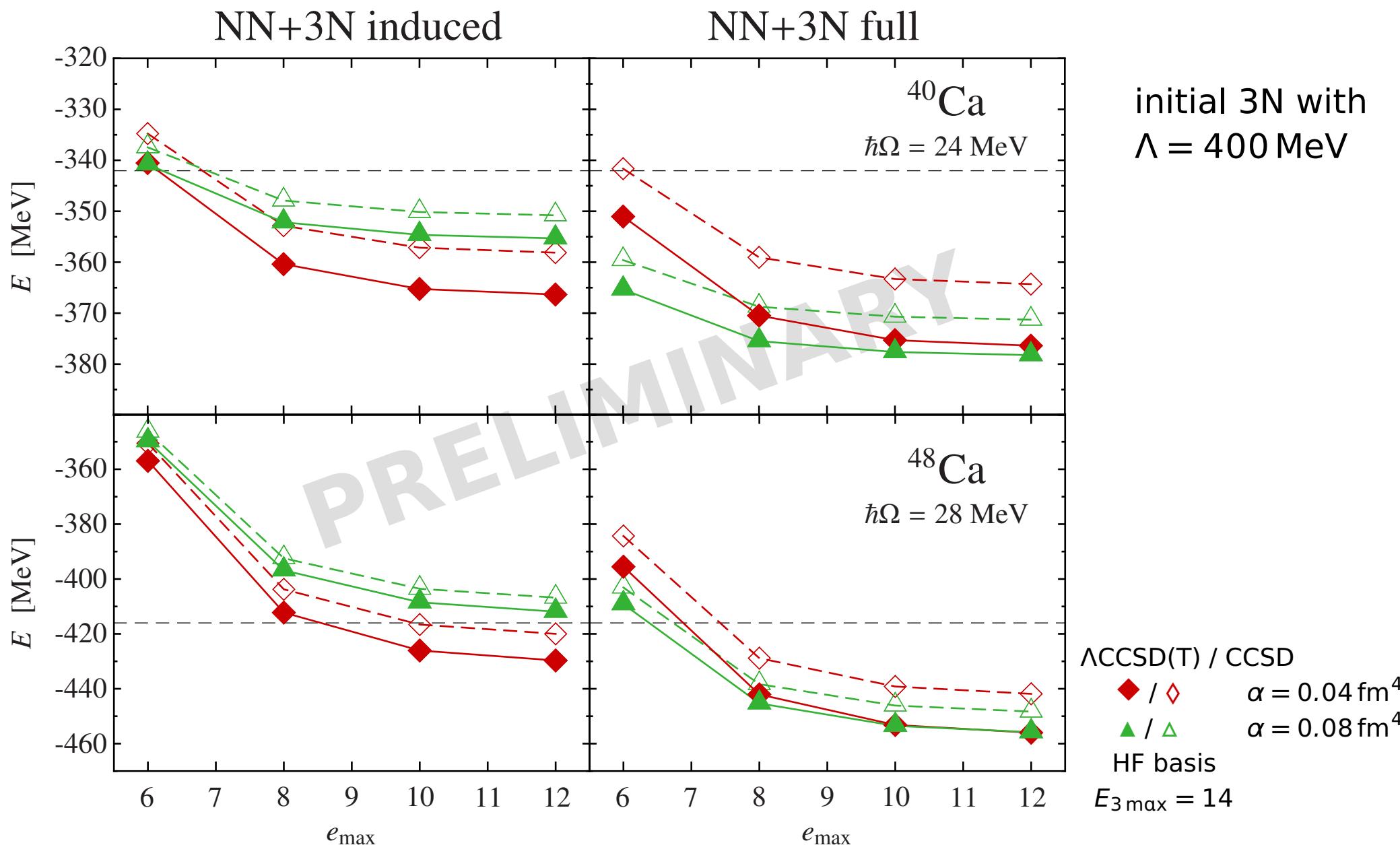
Frequency Dependence



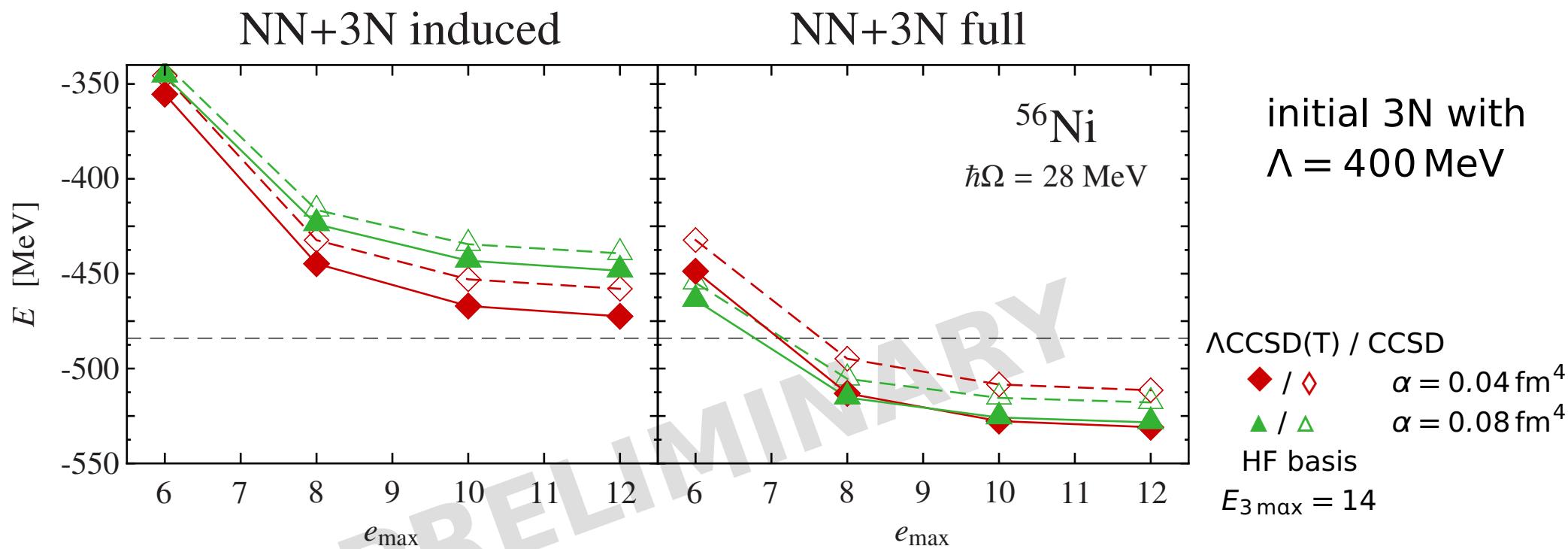
ΛCCSD(T) with 3N_{NO2B} Interaction



ΛCCSD(T) with 3N_{NO2B} Interaction



ΛCCSD(T) with 3N_{NO2B} Interaction



- **ΛCCSD(T) with 3N_{NO2B} currently our best calculation**, since NO2B approximation is 1% accurate
- we find: softer interaction \Rightarrow less triplets corrections
- our results **prove the predictive power of** chiral interactions in the **medium-mass range**
 - interaction fitted entirely in three- and four-body system

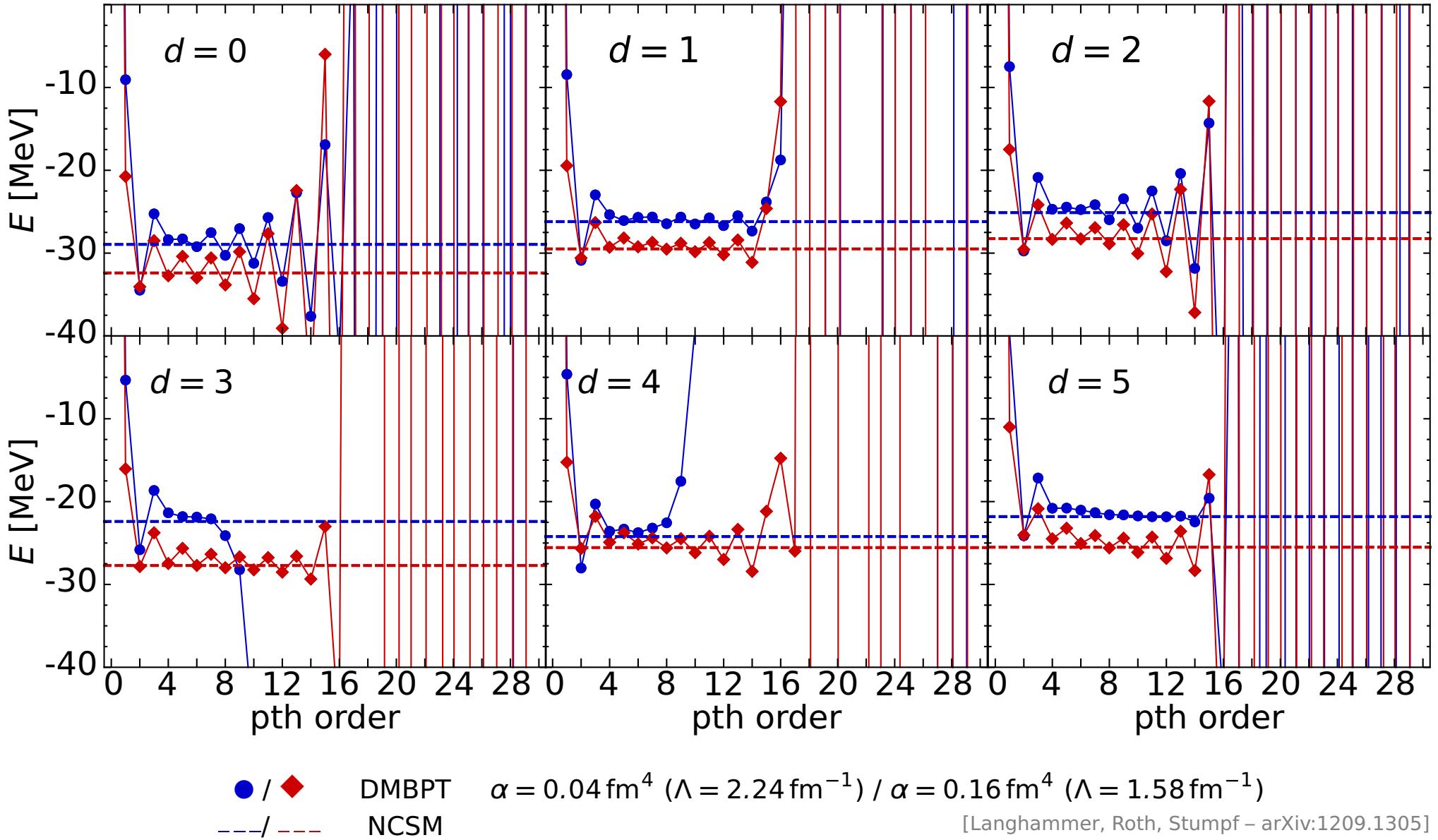
Conclusions — Medium-Mass Nuclei with 3N

- inclusion of **complete 3N interaction in CCSD** calculations for **medium-mass** nuclei feasible
 - benchmark of various approximation schemes possible
- Normal-ordered two-body approximation of 3N
 - accurate on 1% level also in medium-mass nuclei
 - best calculation Λ CCSD(T) with $3N_{NO2B}$
- work in progress:
 - uncertainty quantification for all 'truncations'**,
i.e. dependence on $eMax$, $\hbar\Omega$, $E_{3\max}$, SRG through α variation,
cluster-order through Λ CCSD(T)

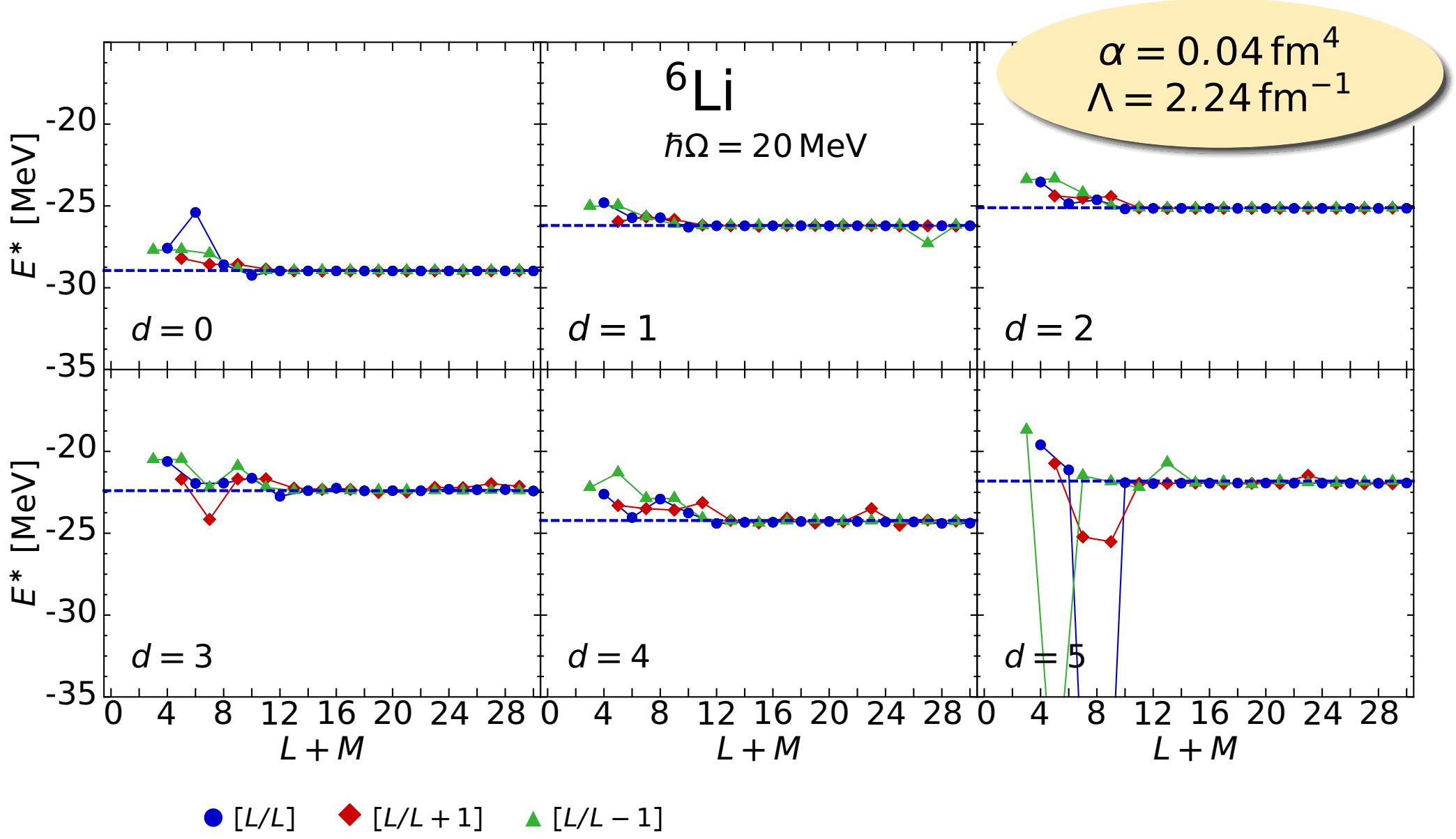
Soft Interactions in Many-Body Perturbation Theory

Langhammer, Roth, Stumpf — arXiv:1209.1305

MBPT ${}^6\text{Li}$: Soft Interaction, but...



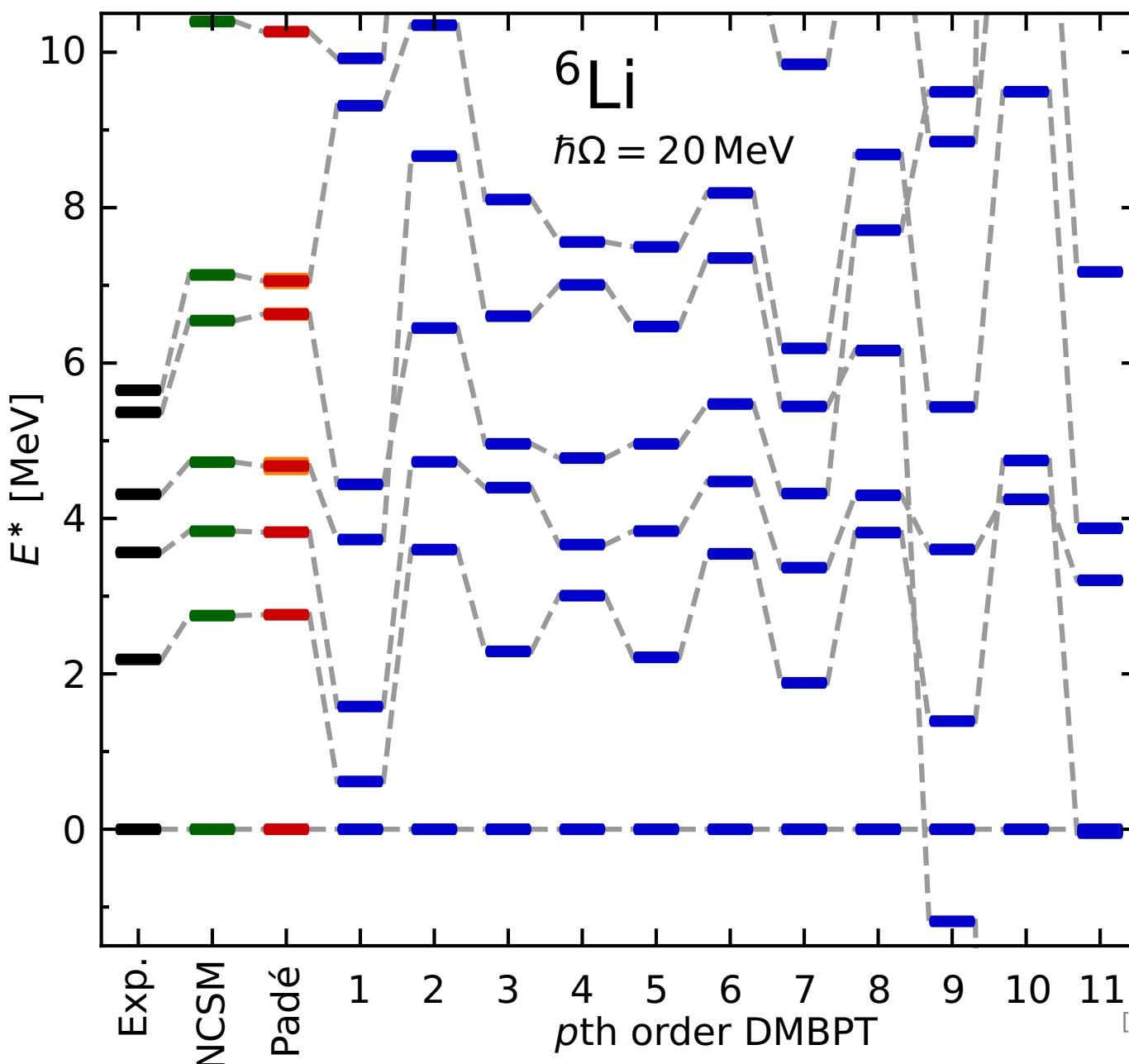
Padé Resummation



[Langhammer, Roth, Stumpf – arXiv:1209.1305]

J.Langhammer - Seattle - October 2012

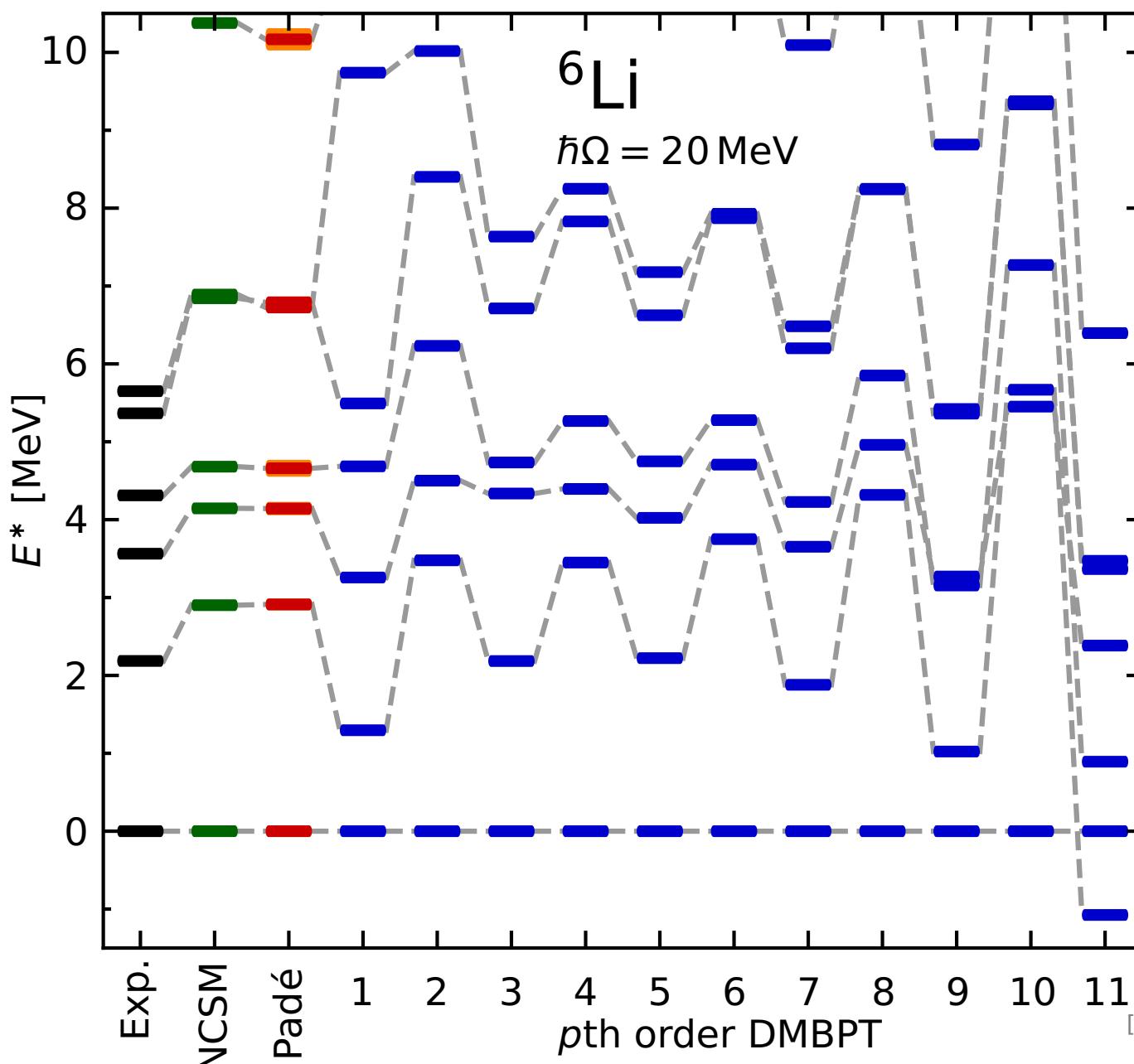
Spectra



$$\alpha = 0.04 \text{ fm}^4$$
$$\Lambda = 2.24 \text{ fm}^{-1}$$

[Langhammer, Roth, Stumpf – arXiv:1209.1305]

Spectra



$$\alpha = 0.16 \text{ fm}^4$$
$$\Lambda = 1.58 \text{ fm}^{-1}$$

[Langhammer, Roth, Stumpf – arXiv:1209.1305]

Epilogue

■ thanks to my group & my collaborators

- **A. Calci, S. Binder** B. Erler, E. Gebrerufael,
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R. Roth, C. Stumpf, R. Trippel, K. Vobig, R. Wirth

Institut für Kernphysik, TU Darmstadt

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- P. Piecuch
Micronova, Poland
- H. Hergert
Ohio State University, USA
- P. Papakonstantinou
IPN Orsay, F
- C. Forssén
Chalmers University, Sweden
- H. Feldmeier, T. Neff
Helmholtzzentrum

Thank you for your
attention!



COMPUTING TIME



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 **LOEWE** – Landes-Offensive
zur Entwicklung Wissenschaftlich-
ökonomischer Exzellenz

