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-^{4}He, n-^{12}C and n-^{16}O 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

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = \left[\eta_\alpha, \widetilde{H}_\alpha\right] \qquad \eta_\alpha = (2\mu)^2 \left[T_{int}, \widetilde{H}_\alpha\right]$$

- NN interaction @ N^3LO [Entem, Machleidt, Phys.Rev C68, 041001(R) (2003)]
- 3N interaction @ N^2LO
  - 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 $\Lambda = 400\,\text{MeV}$ 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

resonances
& scattering states

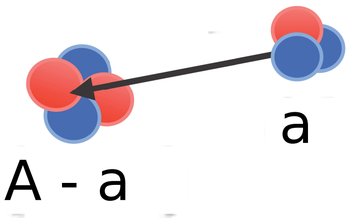
(IT-)NCSM/RGM
approach

(IT-)NCSM

ab-initio description
of nuclear clusters

RGM

cluster technique that as-
sumes clustered nucleons



succesfully applied with NN interac

this talk:
inclusion of
3N interaction

General Approach of NCSM/RGM

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

$$\left|\psi^{J\pi T}\right\rangle = \sum_{\nu}\int \mathrm{d}r r^2 \frac{g_{\nu}^{J\pi T}(r)}{r}\mathcal{A}_{\nu}\left|\phi_{\nu r}^{J\pi T}\right\rangle$$

$g_{\nu}^{J\pi T}(r)$ unknown

with the binary-cluster channel states

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

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

- Solve **generalized eigenvalue** problem

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

Hamiltonian kernel

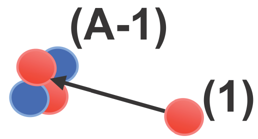
$$\left\langle\phi_{\nu' r'}^{J\pi T}\right|\mathcal{A}_{\nu'}\mathrm{H}\mathcal{A}_{\nu}\left|\phi_{\nu r}^{J\pi T}\right\rangle$$

Norm kernel

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

The Hamiltonian Kernel: NN Diagrams

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



$$\left\langle \phi^{J\pi T}_{\nu' r'} \right| V_{NN} \mathcal{A}^2 \left| \phi^{J\pi T}_{\nu r} \right\rangle = \left\langle \phi^{J\pi T}_{\nu' r'} \right| V_{NN} \left[1 - \sum_{i=1}^{A-1} T_{i,A} \right] \left| \phi^{J\pi T}_{\nu r} \right\rangle$$

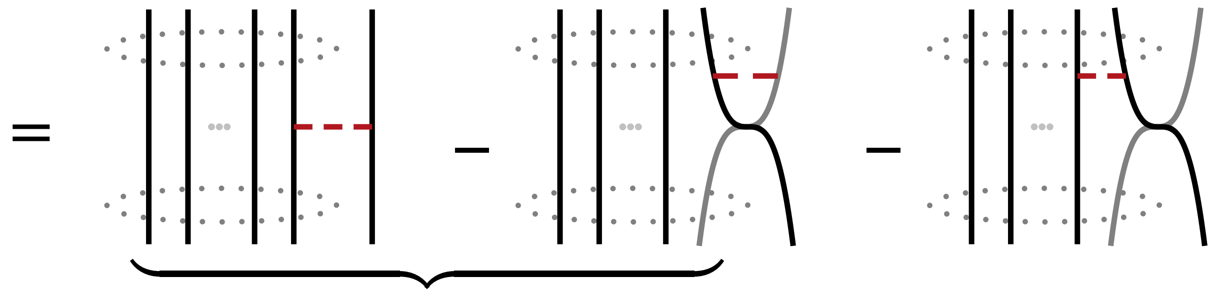
$$= (A-1) \left\langle \phi^{J\pi T}_{\nu' r'} \right| V_{A-1,A} \left| \phi^{J\pi T}_{\nu r} \right\rangle$$

$$- (A-1) \left\langle \phi^{J\pi T}_{\nu' r'} \right| V_{A-1,A} T_{A-1,A} \left| \phi^{J\pi T}_{\nu r} \right\rangle$$

"direct" kernel

$$- (A-1)(A-2) \left\langle \phi^{J\pi T}_{\nu' r'} \right| V_{A-2,A} T_{A-1,A} \left| \phi^{J\pi T}_{\nu r} \right\rangle$$

"exchange" kernel



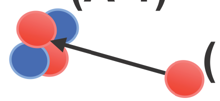
$\propto \left\langle \phi'^{(A-1)} \right| a^\dagger a \left| \phi^{(A-1)} \right\rangle$ $\propto \left\langle \phi'^{(A-1)} \right| a^\dagger a^\dagger a a \left| \phi^{(A-1)} \right\rangle$

densities managable

Towards Inclusion of Full 3N Forces

- Derive expressions for Hamiltonian kernel with 3N interaction

⇒ 3N-interaction kernel



$$\langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{NNN} \mathcal{A}^2 | \phi^{J\pi T}_{\nu r} \rangle = \langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{NNN} [1 - \sum_{i=1}^{A-1} \mathrm{T}_{i,A}] | \phi^{J\pi T}_{\nu r} \rangle$$

$$= \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{A-2,A-1,A} | \phi^{J\pi T}_{\nu r} \rangle$$

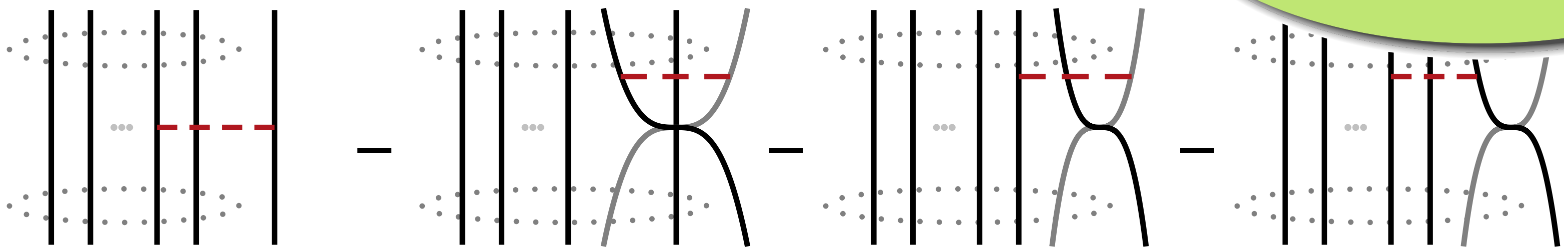
$$- \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{A-2,A-1,A} \mathrm{T}_{\mathrm{A}-2,\mathrm{A}} | \phi^{J\pi T}_{\nu r} \rangle$$

$$- \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{A-1,A-2,A} \mathrm{T}_{\mathrm{A}-1,\mathrm{A}} | \phi^{J\pi T}_{\nu r} \rangle$$

"direct" kernel

$$- \frac{(A-1)(A-2)(A-3)}{2} \langle \phi^{J\pi T}_{\nu' r'} | \mathrm{V}_{A-3,A-2,A} \mathrm{T}_{\mathrm{A}-1,\mathrm{A}} | \phi^{J\pi T}_{\nu r} \rangle$$

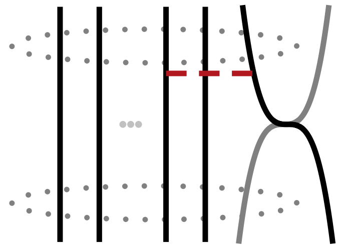
challenge: **handling of 3-body density**

= 

$\propto \langle \phi'^{(A-1)} | a^\dagger a^\dagger a a | \phi^{(A-1)} \rangle$ $\qquad$ $\propto \langle \phi'^{(A-1)} | a^\dagger a^\dagger a^\dagger a a a | \phi^{(A-1)} \rangle$

Two Ways of Handling the Three-Body Density

❶ Precomputed coupled densities



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

$$\begin{Bmatrix} I_1 & K & I_1' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j' & K & j \\ g' & j_0' & J_0 \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T_1' \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \tau & \frac{1}{2} \\ t_g' & t_0' & \ldots \end{Bmatrix}$$

3-body density cannot be stored

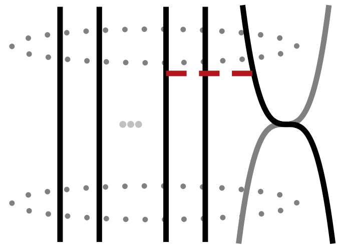
$$\langle \phi'^{(A-1)} I_1' T_1' \| \left[(a^\dagger_{nlj} (a^\dagger_{n_b' l_b' j_b'} a^\dagger_{n_a' l_a' j_a'})^{j_0' t_0'})^{g' t_g'} ((\tilde{a}_{n_\alpha l_\alpha j_\alpha} \tilde{a}_{n_a l_a j_a})^{j_0 t_0} \tilde{a}_{n_b l_b j_b})^{J_0 T_0} \right]^{K\tau} \| \phi^{(A-1)} I_1 T_1 \rangle$$

$${}_a\langle ((n_a' l_a' j_a', n_b' l_b' j_b') j_0' t_0', n' l' j') J_0 T_0 | V_{3N} | ((n_\alpha l_\alpha j_\alpha, n_a l_a j_a) \ldots$$

make use of *JT*-coupled 3N matrix elements

Two Ways of Handling the Three-Body Density

❶ Precomputed coupled densities



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

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

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

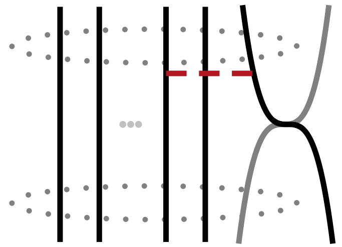
$$\langle \phi''^{(A-4)} I_\beta T_\beta \| ((\tilde{a}_{n_\alpha l_\alpha j_\alpha} \tilde{a}_{n_a l_a j_a})^{j_0 t_0} \tilde{a}_{n_b l_b j_b})^{J_0 T_0} \| \phi^{(A-1)} I_1 T_1 \rangle$$

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

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

Two Ways of Handling the Three-Body Density

❷ Compute uncoupled densities on-the-fly



$$\sum_{jj'}\sum_{M_1 m_j}\sum_{M_{T_1} m_t}\sum_{M_1' m_j'}\sum_{M_{T_1}' m_t'} \tfrac{1}{12}(-1)^{I_1+I_1'+}$$

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

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

$$\left\langle \phi'^{(A-1)} I_1' M_1' T_1' M_{T_1}' \right| \mathrm{a}^{\dagger}_{nljm_j\frac{1}{2}m_t} \mathrm{a}^{\dagger}_{\beta_{A-2}} \mathrm{a}^{\dagger}_{\beta_{A-3}} \mathrm{a}_{\beta_{A-3}'} \mathrm{a}_{\beta_{A-2}'} \mathrm{a}_{\beta_{A-1}'} \left| \phi^{(A-1)} I_1 M_1 T_1 M_{T_1} \right\rangle$$

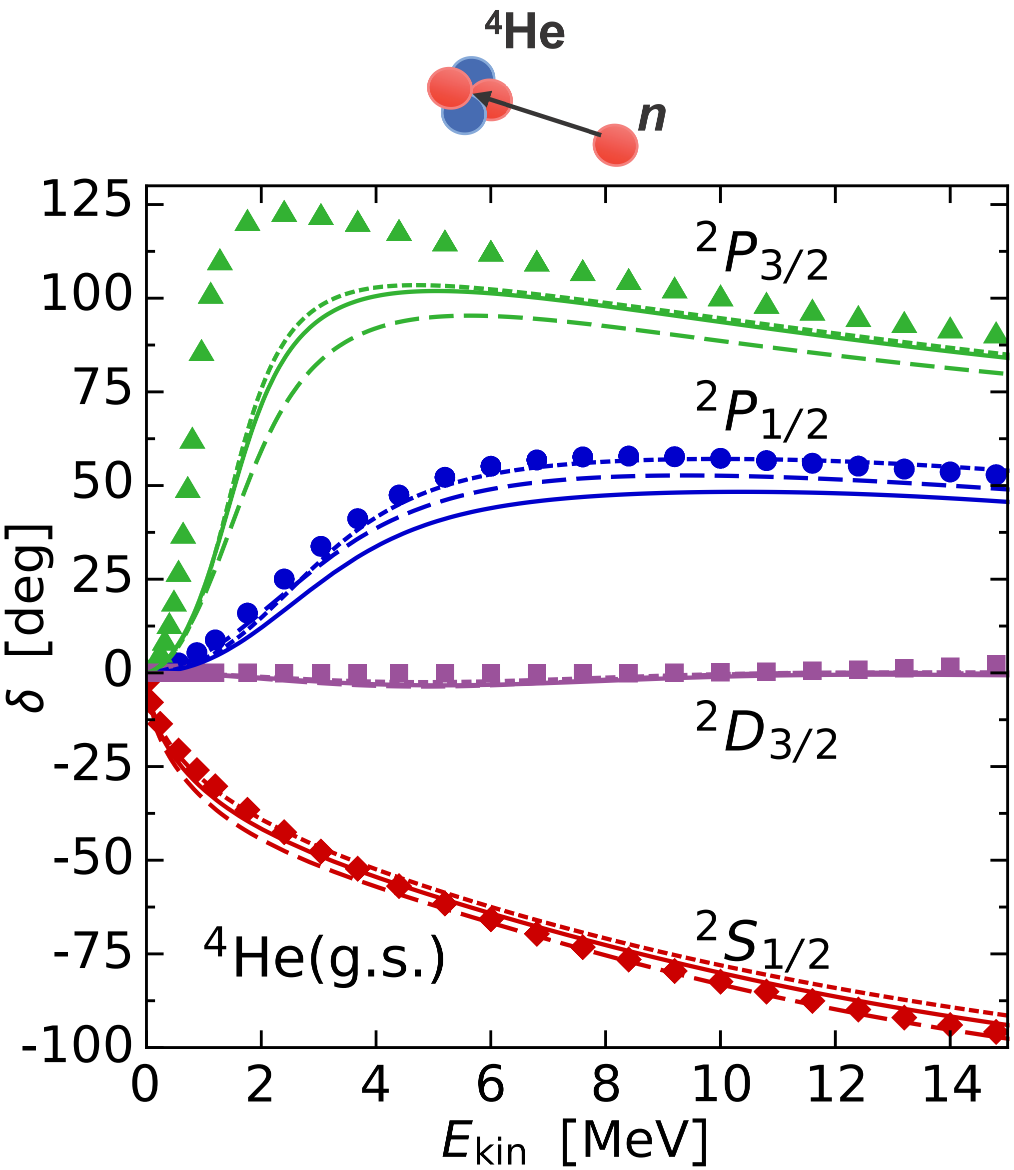
$${}_a\left\langle \beta_{A-3}\beta_{A-2} n' l' j' m_j' \tfrac{1}{2} m_t' \right| \mathrm{V}_{3N} \left| \beta_{A-3}'\beta_{A-2}'\beta_{A-1}' \right\rangle_a$$

+ 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: $n+{}^4\text{He}$



Comparison against experiment

$N_{max} = 13$

◆▲●■ experiment

······· NN-only

--- NN+3N-ind

— NN+3N-full

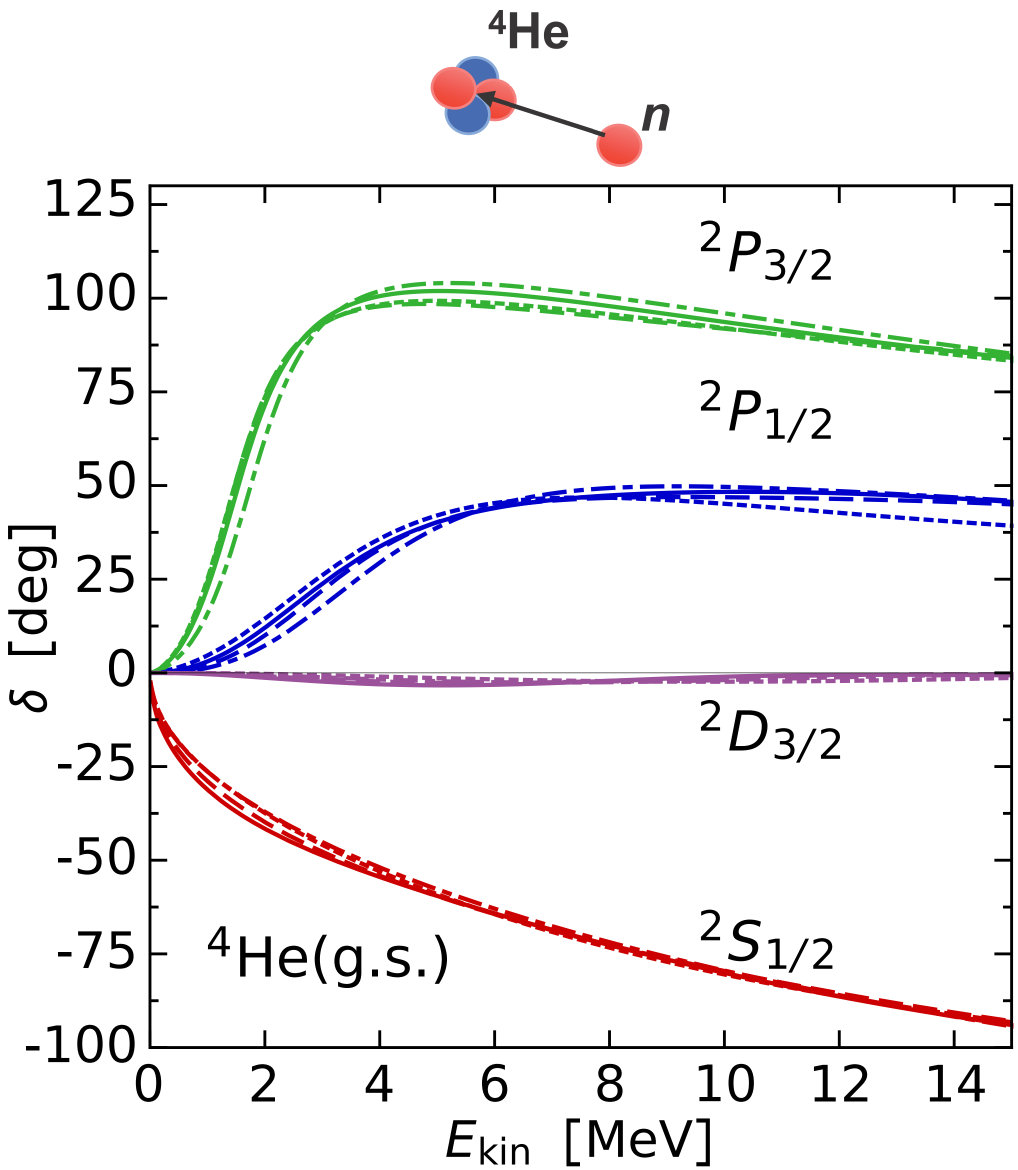
increased spin-orbit splitting by inital 3N

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

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

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

Scattering Phase Shifts: n+^{4}He



Convergence w.r.t. N_{max}

NN+3N-full

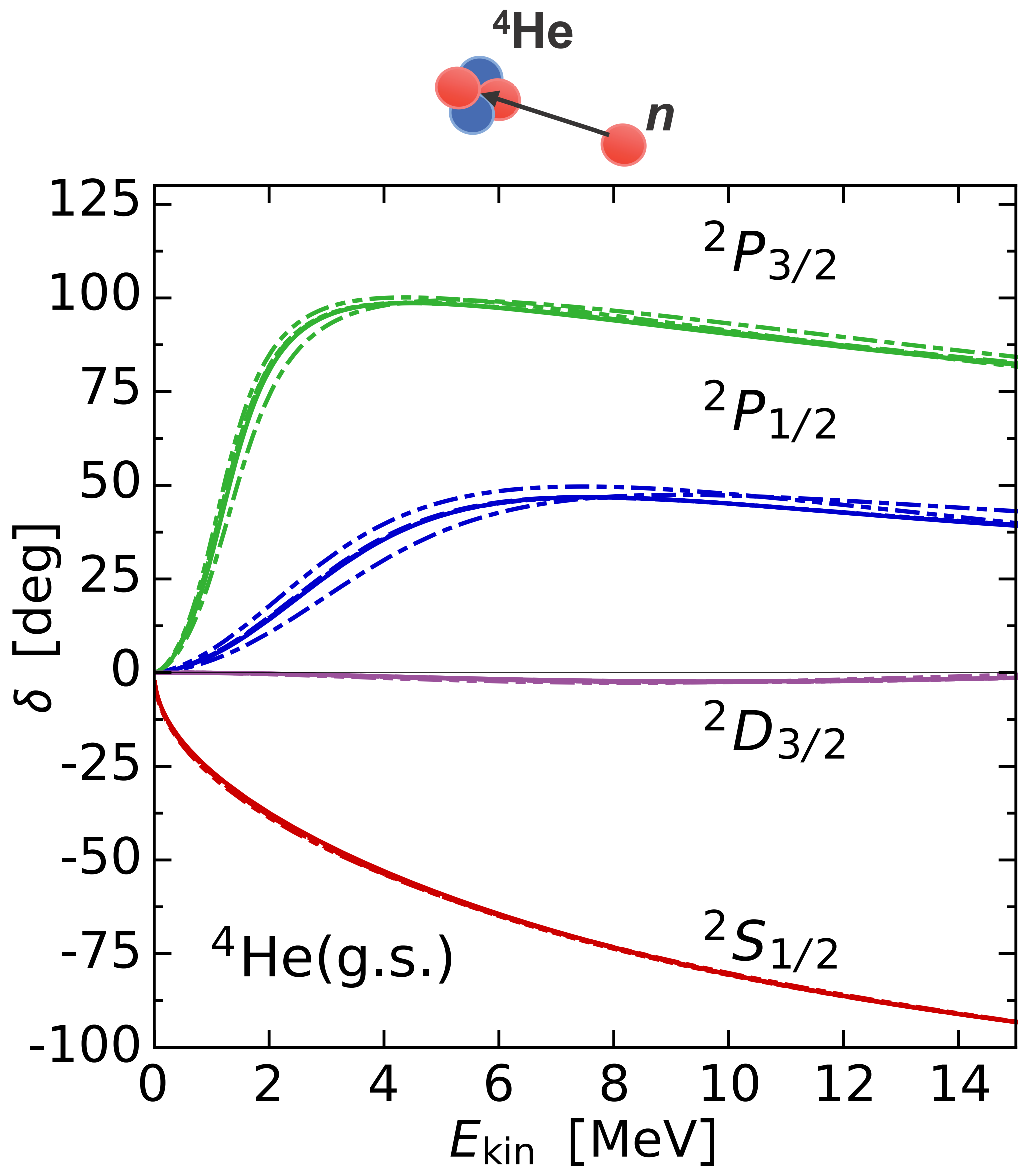
- ······· $N_{max} = 7$
- ·-·-·- $N_{max} = 9$
- - - - $N_{max} = 11$
- —— $N_{max} = 13$

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

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

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

Scattering Phase Shifts: n+^{4}He



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

NN+3N-full

$N_{max} = 7$

$E_{3\,max} = 4$

$E_{3\,max} = 6$

$E_{3\,max} = 8$

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

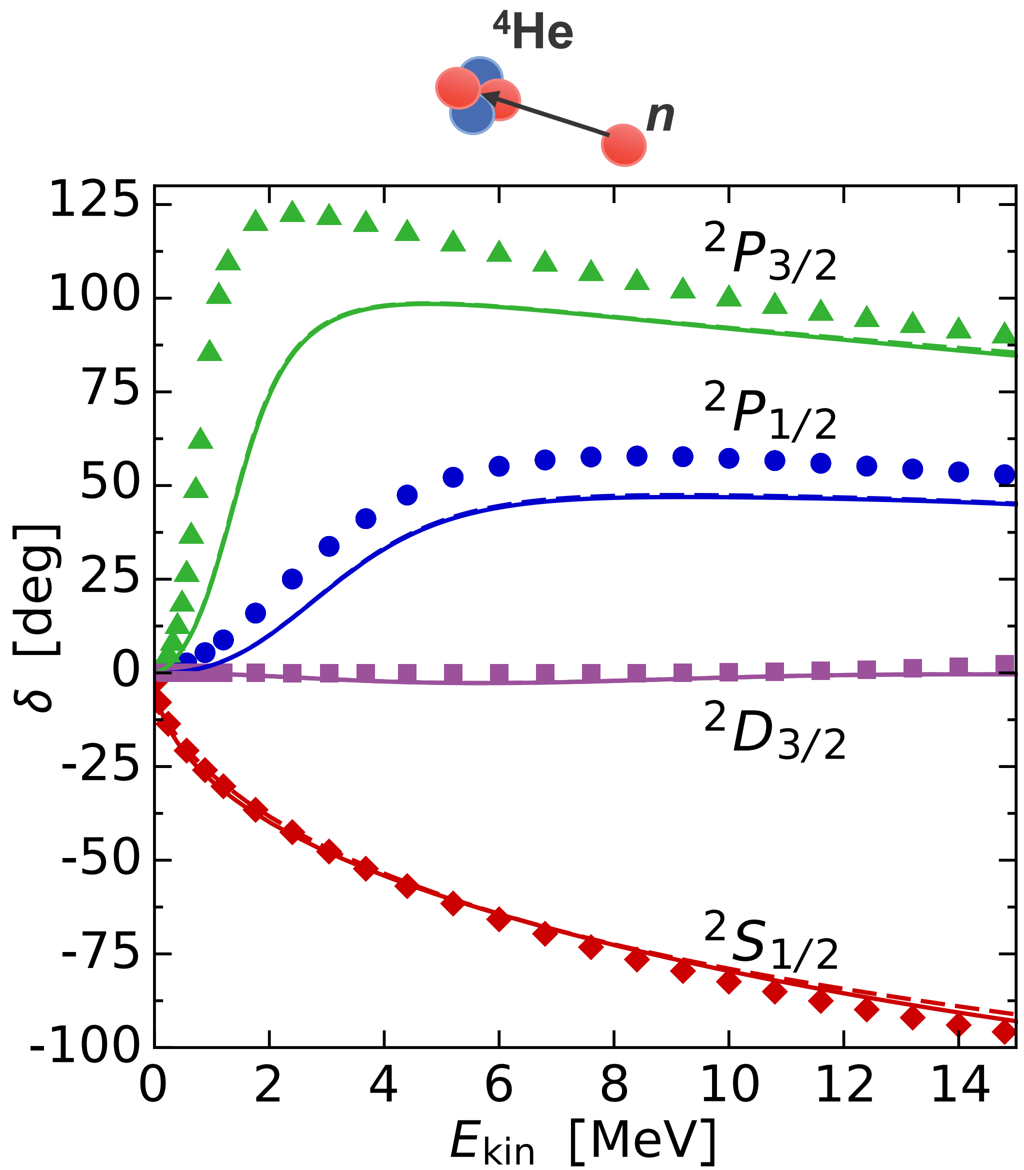
— $E_{3\,max} = 12$

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

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

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

Scattering Phase Shifts: n+^{4}He



Taking into account excited states of ^{4}He

NN+3N-full

$N_{max} = 11$

◆▲●■ experiment

— ^{4}He $0^+(g.s.)$

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

need more excited states...work in progress

$\alpha = 0.0625$

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

$\hbar\Omega = 20\,\mathrm{MeV}$

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+^{4}He results show expected **enhanced spin-orbit splitting**
  - consideration of more ^{4}He 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)

$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

$$= W^{0B} + \sum W^{1B}_{\circ\circ} \{\hat{a}^\dagger_\circ \, \hat{a}_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ} \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \, \hat{a}_\circ \hat{a}_\circ\}$$

$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ} \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ\}$$

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

operator identity

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)

$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

$$= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{\hat{a}^\dagger_\circ\, \hat{a}_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ\}$$

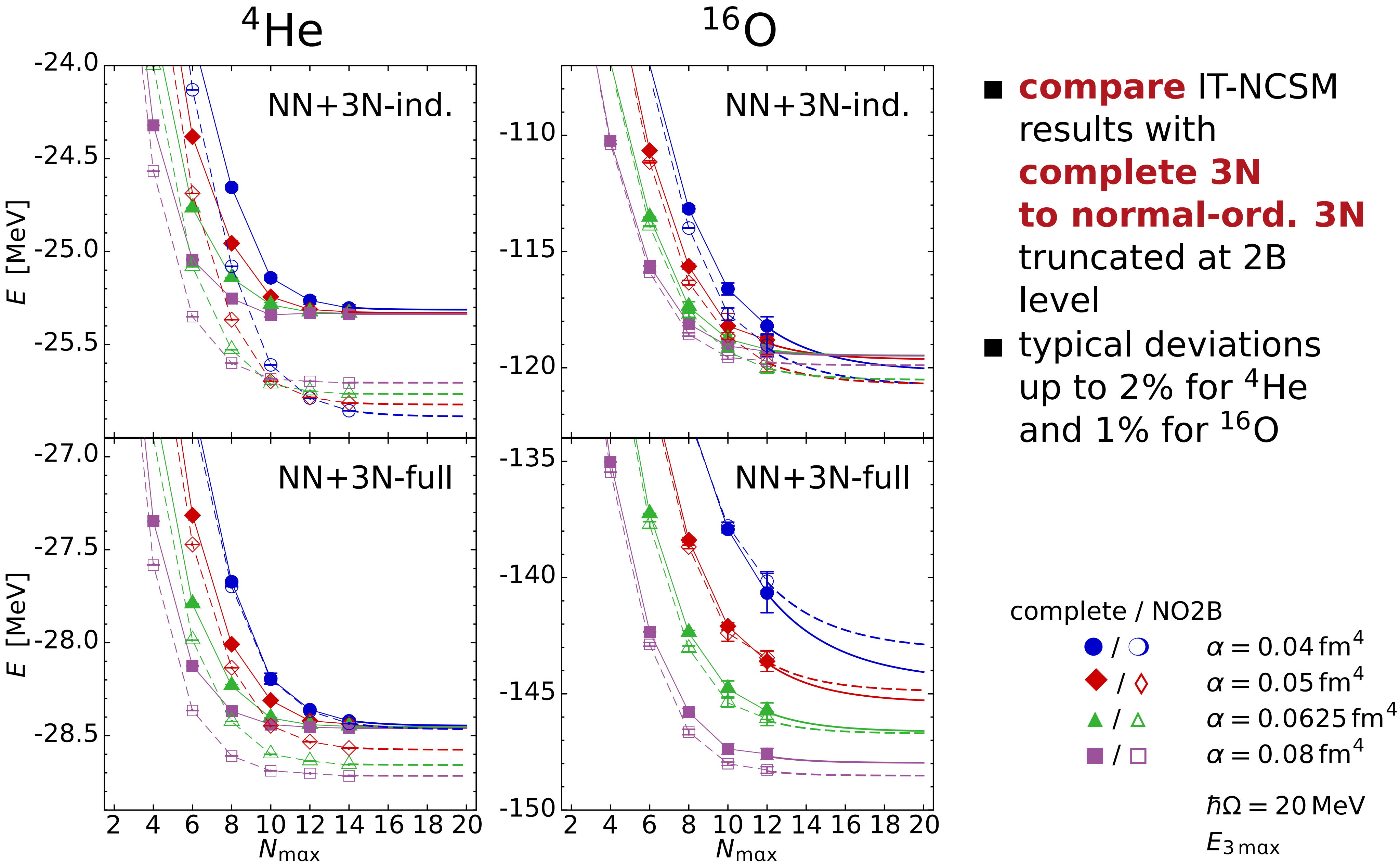
$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ}\, \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ\}$$

operator identity

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

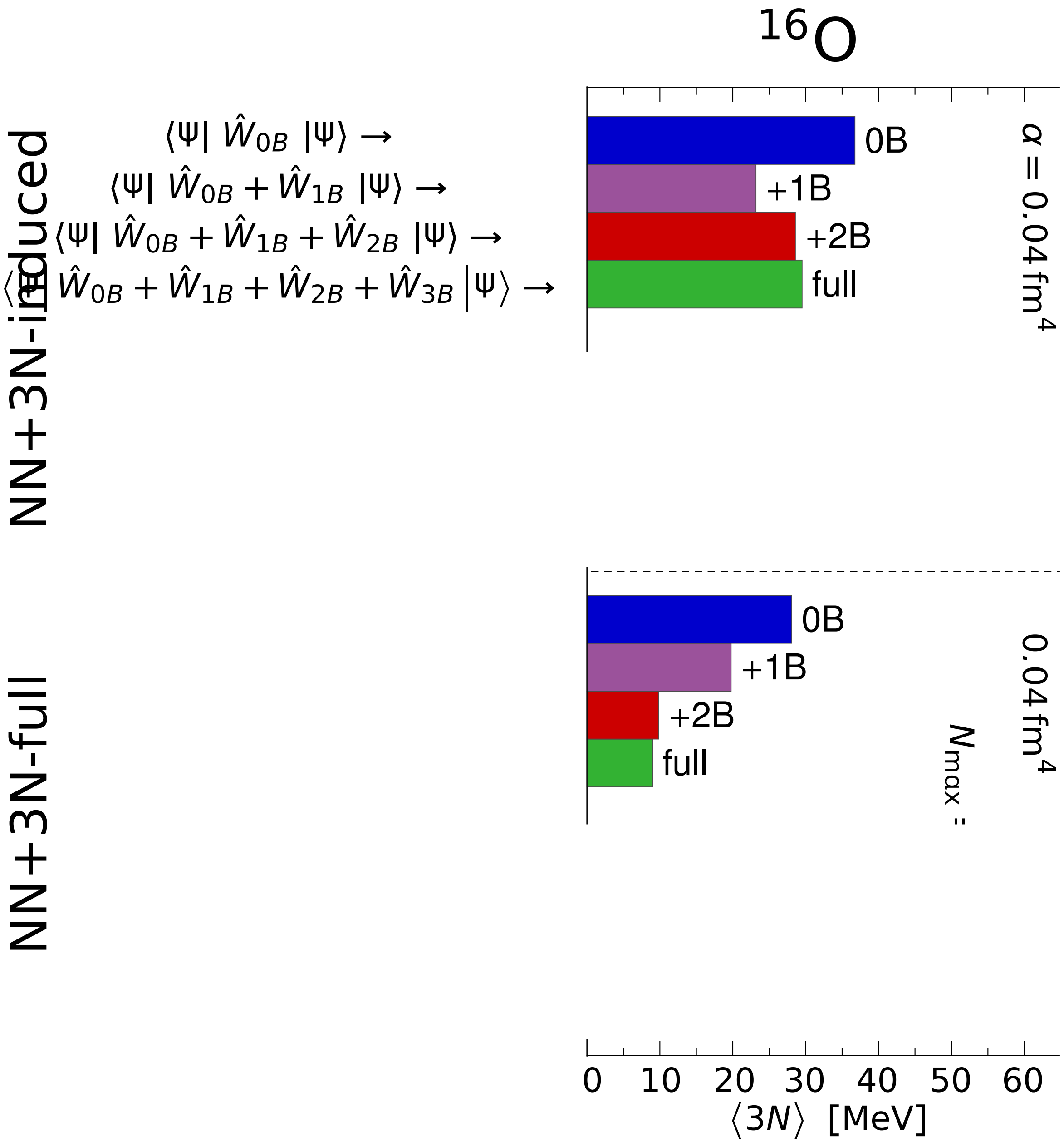
- **question**: if we neglect the normal-ordered $\hat{W}_{3B}$ 3B term, how well does this approximation work?

Benchmark of Normal-Ordered 3N

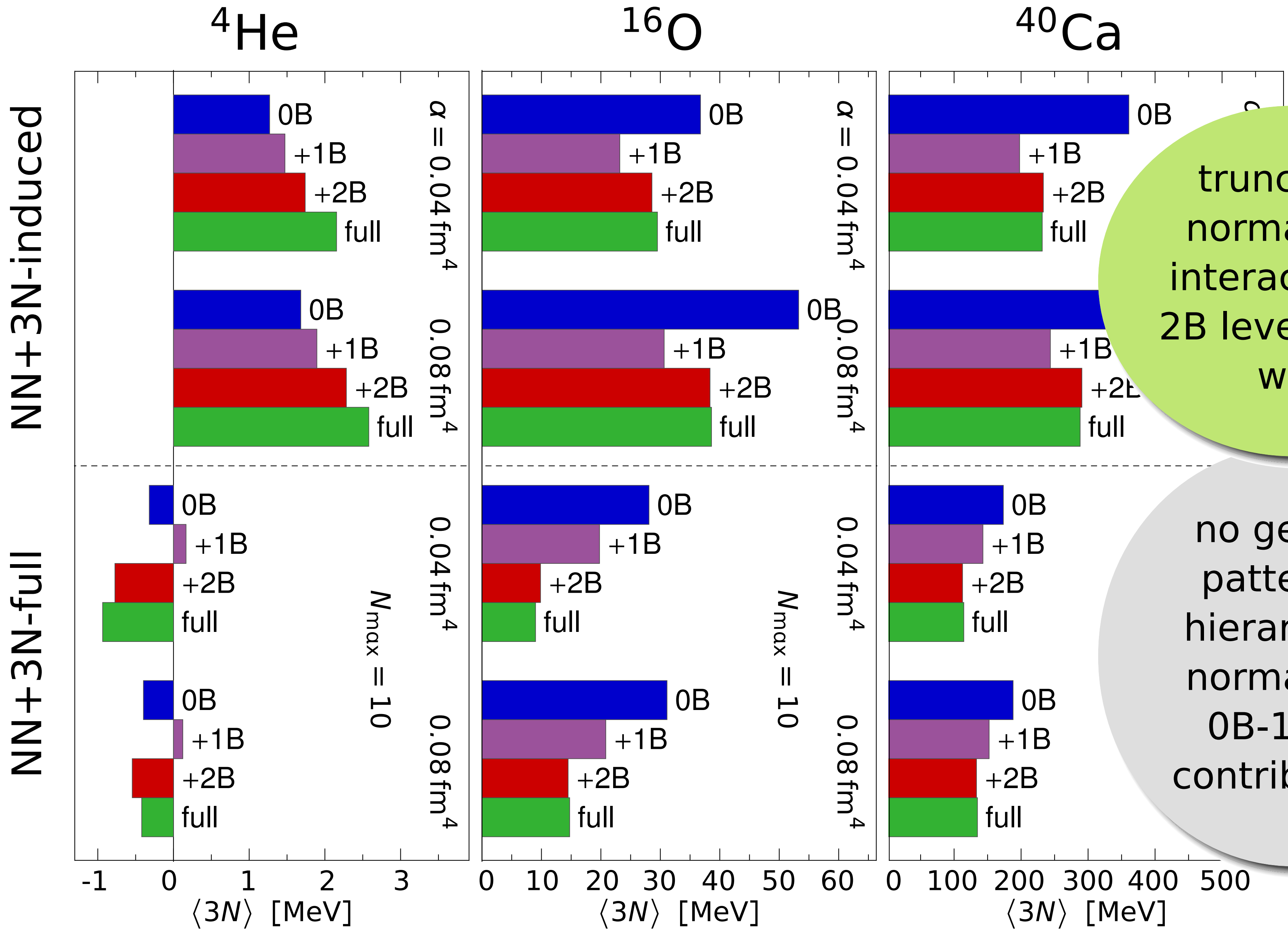


- **compare** IT-NCSM results with **complete 3N** **to normal-ord. 3N** truncated at 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

Anatomy of Normal-Ordered 3N



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

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

- $\hat{T}_n$: ***n*p*n*h excitation** ("cluster") operators

$$\hat{T}_n = \frac{1}{(n!)^2}\sum_{\substack{ijk\ldots\\abc\ldots}} t^{abc\ldots}_{ijk\ldots}\{\hat{a}^\dagger_a\hat{a}^\dagger_b\hat{a}^\dagger_c\ldots\hat{a}_k\hat{a}_j\hat{a}_i\}$$

- **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

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

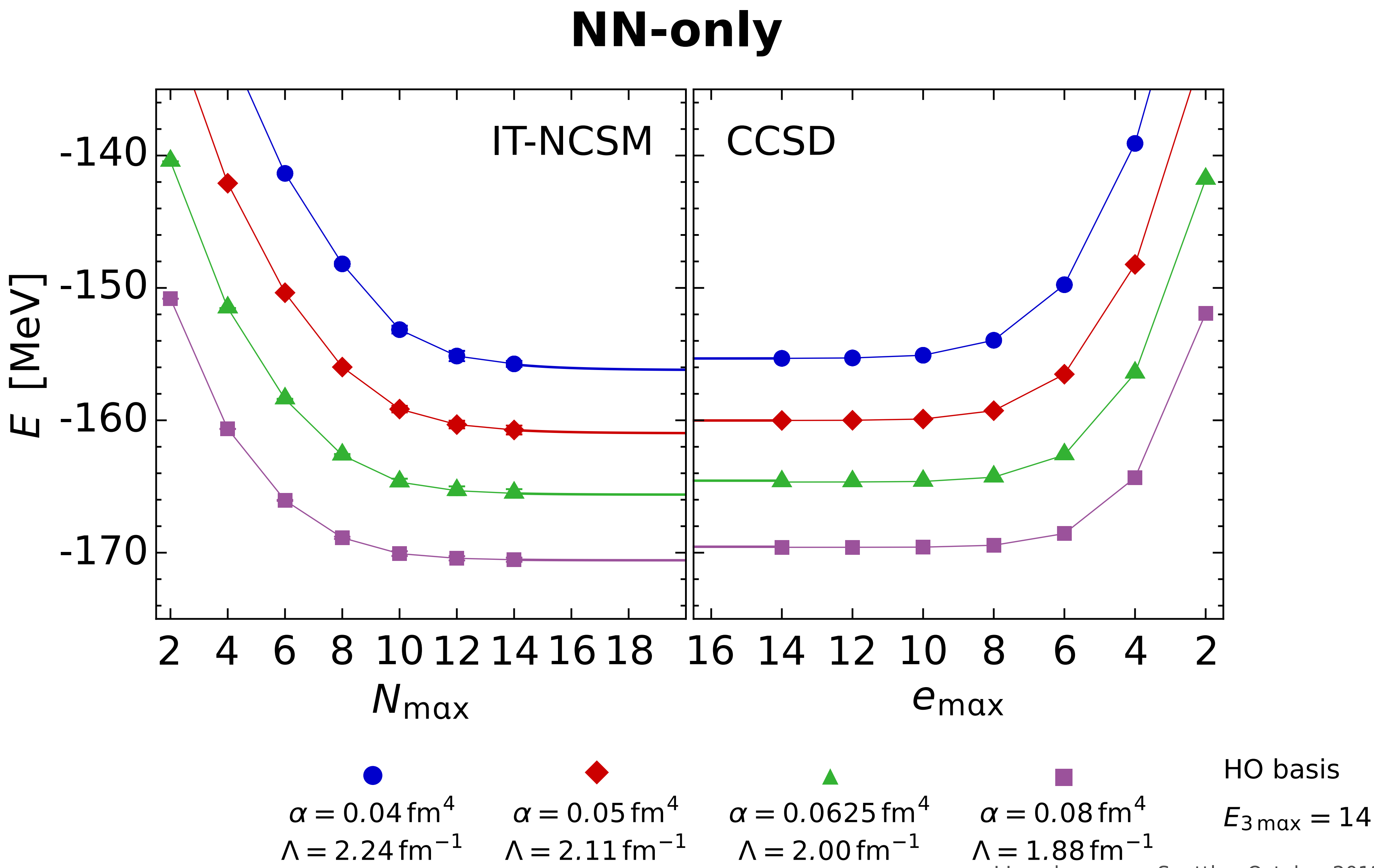
$$\Delta E_{\text{CCSD}}^{NN} = \left\langle \phi_0 \middle| \hat{\mathcal{H}} \middle| \phi_0 \right\rangle = \left\langle \phi_0 \middle| \hat{H}_{NO}(\hat{T}_2 + \hat{T}_1 + \tfrac{1}{2}\hat{T}_1^2) \middle| \phi_0 \right\rangle_C$$

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

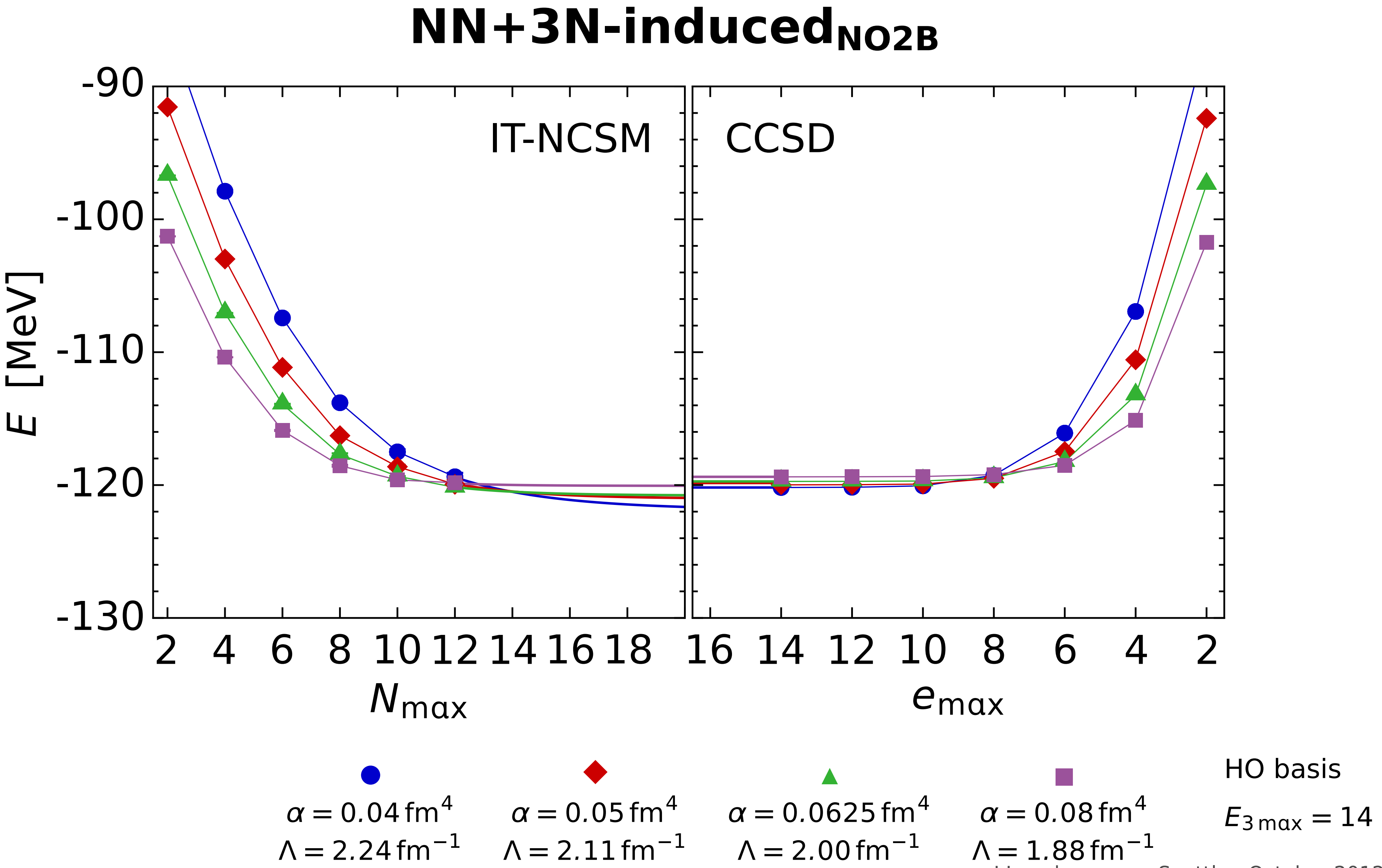
$$0 = \left\langle \phi_{ij}^{ab} \middle| \hat{\mathcal{H}} \middle| \phi_0 \right\rangle = T_{2,CCSD}^{NN} = \left\langle \phi_{ij}^{ab} \middle| \hat{H}_{NO}(1 + \hat{T}_2 + \tfrac{1}{2}\hat{T}_2^2 + \hat{T}_1 + \hat{T}_1\hat{T}_2 \right.$$

$$\left. + \tfrac{1}{2}\hat{T}_1^2 + \tfrac{1}{2}\hat{T}_1^2\hat{T}_2 + \tfrac{1}{3!}\hat{T}_1^3 + \tfrac{1}{4!}\hat{T}_1^4) \middle| \phi_0 \right\rangle_C$$

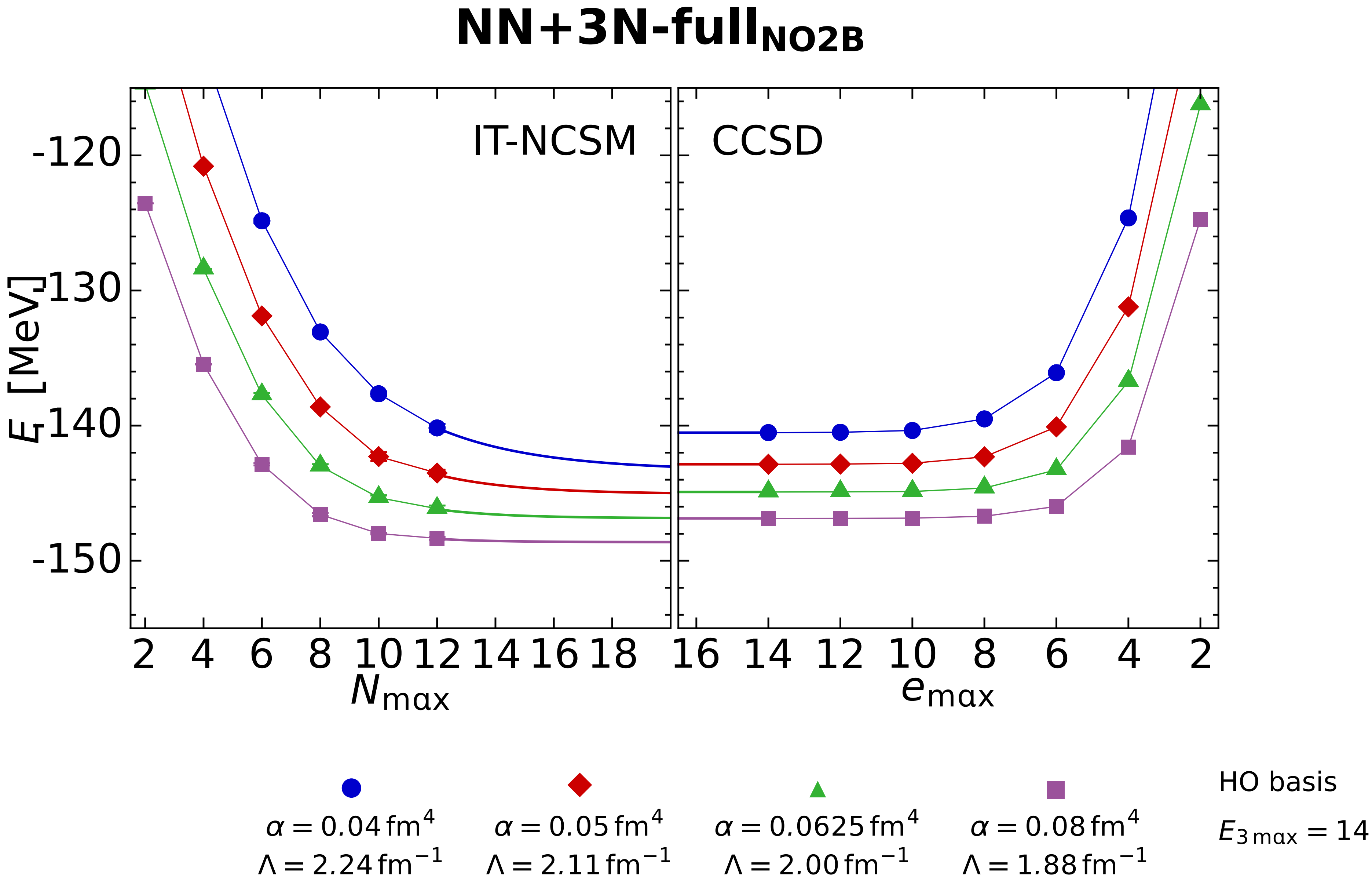
^{16}O: IT-NCSM vs. Coupled-Cluster



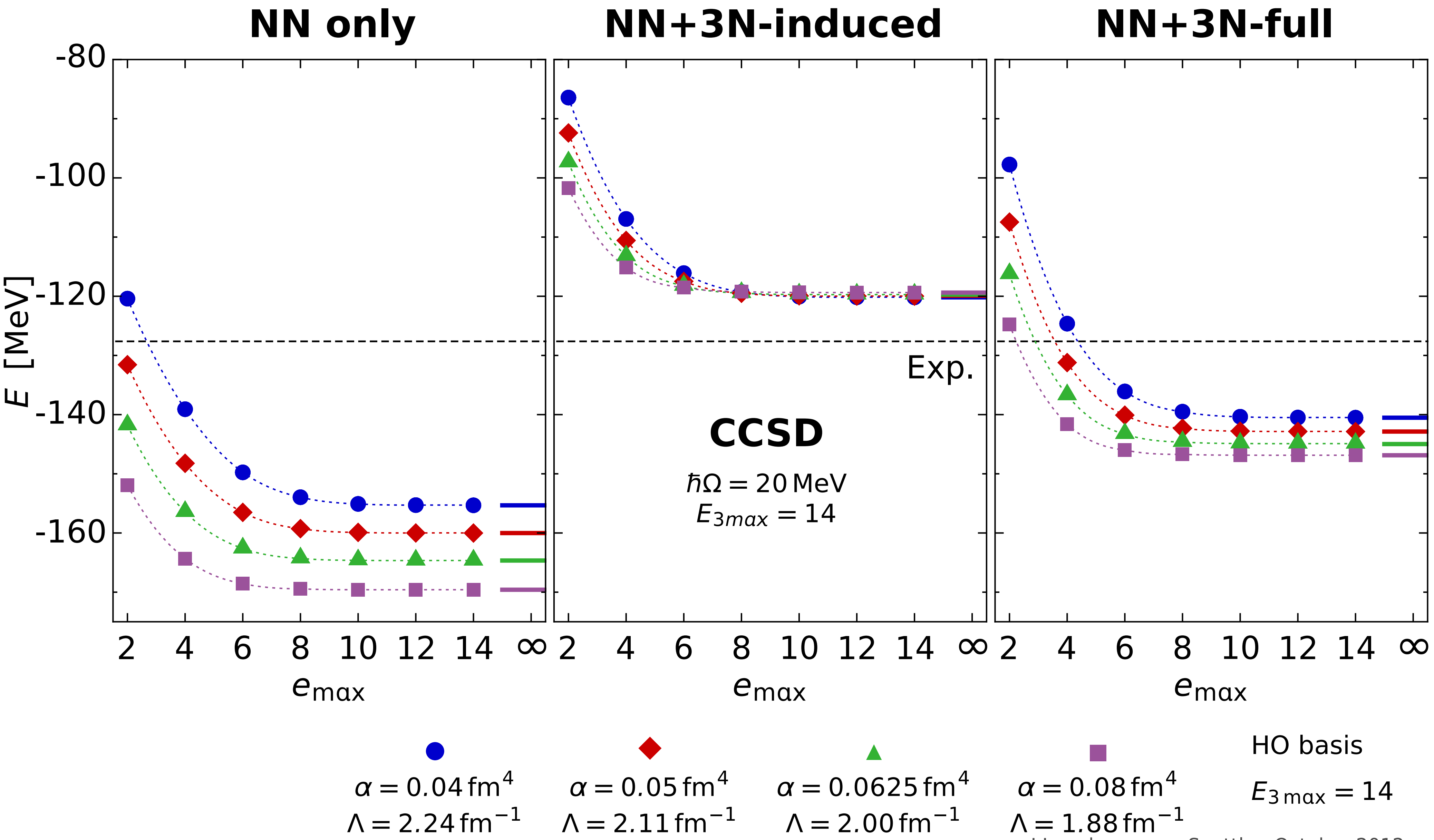
^{16}O: IT-NCSM vs. Coupled-Cluster



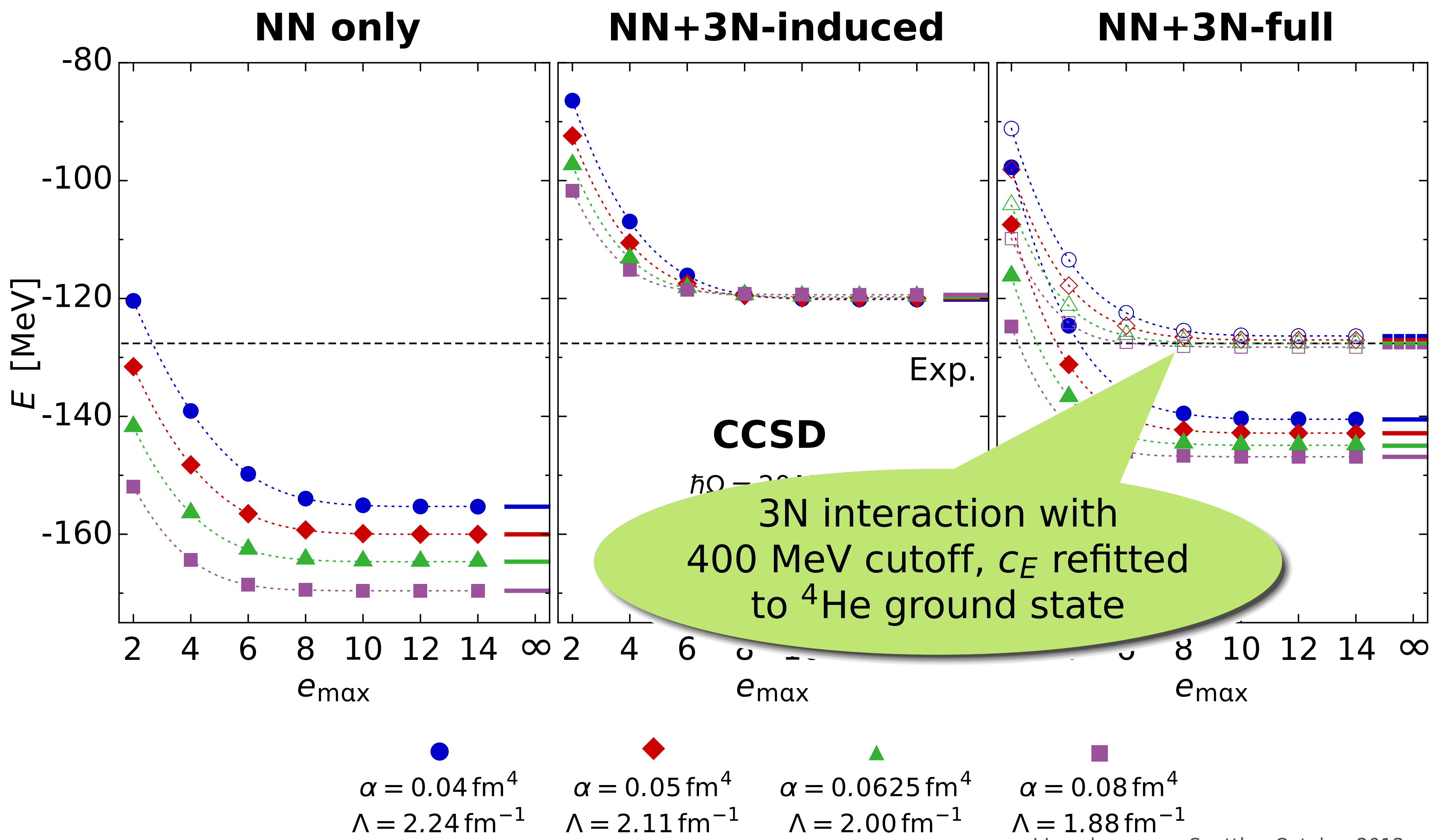
^{16}O: IT-NCSM vs. Coupled-Cluster



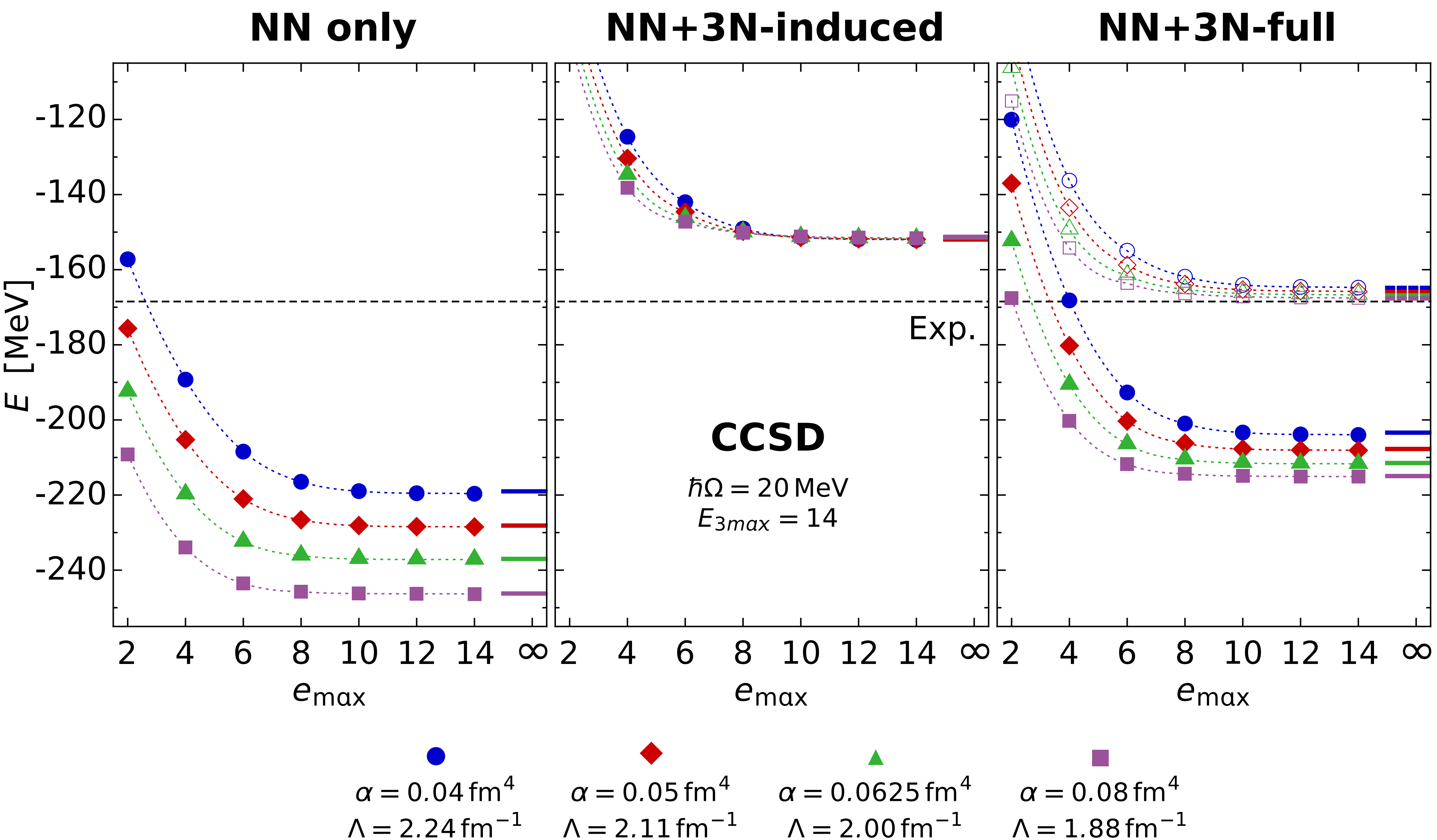
^{16}O: Coupled-Cluster with $3N_{NO2B}$



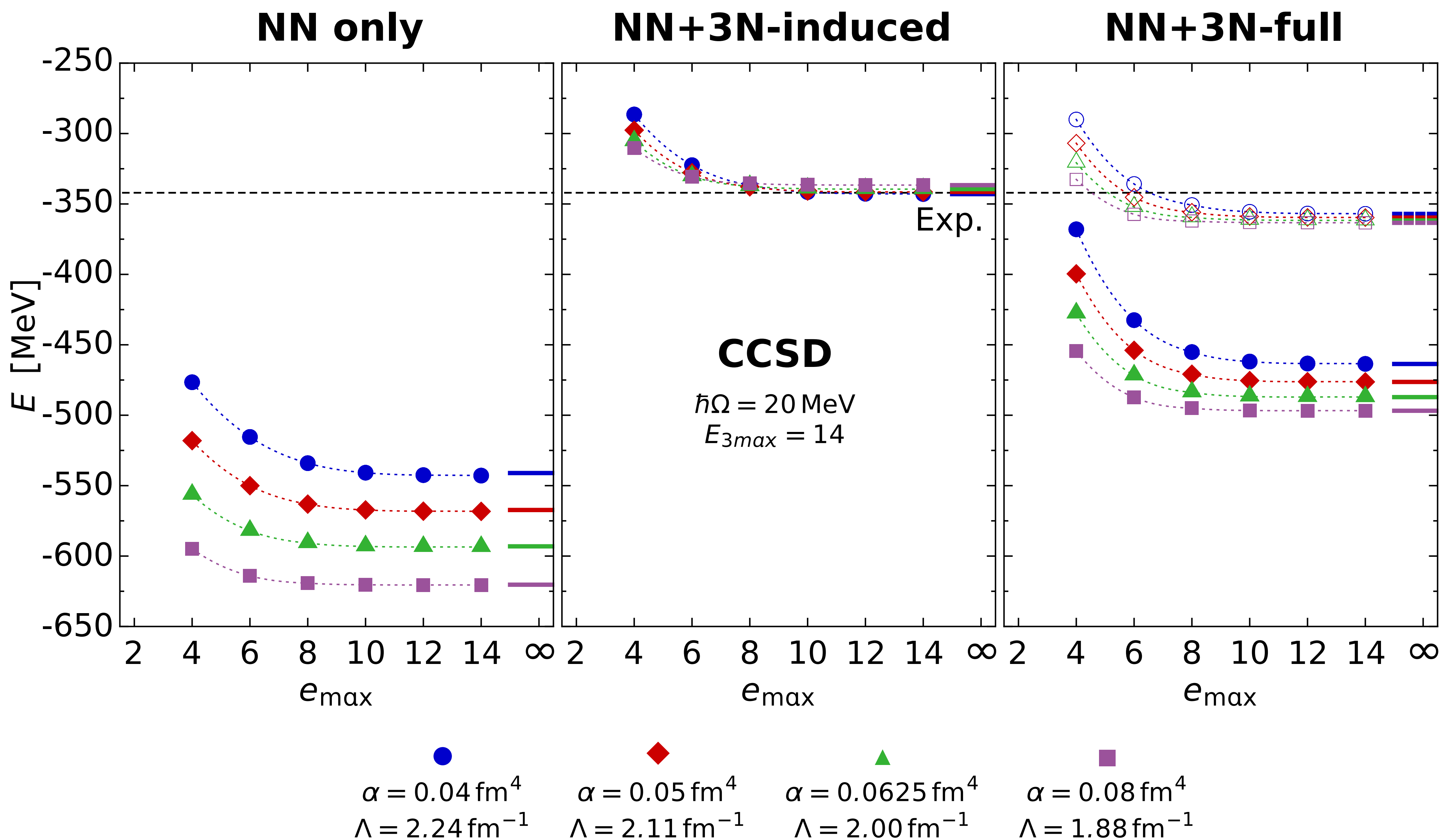
^{16}O: Coupled-Cluster with $3N_{NO2B}$



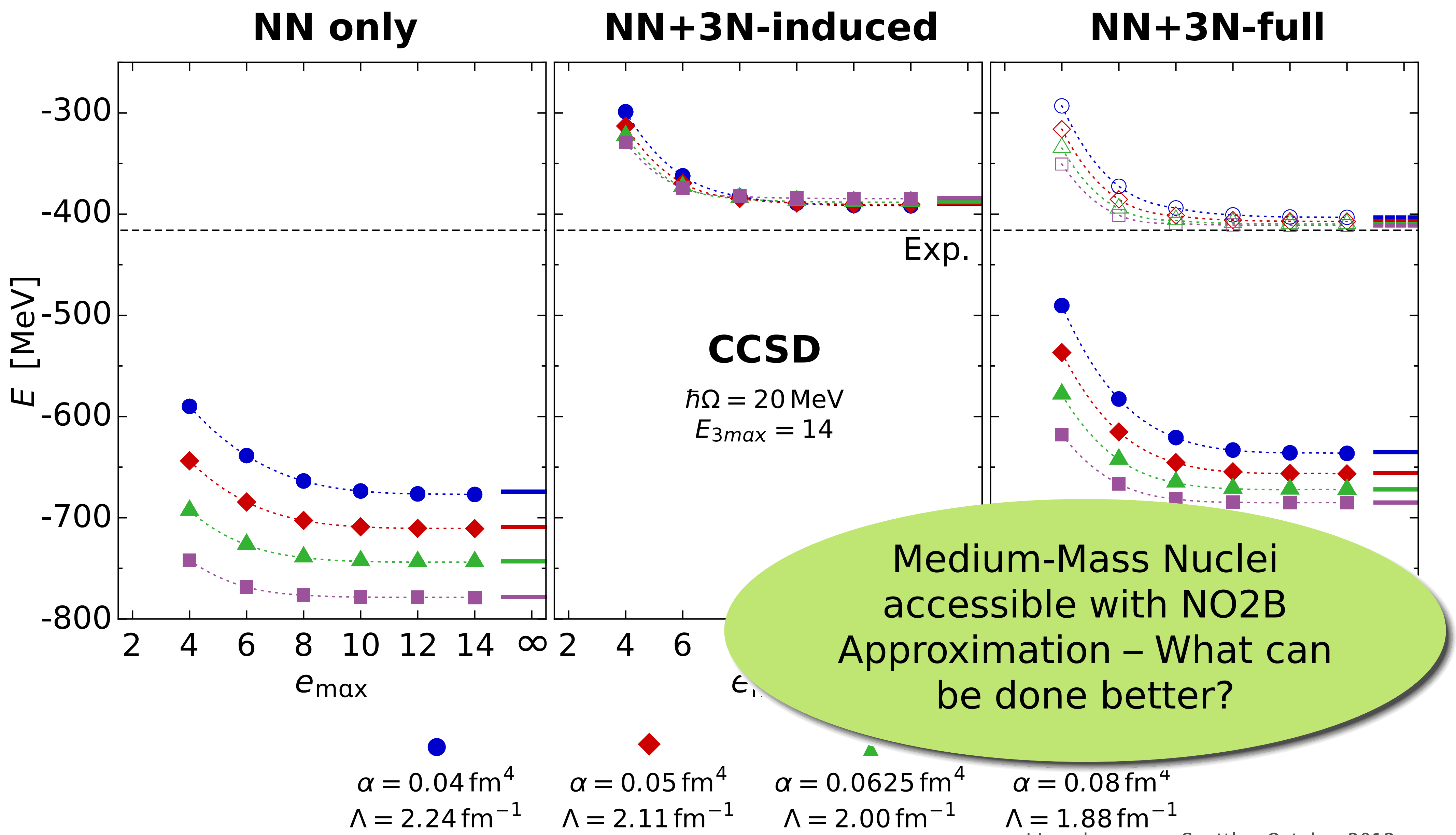
^{24}O: Coupled-Cluster with $3N_{NO2B}$



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



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

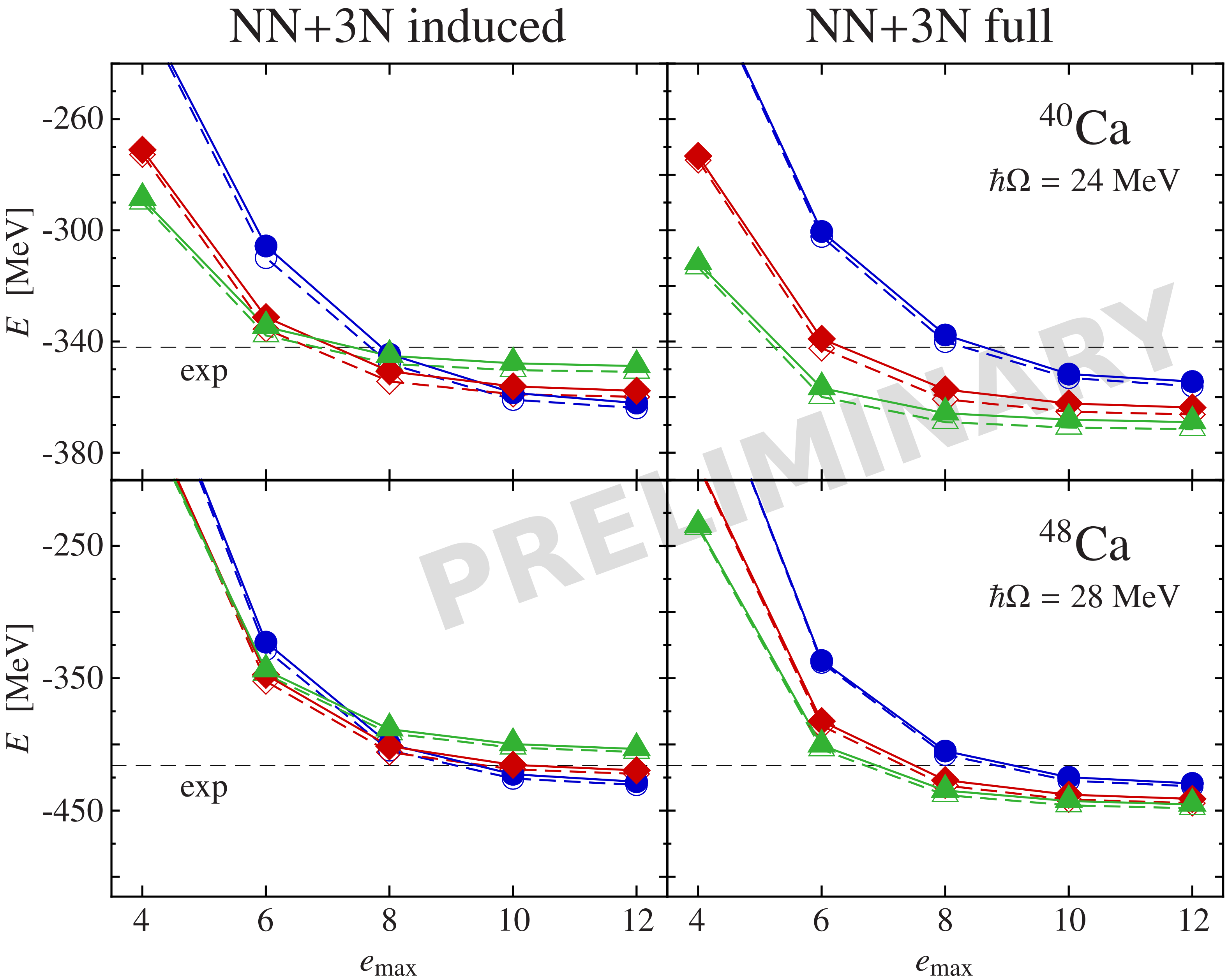


Coupled Cluster Method with Complete 3N Interactions

Binder, Langhammer, Calci, Roth — in prep.

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

CCSD with Complete 3N Interaction



initial 3N with
$\Lambda = 400\,\text{MeV}$

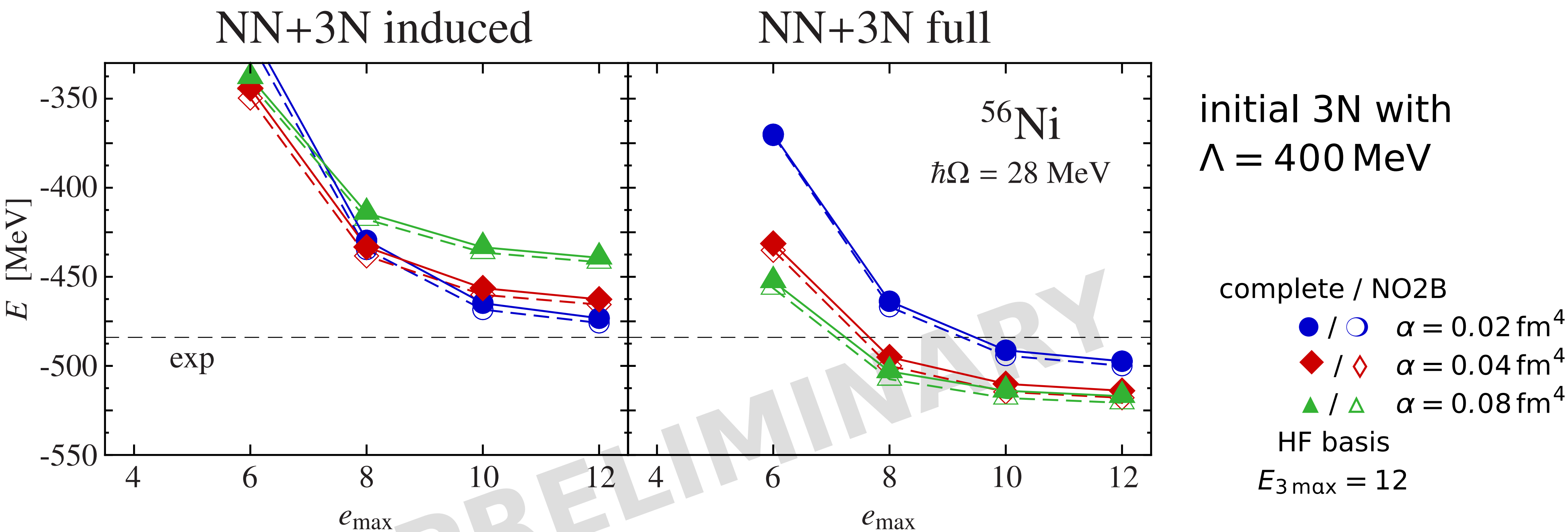
complete / NO2B

- $\alpha = 0.02\,\text{fm}^4$
- $\alpha = 0.04\,\text{fm}^4$
- $\alpha = 0.08\,\text{fm}^4$

HF basis

$E_{3\,max} = 12$

CCSD with Complete 3N Interaction

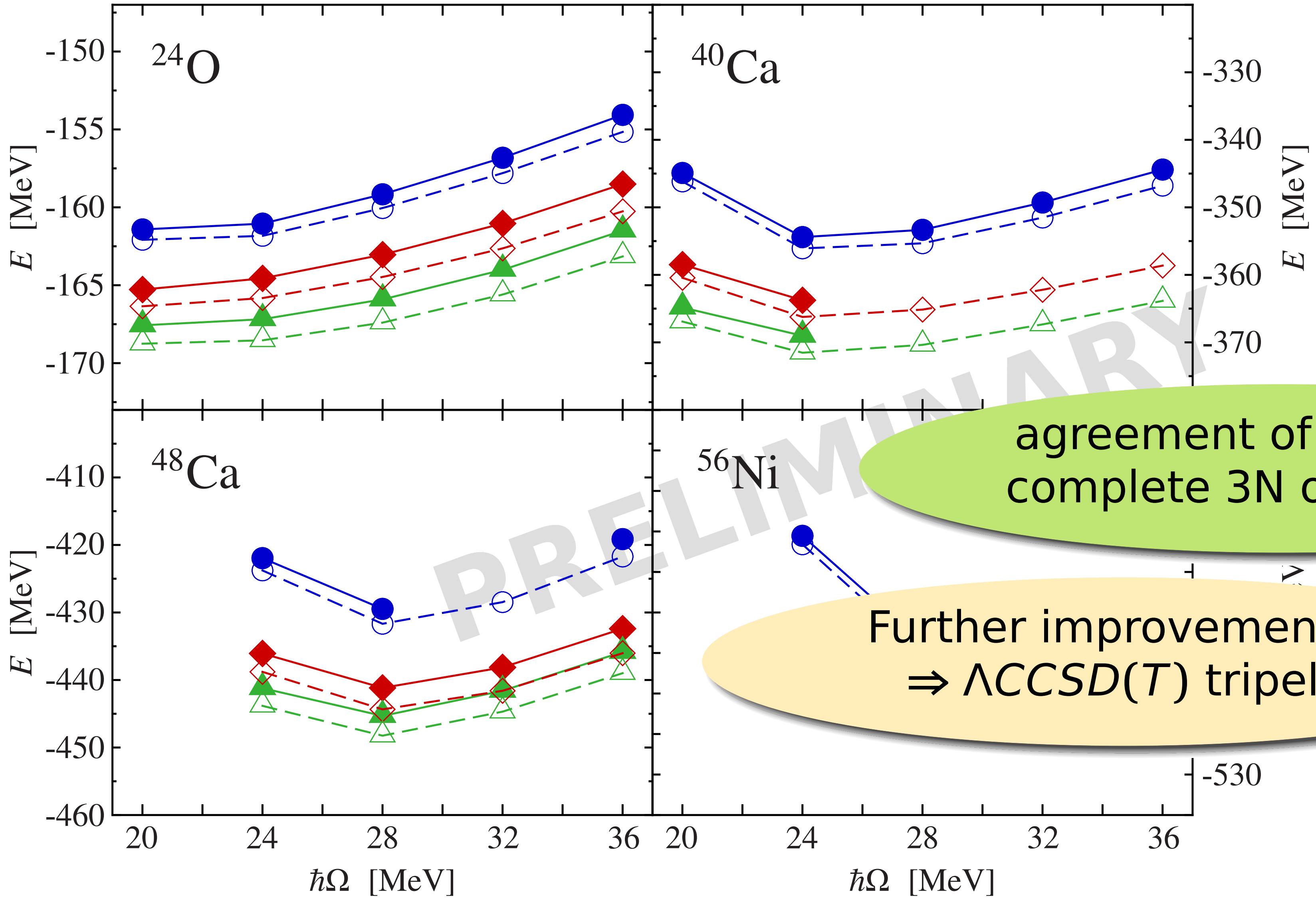


- CCSD calculations with **inclusion of complete 3N interactions for medium-mass nuclei** feasible

  $\Rightarrow$ benchmarking various approximation schemes for 3N interactions in this mass range possible

- ground-state energies: deviation between normal-ordered two-body approximation and complete 3N treatment $\approx$ 1%

Frequency Dependence



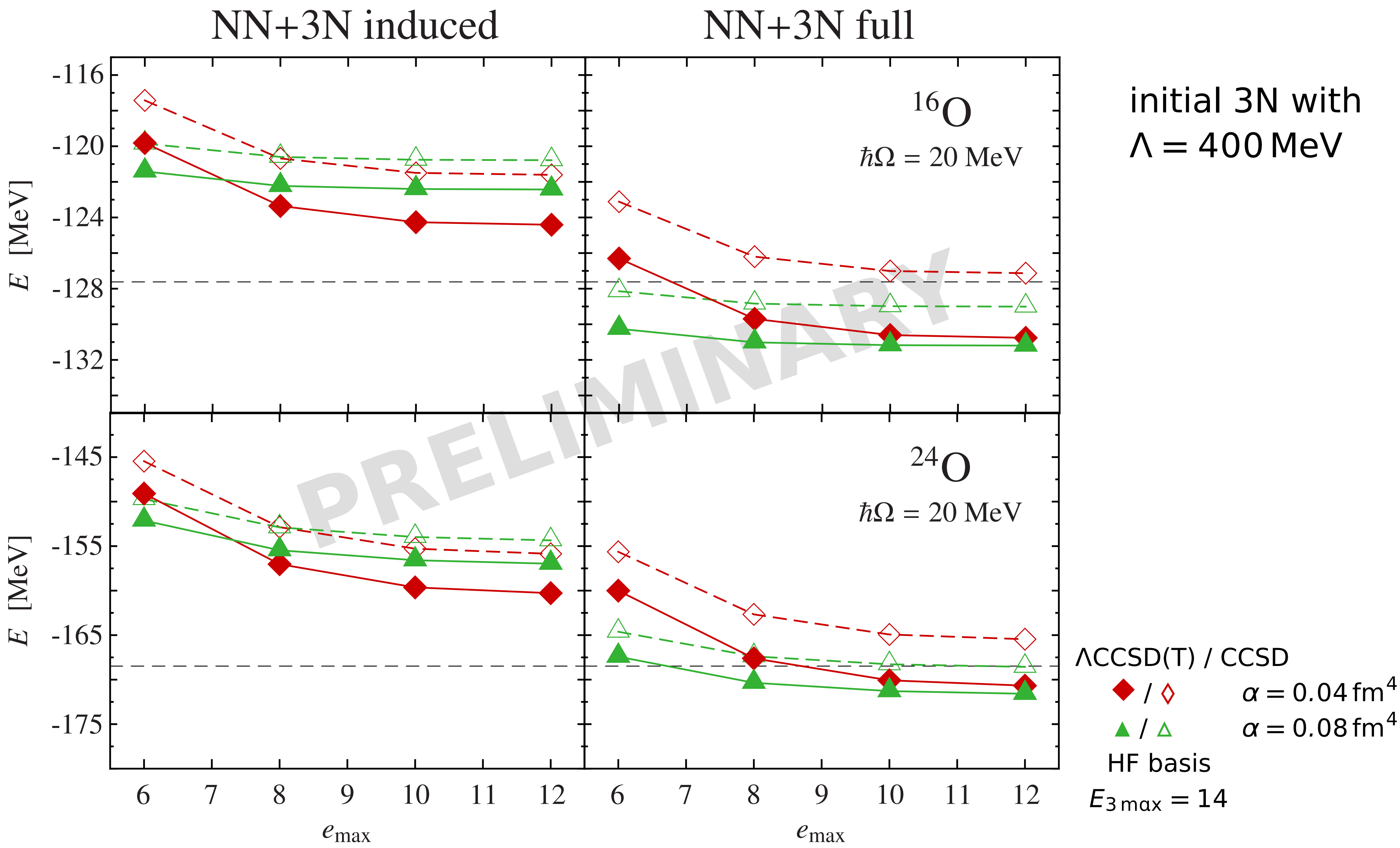
initial 3N with
$\Lambda = 400\,\text{MeV}$

agreement of NO2B and complete 3N on 1% level

Further improvements?
$\Rightarrow \Lambda CCSD(T)$ tripels

complete / NO2B
● / ○ $\alpha = 0.02\,\text{fm}^4$
◆ / ◇ $\alpha = 0.04\,\text{fm}^4$
▲ / △ $\alpha = 0.08\,\text{fm}^4$
HF basis
$E_{3\,max} = 12$

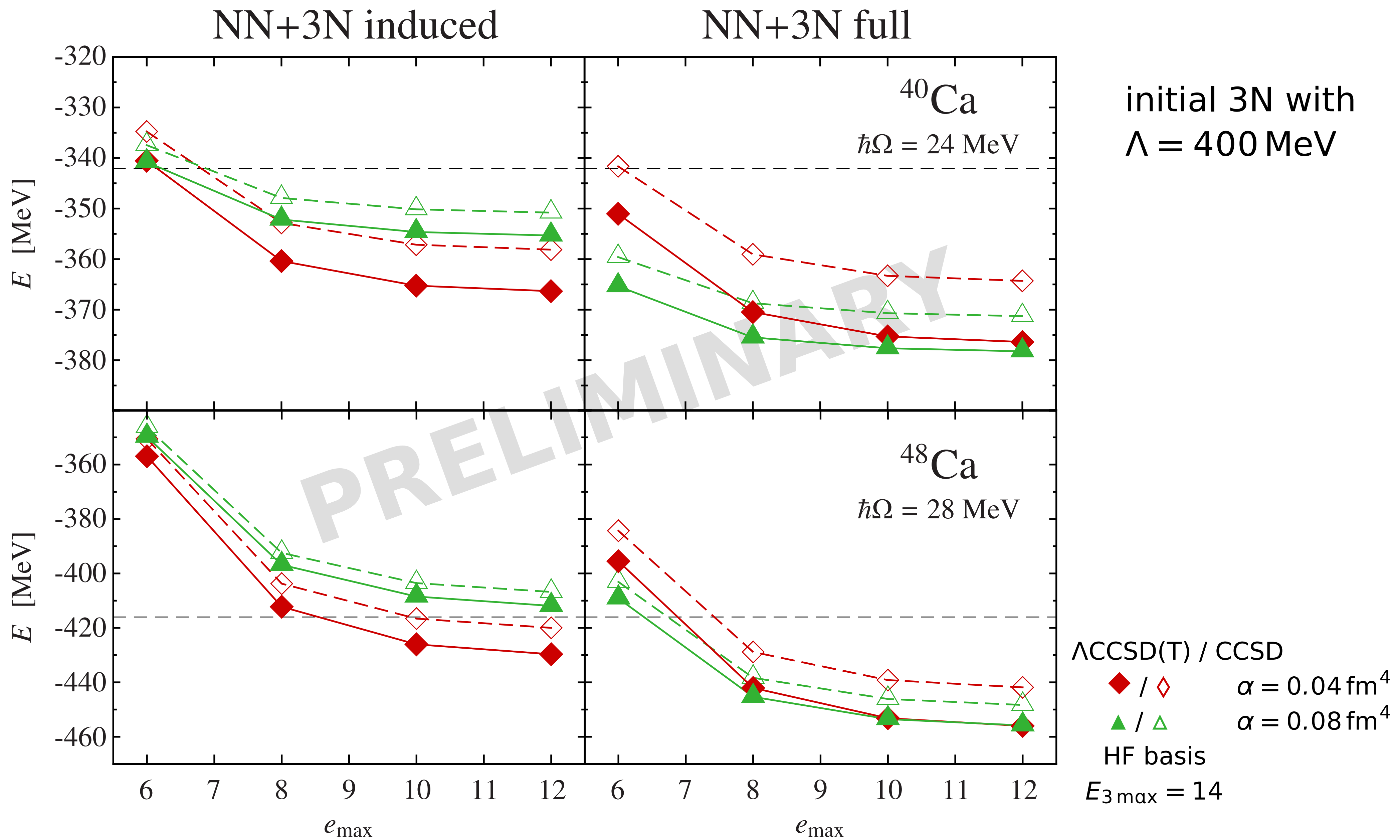
ΛCCSD(T) with $3N_{NO2B}$ Interaction



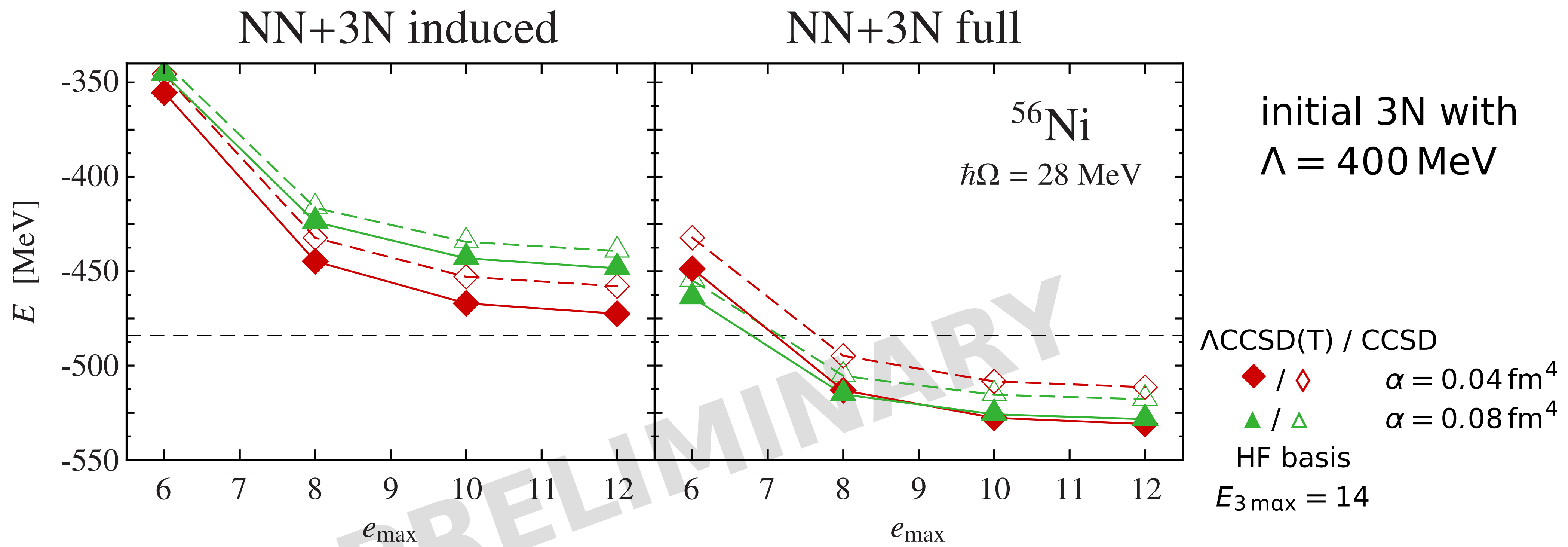
initial 3N with
$\Lambda = 400$ MeV

ΛCCSD(T) with $3N_{NO2B}$ Interaction

initial 3N with
$\Lambda = 400\,\text{MeV}$



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 ⇒ less tripels 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 ΛCCSD(T) with $3N_{NO2B}$

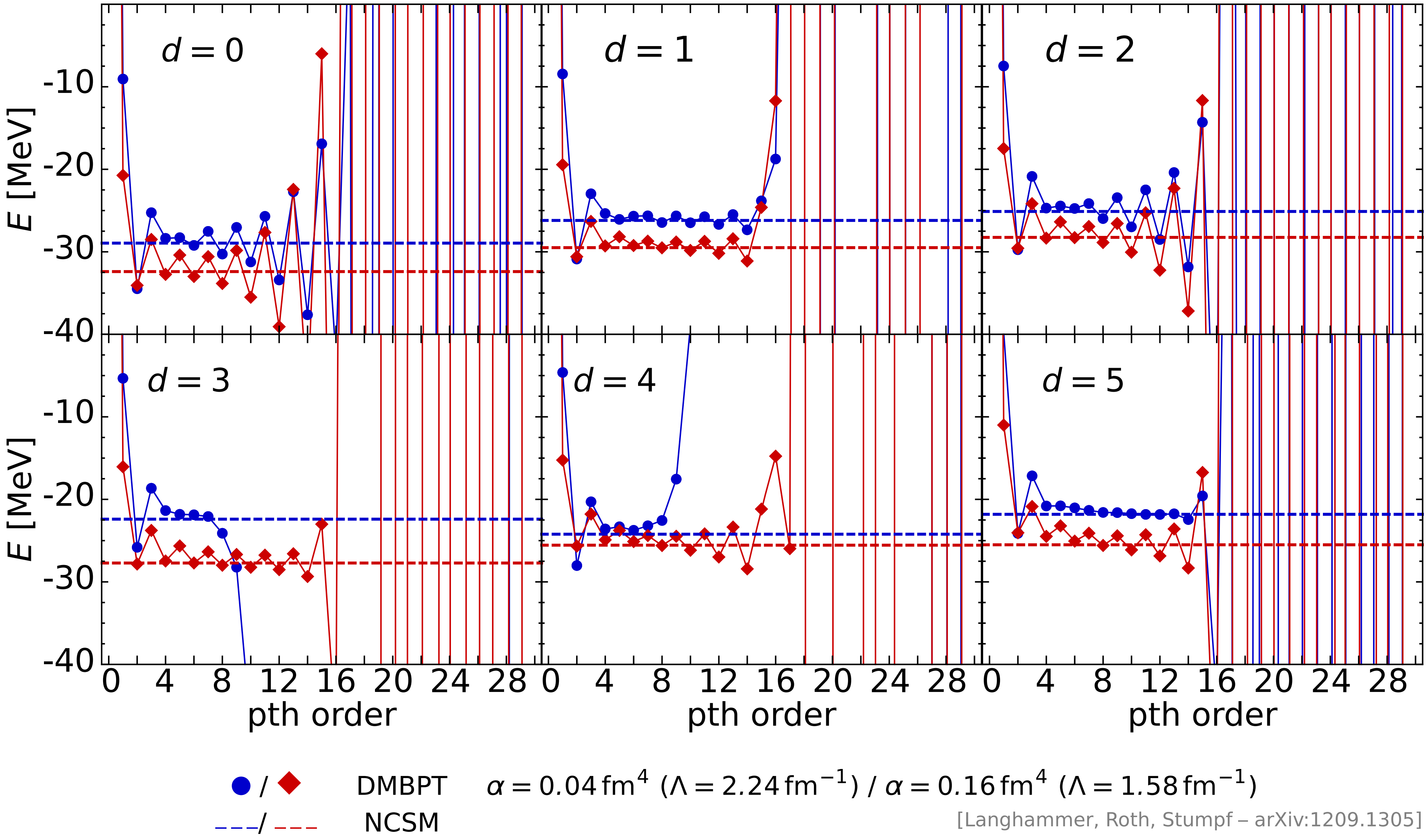
- work in progress:

  uncertainty quantification for all 'truncations',
  i.e. dependence on $eMax$, $\hbar\Omega$, $E_{3\,max}$, SRG through α variation, cluster-order through ΛCCSD(T)

Soft Interactions in Many-Body Perturbation Theory

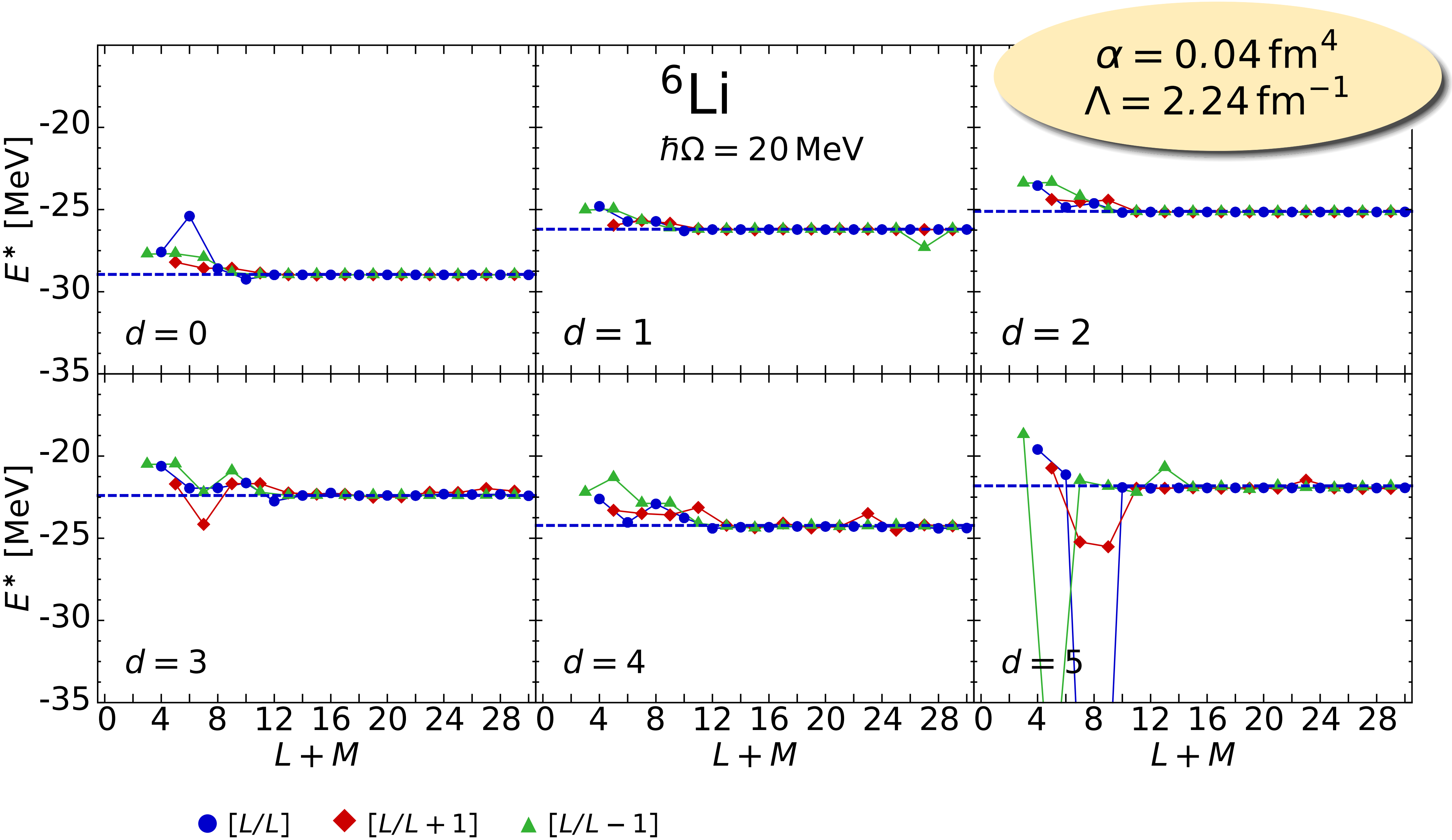
Langhammer, Roth, Stumpf — arXiv:1209.1305

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



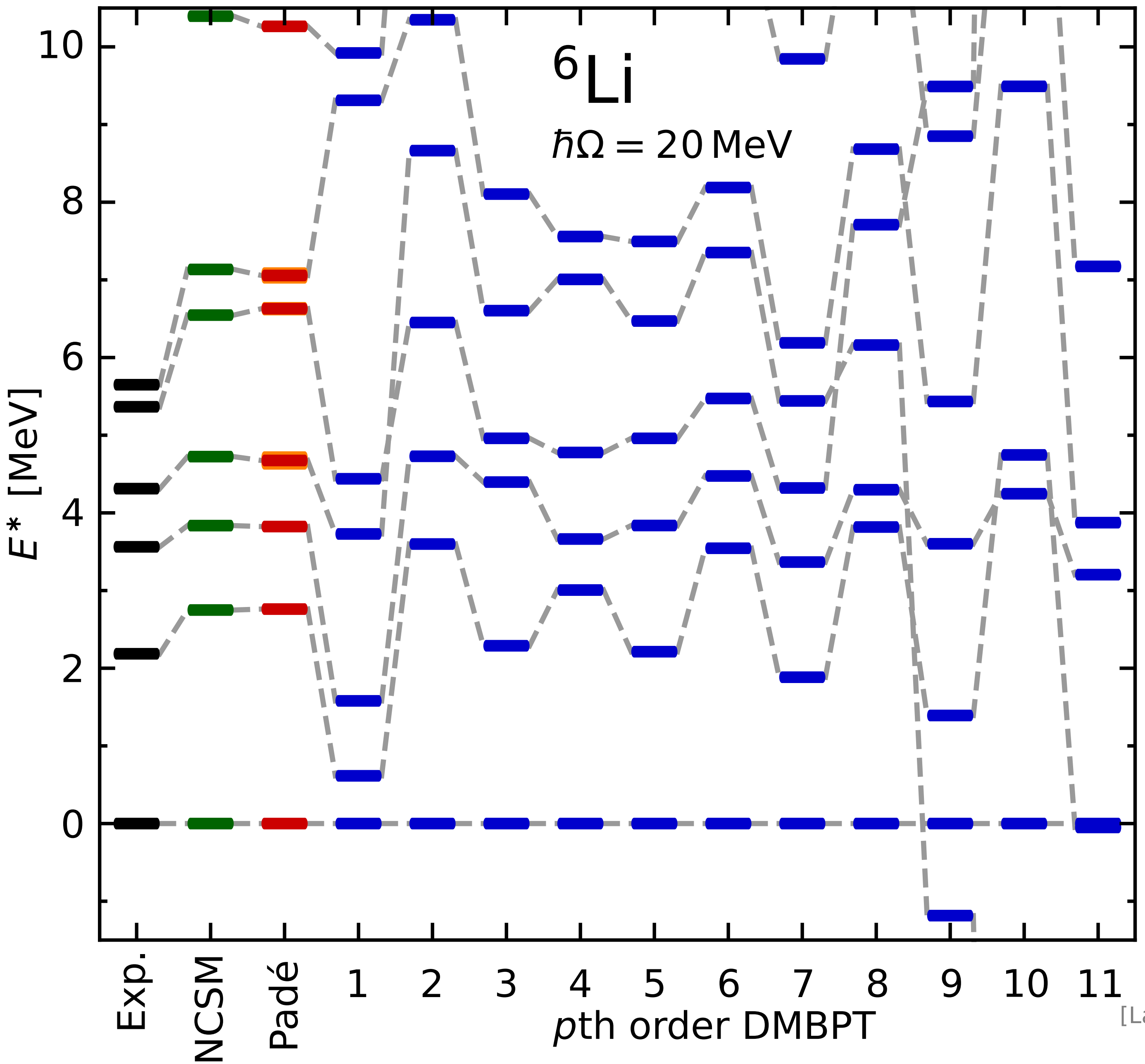
[Langhammer, Roth, Stumpf – arXiv:1209.1305]

Padé Resummation



[Langhammer, Roth, Stumpf – arXiv:1209.1305]

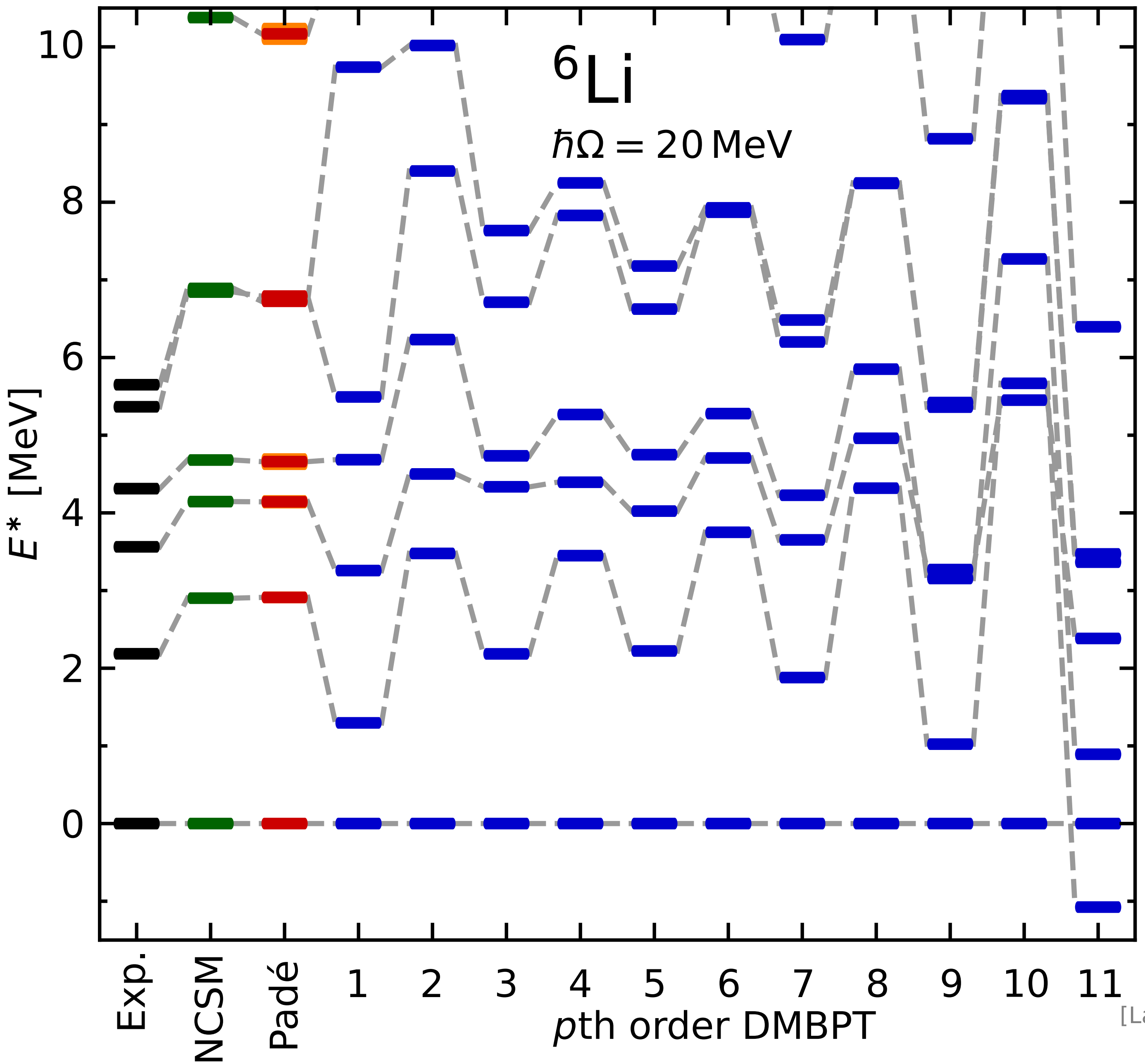
Spectra



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

[Langhammer, Roth, Stumpf – arXiv:1209.1305]

Spectra



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

[Langhammer, Roth, Stumpf – arXiv:1209.1305]

Epilogue

- **thanks to my group & my collaborators**
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    Iowa State University, USA
  - P. Piec
    Mic
  - H. Hergert
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    IPN Orsay, F
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    Chalmers University, Sweden
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    Helmholtzzentrum

Thank you for your attention!

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