Overview & Perspectives "Ab Initio & EFT Programs"

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Projects

- A02: **Effective field theories and ab initio calculations of light nuclei**
  PIs: Hans-Werner Hammer, Robert Roth
- A04: **Strong interactions and structure of medium-mass nuclei**
  PIs: Robert Roth, Achim Schwenk
- B05: **Nuclear matter equation of state for astrophysical applications**
  PIs: Jens Braun, Kai Heleler

- A05: **Halos and clustering in nuclei**
  PIs: Tom Aumann, Pierre Capel, Hans-Werner Hammer
- B01: **Electroweak interactions in nuclei and nuclear matter**
  PIs: Gabriel Martínez-Pinedo, Achim Schwenk
- B04: **Electric dipole response and neutron equation of state**
  PIs: Sonia Bacca, Heiko Scheit

Overview

	A02	A04	B05
Domain	light nuclei (s & p-shell) ^{3}n, ^{4}n systems	medium-mass & heavy nuclei open-shell systems	infinite nuclear/neutron matter
Frontiers	precision calculations of elmag. observables inclusion of continuum resonance physics	observables beyond ground-states multi-reference/deformation heavy nuclei	extension & merging to high-density regime finite temperature arbitrary proton fraction

Uncertainty Quantification

Many-Body Tools

(Chiral) Effective Field Theory

Overview

A02 | A04 | B05

Domain

Frontiers

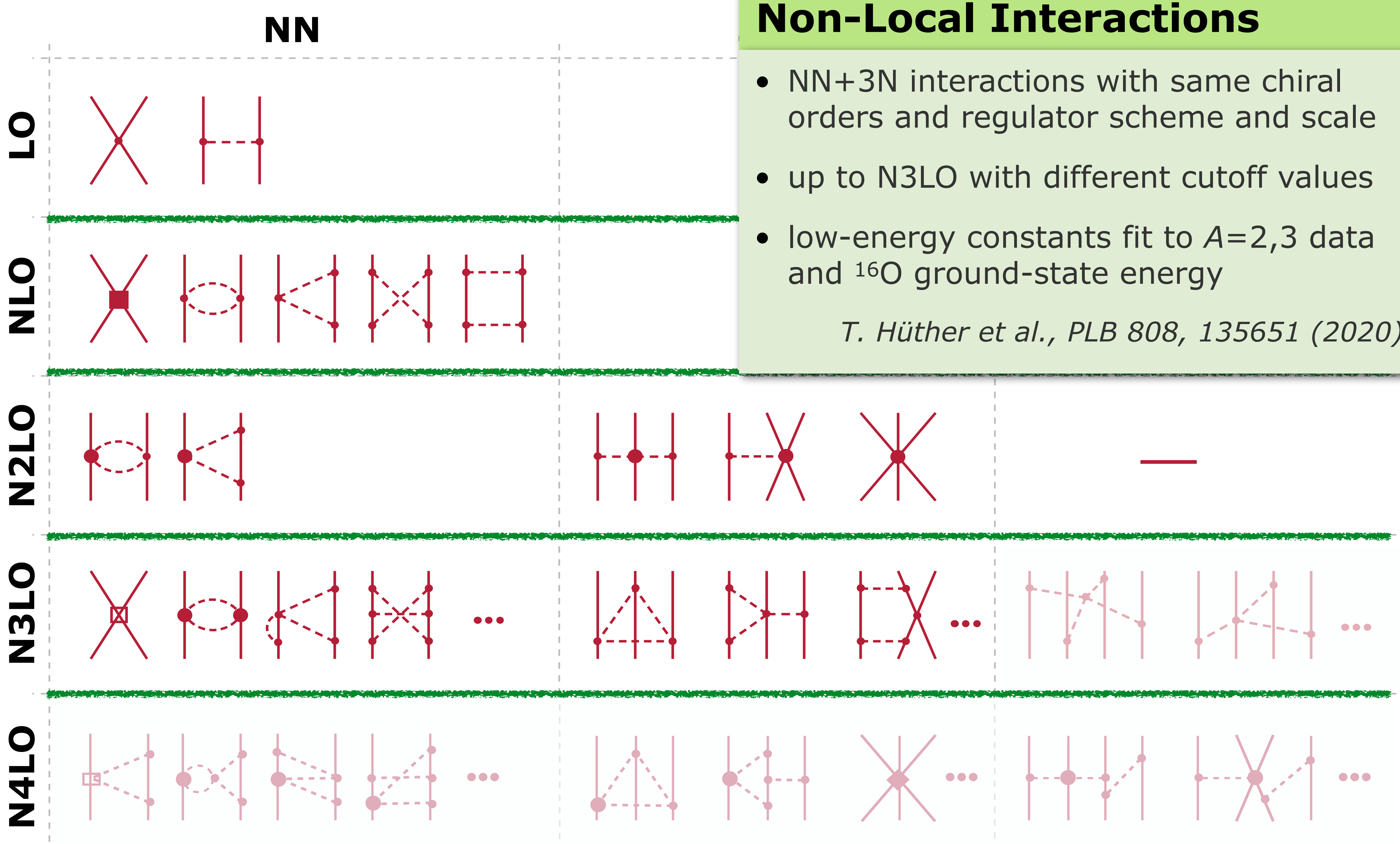
A05	B01	B04
halo nuclei nn system	electroweak transitions neutrino-matter interactions	electric dipole polarizability
inclusion of continuum resonance physics	multi-reference/deformation heavy nuclei	finite temperature arbitrary asymmetry

Uncertainty Quantification

Many-Body Tools

(Chiral) Effective Field Theory

Nuclear Interactions from Chiral EFT

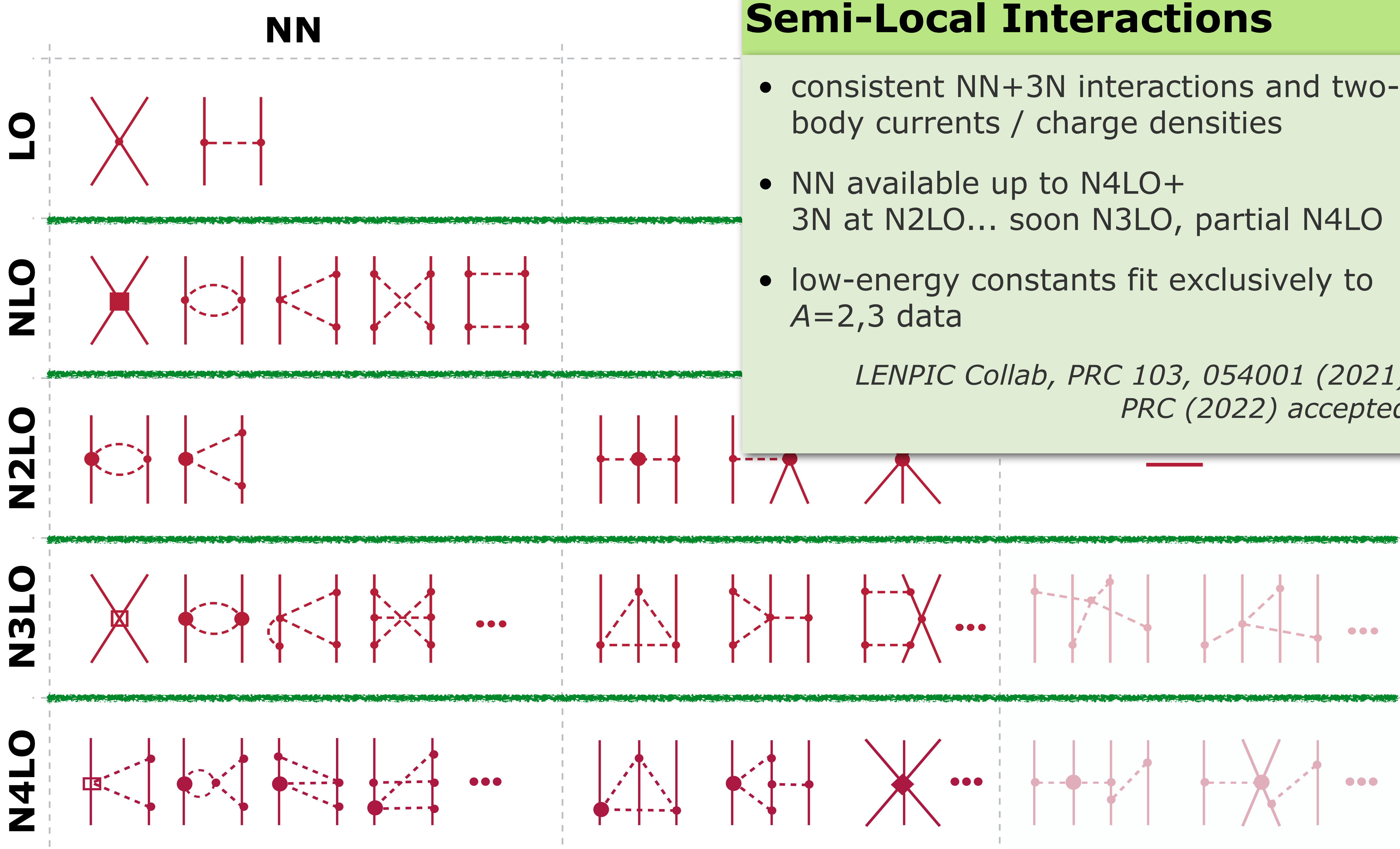


Non-Local Interactions

- NN+3N interactions with same chiral orders and regulator scheme and scale
- up to N3LO with different cutoff values
- low-energy constants fit to A=2,3 data and ^{16}O ground-state energy

T. Hüther et al., PLB 808, 135651 (2020)

Nuclear Interactions from Chiral EFT



Semi-Local Interactions

- consistent NN+3N interactions and two-body currents / charge densities
- NN available up to N4LO+
  3N at N2LO... soon N3LO, partial N4LO
- low-energy constants fit exclusively to *A*=2,3 data

LENPIC Collab, PRC 103, 054001 (2021)
PRC (2022) accepted

Uncertainty Quantification

all theory calculations are affected by systematic uncertainties (some also by statistical uncertainties)

in ab initio methods uncertainties result in a controlled way from truncations

variation of all truncation parameters gives access to systematic UQ

- **chiral EFT uncertainties**
  - assess convergence of observables in dependence of chiral … order
  - convergence affected by regulator scheme and sc…

use Bayesian methods to estimate size of omitted contributions based on known systematics

- **many-body uncertainties**
  - assess convergence of observables with model-space …
  - convergence affected by basis choice, truncation scheme, Hamiltonian

Many-Body Tools

A02	A04	B05

Few-Body Methods

Model / Configuration Interaction

e Shell Model

urbation Theory

Similarity Remormali

In-Medium Similarity Renormalization Group

Functional RG

all methods are computationally limited...

...

Many-Body Tools: Emulators

use emulators to circumvent computationally expensive many-body calculations

real many-body calculations provide the information needed for the construction of the emulator

- **eigenvector continuation for parameter variations**
  - use tiny but highly problem-adapted basis set extracted from full many-body solution (eigenvectors)
  - powerful tool for large-scale parameter variations, e.g. for LEC fitting
- **artificial neural networks for model-space extrapolation**
  - train ANN to predict converged observables based on sequences of non-converged many-body calculations
  - provides robust "extrapolations" with statistically sound uncertainties

. . .

Just one specific example...

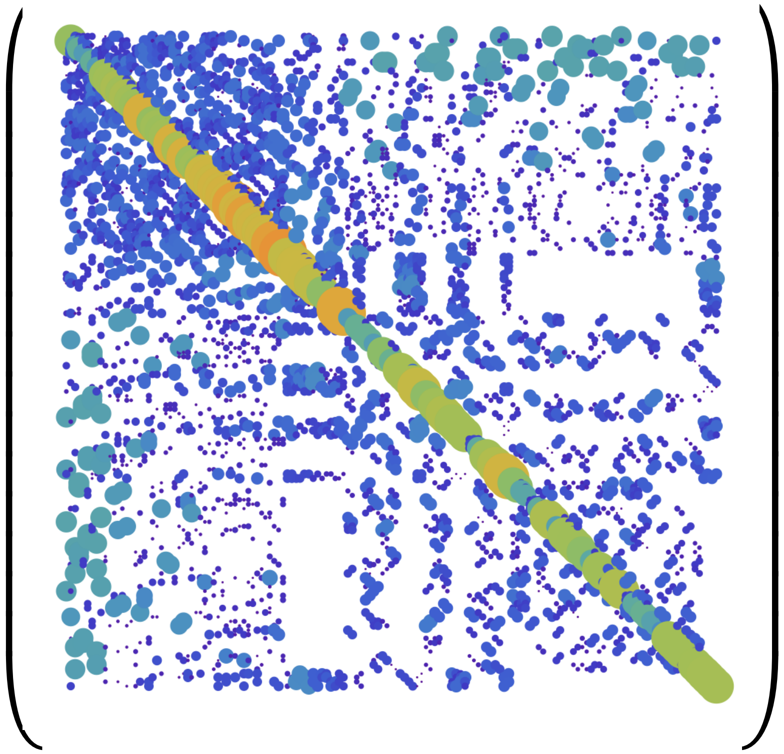
A04: In-Medium NCSM Study of Neon Isotopes

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Nogga, Roth,...

no-core shell model is
universal and powerful ab initio approach for
light nuclei (up to A≈25)

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$



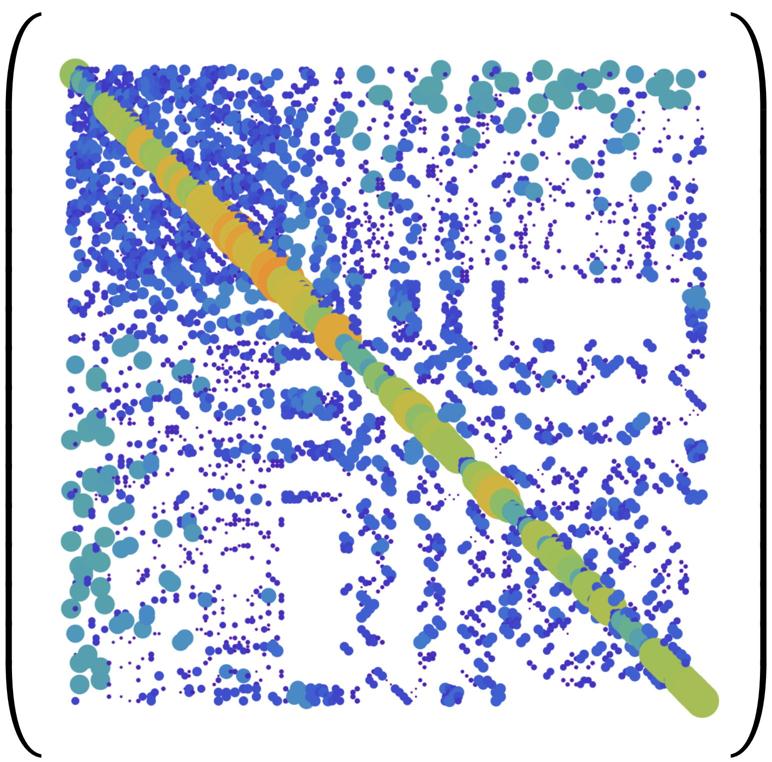
$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

Multi-Reference In-Medium SRG

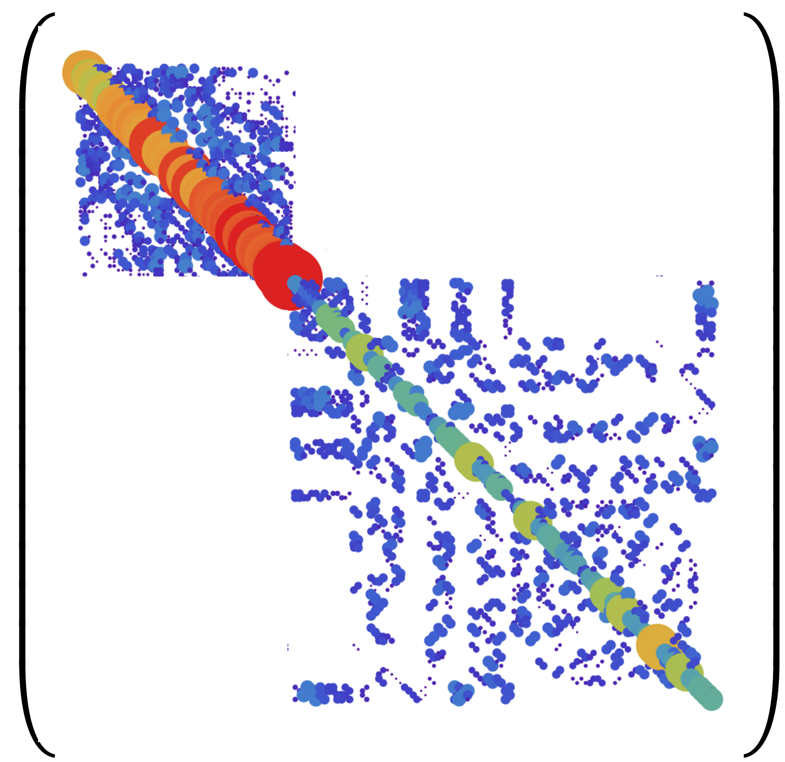
Hergert, Gebrerufael, Vobig, Mongelli, Roth,…

decouple reference state from excitations by a unitary transformation of Hamiltonian and other operators

- **idea**: use multi-reference formulation of IM-SRG to decouple reference space for rest of model space, i.e., block diagonalize *A*-body Hamiltonian



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]$$



In-Medium NCSM

NCSM
reference state

- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- access to all open-shell nuclei and systematically improvable

MR-IM-SRG
decoupling

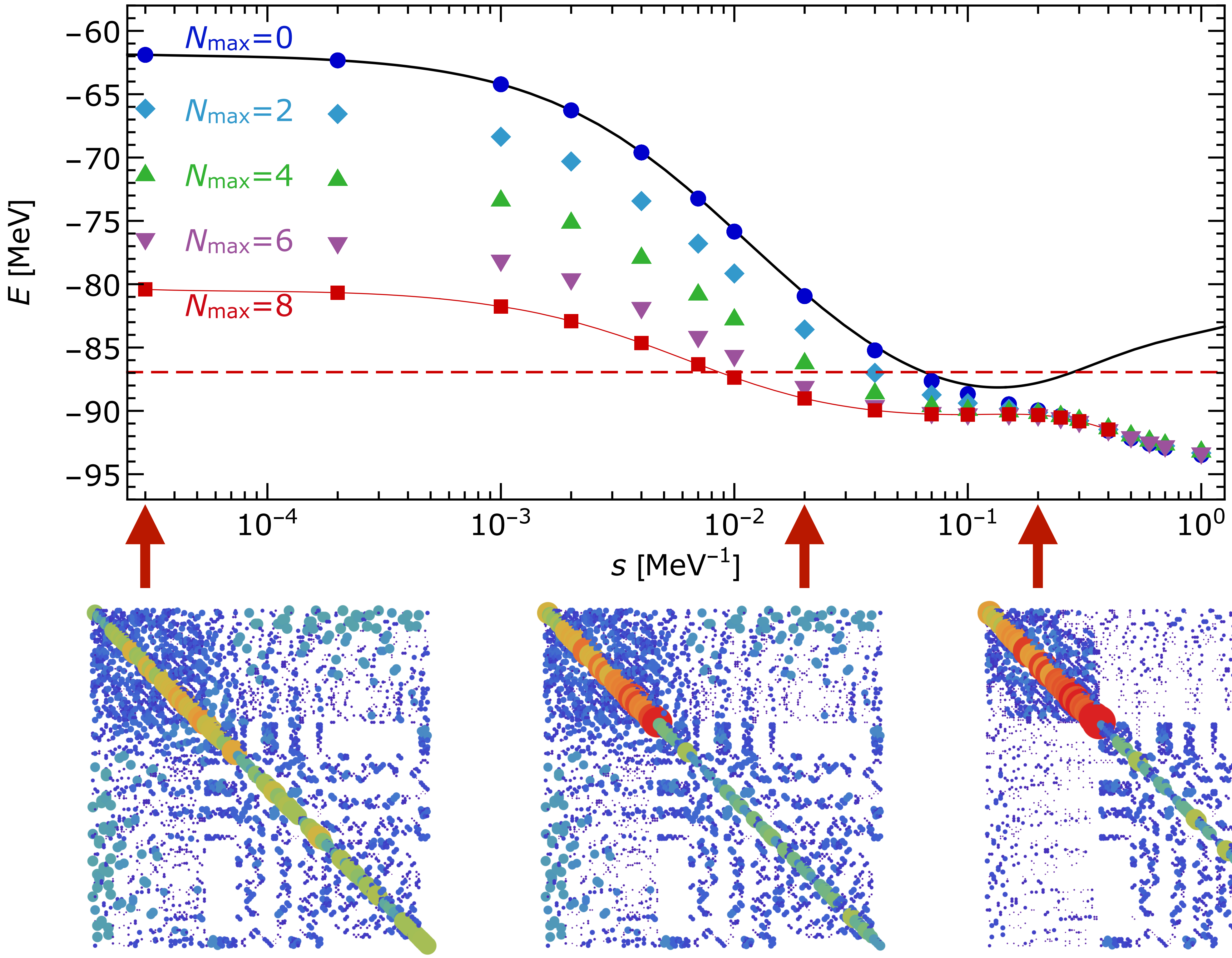
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian and other operators
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

NCSM
many-body solution

- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium NCSM: Flow Evolution

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

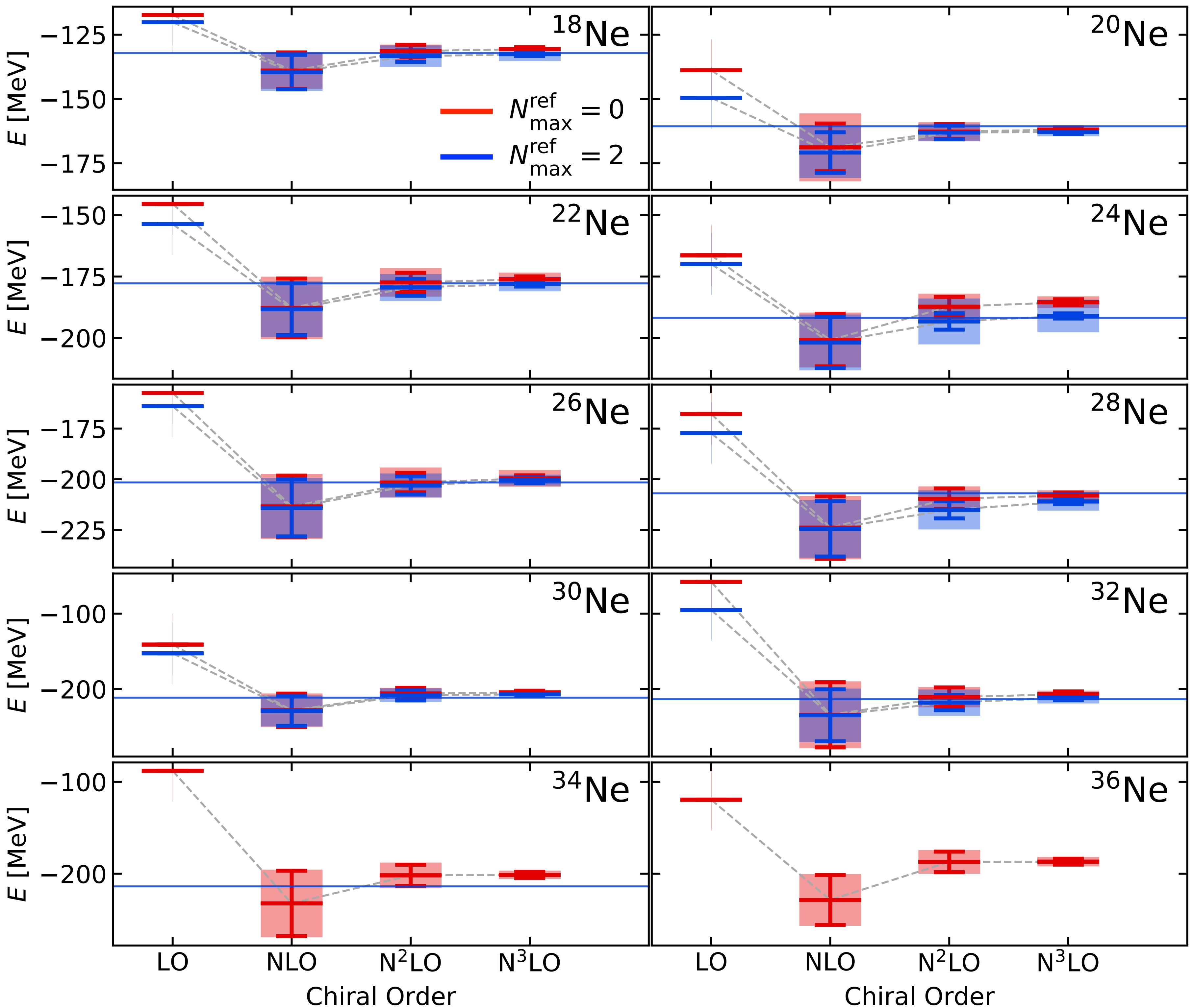
e_{max}=12

N_{max}=0 reference HF basis

Hamilton matrix in N_{max}=2 space

Neon Isotopes: Ground-State Energies

Mongelli et al., in preparation



- amazing reproduction of experimental energies for all isotopes
- uncertainties under control

family of
non-local NN+3N interactions
T. Hüther et al., PLB 808, 135651 (2020)

Λ = 500 MeV
α = 0.04 fm^4
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

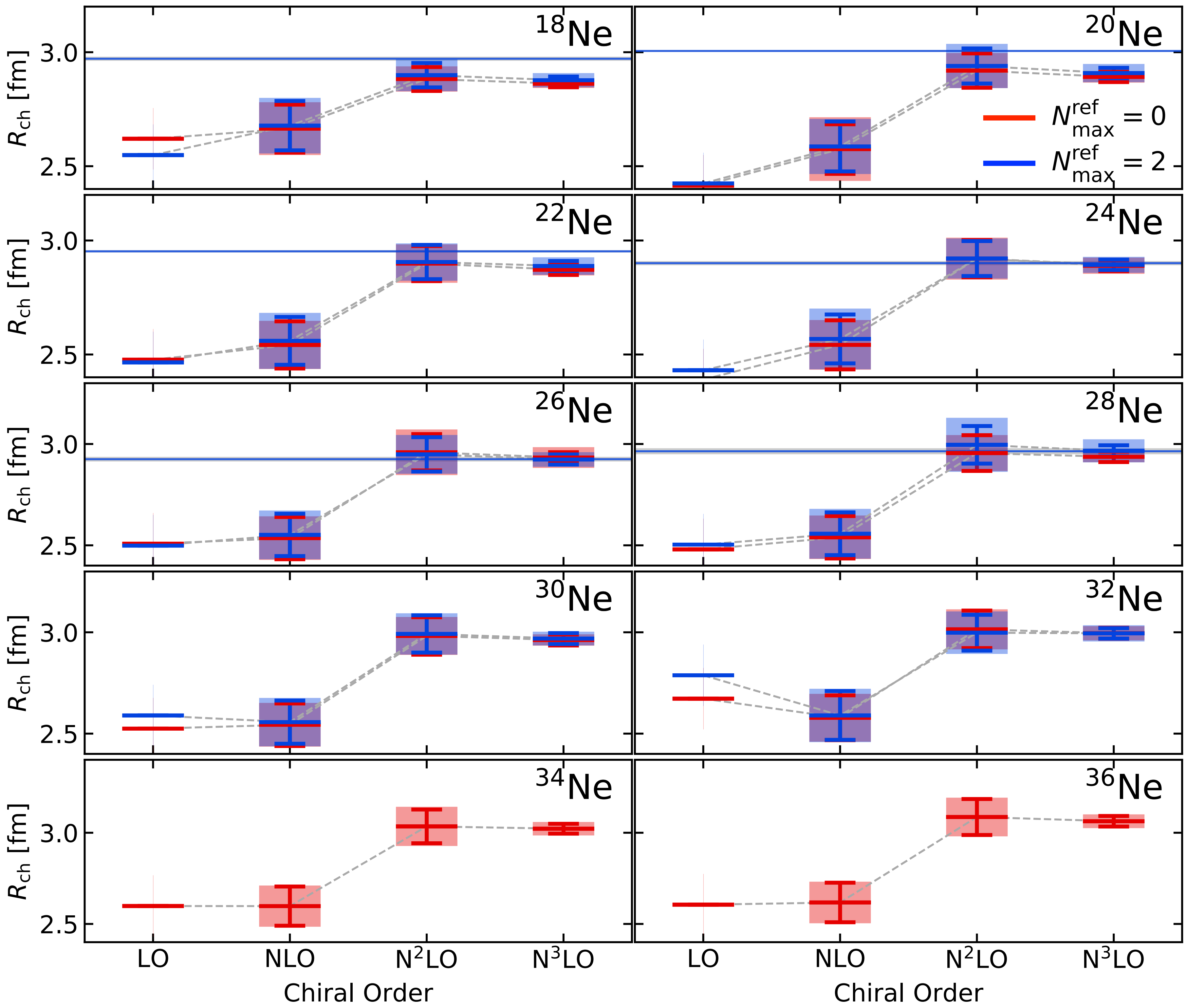
$N^{ref}_{max} = 0, 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

Neon Isotopes: Charge Radii

Mongelli et al., in preparation



- excellent description of radii, slight underestimation for light isotopes
- stable results in N²LO and N³LO

family of non-local NN+3N interactions
T. Hüther et al., PLB 808, 135651 (2020)

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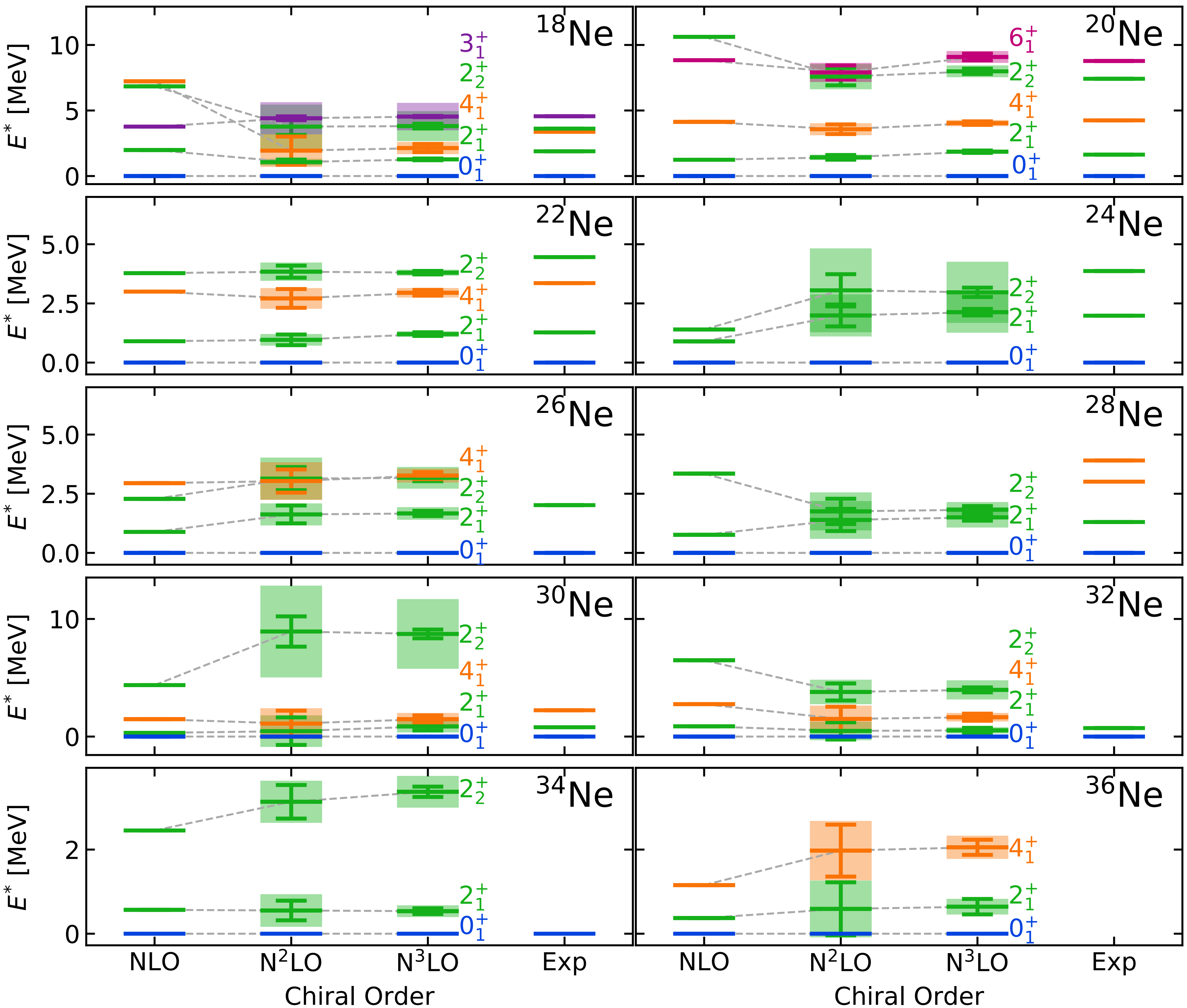
Neon Isotopes: Excitation Energies

Mongelli et al., in preparation



- excellent description of excitation spectra

family of non-local NN+3N interactions
T. Hüther et al., PLB 808, 135651 (2020)

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Following Talks

A02	A04	B05
Sebastian Dietz - *Energy distribution of ^3n systems*	Takayuki Miyagi - *Heavy-mass frontier in nuclear ab initio calculations*	Jonas Keller - *Nuclear EOS for arbitrary proton fraction and temperature*
Tobias Wolfgruber - *From chiral interactions to NCSM observables*		Andreas Geissel - *Towards the EOS of neutron stars*
Julius Müller - *First results from the Gamow-NCSM*		