Light-ion reaction calculations from first principles

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LLNL-PRES- 817357

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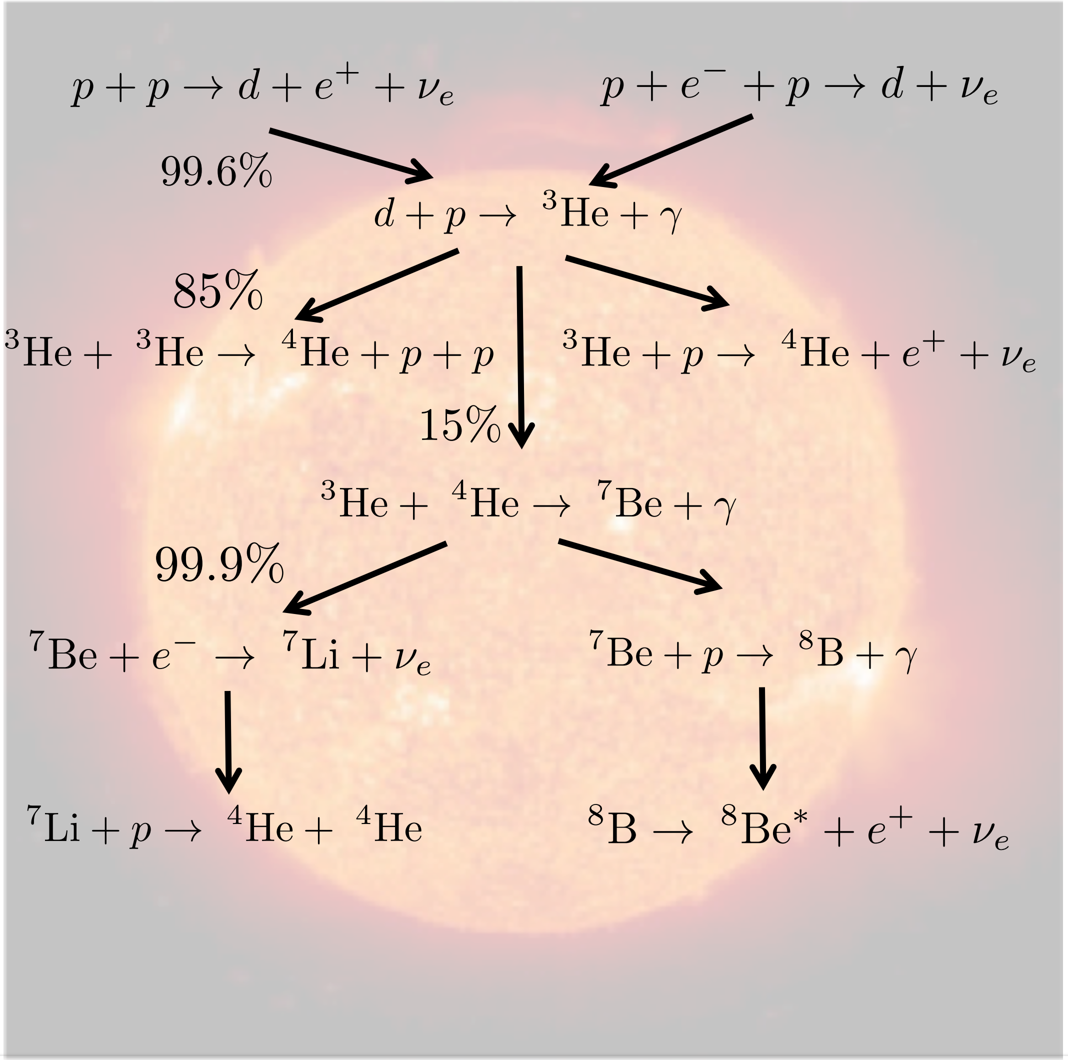
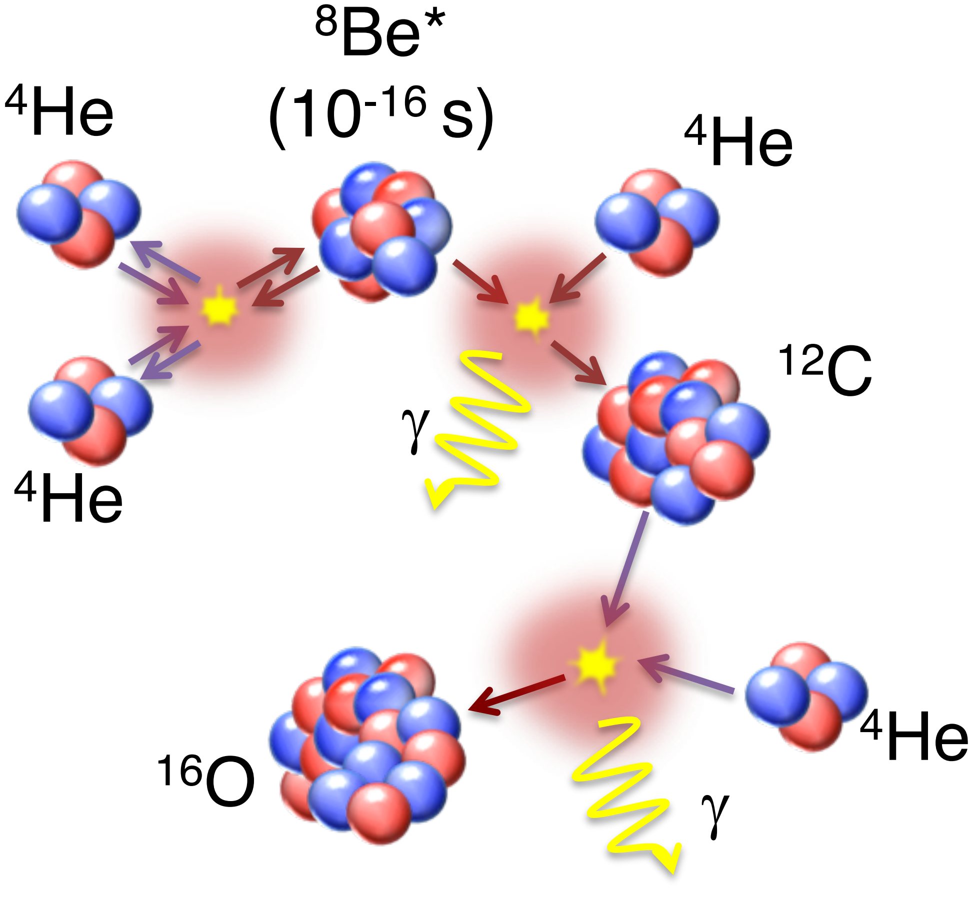
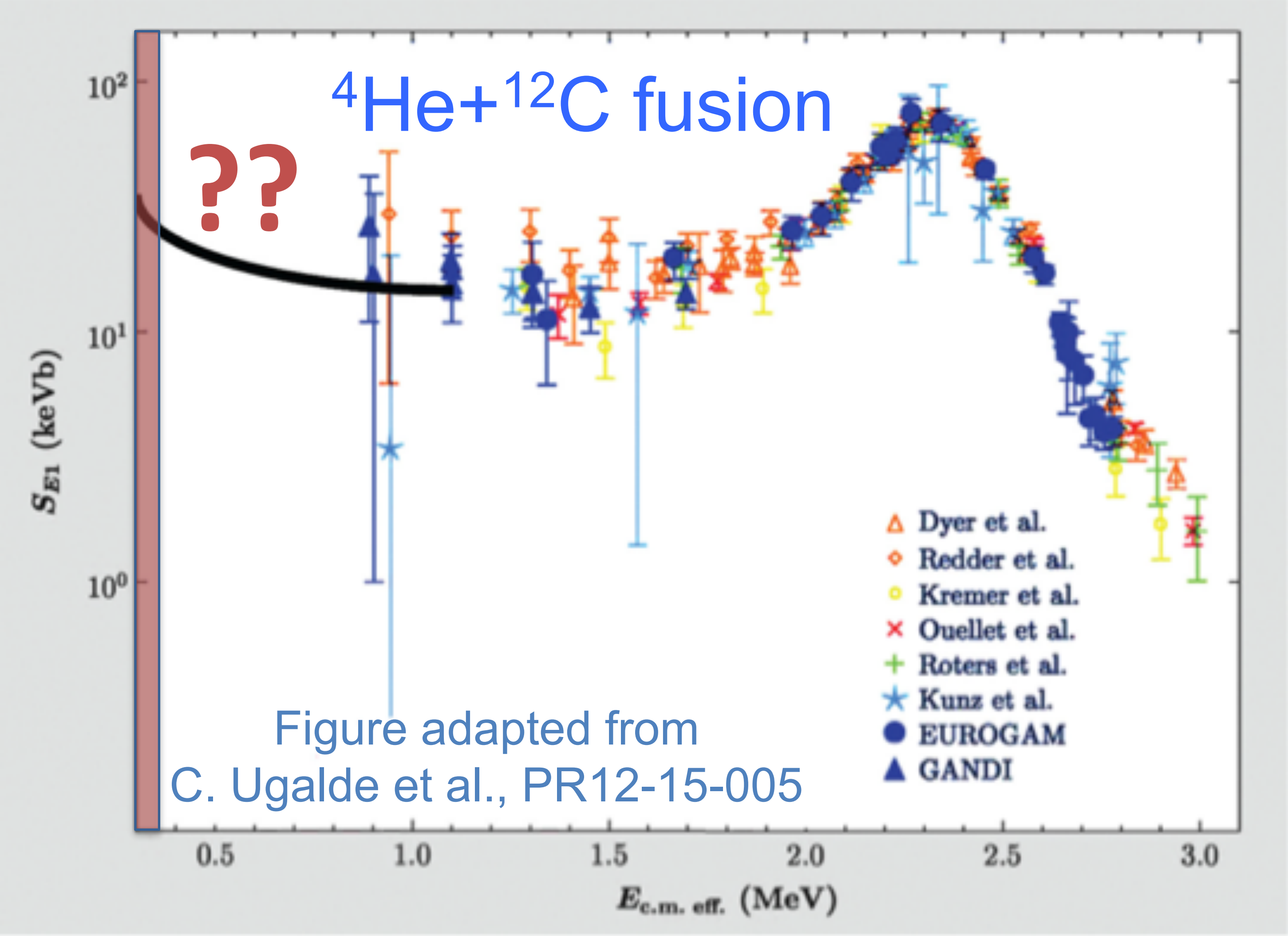
Light-ion reactions in stellar interiors.



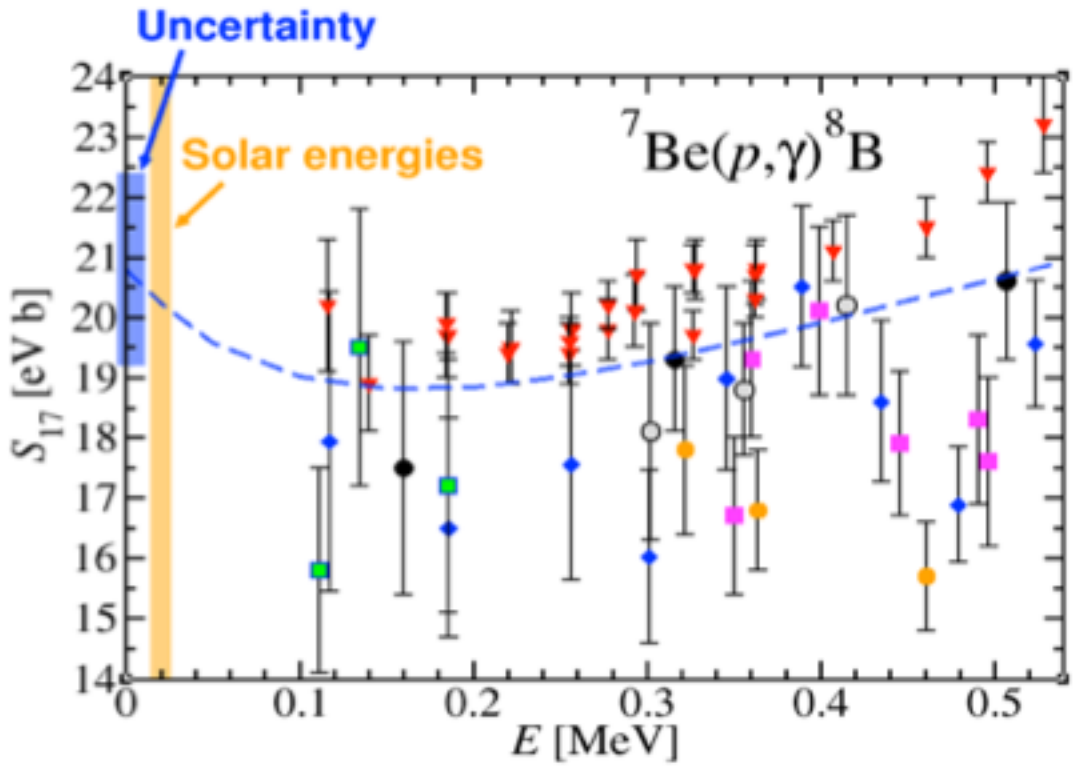


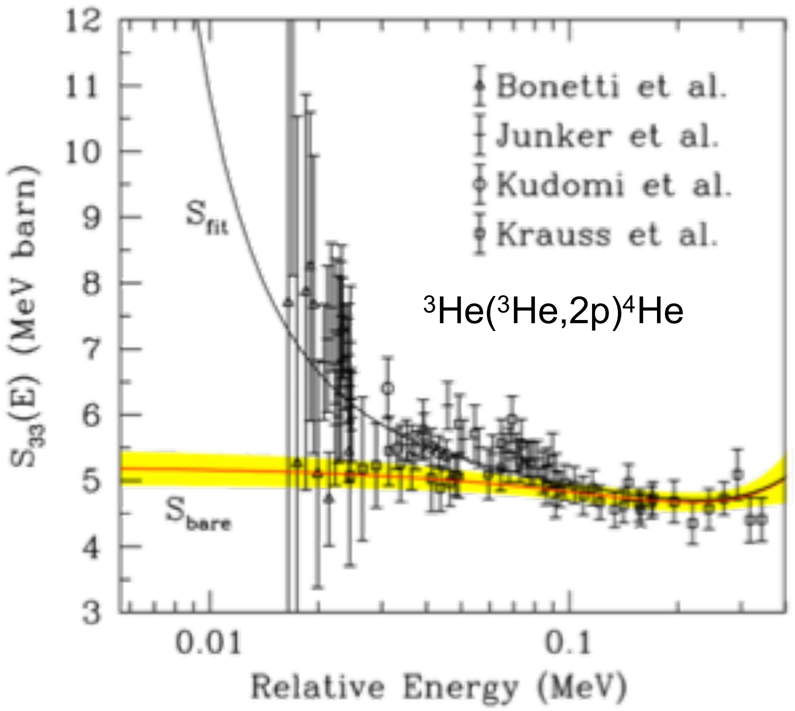
We need reliable theory to estimate the S-factor at stellar energies

- Direct measurements at 300 keV (helium burning conditions) so far impossible
- Major hurdle in precisely determining carbon-to-oxygen ratio produced in stars, introduces large uncertainties in stellar-evolution models and in the predictions of stellar nucleosynthesis

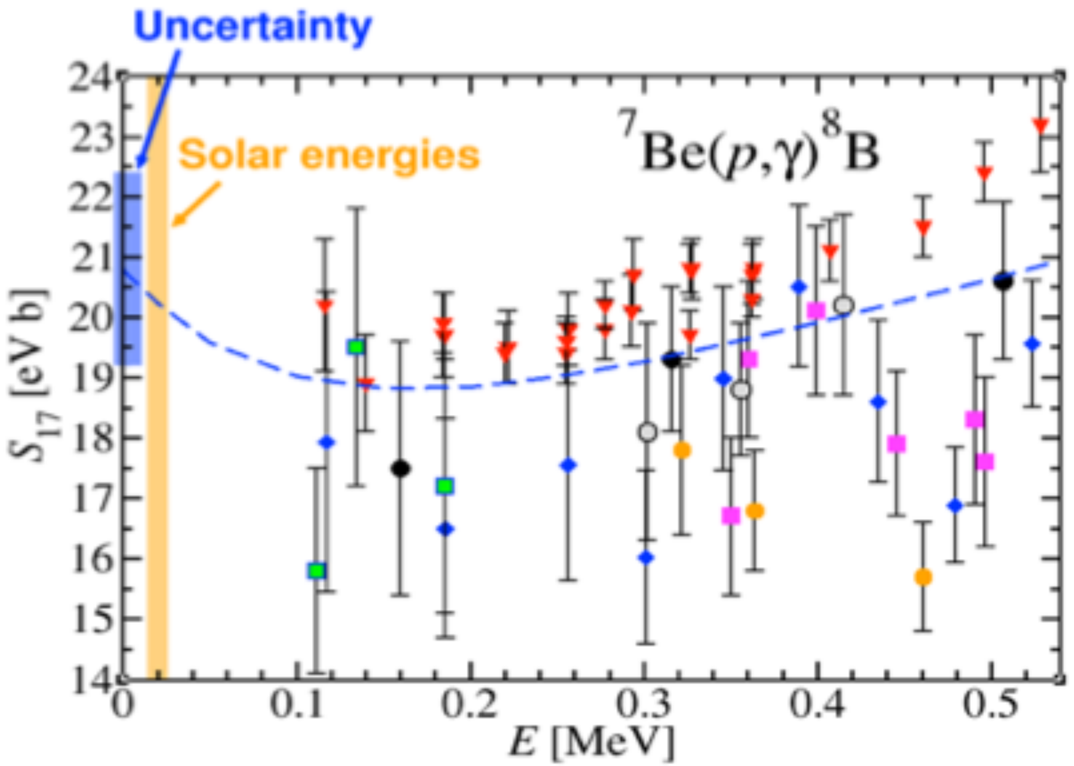


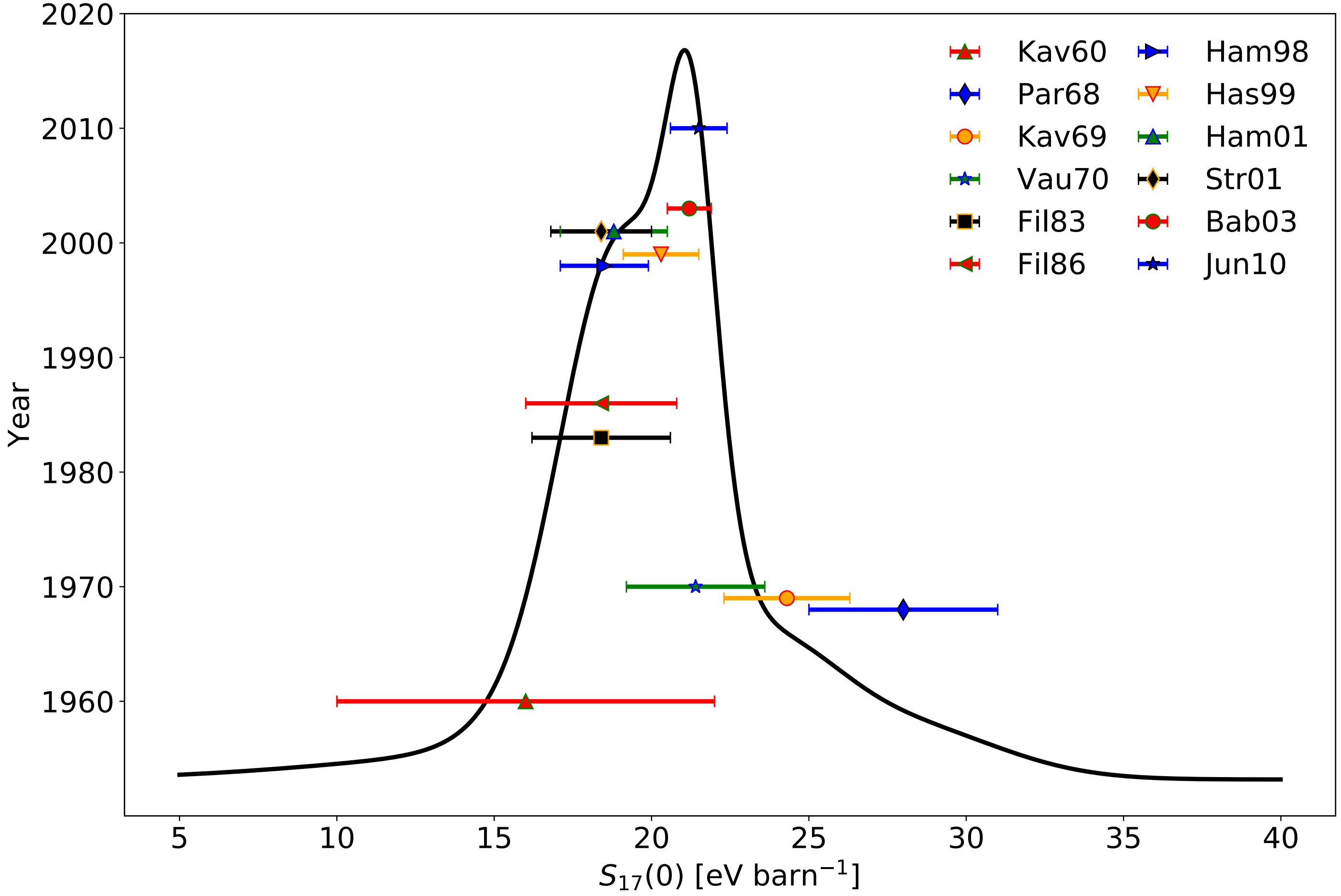
Low-energy charged-particle cross section measurements are nigh impossible



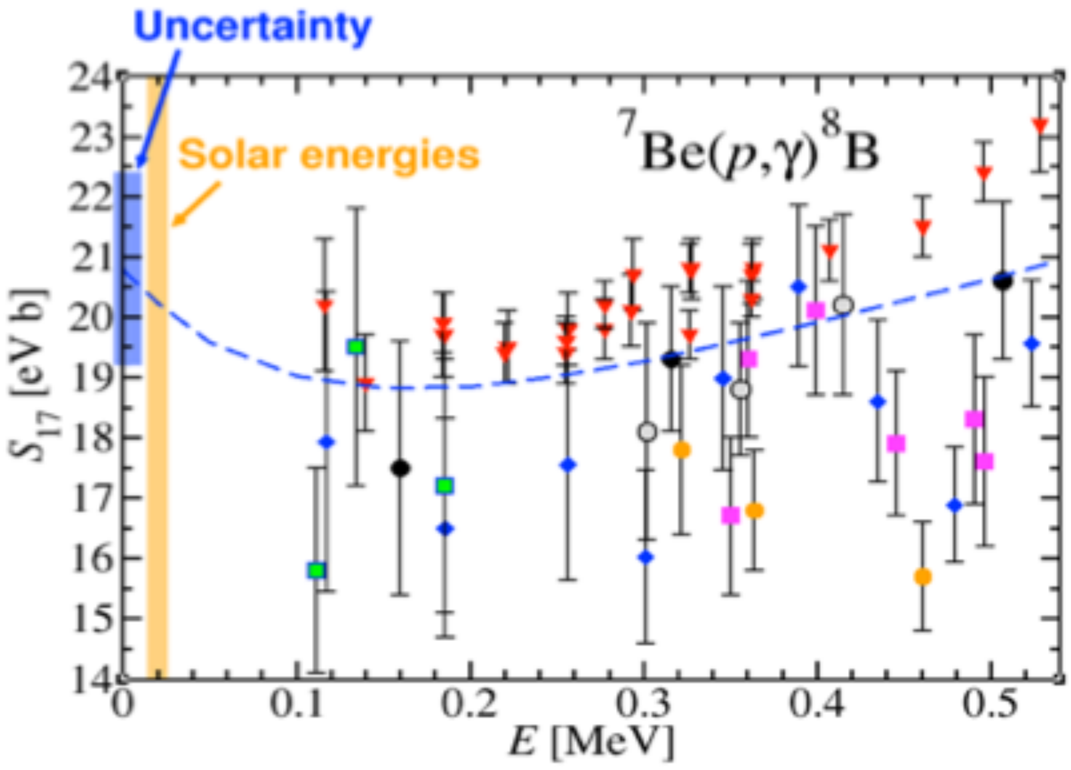


Experiments are getting more precise

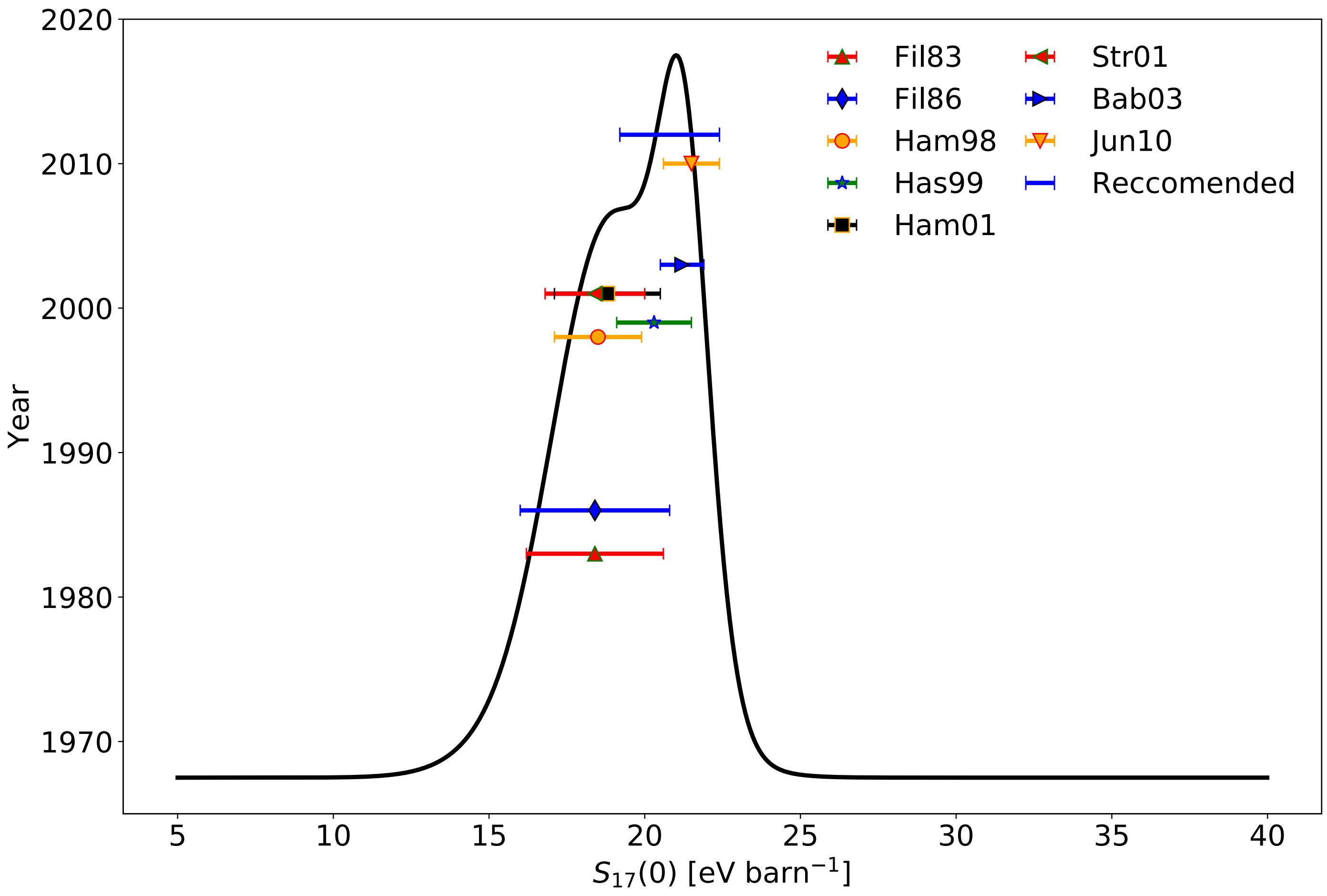




Caveats when blindly fitting to experimental data: single data set with multiple points and small error bars dominates fit.



Recommended value: Rev. Mod. Phys. **83**, 195



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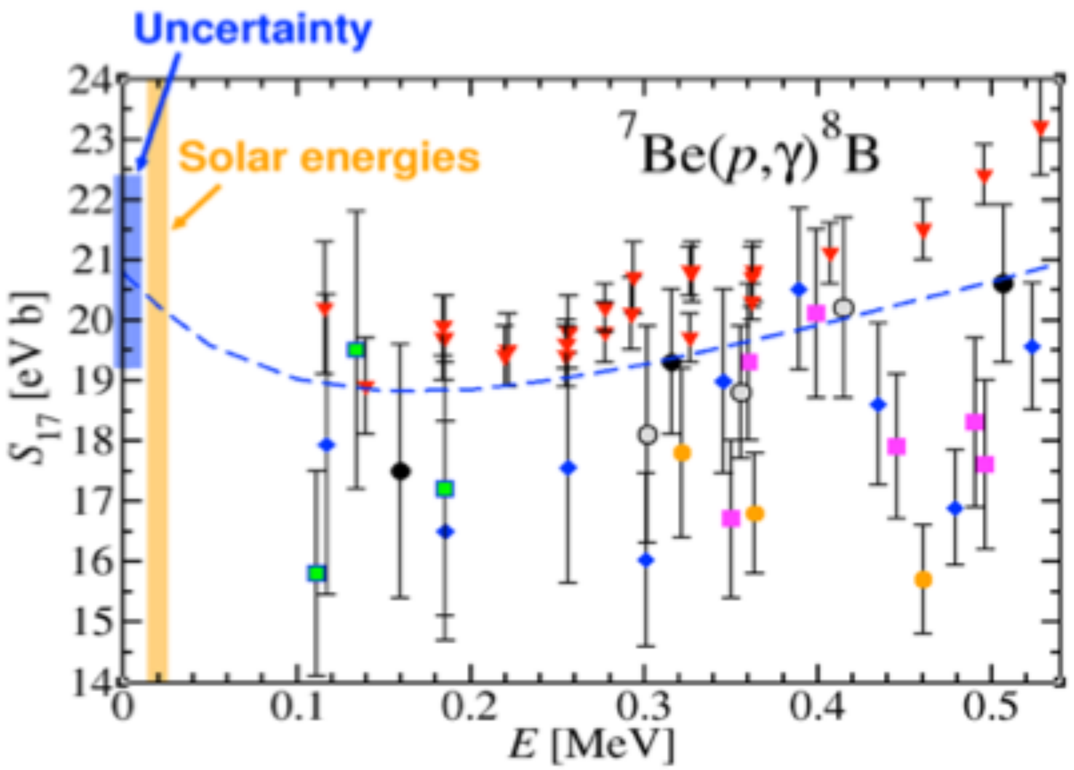
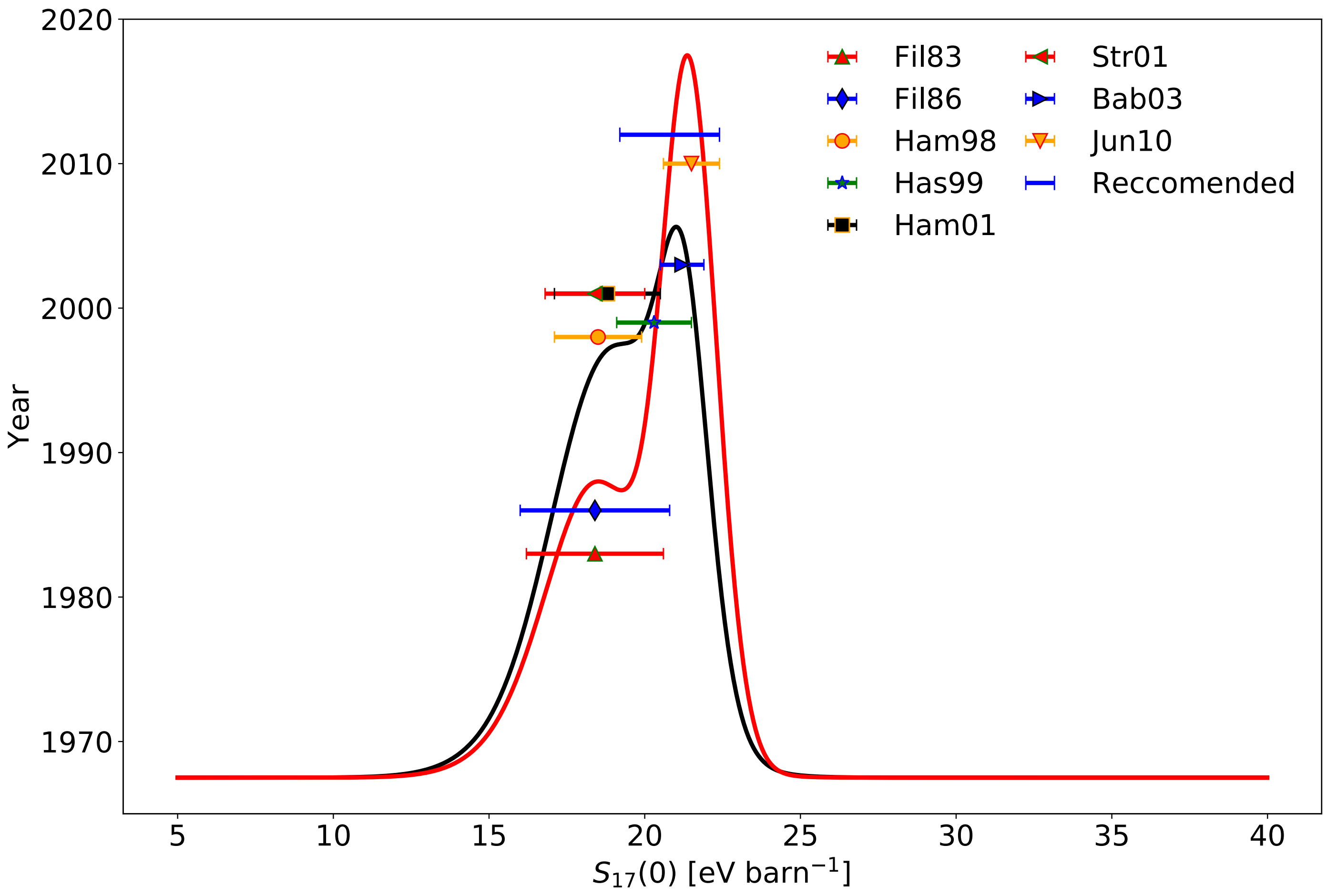


$$\chi^2 = \sum_i \frac{\left(O_i^{\mathrm{th}} - O_i^{\mathrm{exp}}\right)^2}{\sigma_i^2}$$



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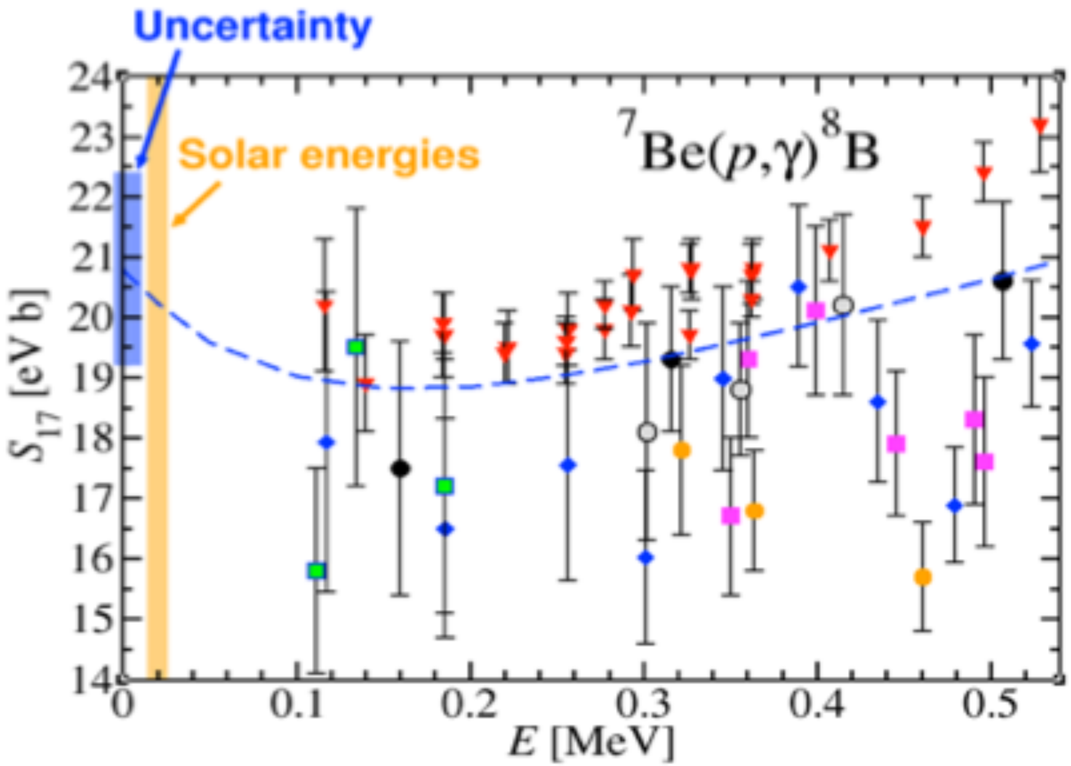

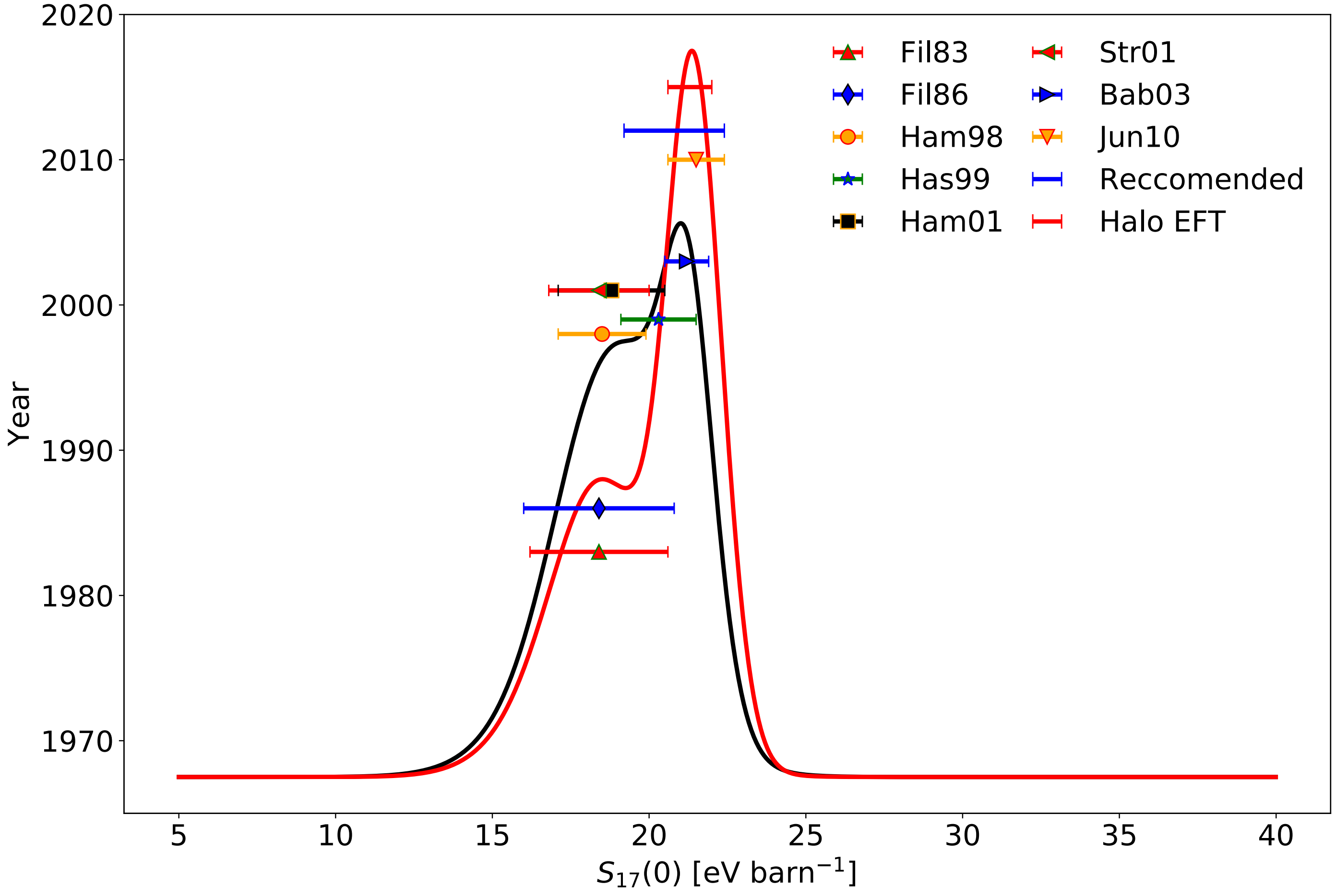

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Halo EFT: Phys. Lett. B **751**, 535-540 (2015)

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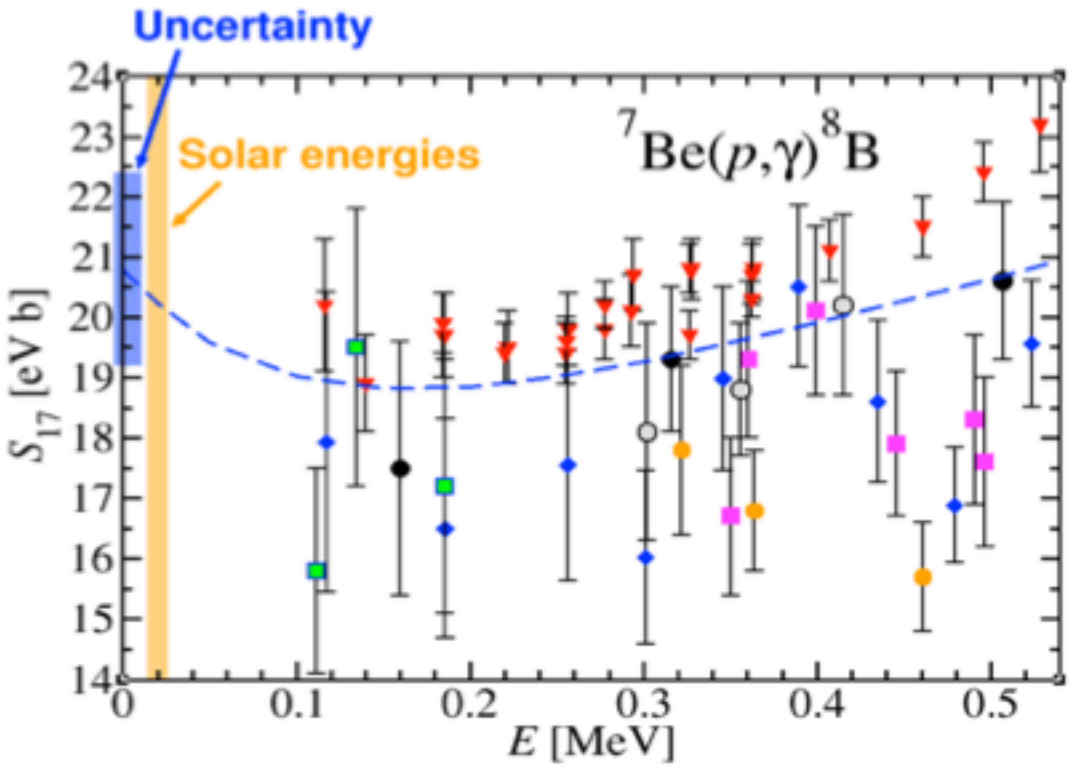

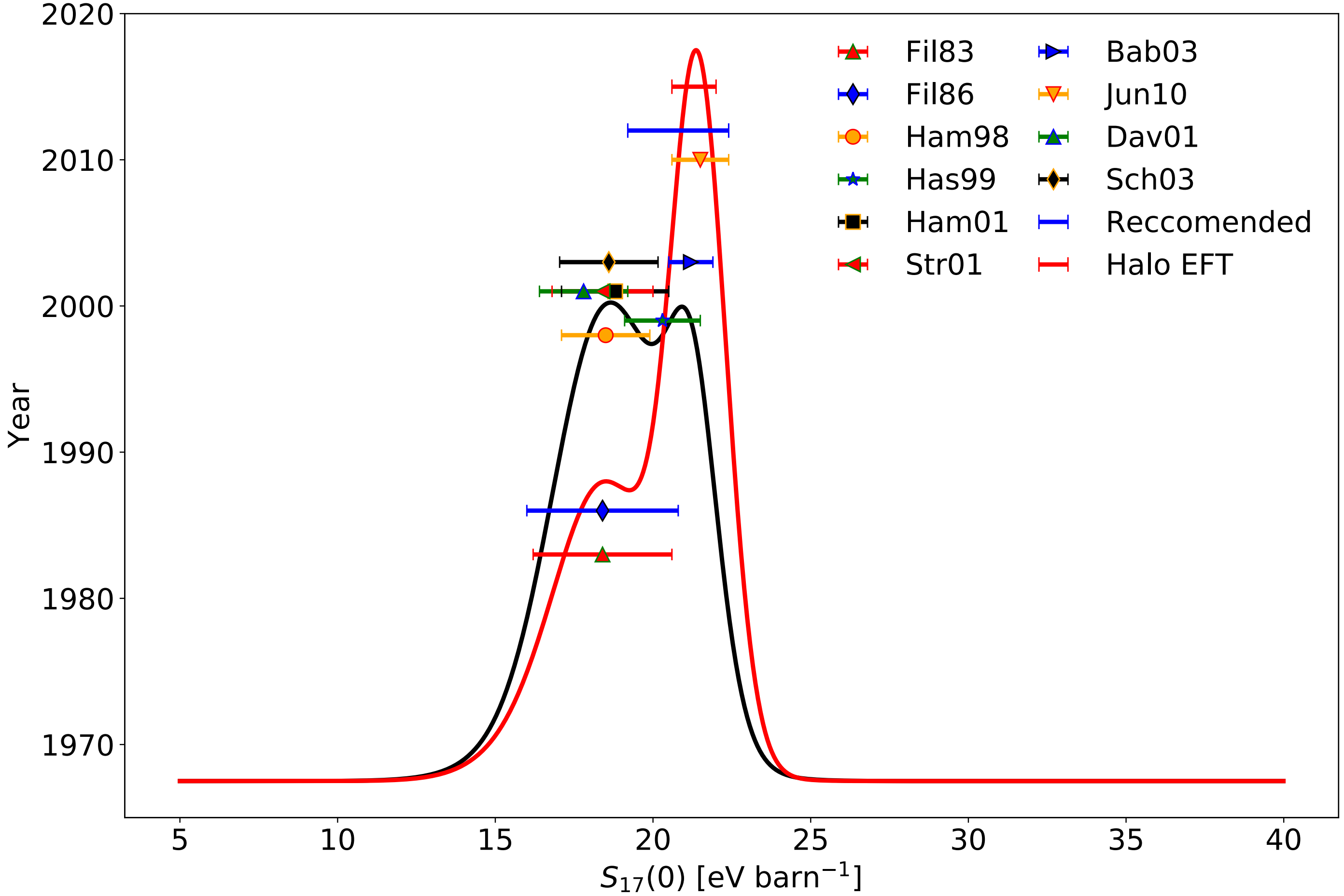

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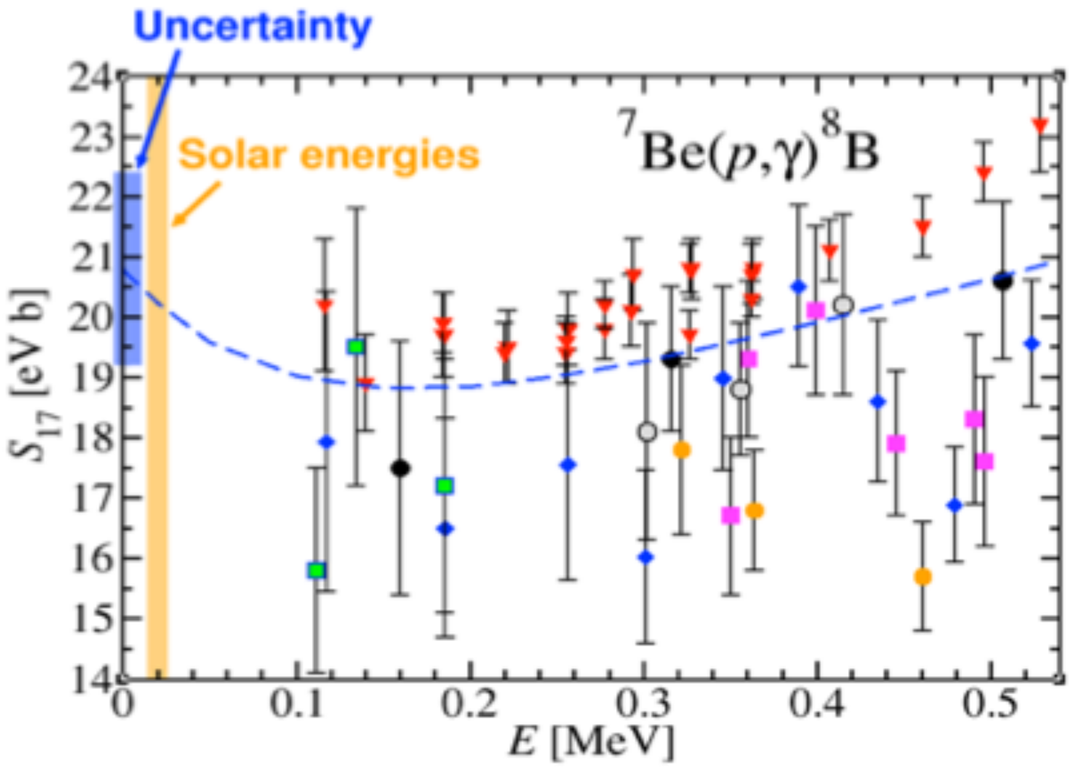

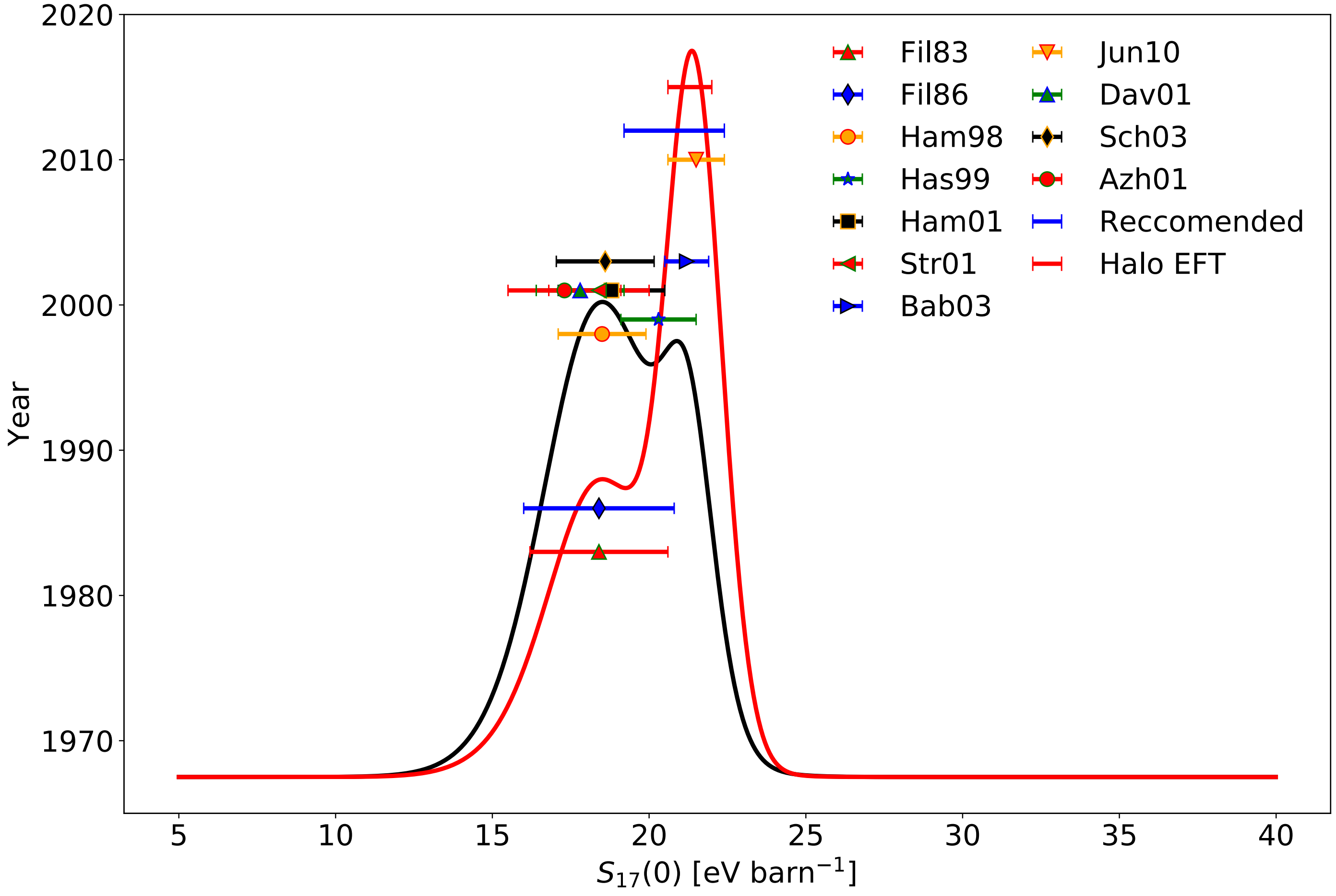

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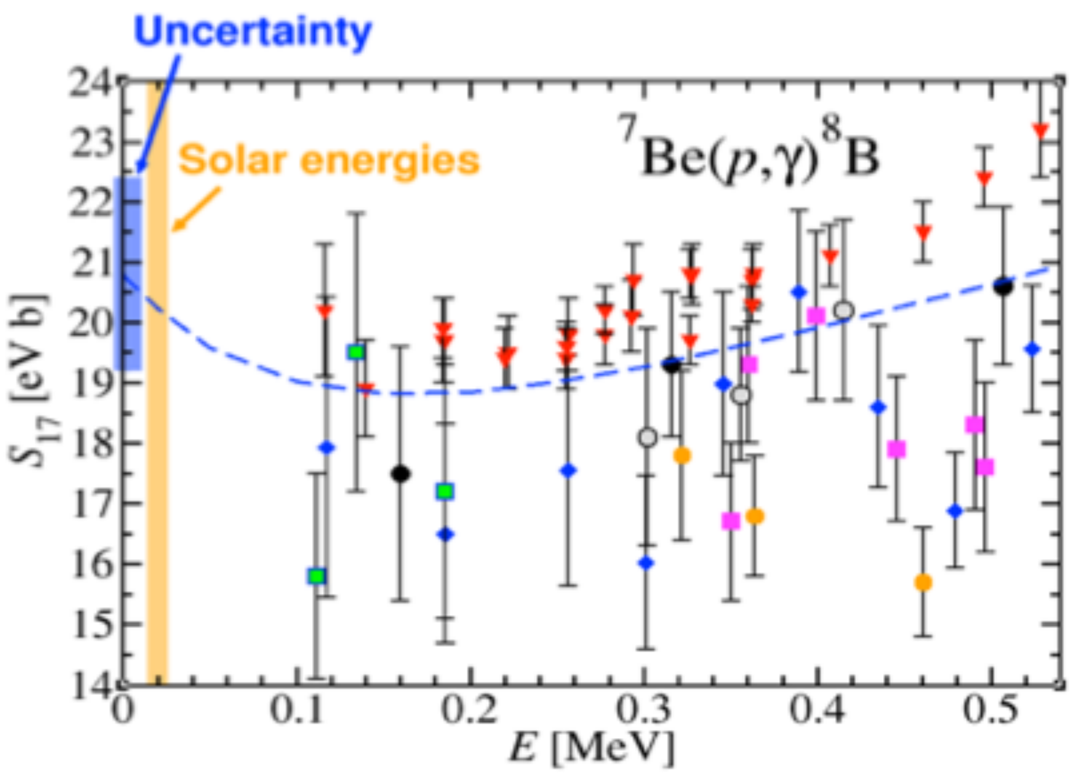

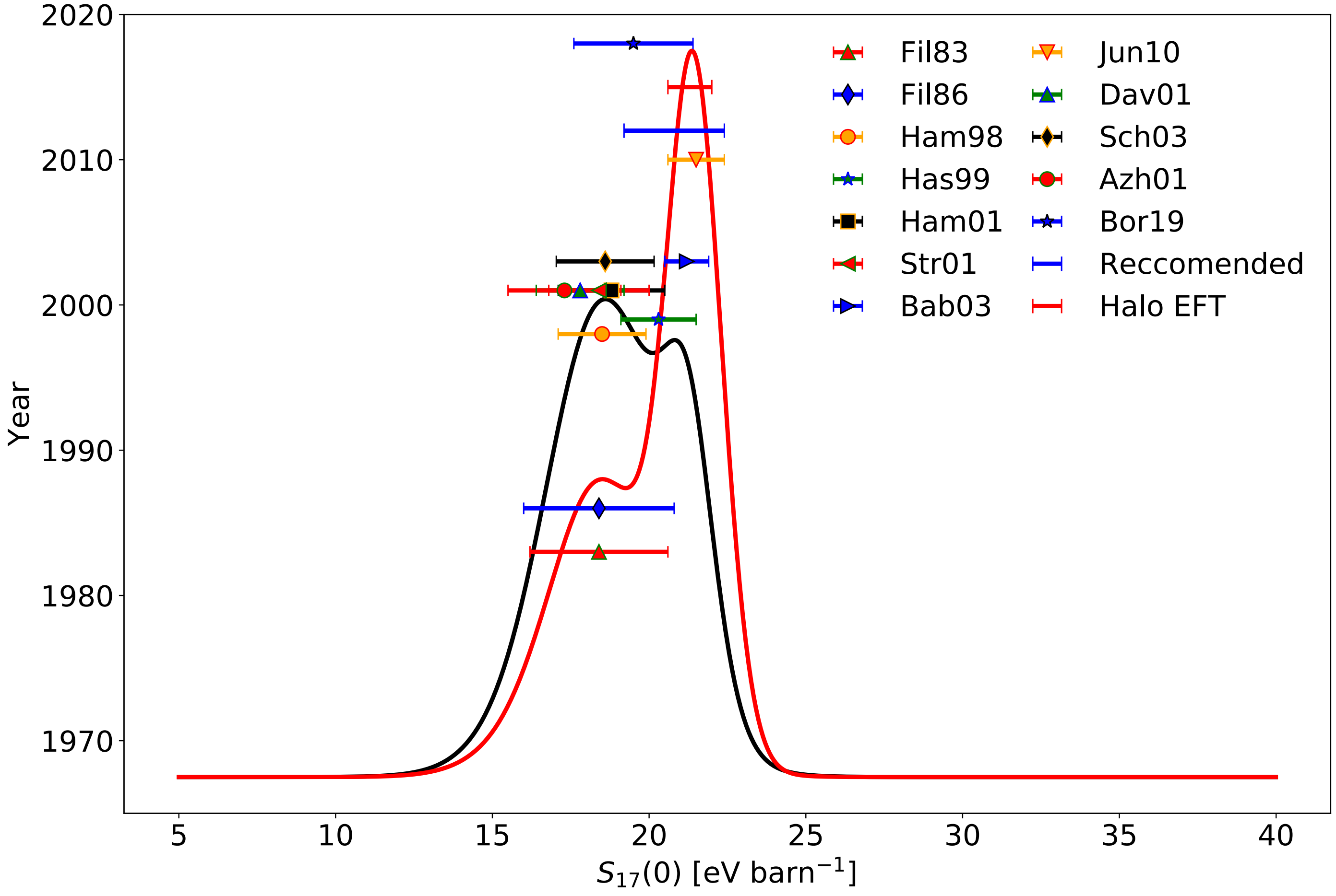

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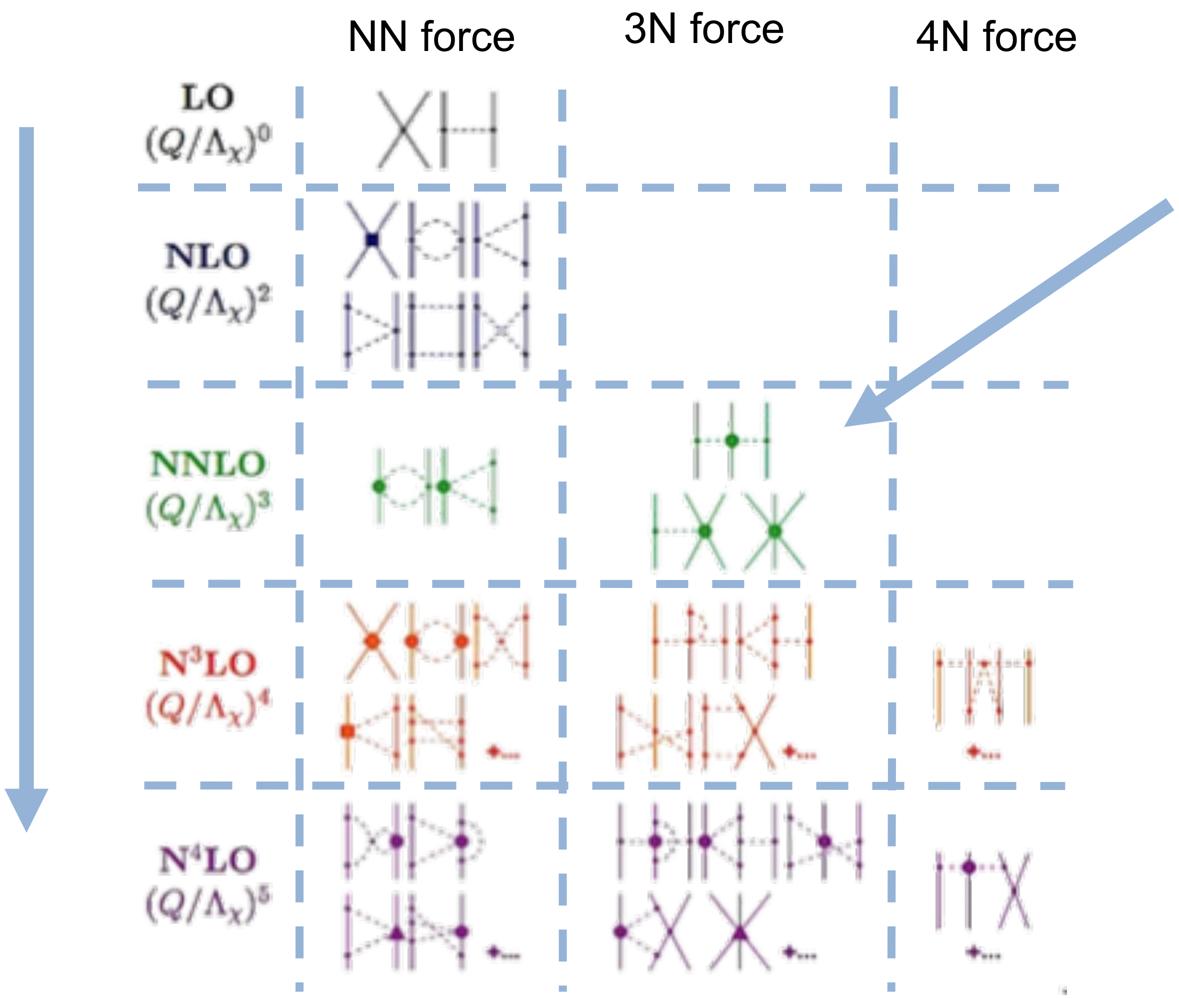
Halo EFT: Phys. Lett. B **751**, 535-540 (2015)

Ab initio nuclear reaction theory can provide predictions without fitting directly to experimental data*

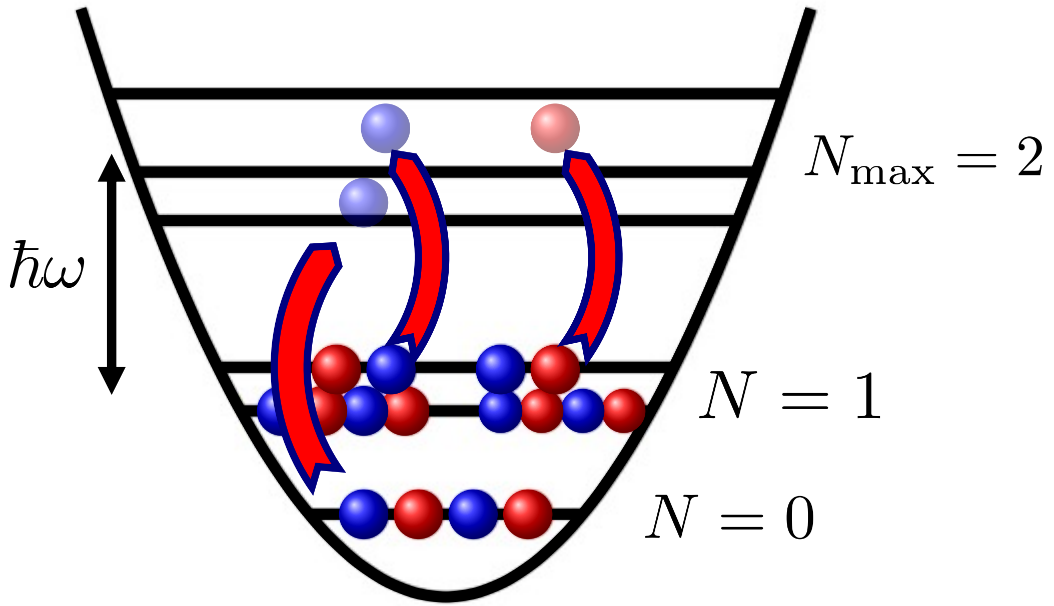
Systematic expansion of the nuclear force means quantifiable uncertainties!



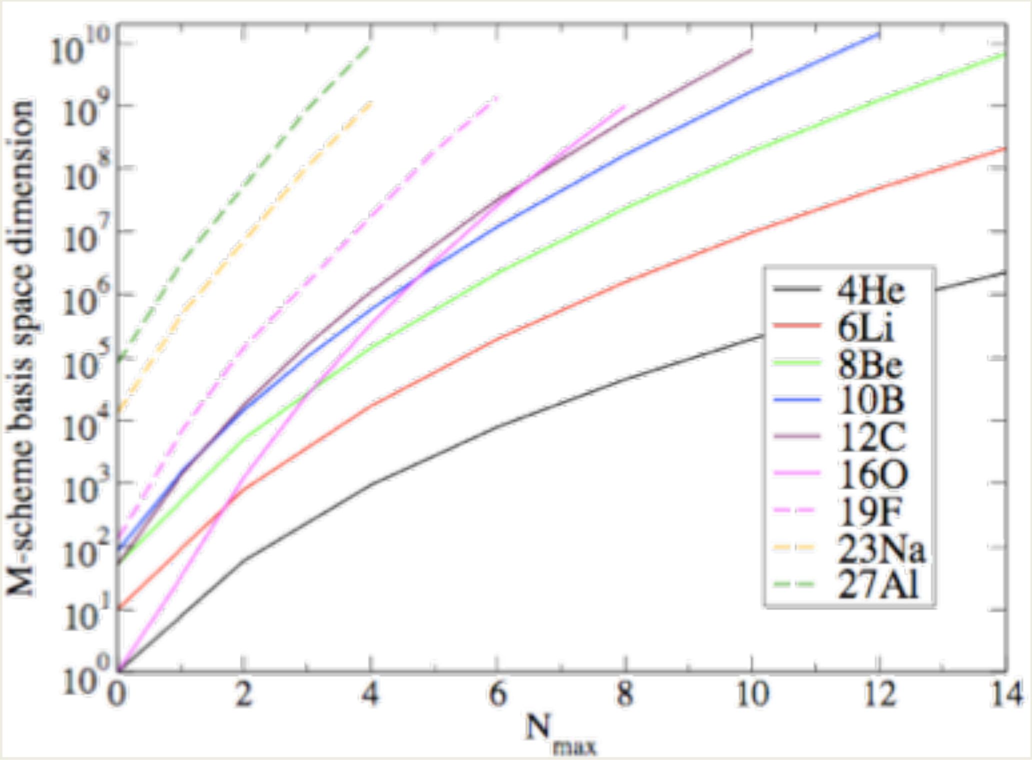
Few diagrams means few parameters that must be constrained from experiments.

Many-nucleon forces appear organically.

For a complete ab initio description we need both structure…

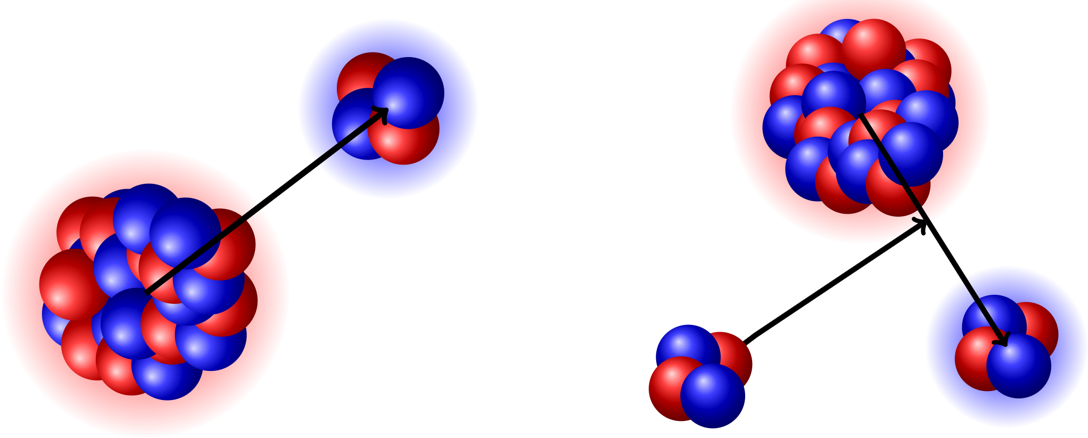


Configuration Interaction
No Core Shell Model (NCSM)



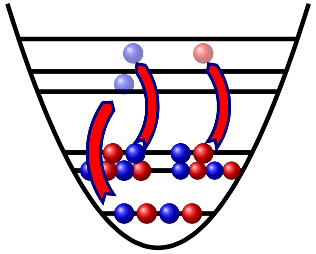
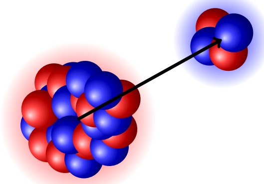
… and dynamical clustered descriptions

- The CI picture is no longer sufficient to describe the many-body system.



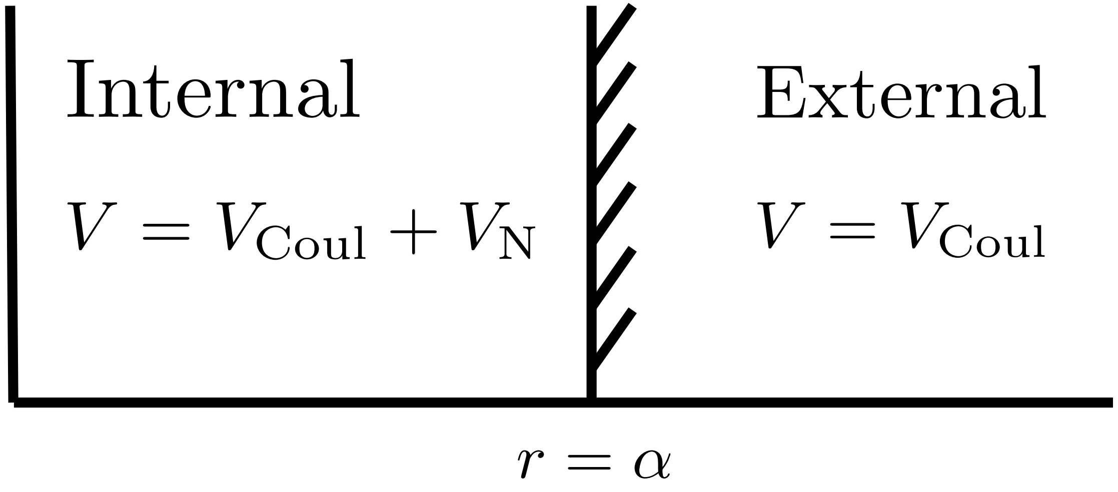
Discrete structure information input

Continuous dynamical input (clustering/reactions)

$$\Psi = \sum_{\lambda} c_{\lambda} |$$

$$\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) |$$

$$\rangle$$

Solving for the unknowns with the R-Matrix.

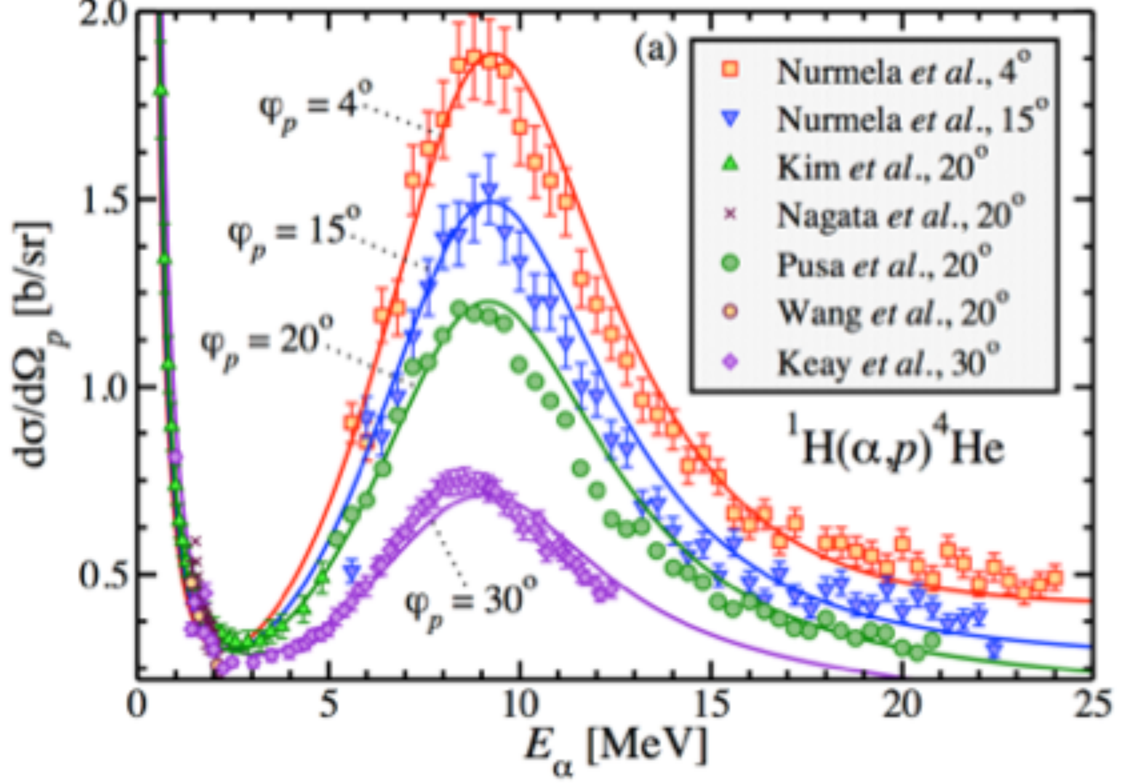
$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{PP}} & \mathcal{H}^{(0)}_{\mathcal{PQ}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{QP}} & \mathcal{H}^{(0)}_{\mathcal{QQ}} \end{array}\right)$$



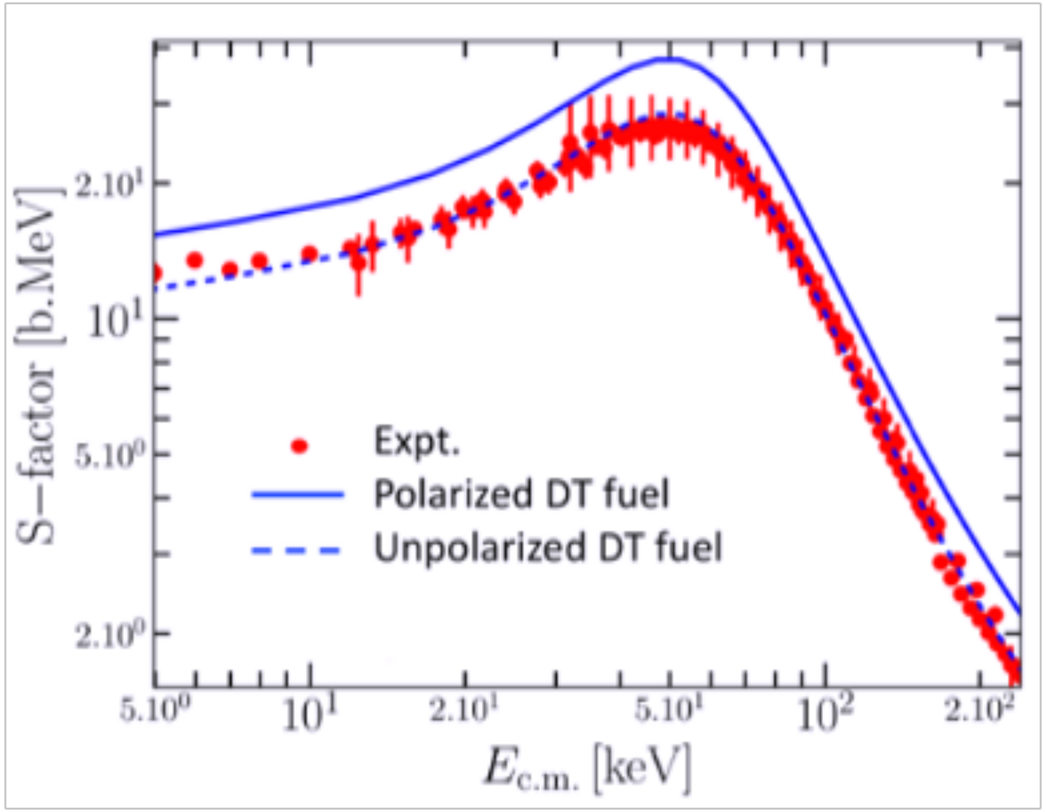
- Need to re-construct the interaction potential seen by the two fragment nuclei.
- Internal P-space Hamiltonian contains interaction potential
- External Q-space only has free components $T + V_{\mathrm{Coul}}$

Can we make accurate predictions?
Proton elastic scattering on ^{4}He and DT fusion

PRC 90, 061601(R)



Nature Comm. 10, 351 (2019)

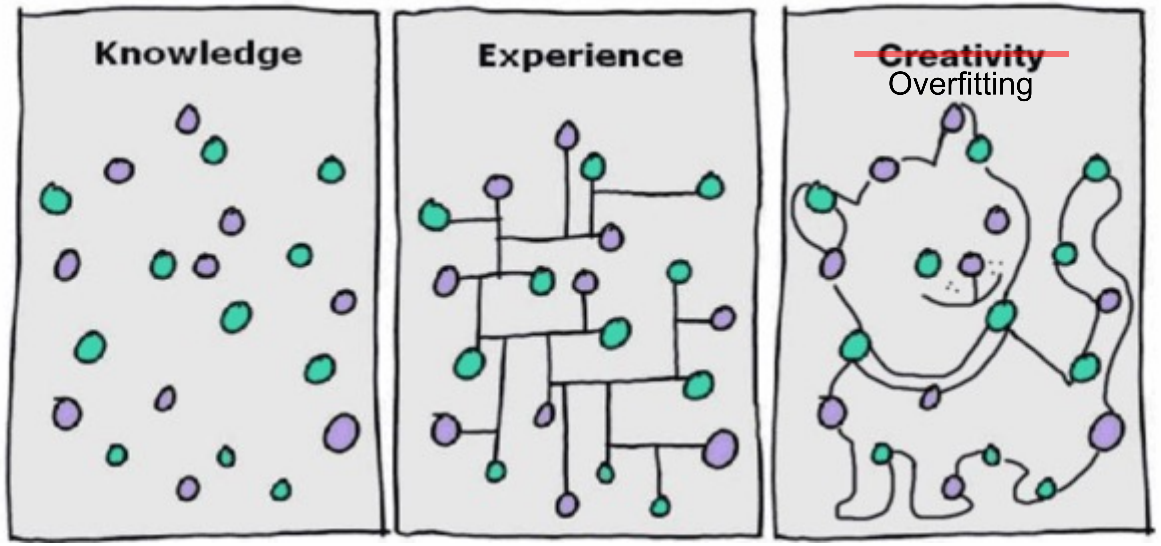


But what about uncertainties? And heavier projectiles?

Sources of uncertainty in ab initio calculations of many-body reactions.

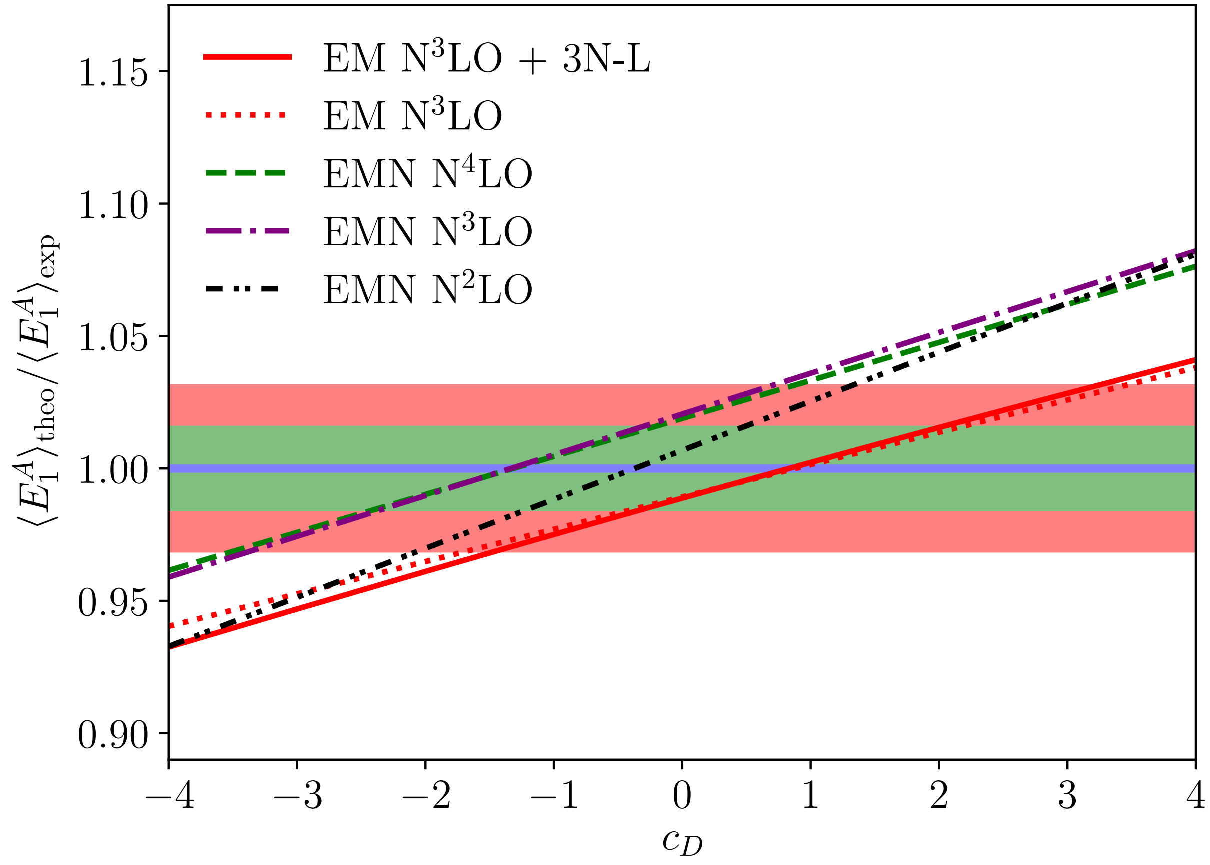
- Uncertainty in the underlying interaction, arising from missing physics, in terms of EFT truncation, exclusion of 4N-forces at N3LO, etc. –Not much we can do to correct for it but, it can be quantified!

- Uncertainty from poorly determined values for LECs, either due to absence of, or large uncertainties in, experimental data. –It can be quantified, if we can propagate it, and if we are not in a very bad minimum.

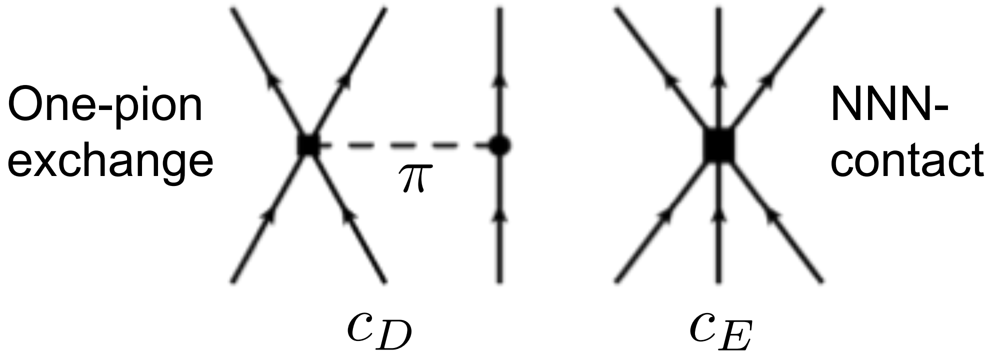


$$\chi^2 = \sum \frac{\left(O^{\rm th} - O^{exp}\right)^2}{\sigma_{exp}^2 + \sigma_{th}^2}$$

Determining low-energy constants from three-body observables

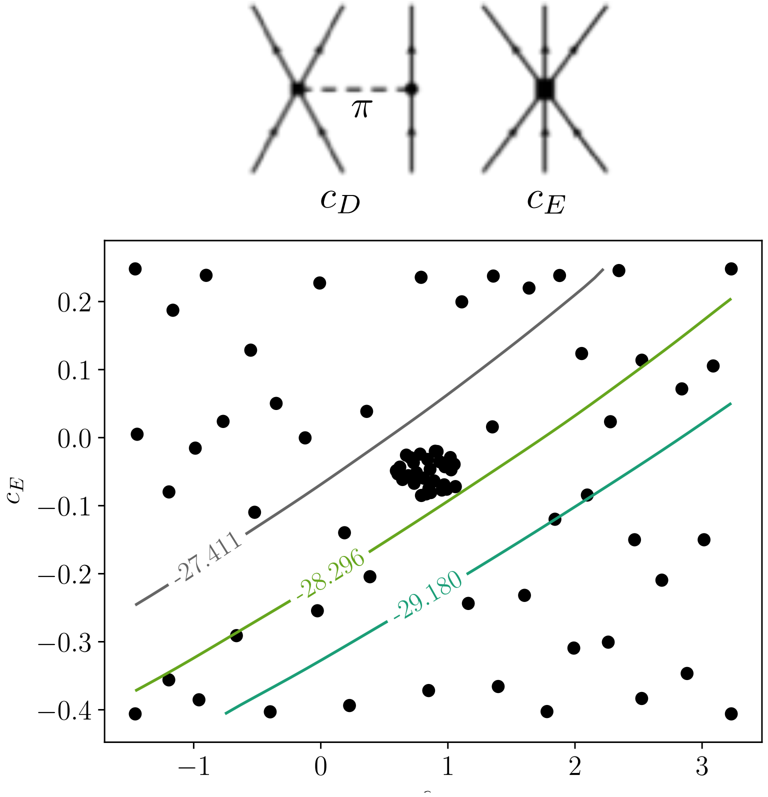


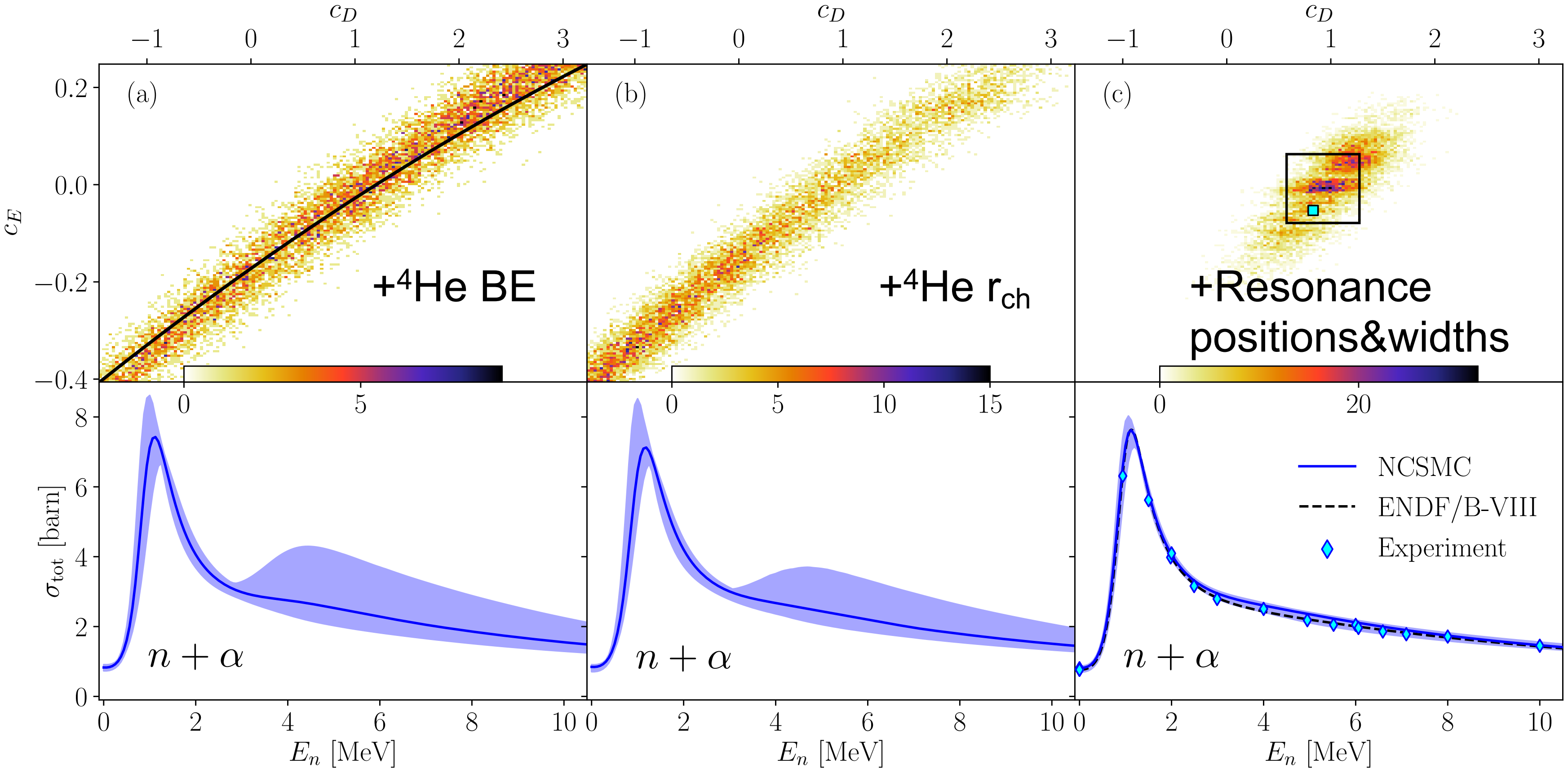
Entem & Machleidt, Phys. Rev. C **68**, 041001(R)
Entem, Machleidt & Nosyk Phys. Rev. C 96, 024004 (2017)



- Estimating theoretical uncertainties is not easy (or pleasant!)
- Even at large chiral order, the theoretical uncertainty completely dominates over experiment, leading to large confidence intervals.

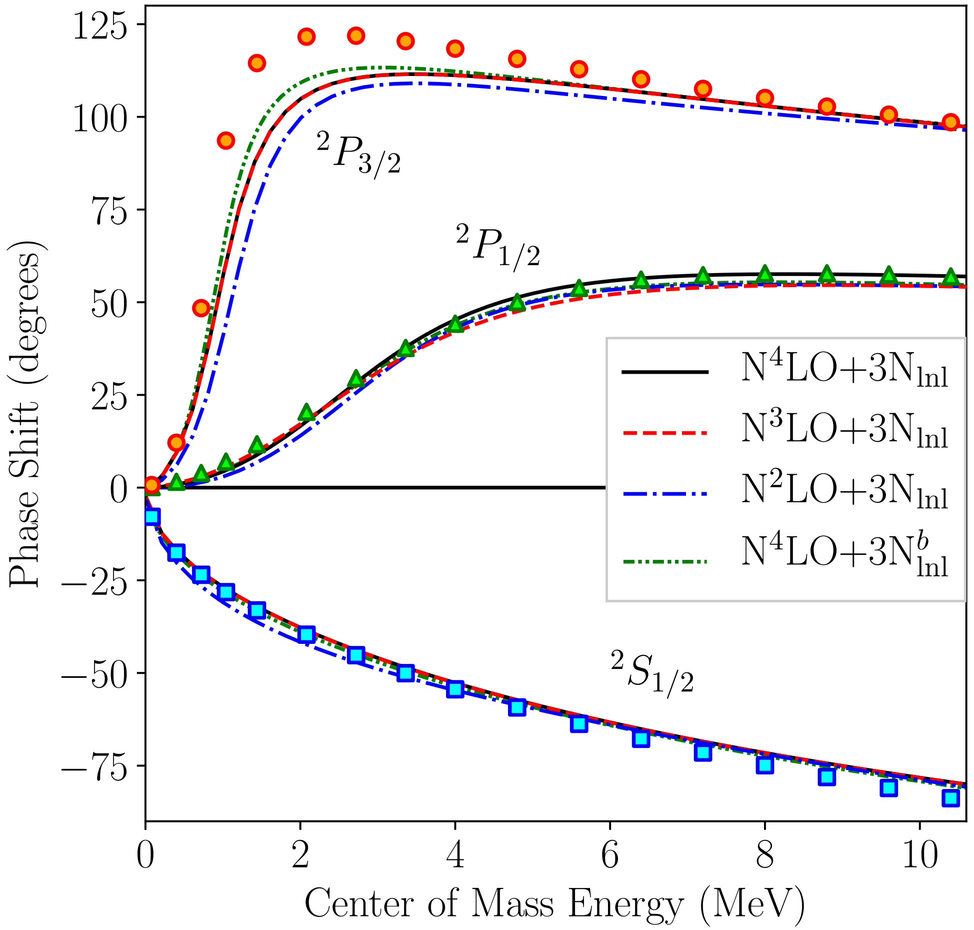
Significant speedups coupled with efficient emulators make uncertainty quantification of theoretical predictions possible.



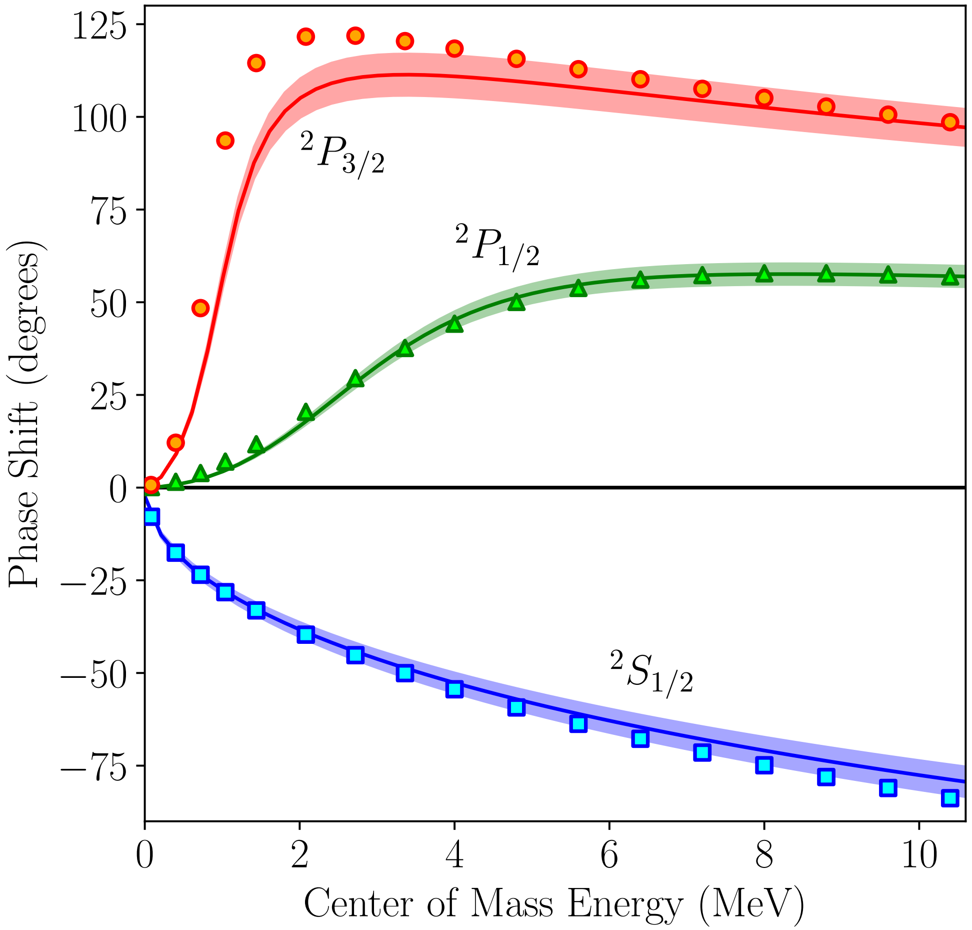


KK, Kevin Quinlan et al, Phys. Rev. C **102**, 024616 (2020)

Consistently constructed order-by-order interactions allow quantification of EFT truncation uncertainty.



NN Potentials from: Phys. Rev. C **96**, 024004 (2017)



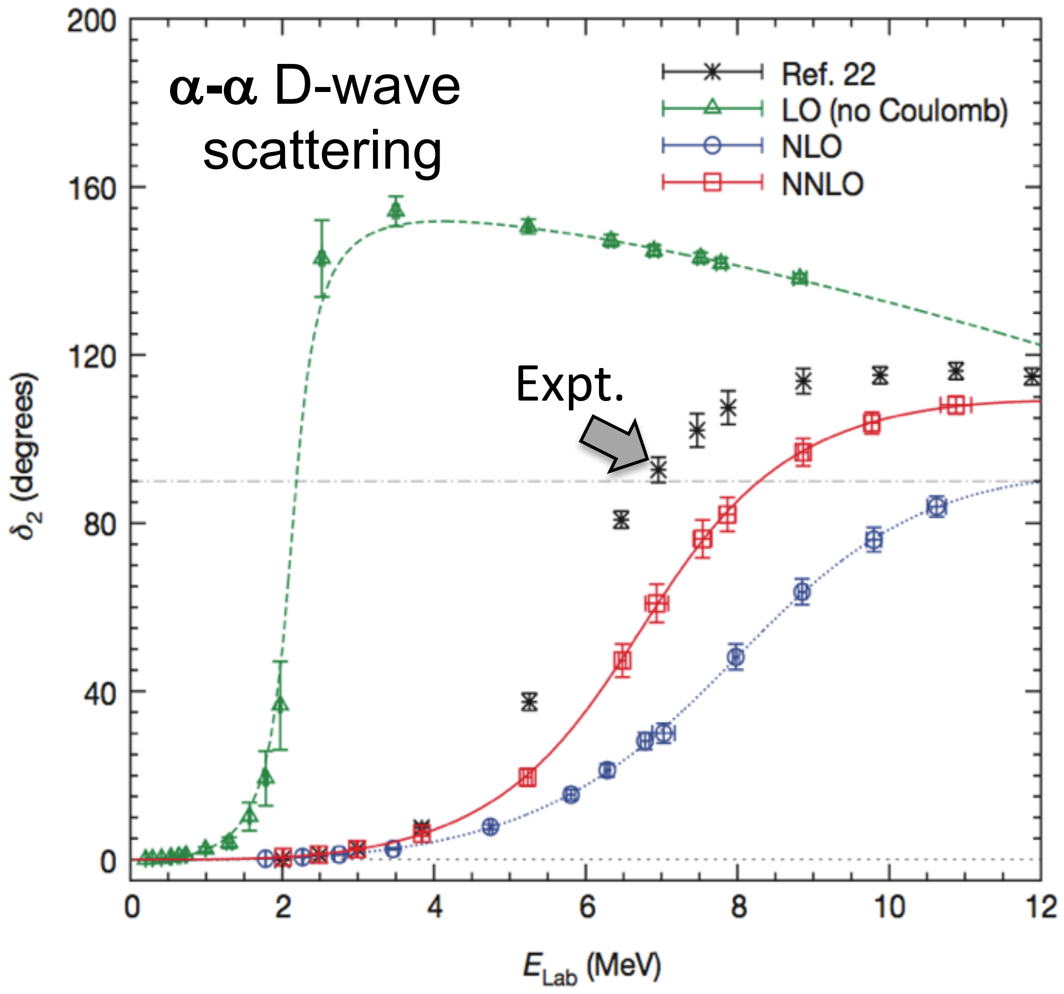
Truncation uncertainties as in: Phys. Rev. C 100, 044001 (2019).

Can ab initio theory treat He burning reactions?

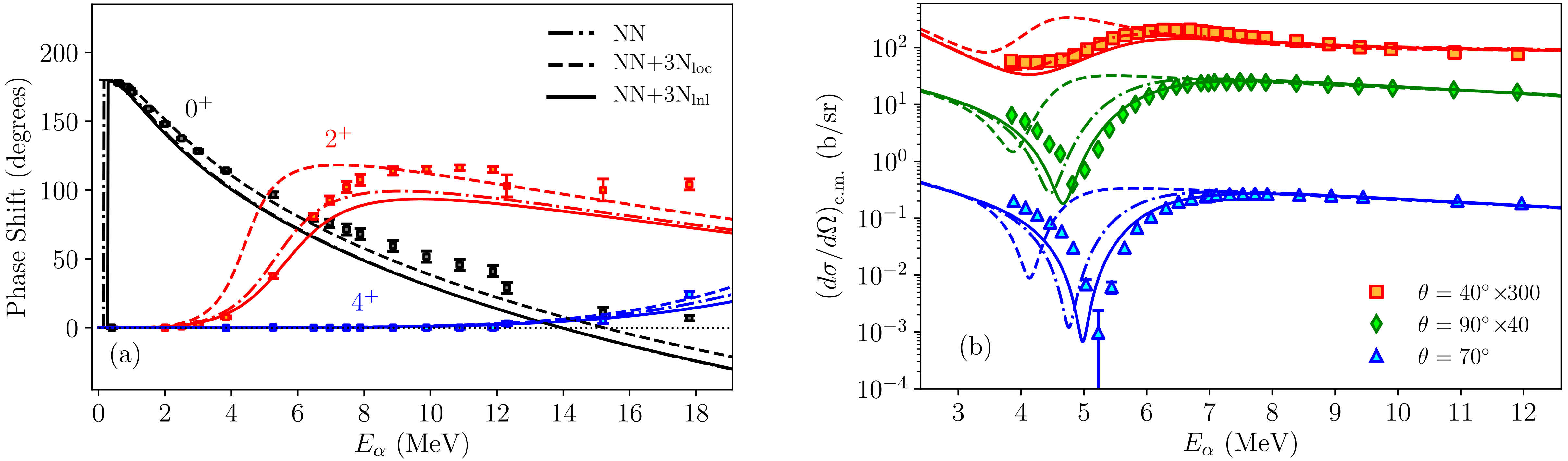
Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111

Nuclear Lattice EFT with the Adiabatic Projection Method

- Promising results for $^4He+^4He$ scattering
- Favorable computational scaling (~A^2)
- $^4He+^{12}C$ fusion becoming possible!
- Extensions to enable treatment of three-cluster dynamics required before the method can be applied to the triple-^4He fusion process

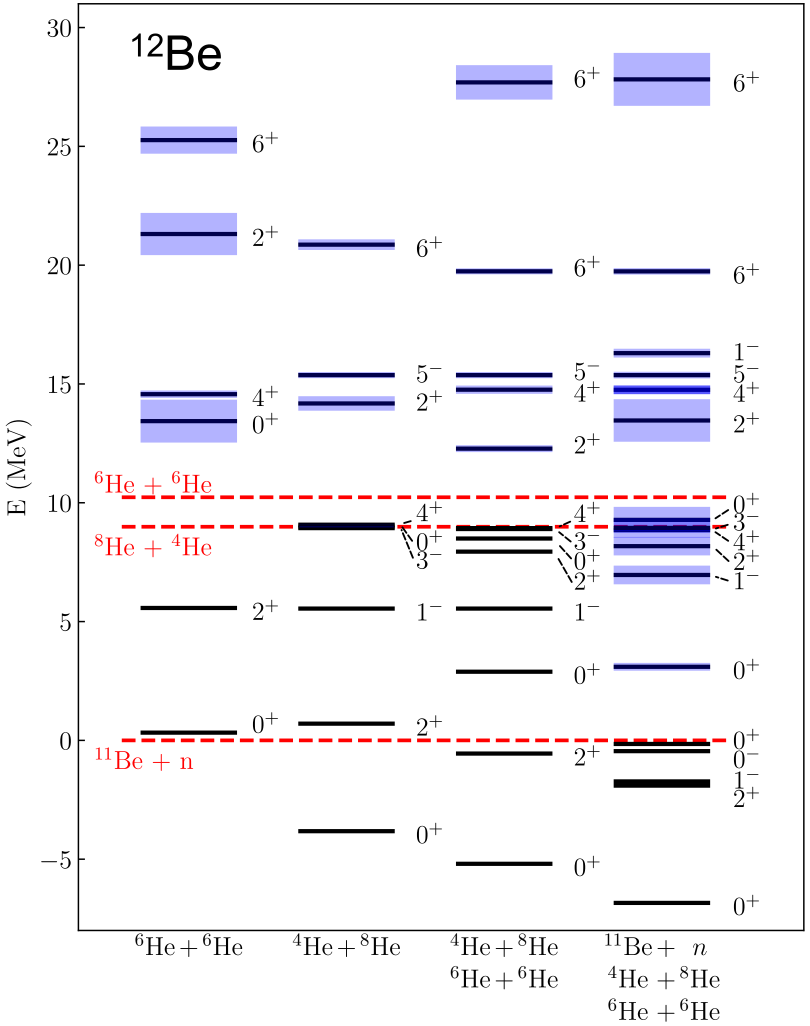


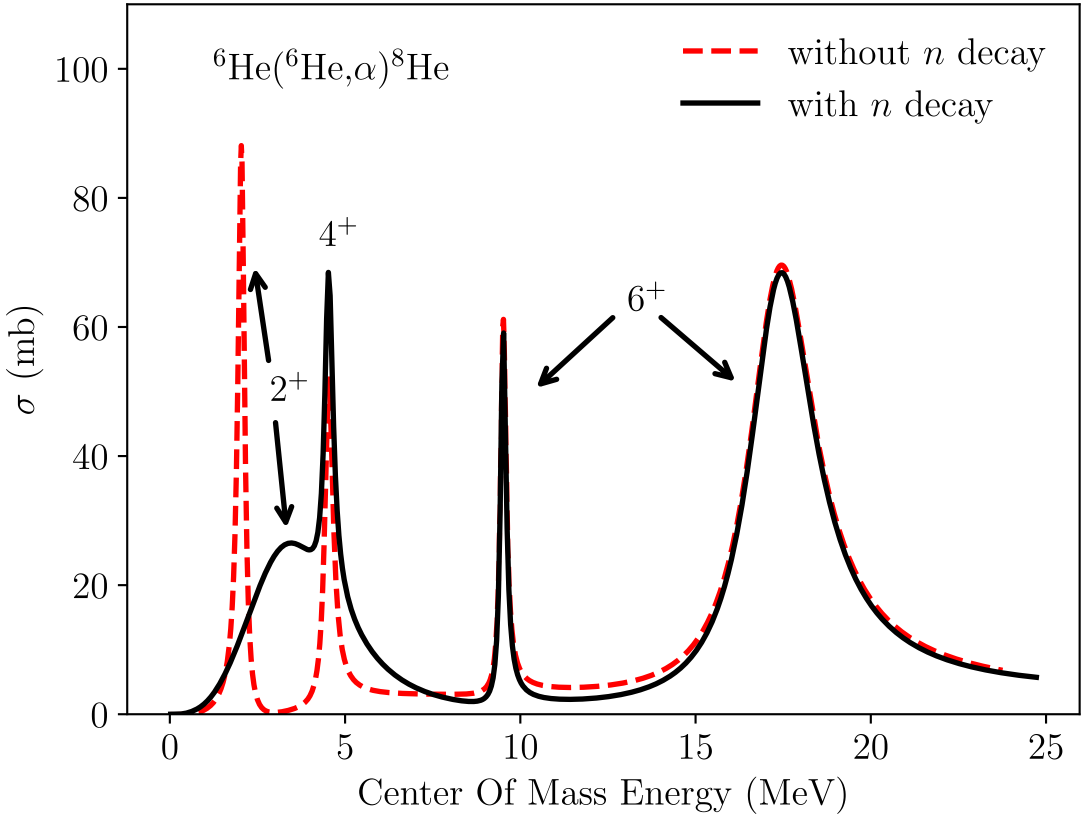
Three-nucleon force effects become significant at higher compound-nucleus masses.



KK, S. Quaglioni, G. Hupin, P. Navratil (arXiv:2012.00228)

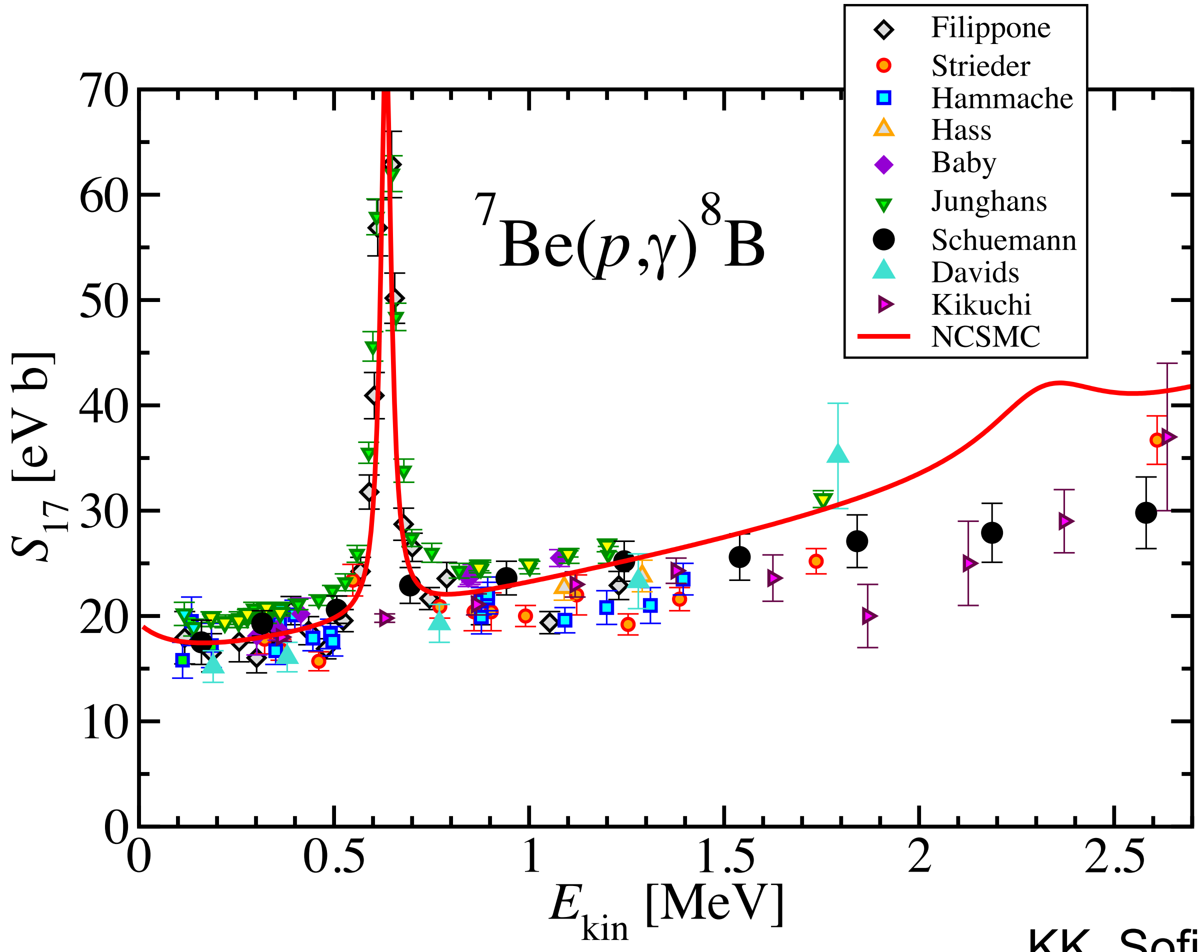
Clustering and reactions with p-shell projectiles





KK, S. Quaglioni, G. Hupin, P. Navratil (arXiv:2012.00228)

Radiative capture from first principles. No uncertainty band yet.



KK, Sofia Quaglioni, Petr Navratil (in prep)

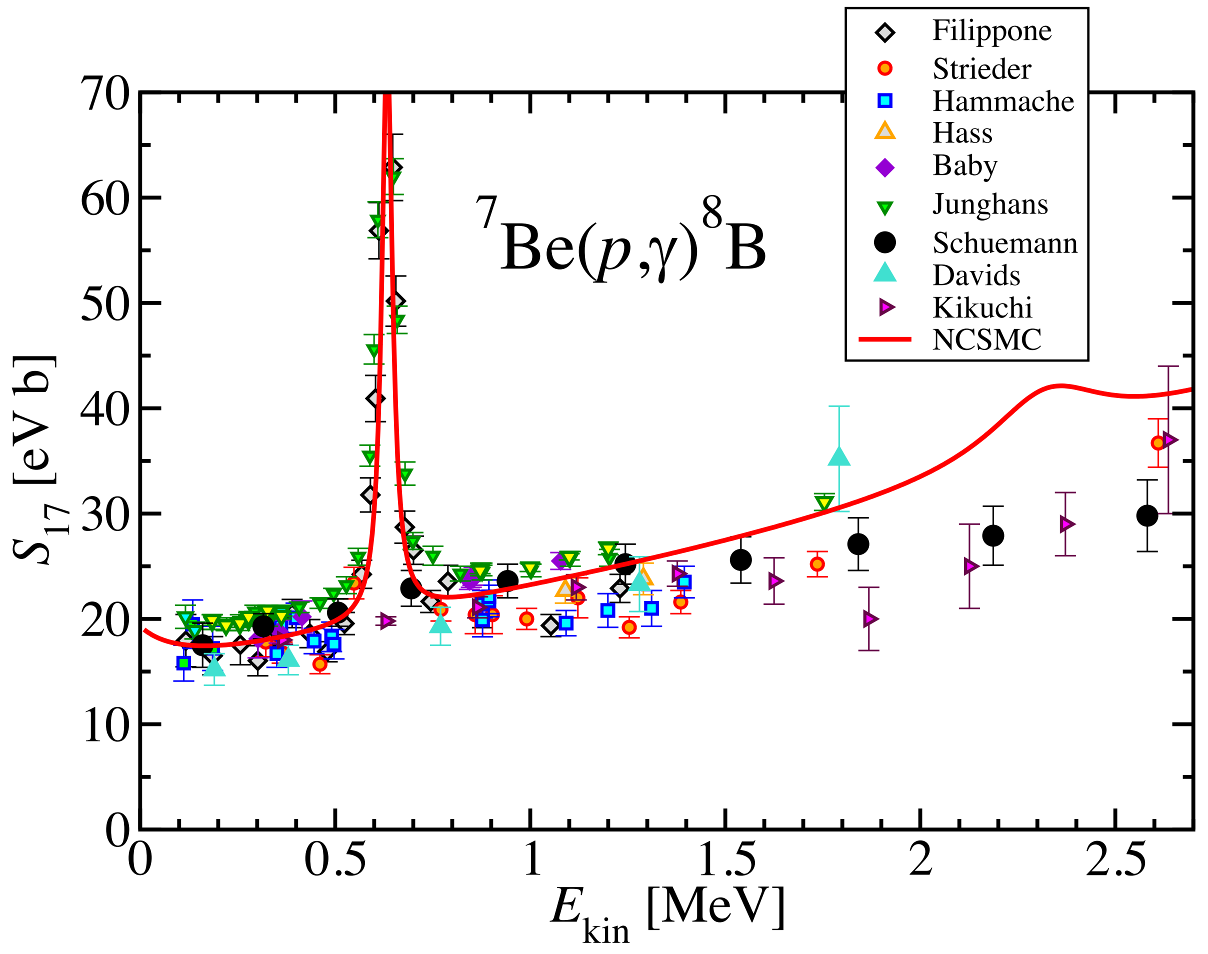
Conclusions

Fitting to experimental data is messy. Potential unrecognized systematic uncertainties can skew results.

Multiple *different* types of experiments are needed to make predictions confidently.

Ab initio nuclear reaction theory can help by providing predictions not directly fitted to data, with quantified uncertainties.

Near Future: Charge-exchange reactions for Big-Bang Nucleosynthesis



Thank you!

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NCSMC vs NCSM/RGM wave functions