Nuclear data generation by combining machine learning and nuclear reaction models

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Nuclear Data Evaluation and Machine Learning

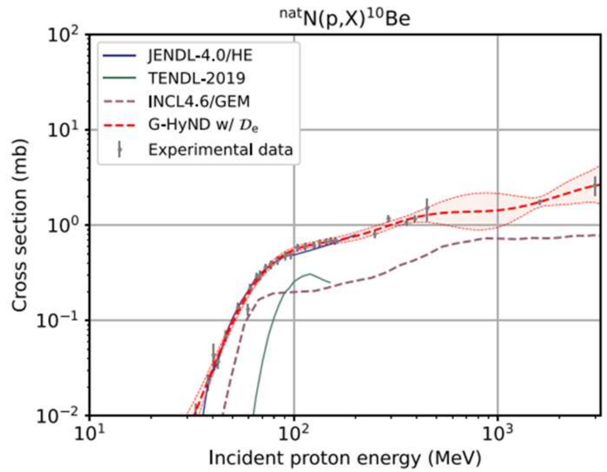
◆ In recent years, many attempts have been made to use machine learning to evaluate nuclear data

・Neural network predictions of inclusive electron-nucleus cross sections

Al Hammal et al, Phys. Rev. C, 107, 065501 (2023)

・G-HyND: a hybrid nuclear data estimator with Gaussian processes.

H. Iwamoto, J. Nucl. Sci. Technol. 59, 334 (2022)



☆ We are studying nuclear data generation by combining nuclear reaction models and Gaussian process regression to find the optimal value of optical potential for nucleon-nucleus scattering.

・Nuclear data generation by machine learning (I)
application to angular distributions for nucleon-nucleus scattering

S. Watanabe et al, J. Nucl. Sci. Technol. 59, 1399 (2022)

・機械学習を用いた核子－原子核散乱に対する最適なポテンシャルの予測

日本原子力学会2022年秋の年会大会 2022/9/8　発表者：渡辺証斗

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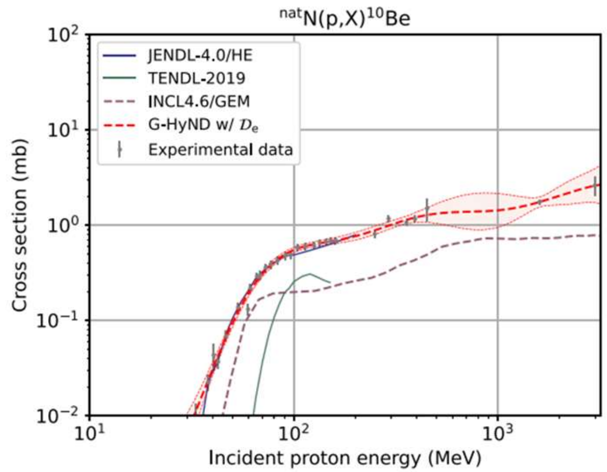

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Framework 1: Nuclear reaction model

- Coupled Channel Optical Model

$$\left(\left[\frac{d^2}{dr^2}-\frac{l_c(l_c+1)}{r^2}+k_c{}^2\right]u_c(r)-\sum_{c'}V_{cc'}u_{c'}(r)\right)=0$$

u_c: Wave function of scattered wave (radial direction)

c : Reaction channel ($\{l_c, j_c, n_c\}$)

$V_{cc'}$: Optical potential(Between c and c' channels)

We solve coupled channel equations using CCONE O. Iwamoto et al., Nucl. Data. Sheets 131, 259 (2016)

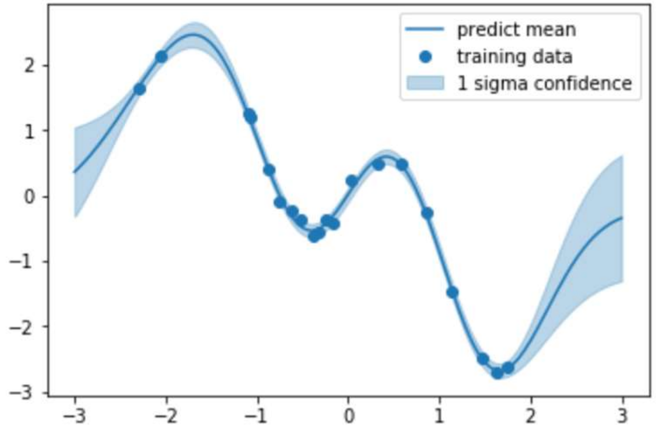
(Neutron-Nucleus Scattering)

$$V(r)=-v_R(E)\ \frac{a}{1+\exp\frac{r-R_R}{a_R}}+[\mathrm{imaginary}]+[\mathrm{LS}]$$

S. Kunieda et al, J. Nucl. Sci. Technol. 44, 838-852 (2007)

Optimize the value of $v_R^0(E)$

Framework 1: Gaussian process regression



○ Gaussian process regression

– A model that estimates a function $y = f(x)$ from inputs x and output y variables, and find the minimum value of the objective function

○ Assuming all inputs-outputs follow a Gaussian distribution and calculating conditional probabilities given training data

○ Gaussian process regression has two characteristics

- No assumption of function form
  - Even Complicated functions can be estimated.
- Estimation results are given by Gaussian distribution
  - Gives the error of the estimate.

Framework 1: Bayesian optimization

○ Bayesian optimization

A method for finding the input x that has the minimum value of the function $y = f(x)$ based on the estimation results of Gaussian process regression

○Objective function describes the deviation between experimental data and theoretical calculation.

$$\frac{1}{data}\sum_{data}\left(\frac{\sigma_{exp}^{(i)}}{\Delta\sigma_{exp}^{(i)}}\log_{10}\frac{\sigma_{th}^{(i)}(x)}{\sigma_{exp}^{(i)}}\right)^2$$

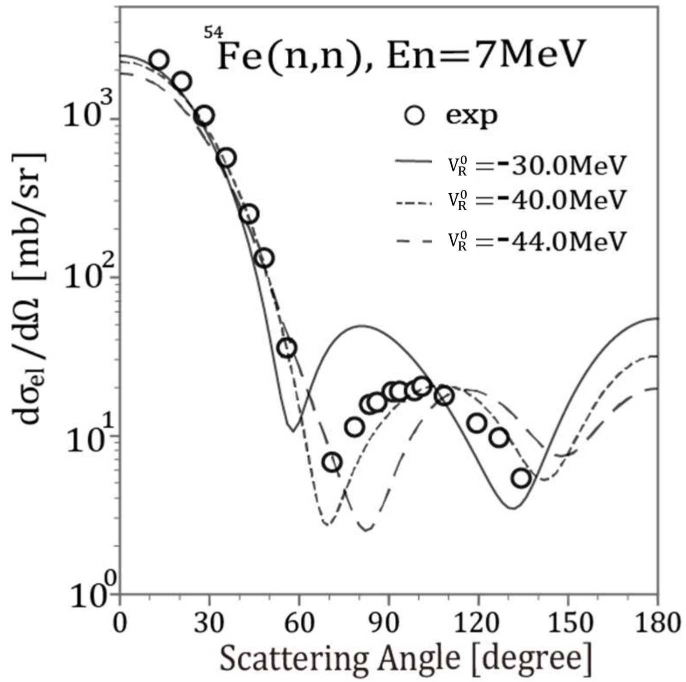
○ Determine the potential parameters x to minimize the Objective function y.

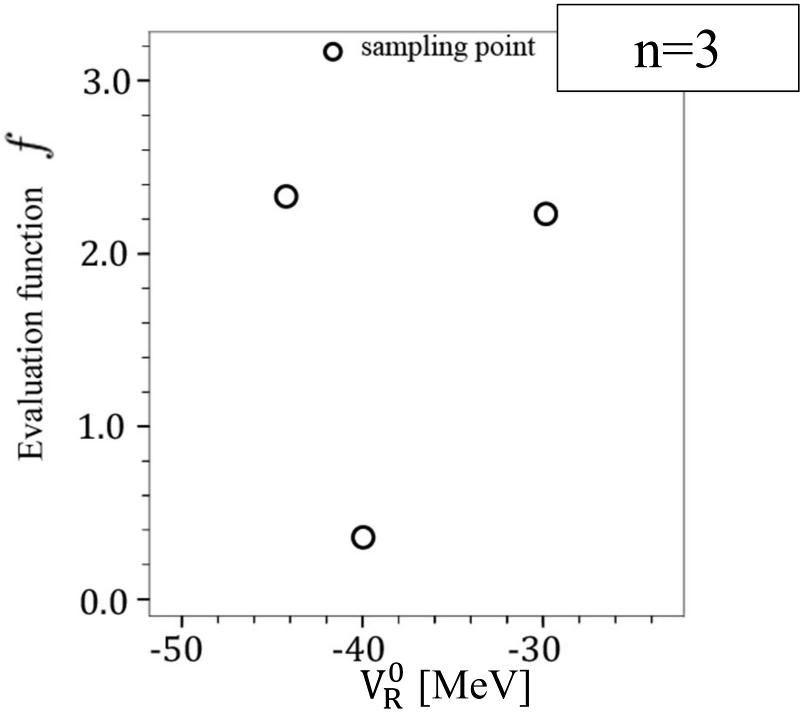
x :Parameter of optical potential
y :Evaluation function

We use GPyOpt as Library of Gaussian process regression
https://sheffieldml.github.io/GPyOpt/

Result 1: An Example of optimization by machine learning

Estimate the evaluation function about optical parameter v_R by Gaussian process regression from the sampling results .
Calculate the evaluation function for v_R , where the large uncertainty and the small predicted value.





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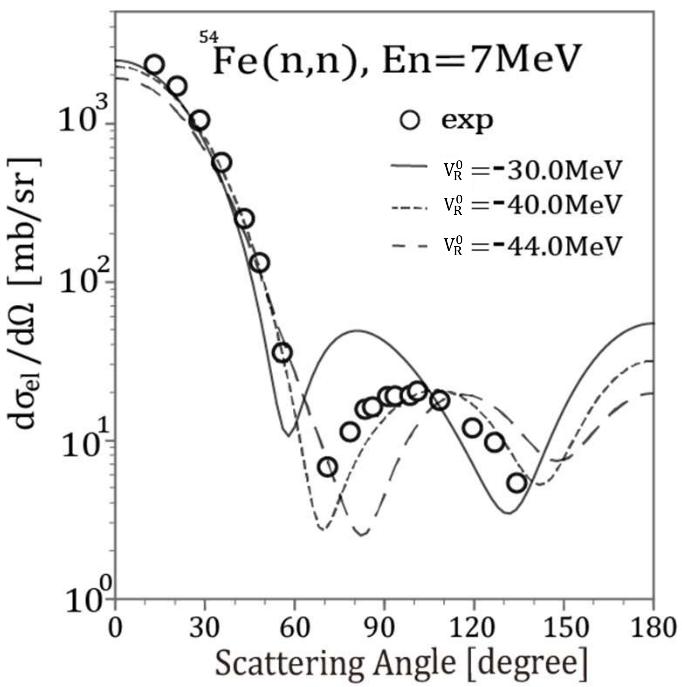

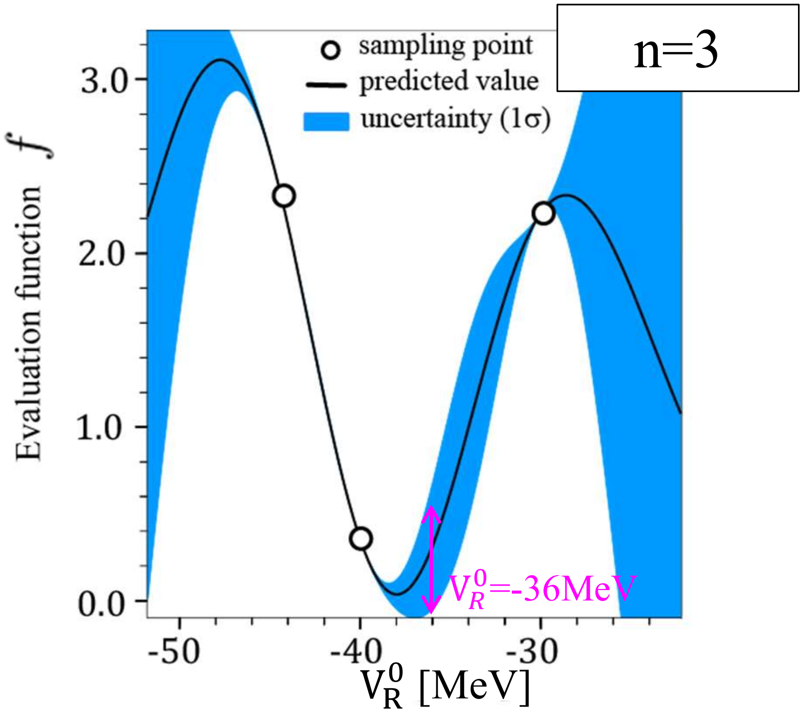

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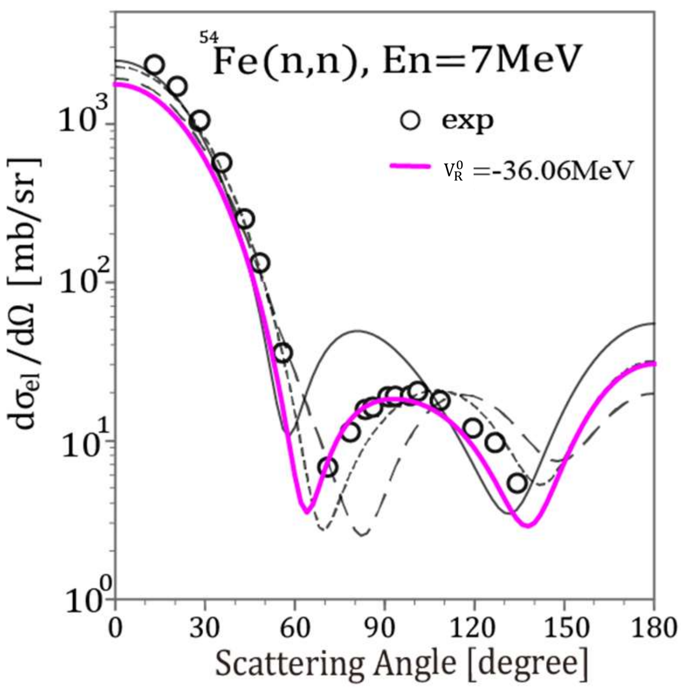

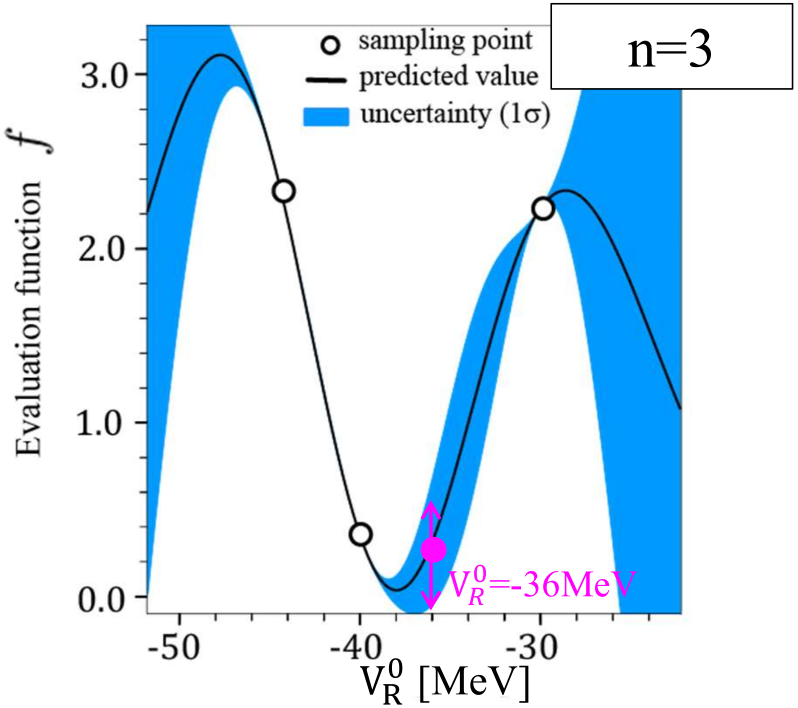

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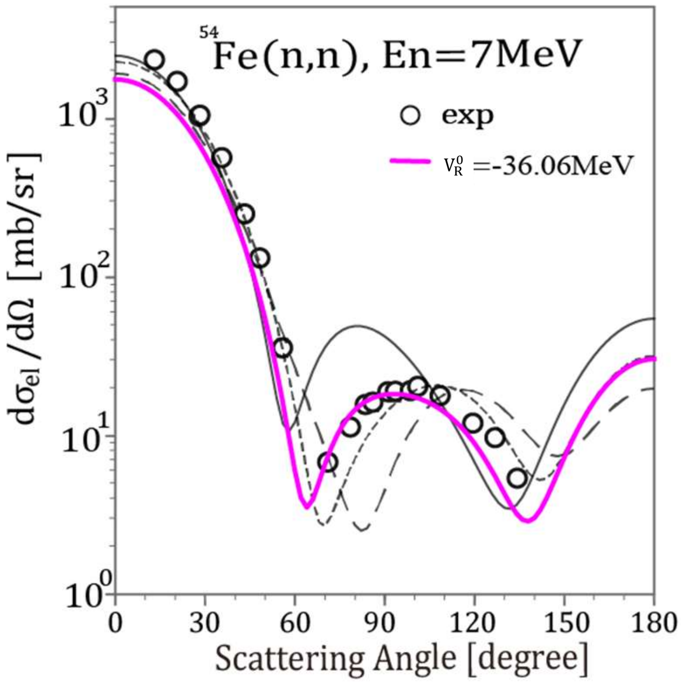

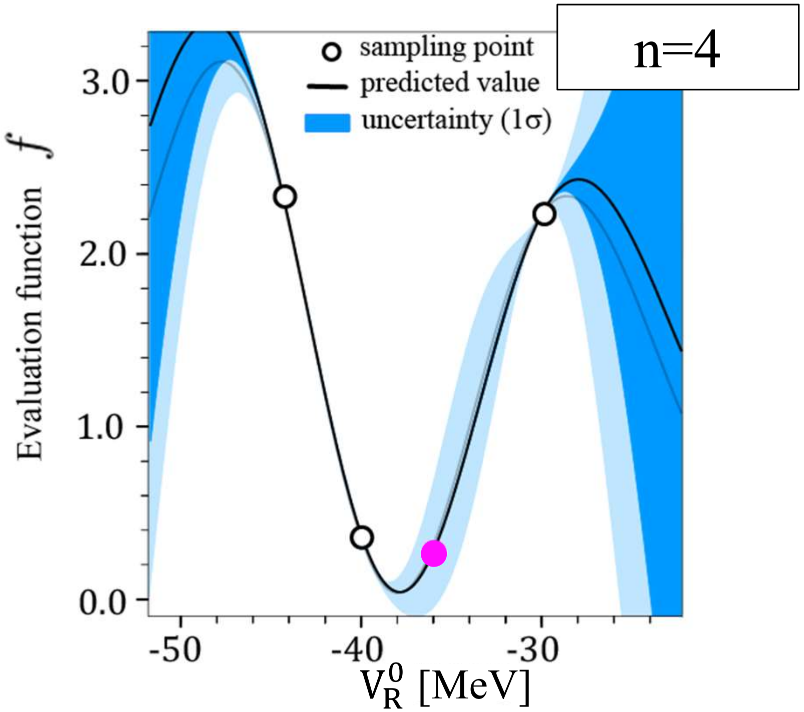

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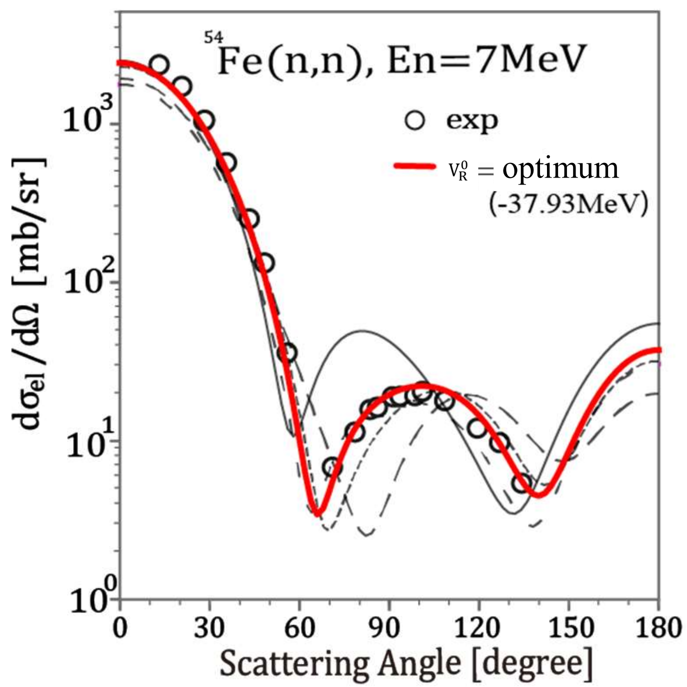
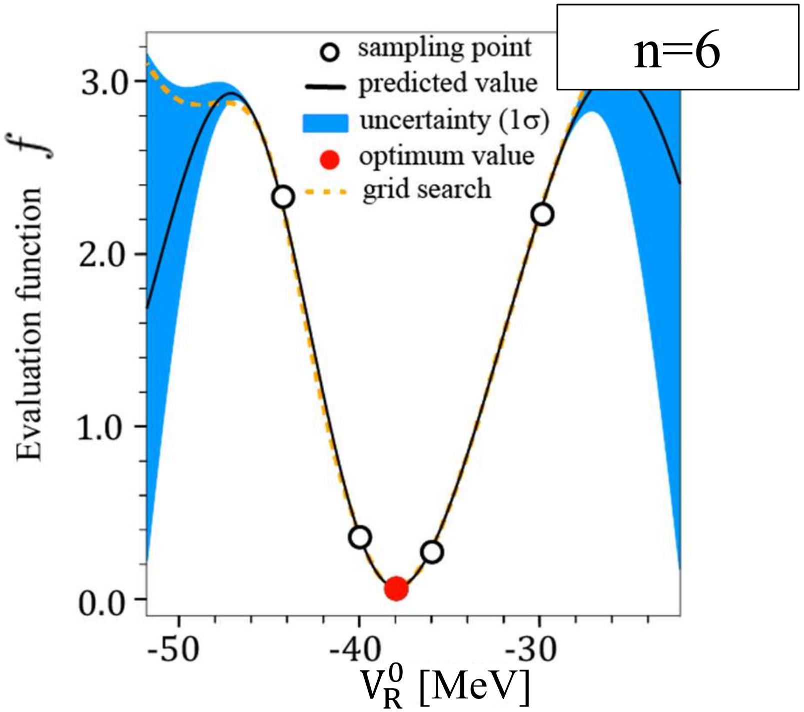
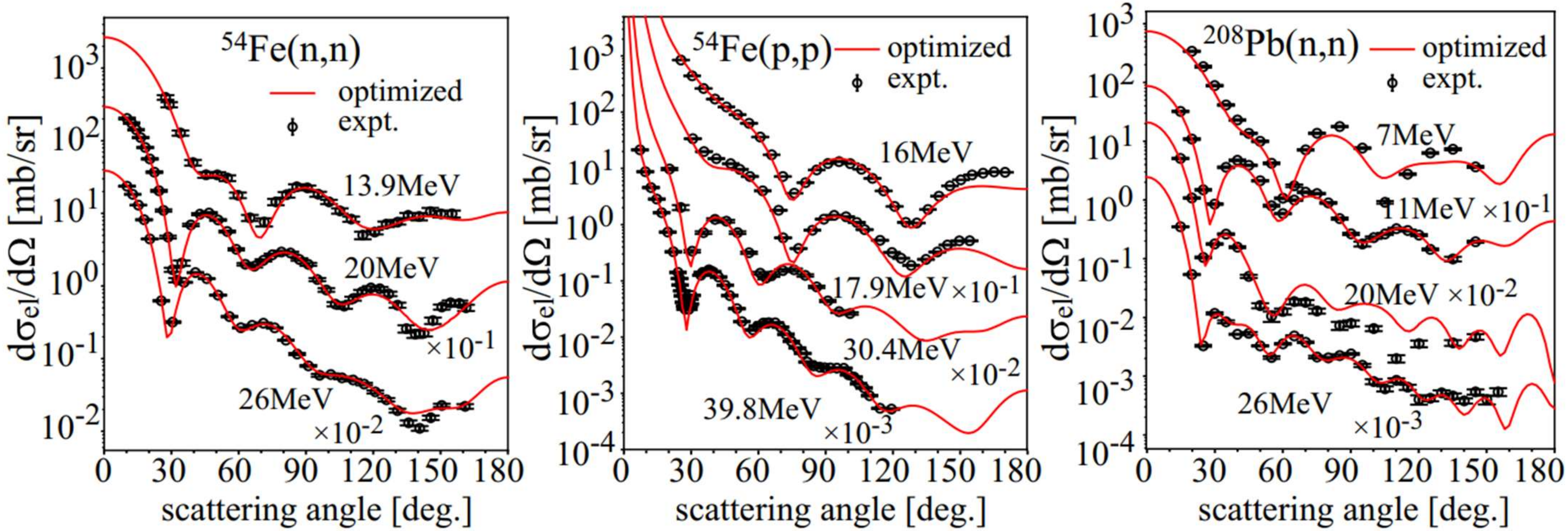




Result 1: Optimization result

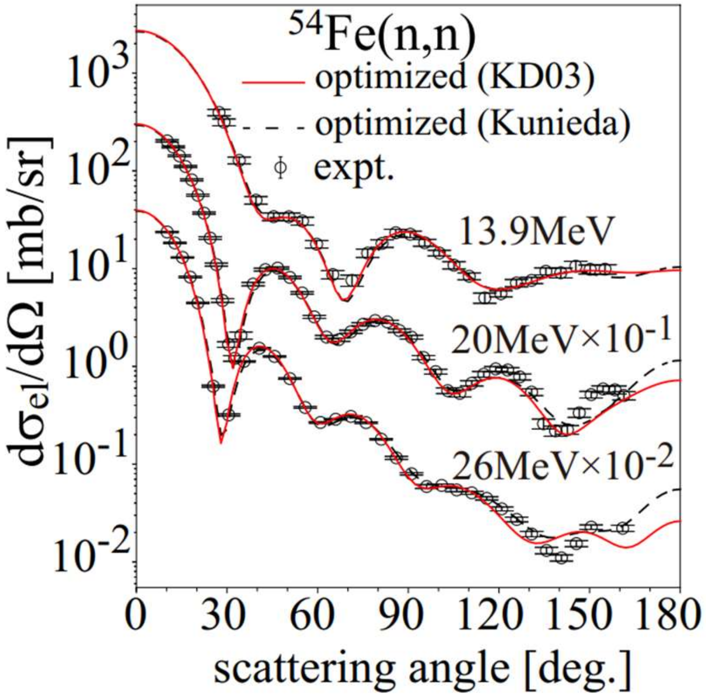
The cross section calculated using obtained v_R in this way is as follows.
Experimental values are reproduced with sufficient accuracy even
for different target nuclei and incident particles.



Result 1: Optimization result

Another model. (only to the depth of the central force part of KD03)

The optimal cross sections are slightly different due to different default values for the model and other parameters. In any case, experimental values are reproduced with sufficient accuracy.



Next motivation

This method can be used to find the optimal value at an energy for which experimental values are available

Conversely, it is not possible to estimate optimal values at energies for which there are no experimental values

The functional form of $v_R(E)$ is phenomenologically and empirically determined

S. Kunieda et al, J. Nucl. Sci. Technol. 44, 838-852 (2007)

$$v_R(E) = V_R^0 + V_R^1(E - E_f) + V_R^2(E - E_f)^2 + V_R^3(E - E_f)^3 + V_R^{DISP}\exp^{-\lambda_R(E-E_f)}$$

A. J. Koning and J. P. Delaroche, Nucl. Phys. A. 713, 231-310 (2003)

$$v_R(E) = V_R^0 + V_R^1(E - E_f) + V_R^2(E - E_f)^2 + V_R^3(E - E_f)^3$$

Using Gaussian process regression, it may be possible to estimate optimal values at arbitrary energies without assuming a functional form.

Framework 2: Research Procedure

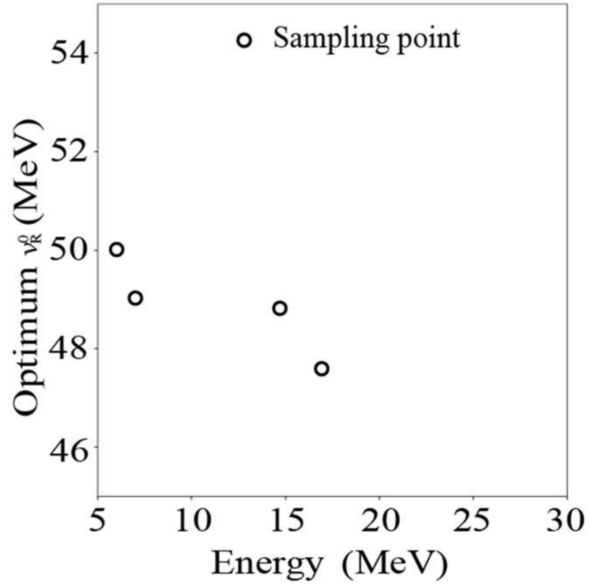
☆ Predict the energy dependence of $v_R\ (E)$ by the following process.

1, Collect the $v_R\ (E)$ list

Input : Energy (MeV)	**Output: v_R^0 (MeV)**
6	**50.0**
7	**49.0**
15	**48.8**
17	**47.6**

⇒

2, Predict the $v_R\ (E)$ using ML



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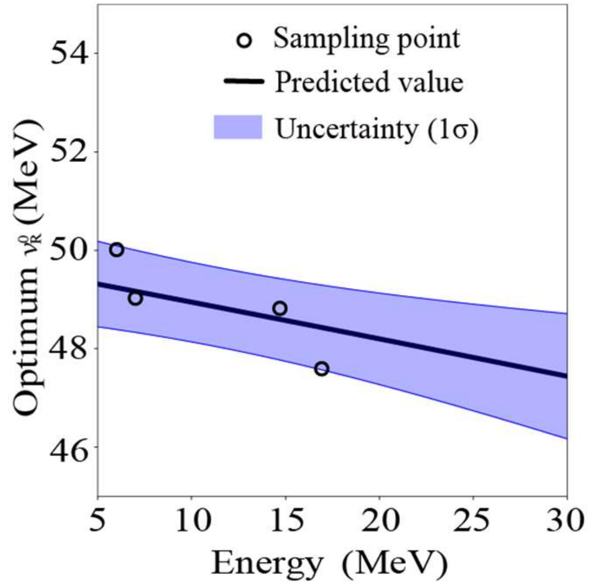
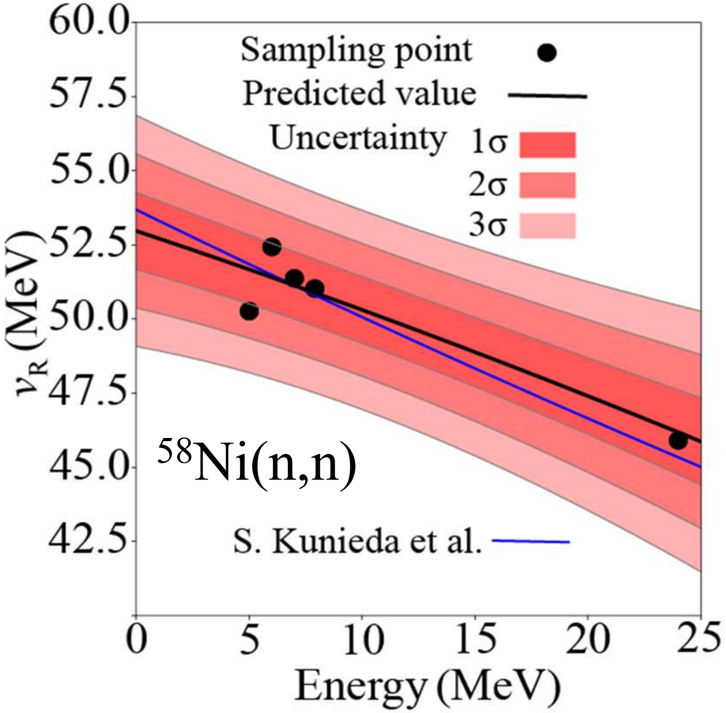
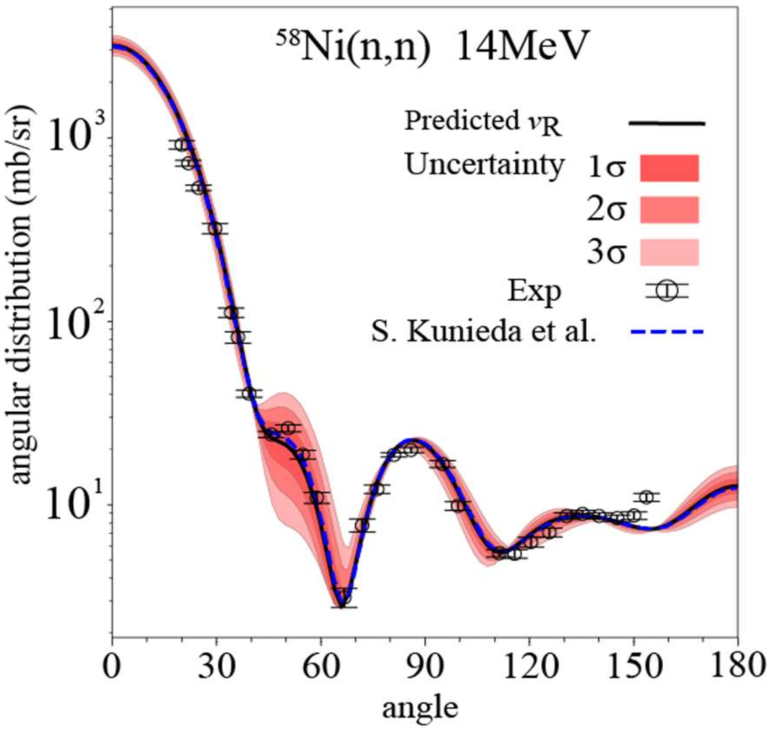


Result 2: ^{58}Ni(n,n) cross section

- Gaussian process regression given as training data the optimal value of v_R that reproduces the experimental data





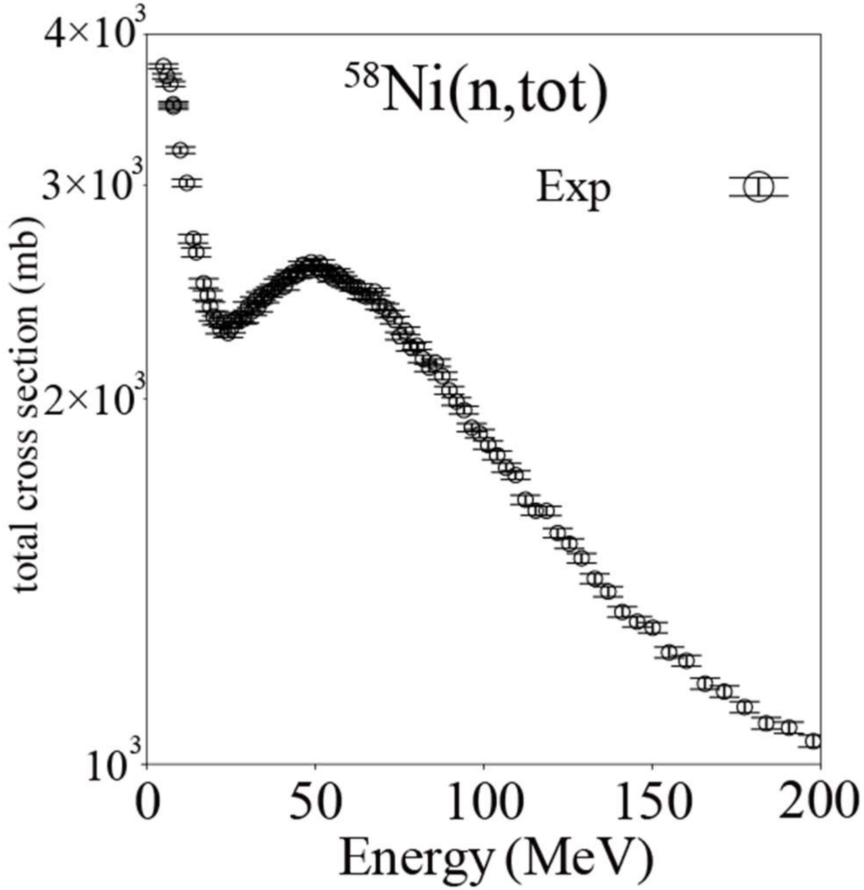
- Angular distribution of ^{58}Ni(n,n) calculated with CCONE using the estimated value of v_R

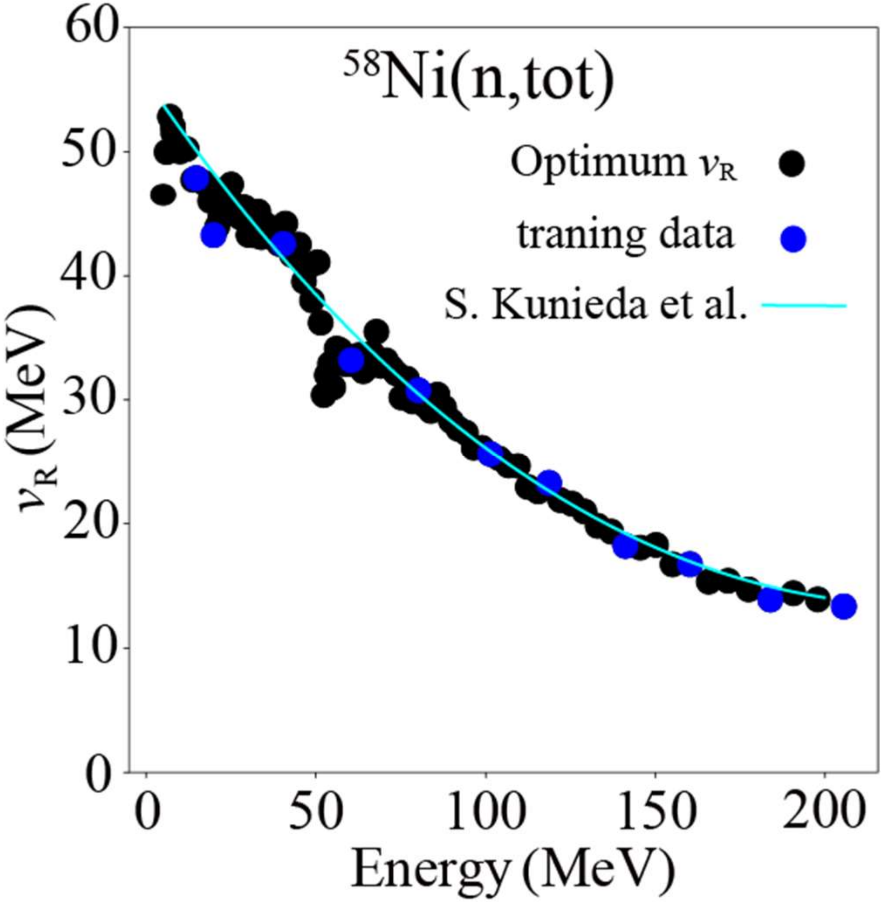
Reproduces the experimental data, showing that the sensitivity is large around 50° .

CCONE: O. Iwamoto et al., Nucl. Data. Sheets 131, 259 (2016)

Result 2: ^{58}Ni(n,tot) cross section

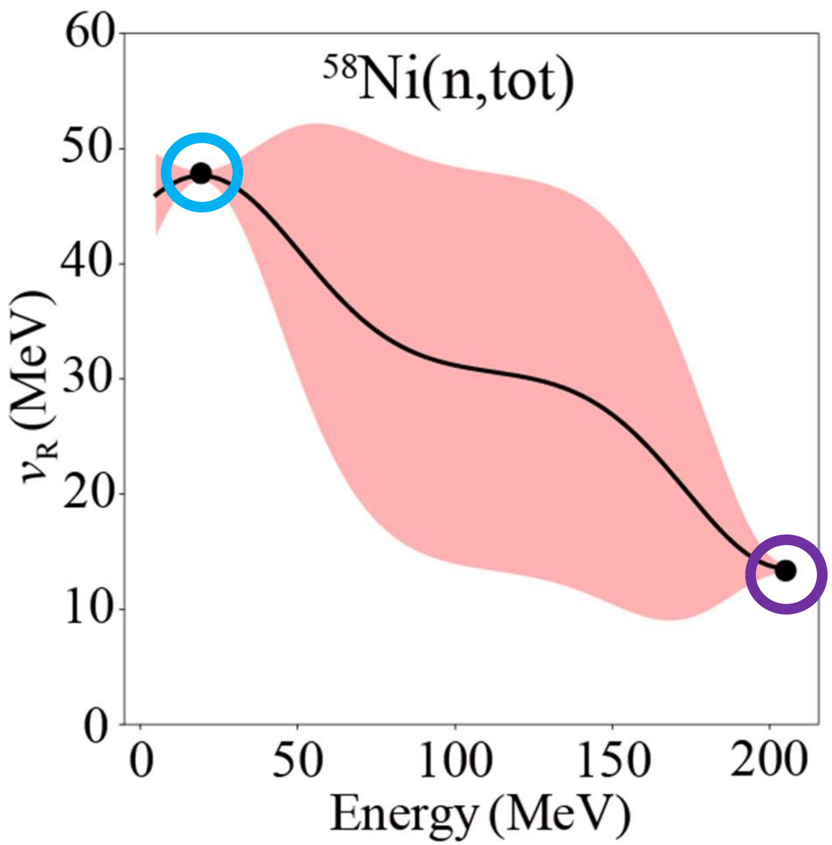
◆ The optimum value of v_R for ^{58}Ni(n,tot) was estimated using the training data

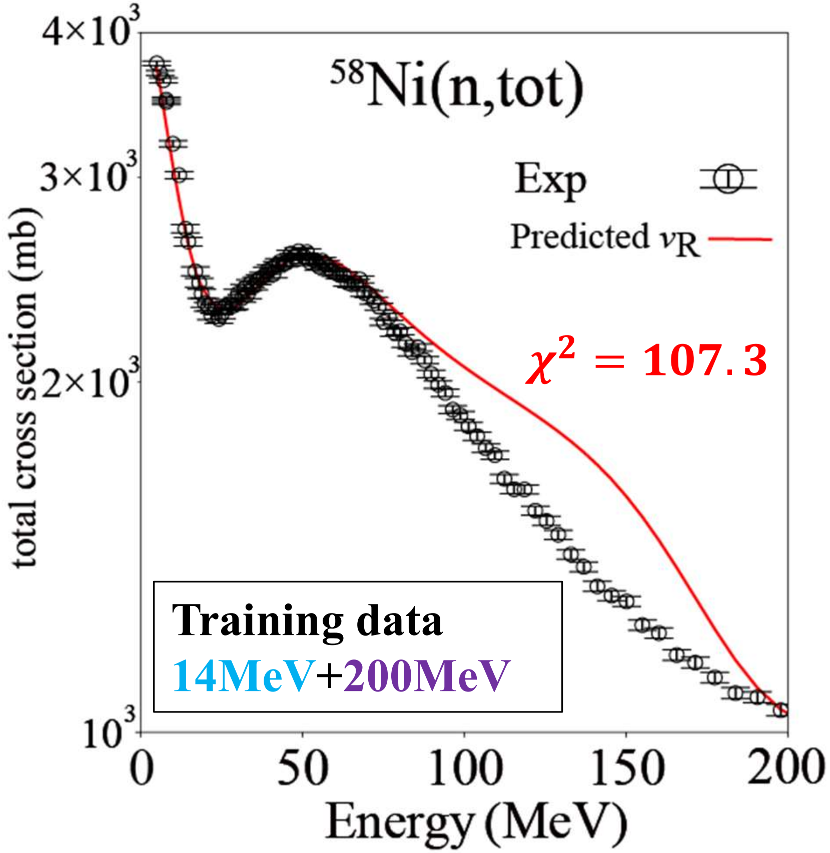




Result 2: ^{58}Ni(n,tot) cross section

◆ Repeat the same operation with different selections as training data.





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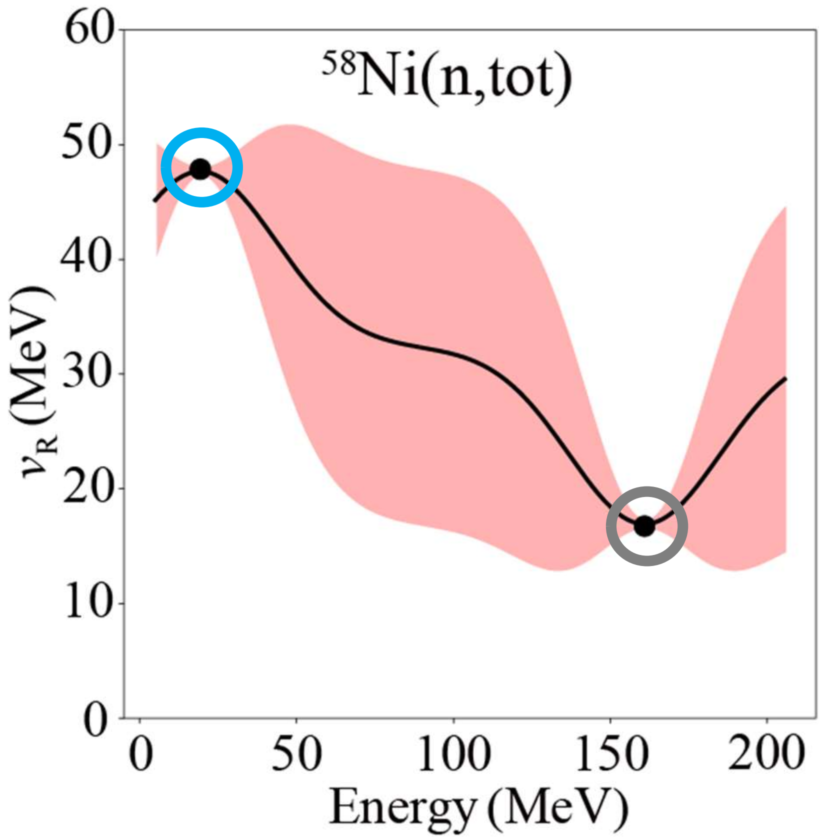
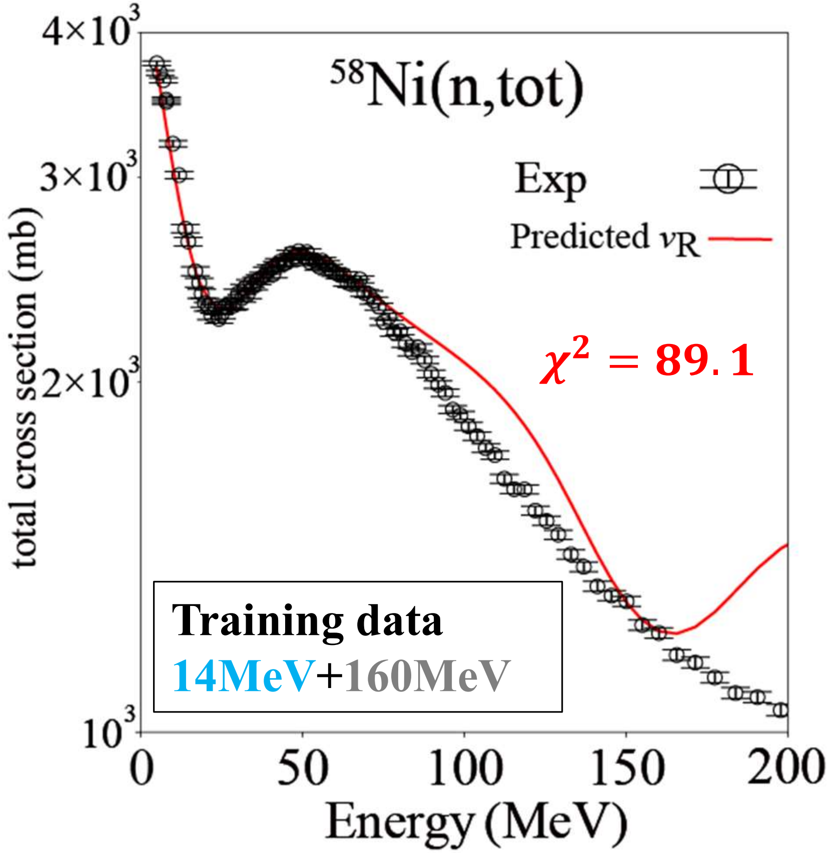
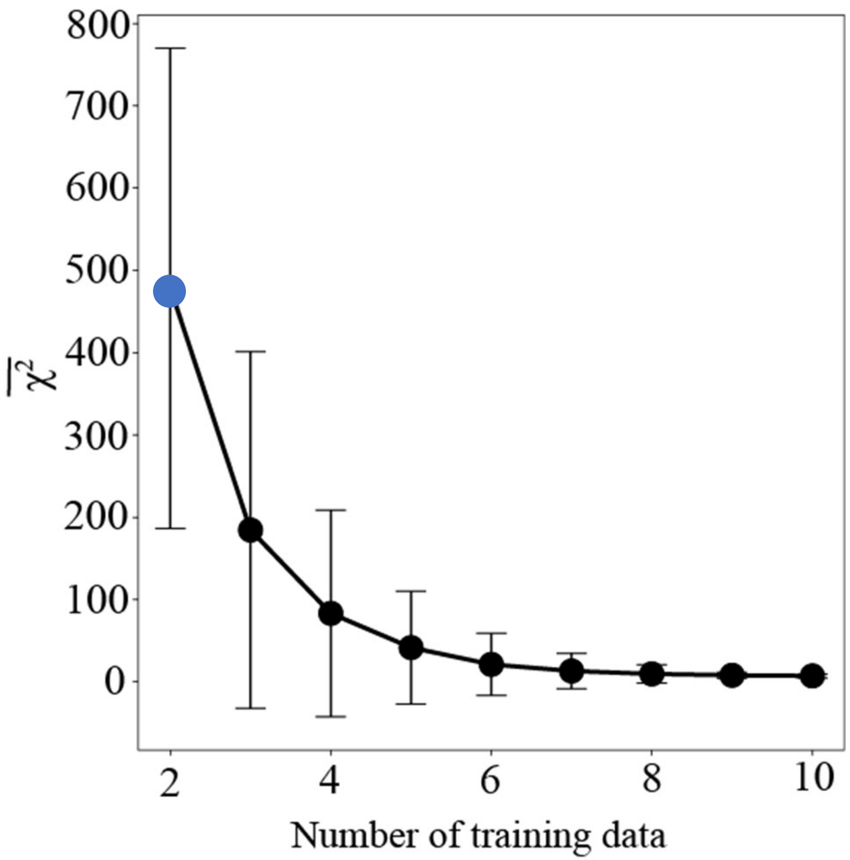
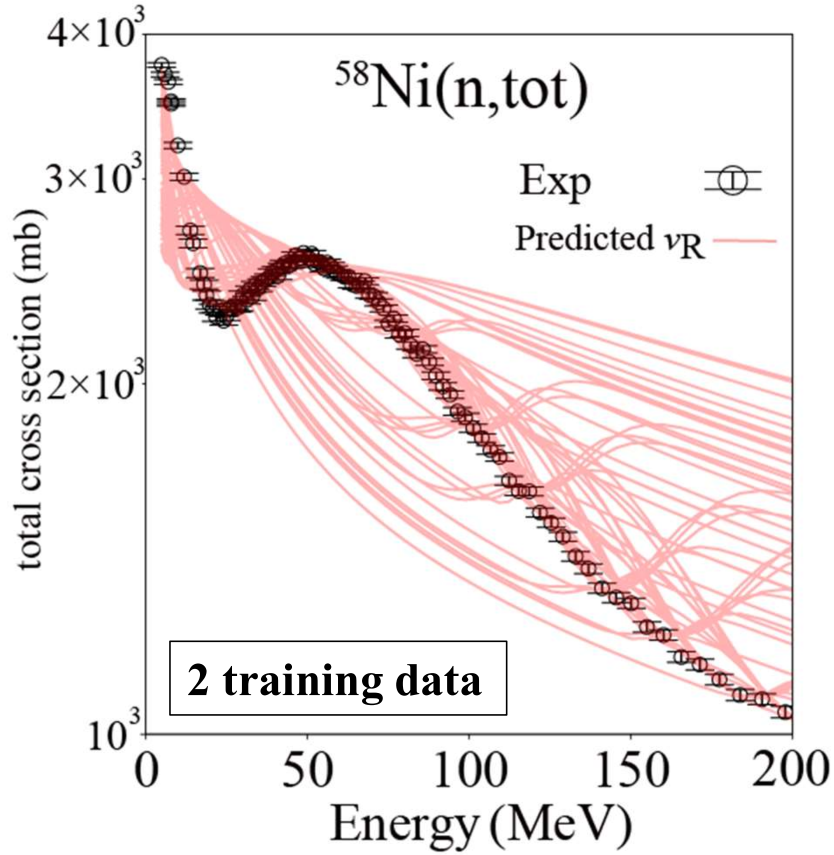




Result 2: ^{58}Ni(n,tot) cross section

◆ Decrease in $\overline{\chi^2}$ and variance relative to experiment as the number of training data increases
Accuracy improves rapidly for 2-5 data sets, and does not improve beyond 7 data sets





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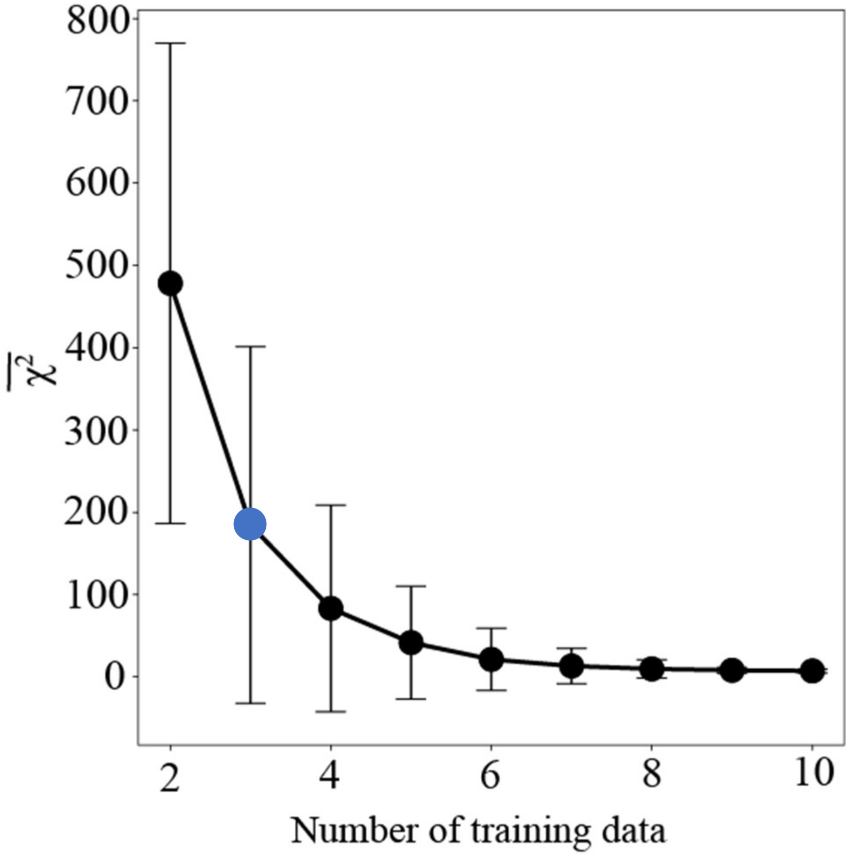

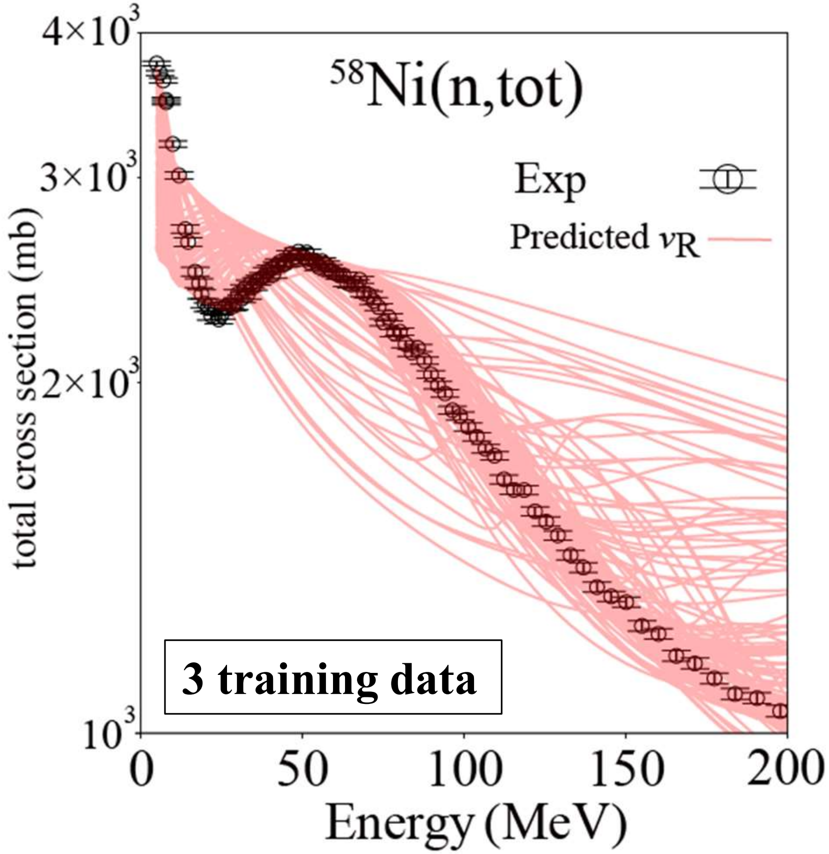

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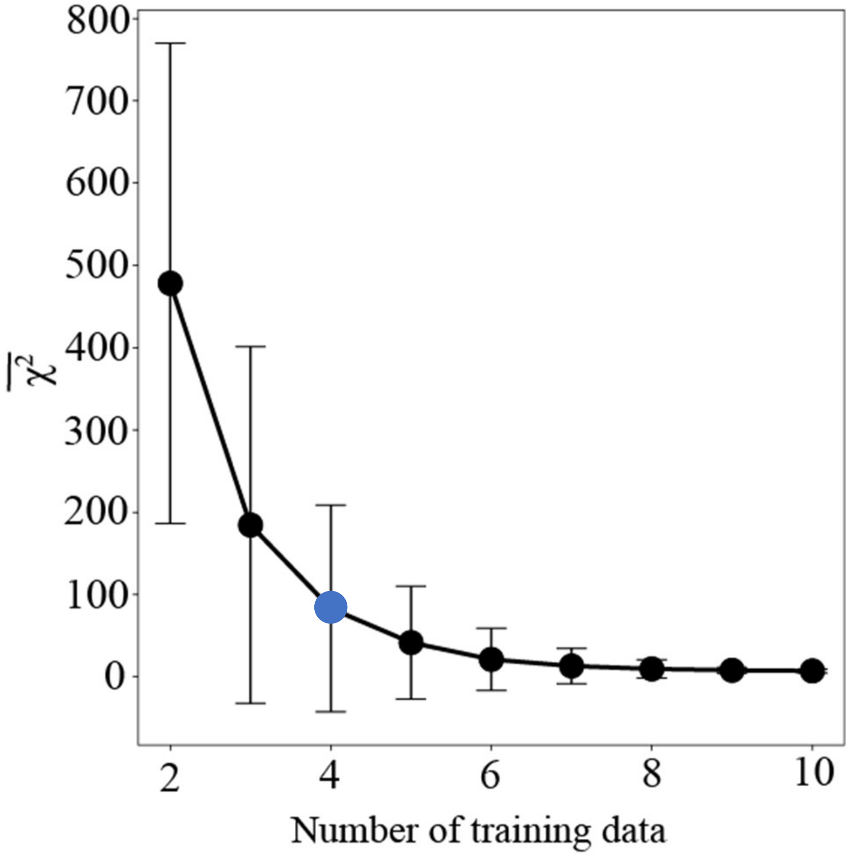

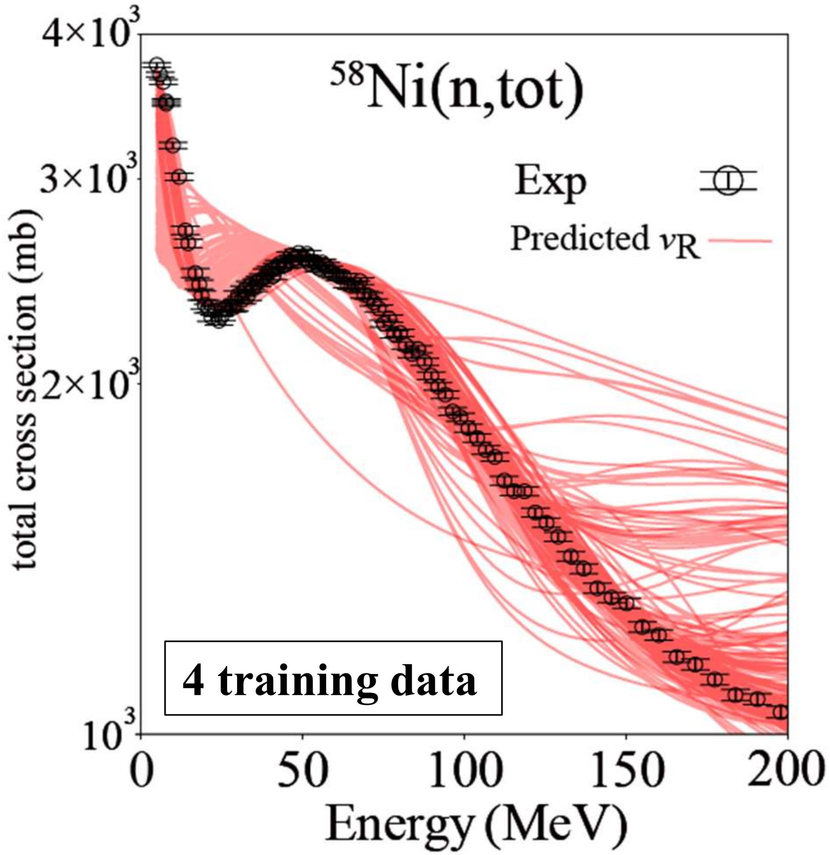

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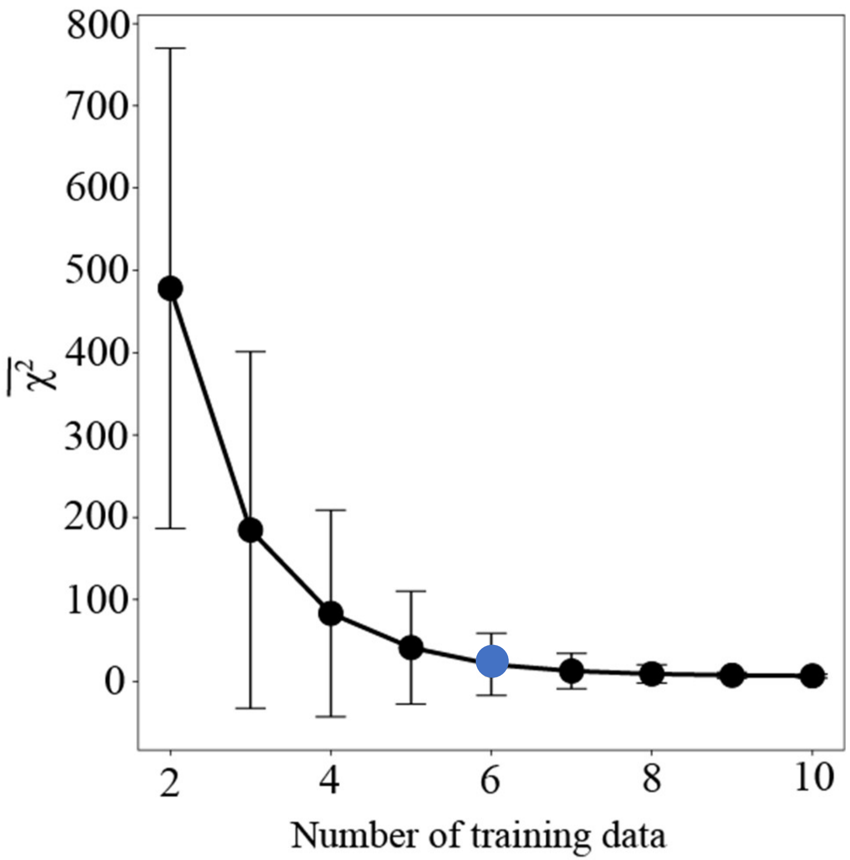

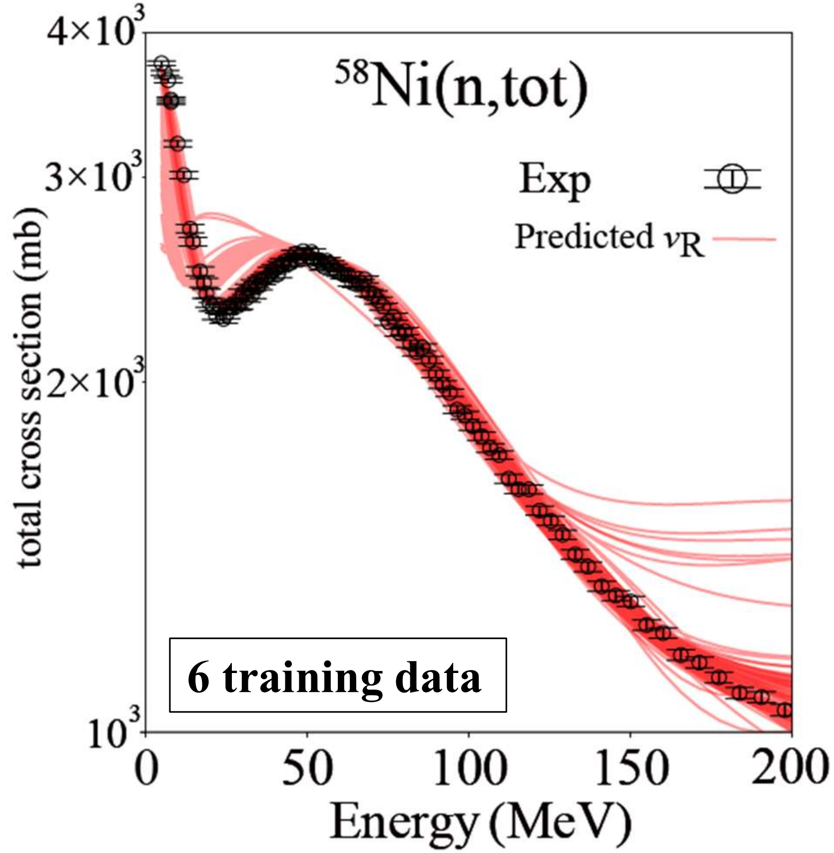

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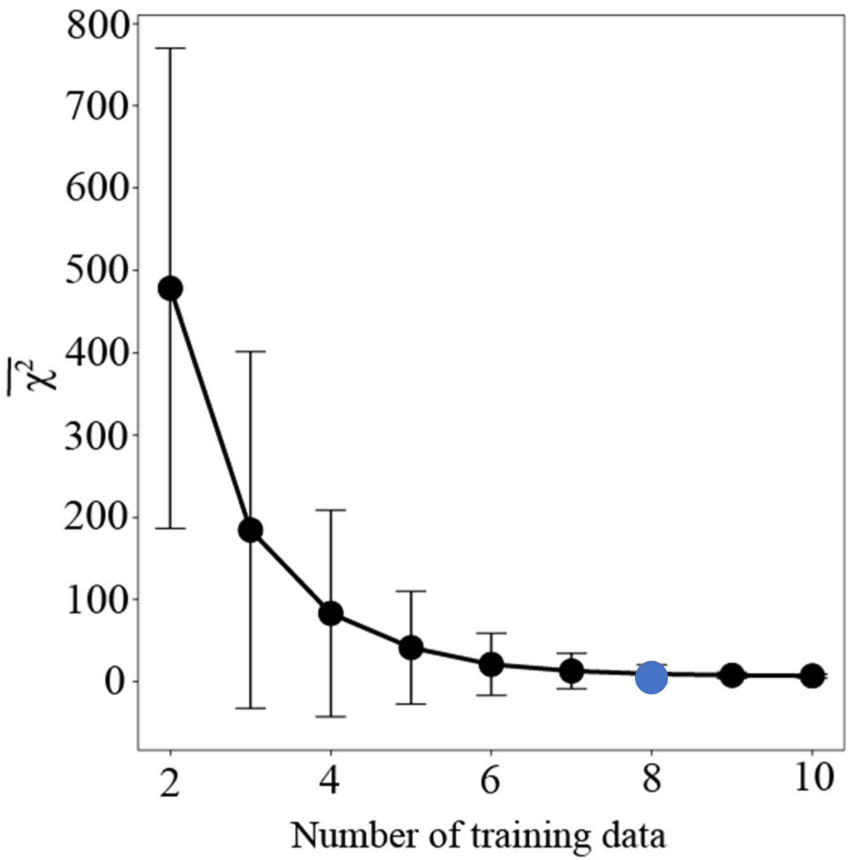
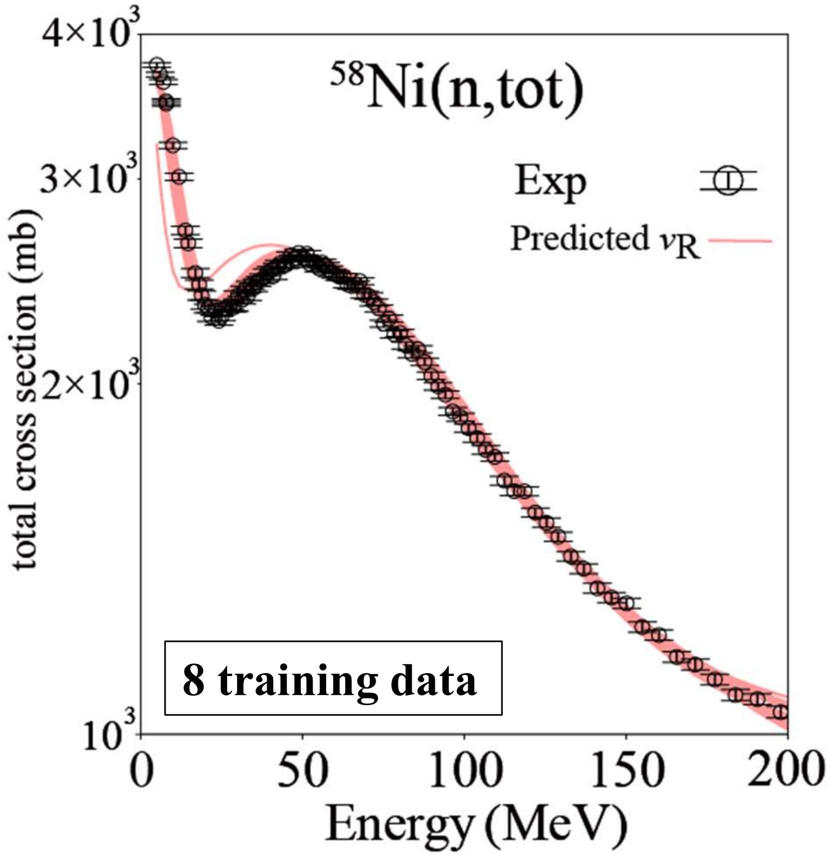
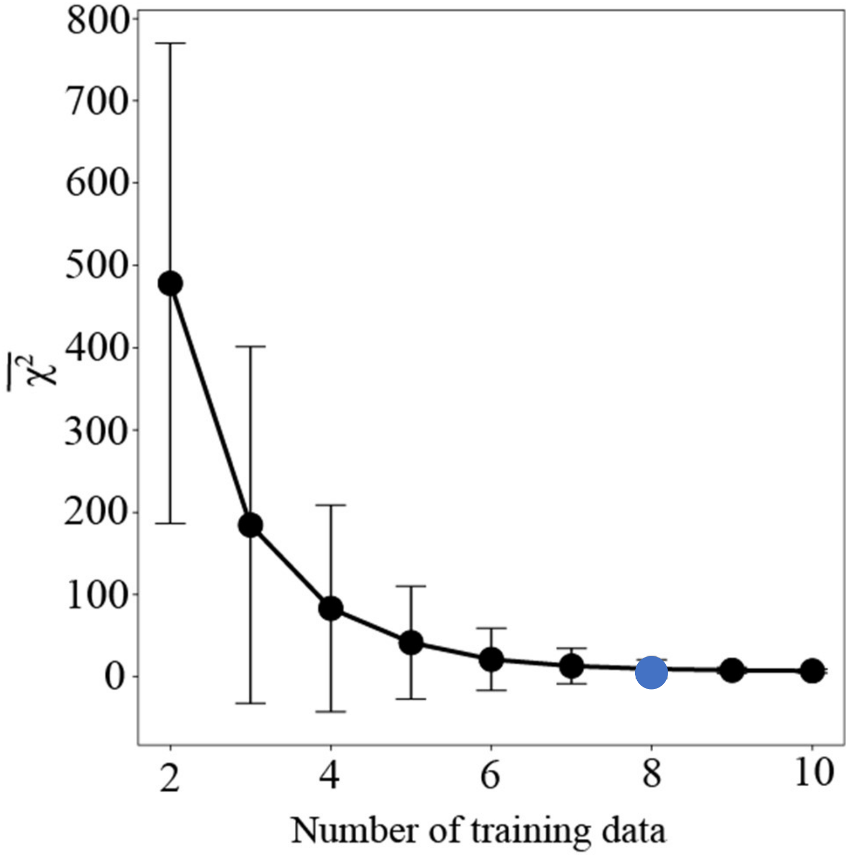
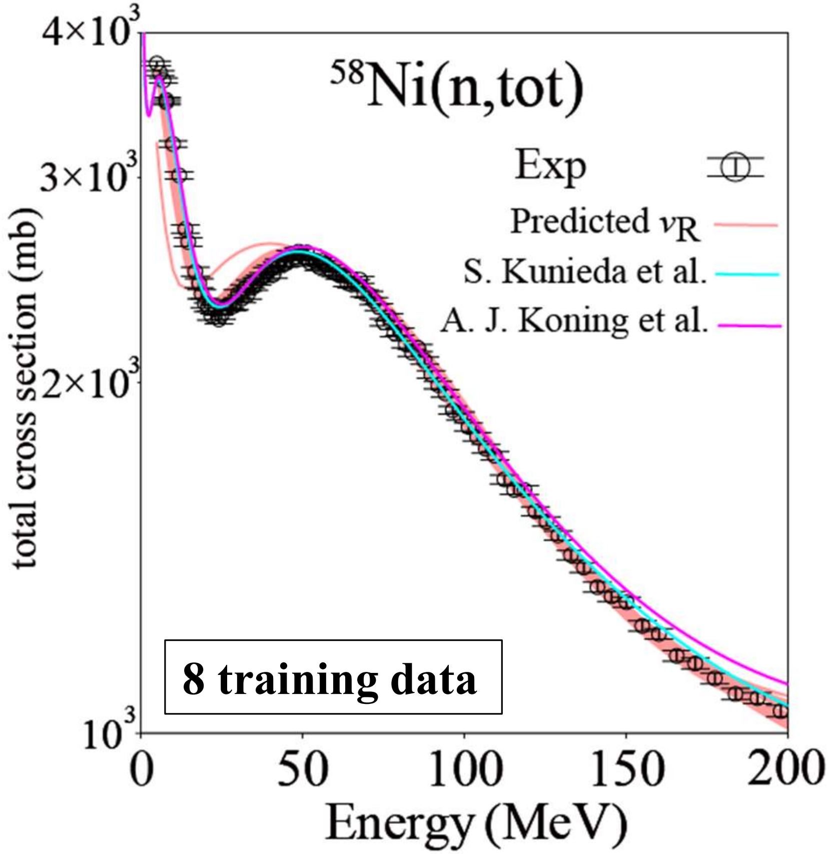




Result 2: ^{58}Ni(n,tot) cross section

◆ No matter how the training data was taken, with 8 points, the cross section could be reproduced with the same accuracy as S. Kunieda and A. J. Koning





Summary & Future work

○Combining machine learning and nuclear reaction models to find the optimum value of $v_R\ (E)$ that reproduces the experimental data

○By using the obtained optimum value as training data, the optimum value of $v_R\ (E)$ at any energy could be obtained

○By estimating $v_R\ (E)$ with more than 7 training data, we were able to reproduce the cross section with the same accuracy as S. Kunieda and A. J. Koning

●Future work will also aim to estimate multiple dependencies of a large number of parameters