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Predictions of $(n, 2n)$ reaction cross section based on a Bayesian neural network approach

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01

Introduction



Introduction



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◆ The (n, 2n) reaction is one of the most common reaction channels for neutron nuclear reactions. It is widely used in **neutron sources**, **neutron scattering** experiments, and **neutron irradiation** studies.

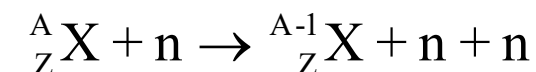
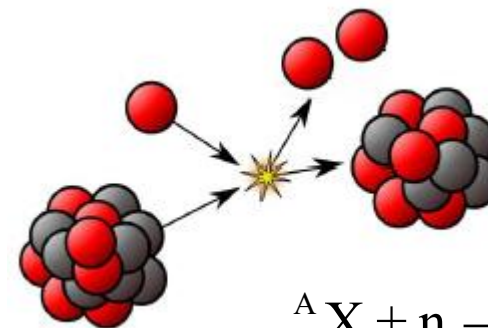
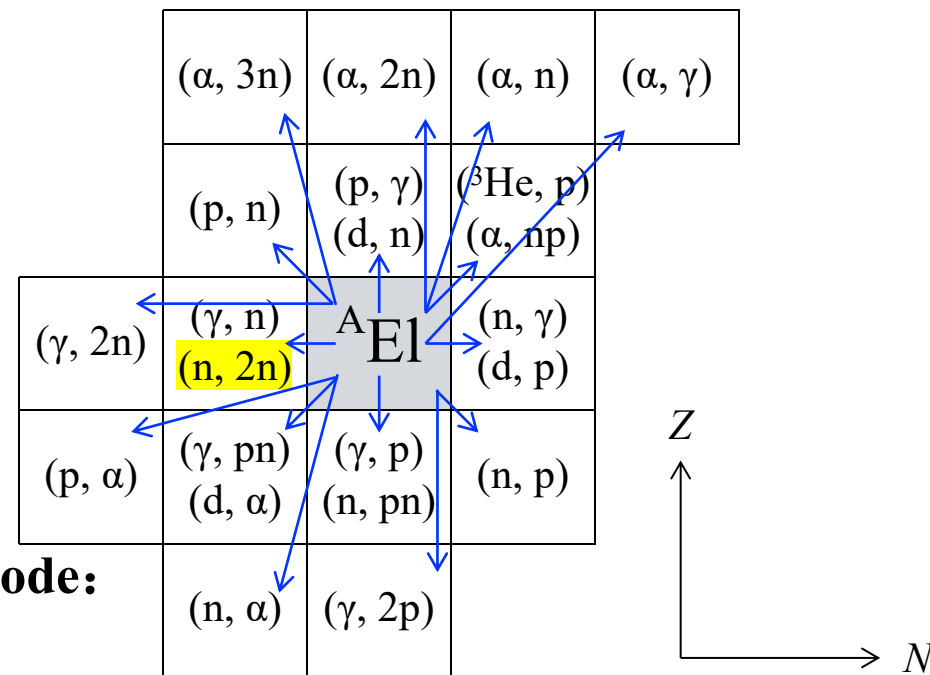
Luo2022EPJA, Kolos2022PRR

Major Nuclear Libraries:

- 1) ENDF/B-VIII.1 (USA, 2024)
- 2) JEFF-3.3 (Europe, 2017)
- 3) JENDL-5 (Japan, 2021)
- 4) CENDL-3.2 (China, 2020)
- 5) BROND-3.1 (Russia, 2016)

Theory-based computer code:

- 1) Talys (Netherlands)
- 2) Empire (USA)
- 3) CCONE (Japan)
- 4) UNF series (China)
- 5)





Introduction



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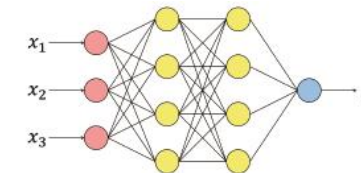
Machine learning in nuclear decays and reactions

- ▲ α -decay half-lives [Saxena2021JPG](#), [Ma2021CPC](#)
- ▲ β -decay half-lives [Niu2019PRC](#), [Li2024JPG](#)
- ▲ Fission yields [Wang2019PRL](#), [Qiao2021PRC](#)
- ▲ Cross-sections in proton induced spallation reactions [Ma2020CPC](#)
- ▲ Neutron-nucleus scattering data [Liang2021Thesis](#)
- ▲ Fusion reaction cross-sections [Akkoyun2020NIMB](#)
- ▲

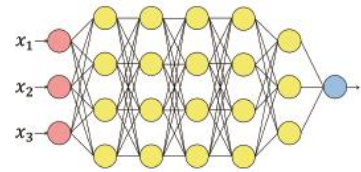
Machine learning in nuclear structure

- ▲ Masses [Niu2018PLB](#), [Niu2022PRC](#), [Wu2022PLB](#)
- ▲ Nuclear spins and parities [Gernoth1993PLB](#), [Clark2006IJMPB](#)
- ▲ charge radii [Wu2020PRC](#), [Ma2020PRC](#), [Dong2023PLB](#)
- ▲ excited states [Bai2021PLB](#), [Wang2021PRC](#), [Wang2022PLB](#)
- ▲

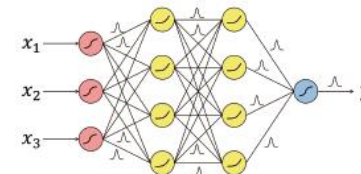
▲ ANN



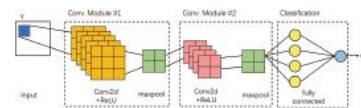
▲ DNN



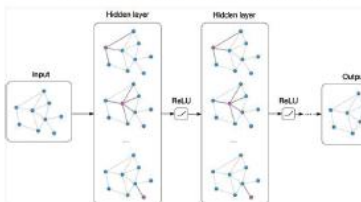
▲ BNN



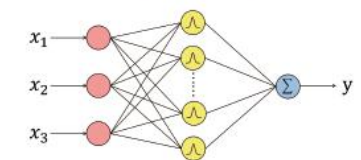
▲ CNN



▲ GNN



▲ RBF



▲

The Figure are taken from [He2023SCPM](#).



02

Theoretical framework

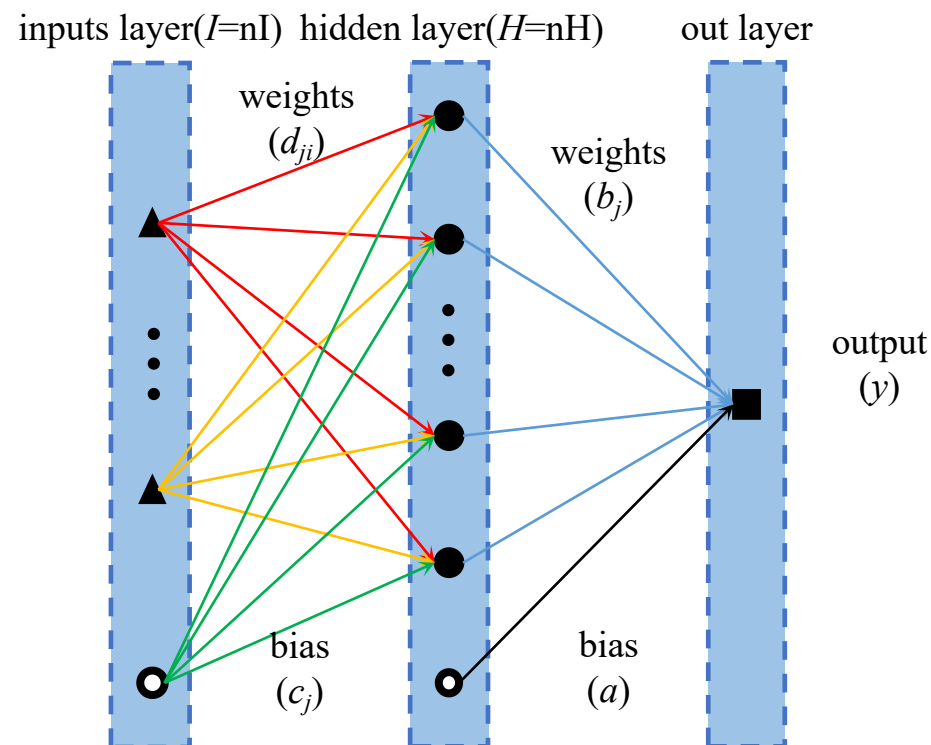


Theoretical framework



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$$y(x, \omega) = a + \sum_j^H b_j \tanh \left(c_j + \sum_{i=1}^I d_{ji} x_i \right)$$

Networks	Input variables	H	Function	Output
BNN-I3	$Z, N, \Delta E$	210	Tanh	σ
BNN-I4 δ	$Z, N, \Delta E, \delta$	175	Tanh	σ
BNN-I4 σ	$Z, N, \Delta E, \sigma_{th}$	175	Tanh	σ
BNN-I5	$Z, N, \Delta E, \delta, \sigma_{th}$	150	Tanh	σ

Z : Proton number;

N : Neutron number;

ΔE : Incident energy – Reaction threshold;

δ : 1, 0, -1 for even-even nuclei, odd- A nuclei, and odd-odd nuclei, respectively;

σ_{th} : Theoretical value of the reaction cross-section.

taken from TENDL-2021



Theoretical framework



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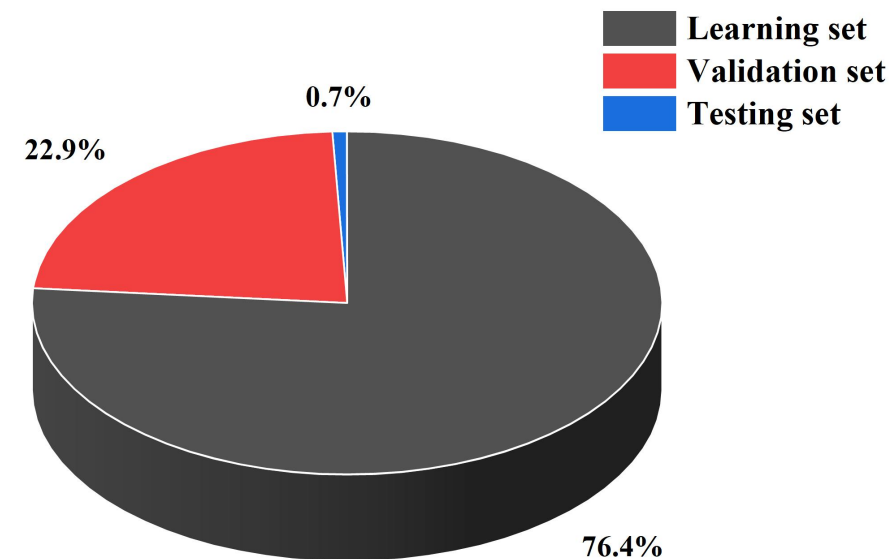
★**Total set:** $Z = 8 - 100$ nuclei region in the energy range from threshold to the region for which data are available or up to 20 MeV. (**519** nuclei, **11349** cross-section data)

All data taken from ENDF/B-VIII.0

★**Testing set:** **85** cross-section data of ^{115}Ag , ^{139}Ba , ^{178}Hf and ^{248}Cm ;

★**Learning set:** No more than 20 cross-section data were randomly selected for each nucleus. (**8666** cross-section data)

★**Validation set:** The remaining **2598** cross-section data.





03

Results and discussion



Results and discussion



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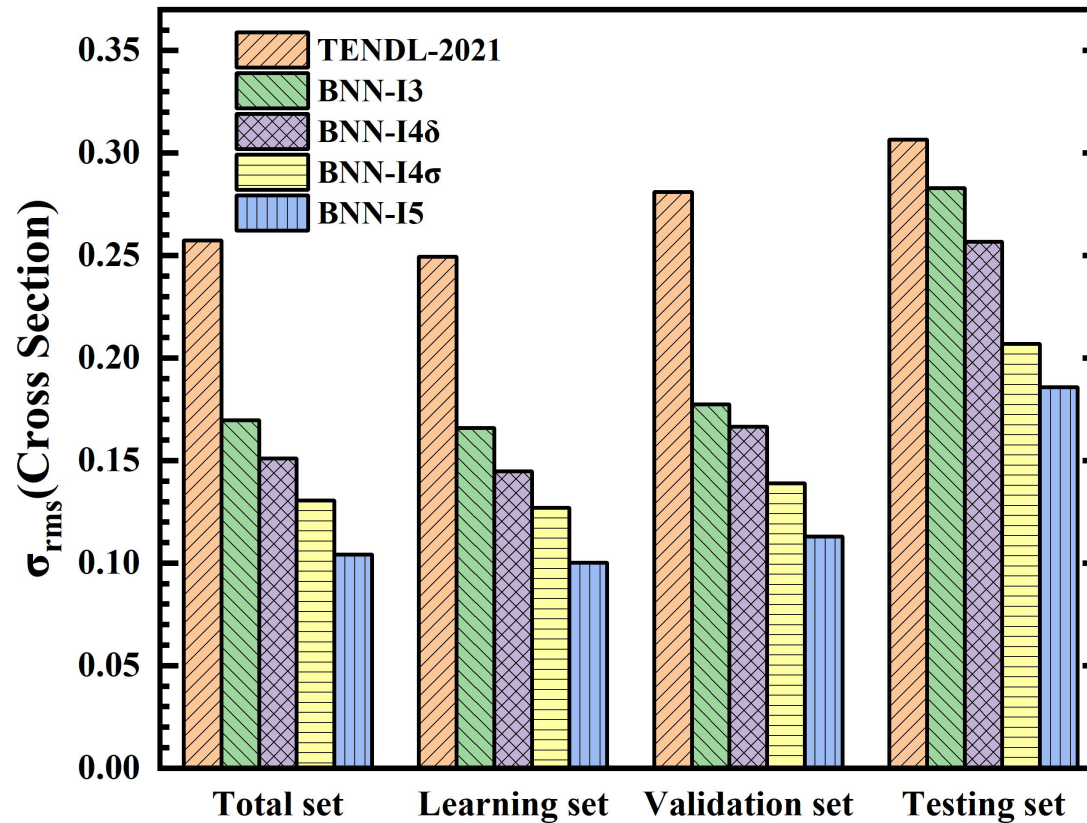


Fig. 1 The rms deviations σ_{rms} (Cross Section) of different BNN predictions with respect to the evaluation data of (n, 2n) reaction cross sections for the total set, learning set, validation set, and testing set.

- ◆ BNN method describes the (n, 2n) reaction cross section with significantly **higher accuracy** than the traditional TALYS approach.
- ◆ Adding relevant physical quantities to the input of the neural network can improve the prediction accuracy of the network to some extent.

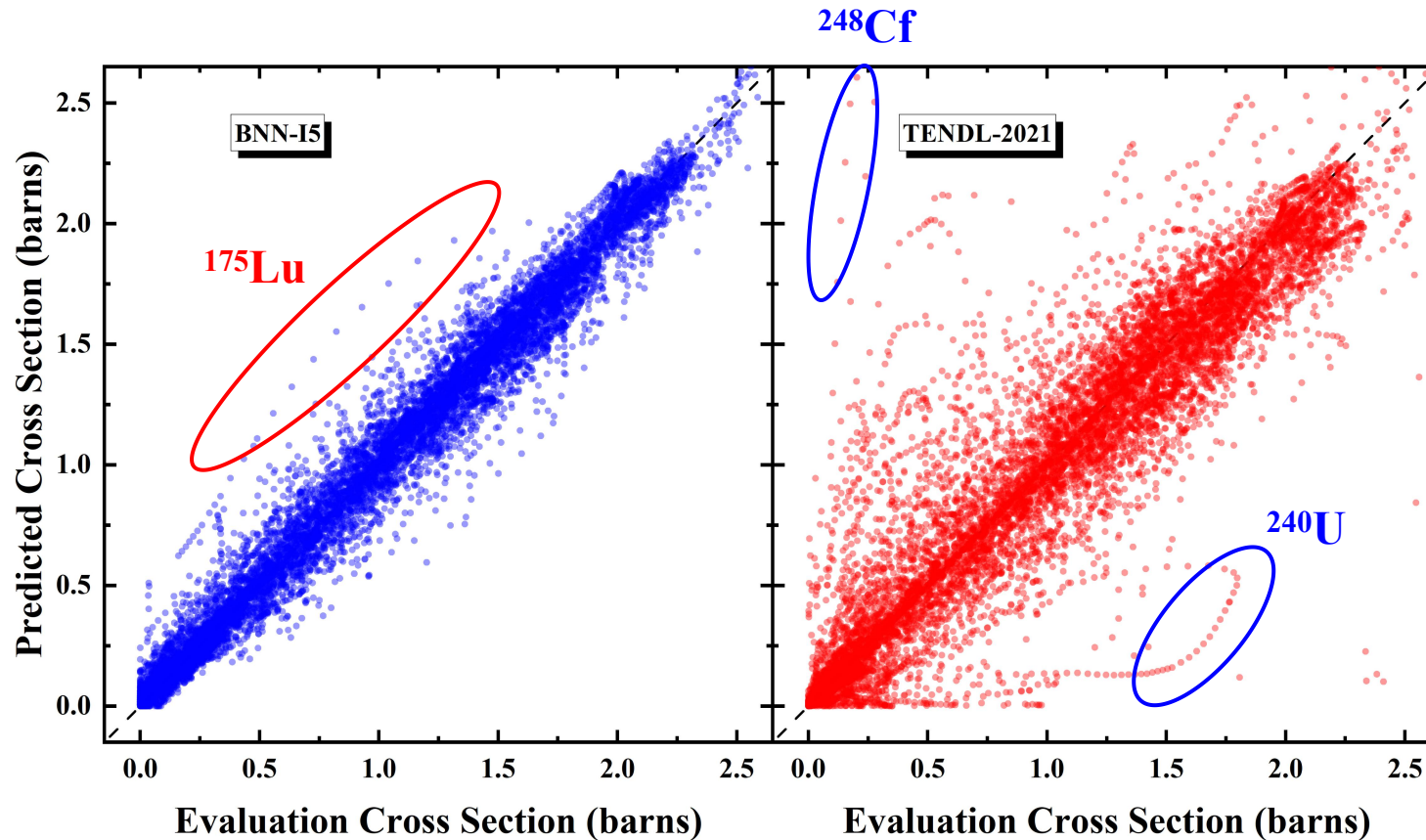


Results and discussion



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◆ The BNN-I5 predictions are in general agreement with the evaluation data for the (n, 2n) cross section and provide better correlation and stability than TENDL-2021.

Fig.2 Scatter distribution of the (n, 2n) reaction cross sections predicted by BNN-I5 approach and TENDL-2021 as a function of the evaluation data.

Results and discussion

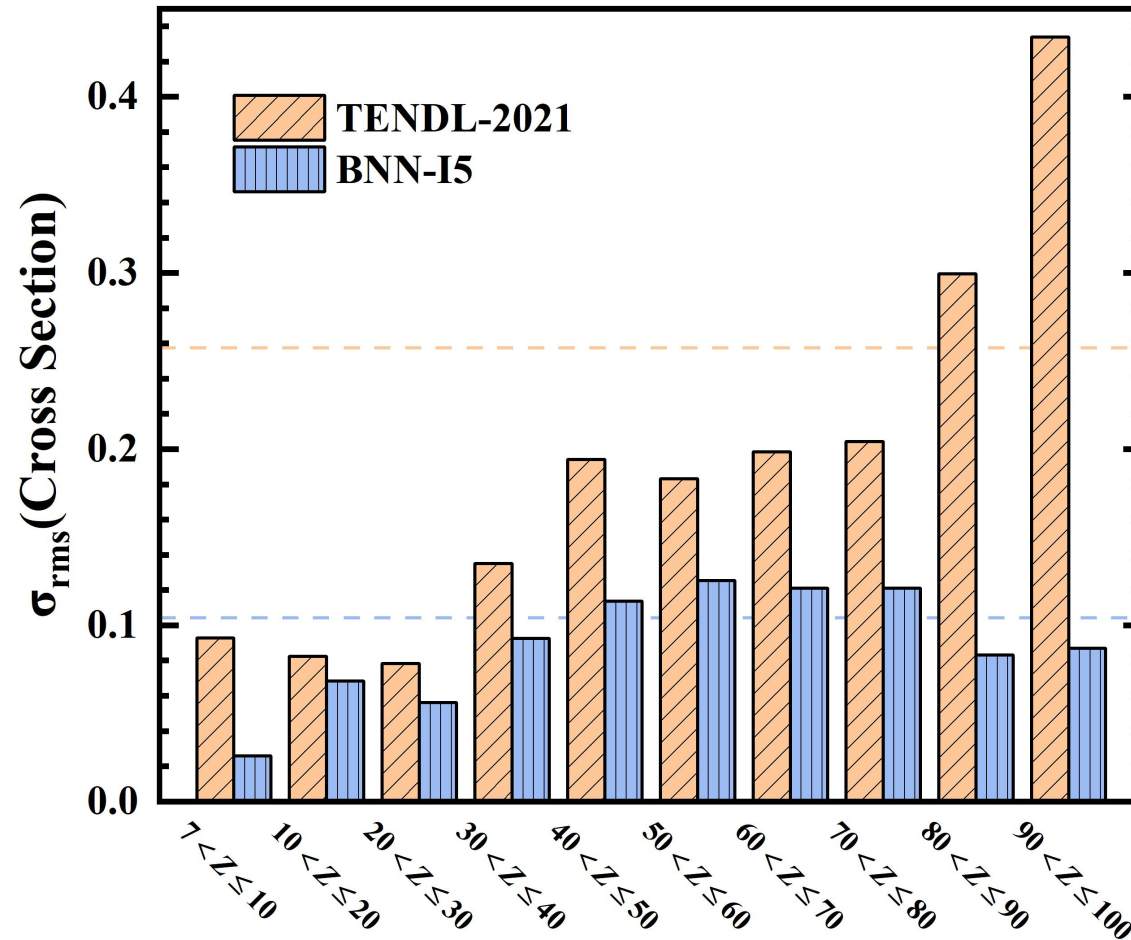


Fig. 3 The rms deviations σ_{rms} (Cross Section) of cross section predictions by BNN-I5 and TENDL-2021 with respect to the evaluation data in different nuclear regions.

◆ The description of the (n, 2n) reaction cross section by TENDL-2021 gets progressively worse with increasing proton number.

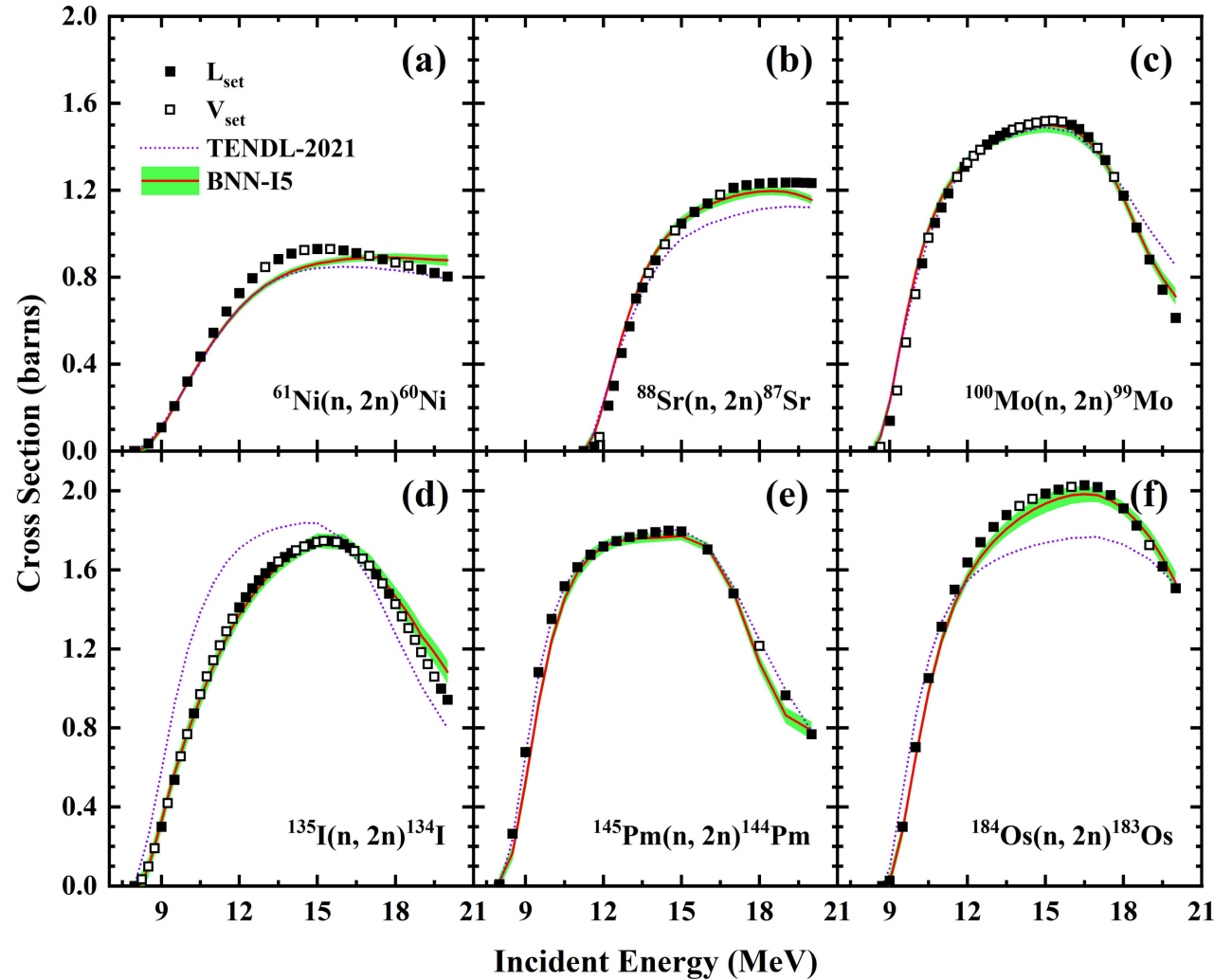
◆ The ability of the neural network to predict the (n, 2n) reaction cross section for $30 < Z \leq 80$ nuclei is relatively weak, but it is still a large improvement compared to the results of TENDL-2021.

Results and discussion



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◆ The BNN-I5 approach has a better ability to describe the (n, 2n) reaction excitation function than TENDL-2021.

◆ The BNN-I5 approach reproduces the (n, 2n) reaction cross section well for both the **learning and validation sets**.

Fig. 4 The (n, 2n) reaction cross sections predicted by the BNN-I5 approach for ^{61}Ni , ^{88}Sr , ^{100}Mo , ^{135}I , ^{145}Pm , and ^{184}Os .



Results and discussion



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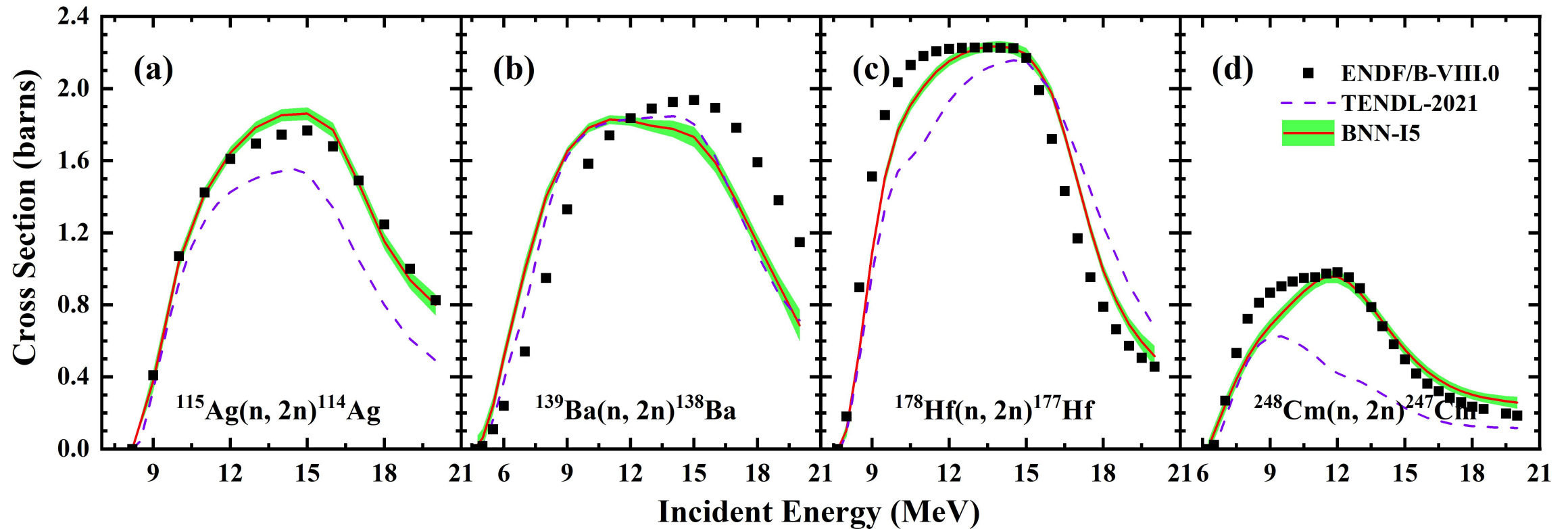


Fig. 5 Same as Fig. 4 but for ^{115}Ag , ^{139}Ba , ^{178}Hf and ^{248}Cm .

◆ The predictive ability of the BNN-I5 approach is also better than that of TENDL-2021 in the **testing set**.

Results and discussion



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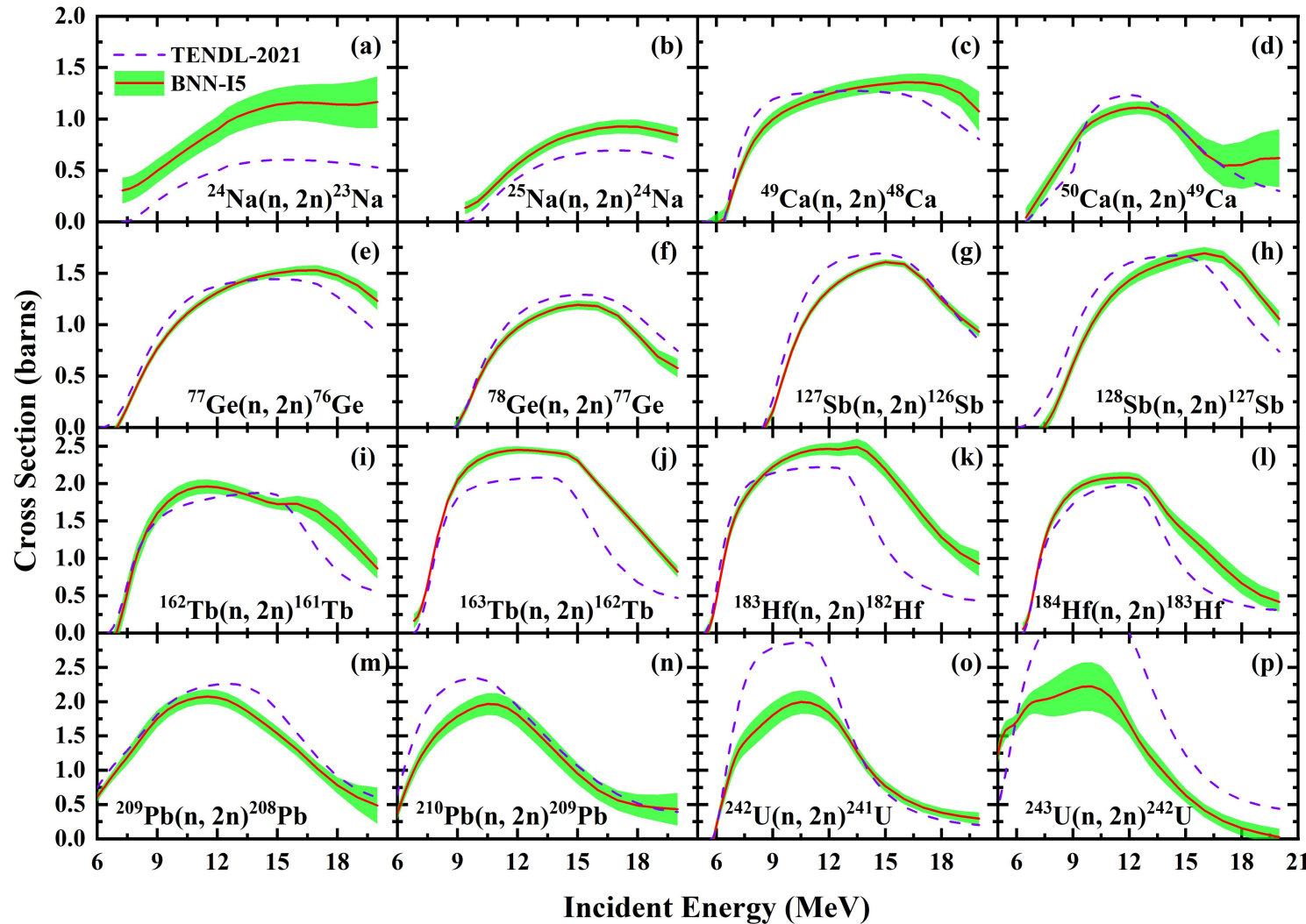


Fig.6 Comparison of the (n, 2n) reaction cross sections from BNN-I5 predictions and TENDL-2021 for various nuclei.

◆ The BNN-I5 approach can well reflect the variation trend of these unknown nuclei (n, 2n) reaction cross section with the incident energy.

◆ The BNN-I5 approach has good extrapolation ability.



Results and discussion



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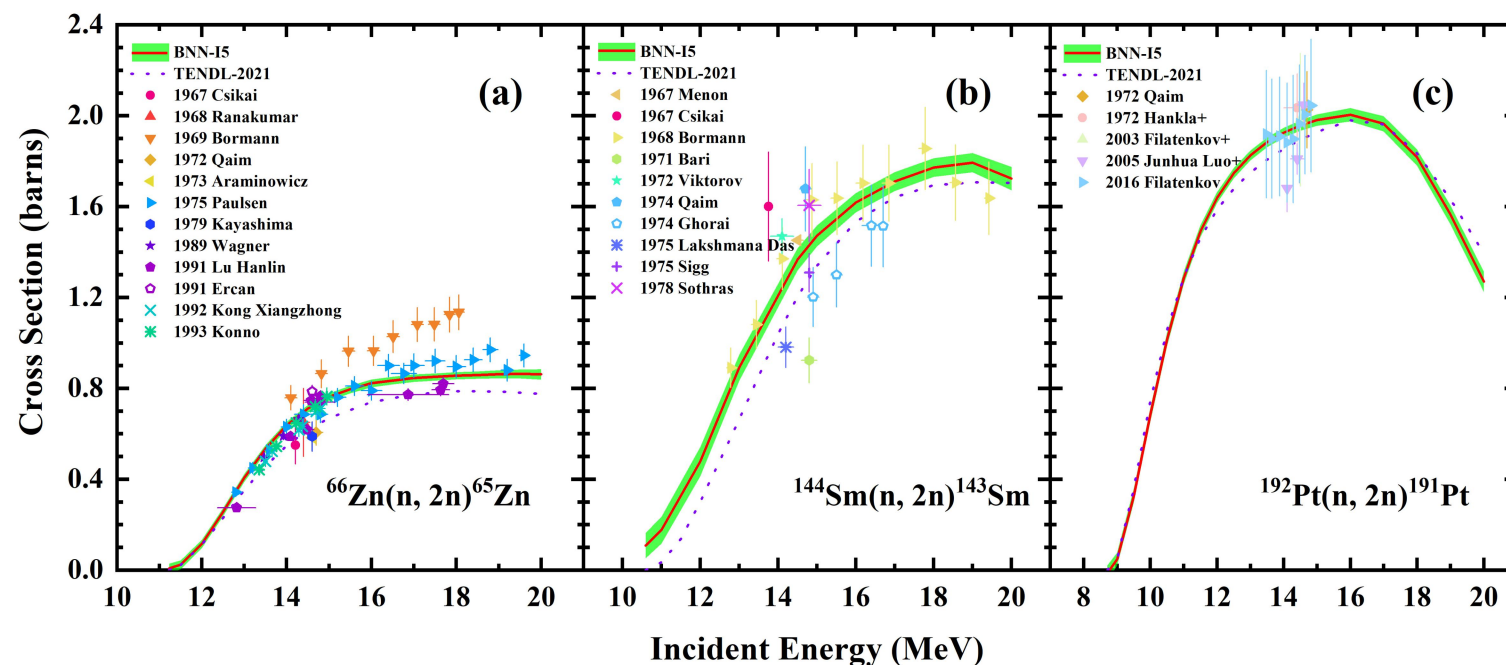


Fig. 7 Comparison of the (n, 2n) reaction cross sections from BNN-I5 predictions with the original experimental data for ^{66}Zn , ^{144}Sm , and ^{192}Pt .

◆ The experimental data from different groups can have significant deviations and may even not agree within the uncertainties.

◆ Near the incident energy of **14.6 MeV**, the BNN-I5 results are in high agreement within the margin of experiment error.



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Summary and perspectives



The nuclear (n, 2n) reaction cross section are investigated and give reasonable uncertainty evaluations with the BNN approach.

- ★ Five physical quantities, including Z , N , ΔE , δ , and σ_{th} , were identified as the best neural network inputs to describe the (n, 2n) reaction excitation function.
- ★ The BNN-I5 approach reproduces the (n, 2n) reaction cross section well for both the learning, validation and **testing sets**.
- ★ When extrapolated to the unknown region, the BNN approach can still well describe the **trend of first increasing and then decreasing** for the (n, 2n) reaction excitation functions with the incident neutron energy predicted by TENDL-2021.



Futtrue perspectives



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In the future, the approach will be extended to more reaction channels and more nuclear regions to provide more data for nuclear reaction studies.

Thank You!

