1，1D-CNN specific parameters

Table S1 Parameters of the 1D-CNN module

	Detail parameters
Input layer	2024 × 1
CNN module	Numbers of layers: 3
	Size of kernels: 3 × 1
	Number of kernels: 64
Pooling layer	Max pooling
	Pool size: 2 × 1
Activation function	ReLU
FC layer	128
Optimizer	Adam optimzer
Intial learning rate	9E-5
Loss function	MSE loss
Epoch	500
Batch size	32
Pruning strategy	agnitude-based pruning
keep ratio	85%

2，Results of the SHAP analysis, showing the top five features with the highest scores, along with their corresponding spectral lines identified based on the NIST public database.

Table S2 Representative wavelengths with high SHAP contributions and their corresponding spectral line assignments under laboratory-data-based and simulation-data-based transfer learning.

Laboratory Data Transfer Learning			Simulate Data Transfer Learning		
Wavelength (nm)	SHAP	Line assignment	Wavelength (nm)	SHAP	Line assignment
306.651	0.064964	Ni I	308.724	0.035009	Ni I
308.724	0.053419	Ni I	308.493	0.029569	Ni I
308.493	0.052537	Ni I	307.342	0.028988	Ni I
308.954	0.049379	Ni I	309.184	0.021786	Ni I
307.342	0.047232	Ni I	310.795	0.018548	Ni I
343.805	0.048175	Mo I	344.033	0.062365	Mo I
344.033	0.040939	Mo I	343.805	0.044766	Mo I
344.262	0.028611	Mo I	344.262	0.043976	Mo I
444.791	0.025539	Mo I	343.348	0.032474	Mo I

578.878	0.024646	Mo I	396.888	0.025548	Mo I
334.661	0.036402	Ti II	334.661	0.023718	Ti II
444.791	0.030545	Ti II	531.457	0.023612	
458.549	0.021487		519.533	0.020457	Ti I
444.124	0.020863	Ti II	322.515	0.016199	Ti II
333.975	0.020007	Ti II	343.805	0.013717	

3，This figure illustrates that, for the laboratory device, effective spectral data cannot be obtained in the region where the two spectral channels overlap.

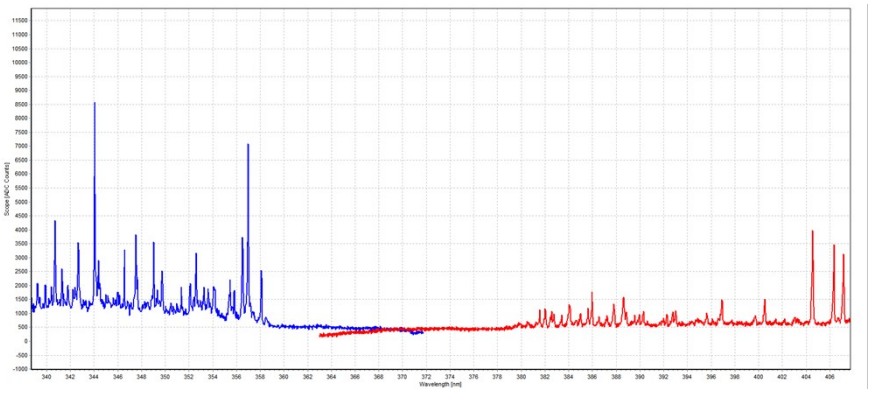


Fig S1 Sample spectrum acquired by the laboratory spectrometer, where blue and red curves correspond to channel 1 and channel 2.

4，This figure presents the SHAP scores obtained under three different conditions: (i) the SHAP scores of the model trained using the full spectral range, (ii) the SHAP scores of the model trained after removing the spectral data in the 360–380 nm range, and (iii) the SHAP scores of the model trained after removing the spectral regions around the Fe-related spectral peaks. along with the corresponding table of regression coefficients.

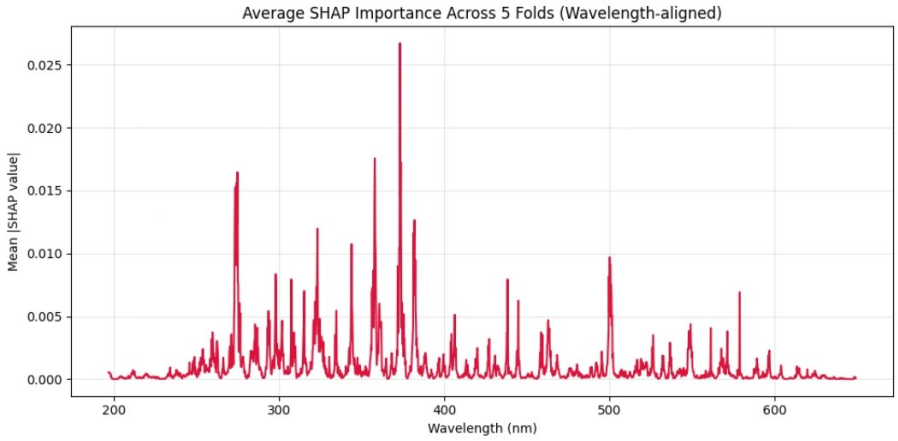


Fig S2 SHAP spectral contribution distributions for Ni

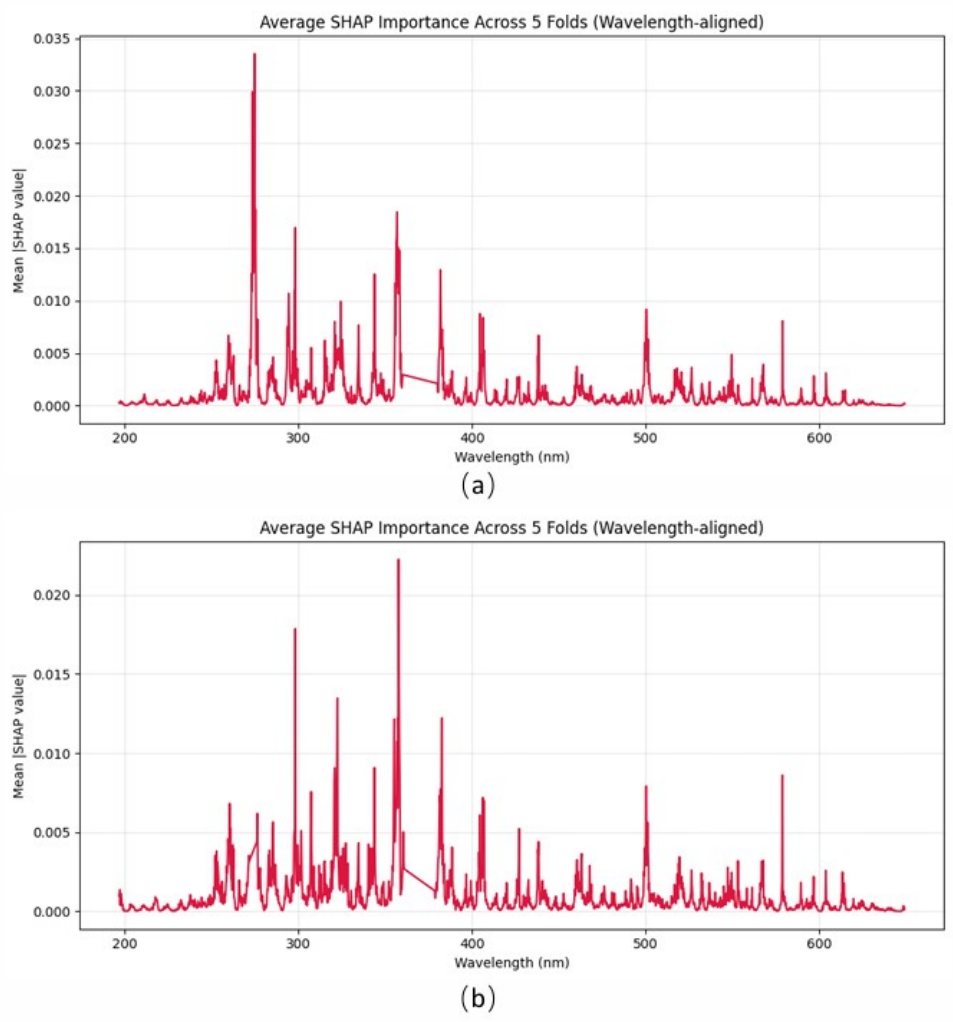
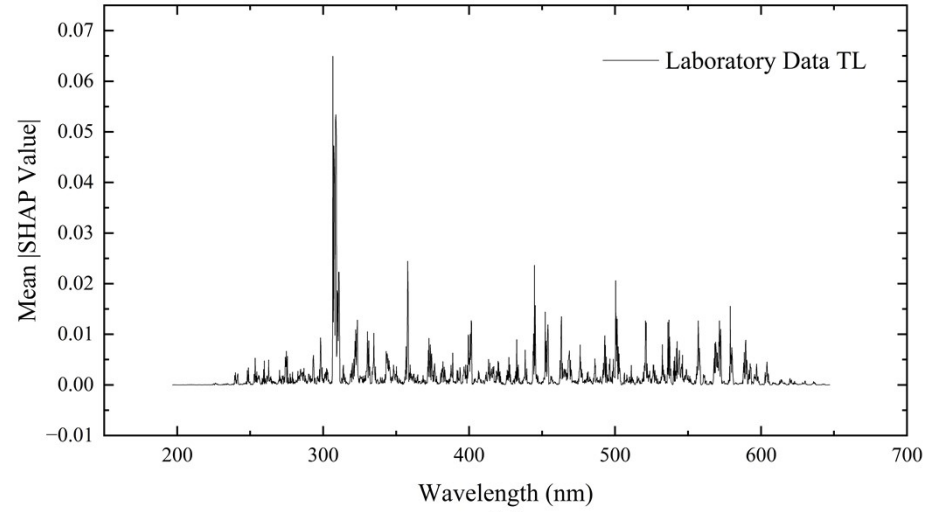


Fig S3 (a)-(b) SHAP spectral contribution distributions for Ni :(a) removing the 360–380 nm wavelength. (b) removing spectral regions associated with the Fe element.

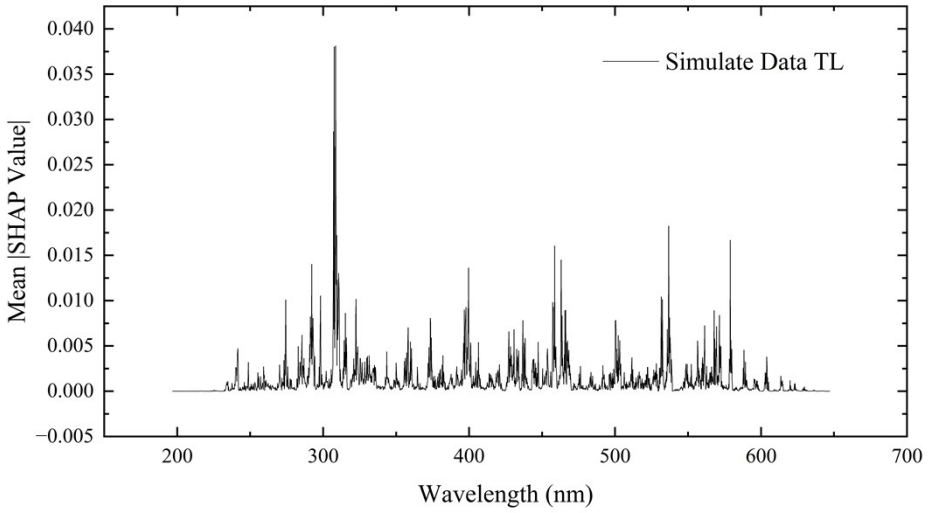
Table S3 Comparison table of regression coefficients

Methods	$R_{cv}{}^2$	$RMSE_{cv}$ (wt.%)
Full spectrum	0.743	0.066
Remove (i)	0.801	0.058
Remove (ii)	0.819	0.052

5，This figure shows the SHAP score results corresponding to the two transfer learning approaches.



(a)



(b)

Fig S4 (a-b) SHAP Spectral Contributions for Ni (a) Laboratory Data Transfer Learning. (b) Simulate Data Transfer Learning