

Supplementary Information

Machine Learning for Accelerated Prediction of Size Distributions of Spherical Nanoparticles from Small-Angle X-ray Scattering

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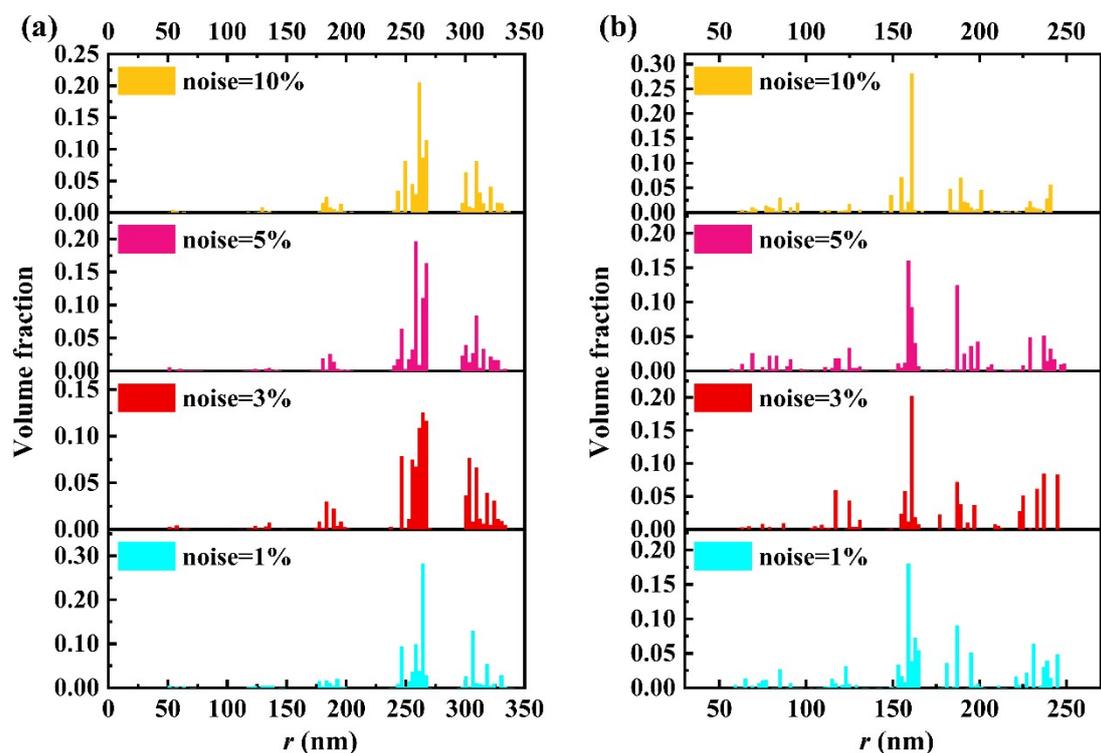


Figure S1. FNN-predicted PSDs under four different noise levels 1%, 3%, 5%, 10% for (a) SiO_2 and (b) polystyrene.

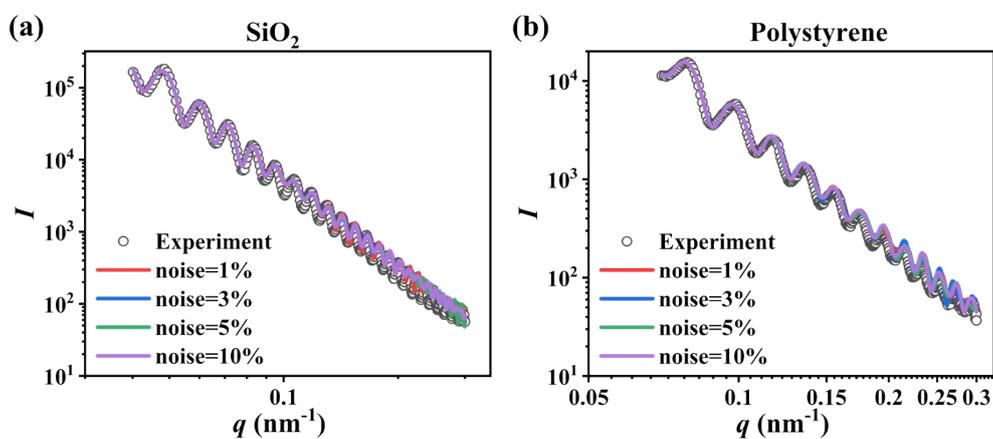


Figure S2. Reconstructed scattering curves from FNN-predicted PSDs under four different noise levels 1%, 3%, 5%, 10% for (a) SiO_2 and (b) polystyrene.

Table S1. Accuracy of fitting scattering curves and the computation time under different noise levels.

Sample	Noise level	R^2	MRE	Time (ms)
SiO ₂	1%	0.9954	0.06401	55.3
	3%	0.9952	0.06528	49.4
	5%	0.9947	0.06857	51.4
	10%	0.9951	0.06568	52.0
Polystyrene	1%	0.9970	0.04885	56.5
	3%	0.9973	0.04638	50.1
	5%	0.9971	0.04795	53.5
	10%	0.9969	0.04975	53.8

Table S2. Accuracy and computational time of the FNN model with varying sizes of hidden layers using simulated SAXS data.

Hidden layer 1 -Hidden layer 2	Average Time (ms)	PSD		SAXS data	
		R^2	MRE	R^2	MRE
512-256	49.2	0.9053	0.2138	0.9921	0.0846
1024-512	48.5	0.9168	0.1971	0.9917	0.0858
2048-1024	52.0	0.9192	0.2057	0.9992	0.0262
4096-2048	49.8	0.7306	0.4029	0.9992	0.0264

Table S3. Computational time of the FNN model with hidden layers 2048-1024 for PSD prediction with different numbers of peaks.

Numbers of Peaks	Average Time (ms)
1	49.9
2	50.6
3	50.6
4	50.3

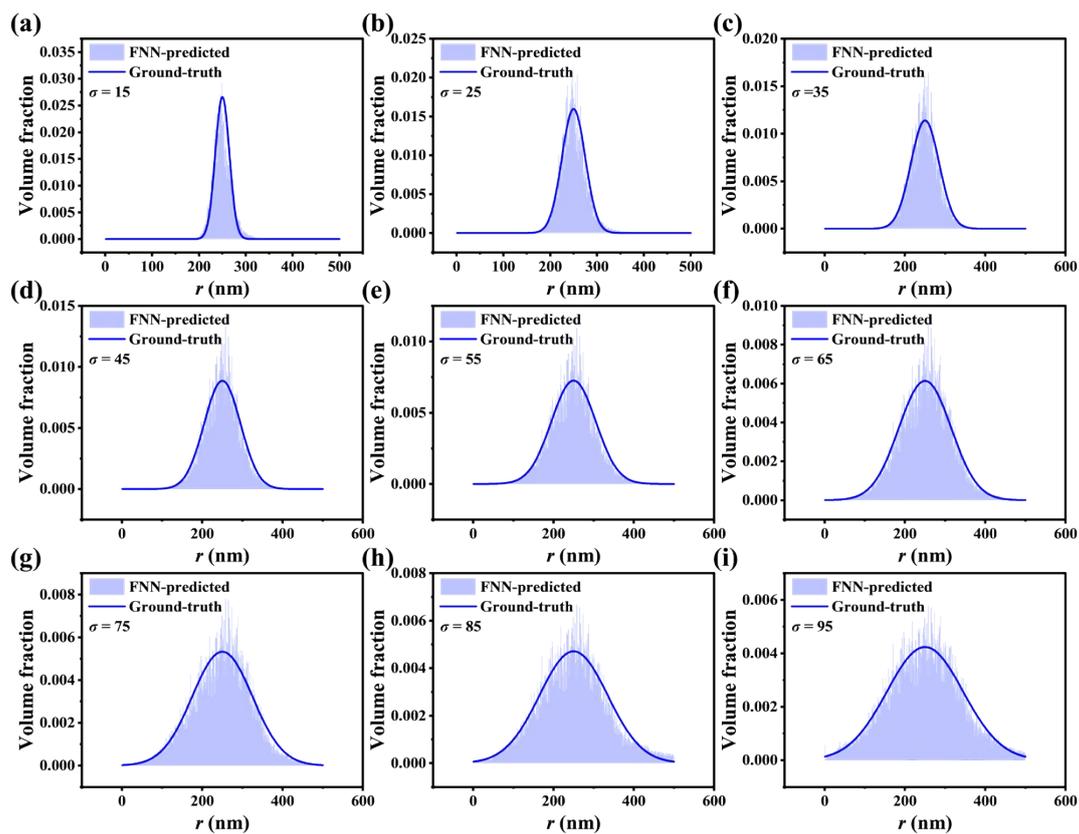


Figure S3. Comparison of FNN-predicted and ground-truth PSDs under different peak broadening conditions. The peak position is 250 nm and the Gaussian standard deviations (σ) for ground-truth PSDs (a)-(i) are 15, 25, 35, 45, 55, 65, 75, 85, 95, respectively.

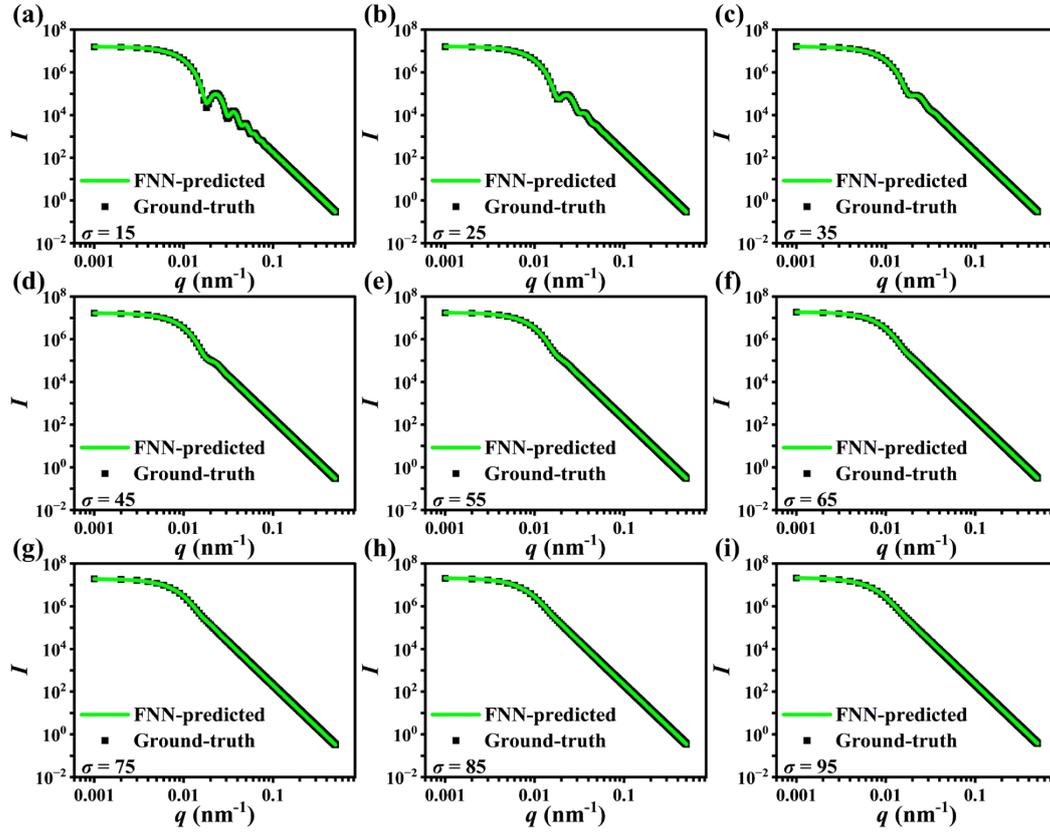


Figure S4. Comparison of FNN-generated and ground-truth SAXS curves under different peak broadening conditions. The peak position is 250 nm and the Gaussian standard deviations (σ) for ground-truth PSDs (a)-(i) are 15, 25, 35, 45, 55, 65, 75, 85, 95, respectively.

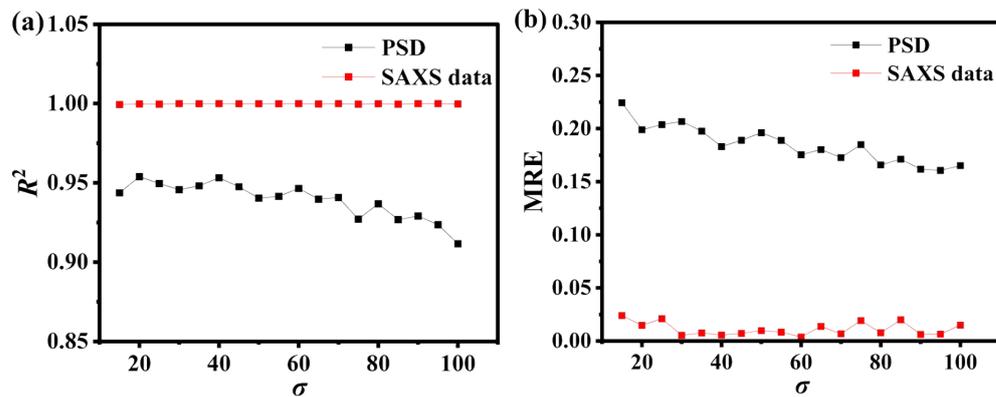


Figure S5. (a) R^2 and (b) MRE of the FNN model for predicting PSD and reconstructing SAXS curves under different peak broadening conditions.