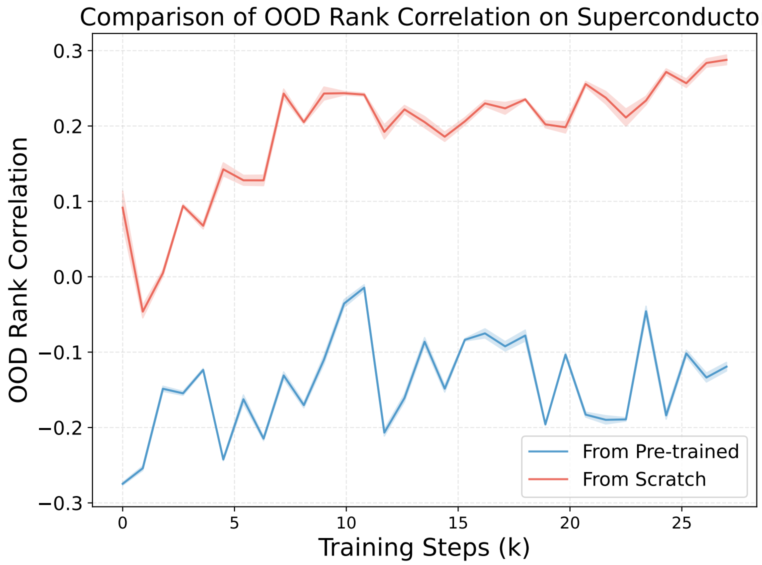

Figure 1. Comparison of OOD Spearman rank correlation on Superconductor task between UniSO-N from pre-trained embedder (blue) and from scratch (red). The OOD dataset is constructed following Chen et al. (2023). Higher correlation indicates better surrogate model for offline BBO (Tan et al., 2025).

Table S1. Computational resources comparison between improved UniSO-N and UniSO-T. All measurements are conducted on a machine with 4 RTX 4090 D GPUs and AMD EPYC 9754 128-Core Processor.

	Training	Search (one task)	GPU memory
UniSO-N	22530s	44s	21G
UniSO-T	71225s	203s	89G

Table S2. Ablation studies on different metadata components (name, description, and objective) on various tasks. All experiments are conducted based on improved UniSO-T. The first part includes tasks appearing in training dataset, i.e., unconstrained tasks from Design-Bench and SOO-Bench. The remaining two parts contain unseen tasks during training, where we compare them under both zero-shot and few-shot settings. The best and runner-up results on each task are **Blue** and **Violet**. $\mathcal{D}$(best) denotes the best score in the offline dataset.

Task	$\mathcal{D}$(best)	UniSO-T	w/o name	w/o desc.	w/o obj.	w/o metadata
Ant	165.326	**374.665 ± 56.057**	345.369 ± 40.675	362.842 ± 33.008	**363.812 ± 59.380**	358.379 ± 64.211
D'Kitty	199.363	225.752 ± 8.521	**235.715 ± 11.617**	226.479 ± 15.311	**245.135 ± 15.571**	227.169 ± 12.278
Superconductor	74.000	92.200 ± 15.209	85.207 ± 6.261	**99.113 ± 12.742**	**97.610 ± 10.297**	90.871 ± 10.611
TF Bind 8	0.439	0.903 ± 0.041	**0.954 ± 0.025**	0.935 ± 0.041	0.937 ± 0.012	**0.950 ± 0.025**
TF Bind 10	0.005	**0.823 ± 0.542**	**0.696 ± 0.126**	0.664 ± 0.141	0.596 ± 0.148	0.651 ± 0.121
GTOPX 2	-195.586	**-72.848 ± 9.576**	-97.806 ± 40.646	**-63.670 ± 20.381**	-80.789 ± 8.908	-79.864 ± 13.338
GTOPX 3	-151.190	**-45.602 ± 8.433**	-50.788 ± 8.706	**-45.981 ± 4.211**	-50.660 ± 10.713	-48.178 ± 12.638
GTOPX 4	-215.716	-84.271 ± 8.307	-84.962 ± 11.300	-92.163 ± 9.529	**-75.233 ± 5.734**	**-79.887 ± 14.729**
GTOPX 6	-112.599	-47.794 ± 11.943	**-42.181 ± 11.671**	**-45.591 ± 12.310**	-48.050 ± 13.901	-45.764 ± 7.685
RobotPush (zero-shot)	0.102	**3.171 ± 0.984**	2.747 ± 1.455	**3.416 ± 1.455**	2.634 ± 0.953	2.517 ± 1.640
Rover (zero-shot)	-16.148	**-8.888 ± 2.119**	-11.009 ± 0.598	-10.854 ± 0.859	**-9.099 ± 2.202**	-9.089 ± 3.070
LunarLander (zero-shot)	7.038	**31.186 ± 27.971**	30.105 ± 57.577	30.892 ± 54.657	**52.108 ± 47.941**	6.251 ± 53.042
RobotPush (few-shot)	0.102	**7.067 ± 0.169**	7.026 ± 0.219	**7.129 ± 0.486**	6.310 ± 1.677	6.155 ± 1.495
Rover (few-shot)	-16.148	**-8.239 ± 1.270**	-8.850 ± 0.703	**-8.084 ± 0.569**	-8.342 ± 1.573	-10.511 ± 2.070
LunarLander (few-shot)	7.038	**248.573 ± 45.386**	226.726 ± 65.244	**244.252 ± 38.329**	233.169 ± 51.037	233.919 ± 60.467
Avg. Rank	/	**2.333 ± 1.350**	3.600 ± 1.451	**2.467 ± 1.310**	3.067 ± 1.340	3.533 ± 1.087

Table S3. Ablation studies of loss balancing strategy in improved UniSO-T on unconstrained tasks from Design-Bench and SOO-Bench, where the better one is **Bold**. $\mathcal{D}$(best) denotes the best score in the offline dataset.

Task	$\mathcal{D}$(best)	UniSO-T w/ balance	UniSO-T w/o balance
Ant	165.326	**374.665 ± 56.057**	185.597 ± 165.661
D'Kitty	199.363	**225.752 ± 8.521**	203.553 ± 32.507
Superconductor	74.000	**92.200 ± 15.209**	79.635 ± 5.777
TF Bind 8	0.439	0.903 ± 0.041	**0.929 ± 0.049**
TF Bind 10	0.005	**0.823 ± 0.542**	0.696 ± 0.126
GTOPX 2	-195.586	**-72.848 ± 9.576**	-175.327 ± 73.053
GTOPX 3	-151.190	**-45.602 ± 8.433**	-56.221 ± 18.342
GTOPX 4	-215.716	**-84.271 ± 8.307**	-122.291 ± 54.913
GTOPX 6	-112.599	**-47.794 ± 11.943**	-70.352 ± 25.870
Avg. Rank	/	**1.111 ± 0.314**	1.889 ± 0.314

Table S4. Performance comparison between UniSO-N with pre-trained and randomly initialized embedders on Design-Bench and SOO-Bench unconstrained tasks, where the better one is **Bold**. $\mathcal{D}$(best) denotes the best score in the offline dataset.

Task	$\mathcal{D}$(best)	UniSO-N from scratch	UniSO-N from pre-trained
Ant	165.326	**305.576 ± 120.465**	269.691 ± 77.425
D'Kitty	199.363	**223.104 ± 23.838**	173.911 ± 46.662
Superconductor	74.000	**101.754 ± 6.972**	67.333 ± 10.838
TF Bind 8	0.439	**0.883 ± 0.048**	0.833 ± 0.005
TF Bind 10	0.005	0.578 ± 0.108	**0.959 ± 0.115**
GTOPX 2	-195.586	**-102.632 ± 22.635**	-124.995 ± 56.170
GTOPX 3	-151.190	**-55.743 ± 7.490**	-62.622 ± 22.261
GTOPX 4	-215.716	**-102.684 ± 19.227**	-110.284 ± 17.559
GTOPX 6	-112.599	**-56.469 ± 10.337**	-57.435 ± 18.832
Avg. Rank	/	**1.111 ± 0.314**	1.889 ± 0.314