Table 1: Evaluation results on the COLL test set. Now moved to main text (previously in appendix)

		COLL test set			
	Model	Energy MAE meV ↓	Force MAE meV/Å ↓	Force cos ↑	EFwT % ↑
same	Student (PaiNN-small)	104.0	80.9	0.984	5.4
	Teacher (PaiNN-big)	85.8	64.1	0.988	10.1
	Vanilla KD (1)	106.1(-11.5%)	82.0(-6.5%)	0.984(2.3%)	4.46(-20.2%)
	Vanilla KD (2)	**86.4 (96.7%)**	80.9(0%)	0.983(-2.3%)	4.3(-23.7%)
	n2n	92.5(63.2%)	77.8(18.5%)	0.984(18.2%)	**6.63 (26.5%)**
	v2v	90.4(74.7%)	**70.4 (62.5%)**	**0.986 (45.5%)**	5.8(8.4%)
similar	Student (SchNet)	146.5	121.2	0.970	2.75
	Teacher (PaiNN-big)	85.8	64.1	0.988	10.1
	Vanilla KD (1)	146.1(0.7%)	120.8(0.7%)	0.970(1.1%)	2.54(-2.9%)
	Vanilla KD (2)	**104.1 (69.9%)**	120.9(0.5%)	0.970(1.1%)	**6.45 (50.7%)**
	n2n	141.6(8.1%)	**117.2 (7.0%)**	**0.971 (5.4%)**	2.63(-1.6%)
different	Student (PaiNN-big)	85.8	64.1	0.988	10.1
	Teacher (GemNet-OC)	44.8	38.2	0.994	20.2
	Vanilla KD (1)	86.2(-1.1%)	63.9(0.6%)	0.988(1.5%)	10.1(0.1%)
	Vanilla KD (2)	61.4(59.5%)	62.9(4.6%)	0.988(5.2%)	13.0(29.2%)
	n2n	**60.4 (62.0%)**	**61.2 (11.3%)**	**0.989 (14.9%)**	**13.6 (34.6%)**
	e2n	77.3(20.8%)	63.3(3.0%)	0.988(7.9%)	11.0(9.2%)
	v2v	81.2(11.2%)	63.3(3.1%)	0.988(3.4%)	10.5(4.6%)

Table 2: Comparing MSE, LSP and GSP with GemNet-OC as teacher and PaiNN-big as student.

		OC20 validation set			
	Loss	Energy MAE meV ↓	Force MAE meV/Å ↓	Force cos ↑	EFwT % ↑
n2n	MSE	349	43.5	0.379	0.227
	GSP	446	48.1	0.335	0.098
	LSP	413	46.9	0.348	0.128
e2n	MSE	439	42.1	0.391	0.186
	GSP	483	46.4	0.350	0.108
	LSP	458	44.8	0.366	0.113

Table 3: Performance of KD from GemNet-OC into PaiNN-big across 3 different seeds.

	OC20 validation set			
Loss	Energy MAE meV ↓	Force MAE meV/Å ↓	Force cos ↑	EFwT % ↑
None (baseline)	440 ± 8	-	0.376 ± 0.0018	0.143 ± 0.0051
n2n	349 ± 0.9	43.5 ± 0.4	0.378 ± 0.0016	0.222 ± 0.0086
e2n	437 ± 3	42.5 ± 0.4	0.390 ± 0.0022	0.185 ± 0.0044