

Training set	Model	Throughput	S2EF validation		S2EF test		IS2RS test		IS2RE test
		Samples / GPU sec. \uparrow	Energy MAE (meV) \downarrow	Force MAE (meV/Å) \downarrow	Energy MAE (meV) \downarrow	Force MAE (meV/Å) \downarrow	AFbT (%) \uparrow	ADwT (%) \uparrow	Energy MAE (meV) \downarrow
OC20 All	CGCNN [44]	-	590	74.0	608	73.3	-	-	-
	SchNet [43]	-	549	56.8	540	54.7	-	14.4	764
	ForceNet-large [63]	15.3	-	33.5	-	32.0	12.7	49.6	-
	DimeNet++-L-F+E [4]	4.6	515	32.8	480	31.3	21.7	51.7	559
	SpinConv [49]	6.0	371	41.2	336	29.7	16.7	53.6	437
	GemNet-dT [50]	25.8	315	27.2	292	24.2	27.6	58.7	400
	GemNet-XL [8]	1.5	-	-	270	20.5	30.8	62.7	371
	GemNet-OC [51]	18.3	244	21.7	233	20.7	35.3	60.3	355
	SCN L=8 K=20 [42]	-	-	-	244	17.7	40.3	67.1	330
	eSCN L=6 K=20 [18]	2.9	-	-	242	17.1	48.5	65.7	341
	EquiformerV2 ($\lambda_E = 2$, 153M)	1.8	236	15.7	229	14.8	53.0	69.0	316
OC20 All+MD	GemNet-OC-L-E [51]	7.5	239	22.1	230	21.0	-	-	-
	GemNet-OC-L-F [51]	3.2	252	20.0	241	19.0	40.6	60.4	-
	GemNet-OC-L-F+E [51]	-	-	-	-	-	-	-	348
	SCN L=6 K=16 (4-tap 2-band) [42]	-	-	-	228	17.8	43.3	64.9	328
	SCN L=8 K=20 [42]	-	-	-	237	17.2	43.6	67.5	321
	eSCN L=6 K=20 [18]	2.9	243	17.1	236	16.2	50.3	66.7	327
	EquiformerV2 ($\lambda_E = 4$, 31M)	7.1	232	16.3	228	15.5	47.6	68.3	315
	EquiformerV2 ($\lambda_E = 2$, 153M)	1.8	230	14.6	227	13.8	55.4	69.8	311
	EquiformerV2 ($\lambda_E = 4$, 153M)	1.8	227	15.0	219	14.2	54.4	69.4	309