

OC20 2M Validation

Model	Samples / GPU sec.				S2EF				IS2RE	
					Energy MAE [meV] ↓	Force MAE [meV/Å] ↓	Force Cos ↑	EFwT [%] ↑	Energy MAE [meV] ↓	EwT [%] ↑
SchNet (Schütt et al., 2018)					1400	78.3	0.109	0.00	-	-
DimeNet++ (Gasteiger et al., 2020a)					805	65.7	0.217	0.01	-	-
SpinConv (Shuaibi et al., 2021)					406	36.2	0.479	0.13	-	-
GemNet-dT (Gasteiger et al., 2021)	25.8				358	29.5	0.557	0.61	438	-
GemNet-OC (Gasteiger et al., 2022)	18.3				286	25.7	0.598	1.06	407	-
<i>L</i> # layers # batch										
SCN 1-tap 1-band (Zitnick et al., 2022)	6	12	64	7.7	299	24.3	0.605	0.98	-	-
SCN 4-tap 2-band (Zitnick et al., 2022)	6	12	64	3.5	279	22.2	0.643	1.41	371	11.0
SCN 4-tap 2-band (Zitnick et al., 2022)	6	16	64	2.3	279	21.9	0.650	1.46	373	11.0
eSCN linear	6	12	96	6.8	301	21.9	0.646	1.28	-	-
eSCN	2	12	96	9.7	307	26.7	0.577	0.94	-	-
eSCN	4	12	96	7.8	291	22.2	0.637	1.39	-	-
eSCN	6	12	96	6.8	294	21.3	0.653	1.45	376	10.9
eSCN	8	12	96	4.4	296	21.3	0.654	1.47	-	-
eSCN m=0	6	12	96	13.8	316	26.5	0.584	0.88	-	-
eSCN m=1	6	12	96	8.7	309	23.4	0.626	1.13	-	-
eSCN m=2	6	12	96	6.8	294	21.3	0.653	1.45	376	10.9
eSCN m=3	6	12	96	4.8	295	21.2	0.656	1.38	-	-
eSCN m=4	6	12	96	3.8	298	21.2	0.657	1.41	-	-
eSCN	6	4	96	14.3	338	25.6	0.591	0.76	-	-
eSCN	6	8	96	8.7	306	22.4	0.634	1.16	-	-
eSCN	6	12	96	6.8	294	21.3	0.653	1.45	376	10.9
eSCN	6	16	64	4.2	283	20.5	0.662	1.67	371	11.2