Model	Validity (%) ↑		Stability Rate - DFT (%) \uparrow		S.U.N. Rate (%) ↑
	Composition	Structural	$E_{hull} < 0.0$	$E_{hull} < 0.1$	MP
CDVAE	<u>86.7</u> %	100 %	1.57%	-	1.4%
DiffCSP	83.3 %	100 %	5.06%	-	3.3%
FlowMM (ICML 24)	83.2 %	96.9 %	4.19%	-	2.5%
Mat2Seq (temp=1.35) Mat2Seq (temp=1.65)	88.5 % 81.7 %	94.2 % 88.6 %	4.10% <u>4.50</u> %	49.2 % <u>46.6</u> %	2.0% <u>3.2</u> %

Table 8: Comparison of Validity (%), Stability (%). and Stable, Unique, and Novel (S.U.N) (%). The unit of E_{hull} is eV/atom.

Table 9: Ability to generate crystal structures with desired band gap properties. We measure the success rate of generating crystal structures with band gap value < 0.5 eV and band gap value > 3.0 eV, measured by the state-of-the-art band gap predictor ComFormer [13].

Success rate	band gap $< 0.5 \text{ eV}$	band gap > 3.0 eV	Validity (%)	Uniqueness (%)	Novelty (%)
Ours-band gap \downarrow	83.6%	12.0%	88.0%	98.0 %	86.2%
Ours-band gap \uparrow	6.4%	90.7%	89.8 %	92.2%	98.6 %

Table 10: Mat2Seq match rate (%) and RMSE for **experimentally observed** crystal structures in MP-20 test set.

MP-20	number of crystals	Match Rate (%)	RMSE
Ours - exp observed	3819	65.2 %	0.042
Ours - the whole test set	9046	61.3 %	0.040

Table 11: Efficiency and model complexity comparisons.

MP-20 test set	number of parameters	RMSE	20 shots generation speed (sec./crystal)
CDVAE	4.5 M	0.103	37.9 s
DiffCSP	Similar to CDVAE	0.049	7.3 s
Ours-small	25 M	0.039	2.1 s
Ours-large	200 M	0.037	<u>5.7 s</u>

Table 12: Comparison of Hit Rate (%) and RMSE for ten recently discovered crystal structures from literature.

Model	Hit Rate (%) \uparrow	$RMSE\downarrow$
CrystaLLM	<mark>0</mark>	nan
Mat2Seq	10.0 %	0.0388