Crystalline Material Experiment

Method	NFE	Validity (%) ↑		Coverage (%) ↑		Property ↓		Stability Rate (%) ↑
		Structural	Composition	Recall	Precision	wdist (ρ)	wdist (N_{el})	
CDVAE (Xie et al., 2021)	5000	100.00	86.70	99.15	99.49	0.688	0.278	1.57
DiffCSP (Jiao et al., 2023)	1000	100.00	83.25	99.71	99.76	0.350	0.125	5.06
FlowMM (Miller et al., 2024)	1000	96.85	83.19	99.49	99.58	0.239	0.083	4.65
CrystalLLM (70B) (Gruver et al., 2024)	–	99.6	95.4	85.8	98.9	0.81	0.44	5.28
Autoregressive	–	86.43	89.33	63.31	99.74	0.088	0.030	1.99
Perm. invariant DFM - Mask w/ Cubic	250	94.40	84.40	98.25	99.40	0.244	0.144	6.90
Perm. invariant DFM - Mask w/ Kinetic Optimal	250	95.79	88.50	90.11	99.29	0.542	0.154	**7.02**

Conclusions

1. Kinetic energy for CTMC velocity.
2. Closed form solution for symmetric weights.
3. Instantiate on two probability paths and validate empirically.