Periodic Materials Generation using Text-Guided Joint Diffusion Model

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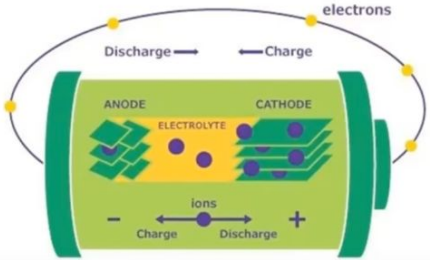
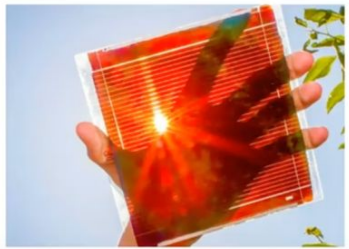
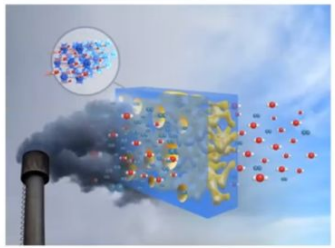
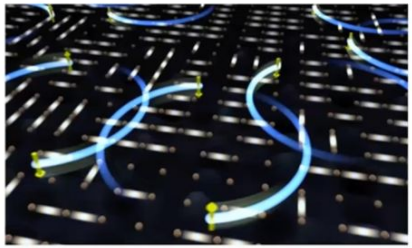
3D Crystal Materials form the Foundation of Modern Technology





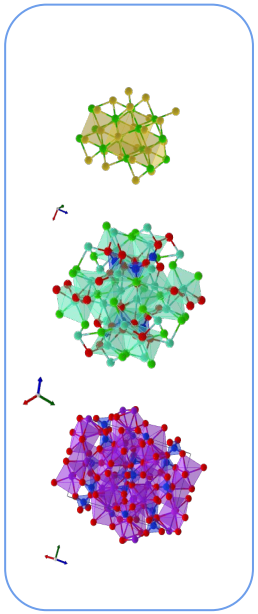




Batteries | Solar cells | Carbon Capture | Quantum Computer

Image: Tian Xie

Material Design Pipeline



Material Database

Screening Generate

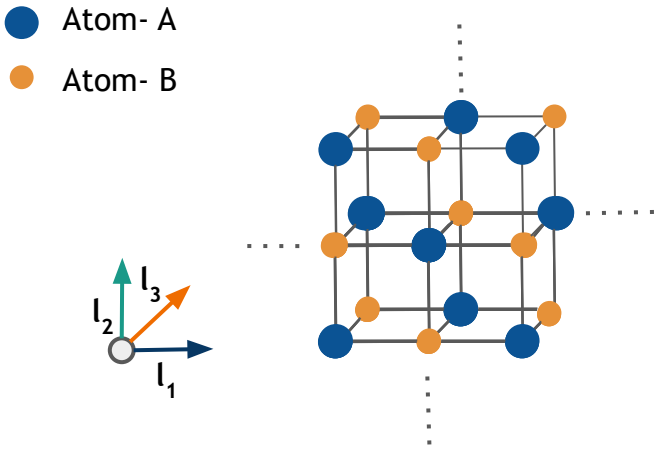
Generative Models : Diffusion/Flow Matching

10k Candidate Materials

Check Properties

5-10 Materials For Synthesis in Lab

Periodic Crystal Material



- Crystal Material $\mathbf{M} = (\mathbf{A}, \mathbf{X}, \mathbf{L})$
- Atom Type Matrix $(\mathbf{A}) = [\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_N]^T \in \mathbb{R}^{N \times k}$ denotes set of atomic type in one hot representation.
- Coordinate Matrix $(\mathbf{X}) = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N]^T \in \mathbb{R}^{N \times 3}$ denotes atomic coordinate positions
- Lattice Matrix $(\mathbf{L}) = [\mathbf{l}_1, \mathbf{l}_2, \mathbf{l}_3]^T \in \mathbb{R}^{3 \times 3}$, which describes how a unit cell repeats itself in the 3D space.

Limitation in Existing Works

- No SOTA model learns the **joint distribution of atom coordinates, types, and lattice** structure end-to-end via diffusion.
- Most popular studies follow **unconditional generation**.
- **Without imposing any external constraints** related to physical or chemical properties.

Un-Realistic !!

Research Question - Text Guided Generation

- **Join distribution of atom coordinates, types, and lattice** structure end-to-end via diffusion model.
- **Leverage textual descriptions (prompts)** of a given material to generate materials with **desired target properties.**
- A key benefit of using textual descriptions is they provide **a diverse set of structural (global and local) information** and encompass different conditions effectively and flexibly.

Joint Diffusion Framework

- **Diffusion on (A)**
  - Discrete Denoising Diffusion Probabilistic Model (D3PM).
- **Diffusion on (X)**
  - Quotient space $\mathbb{R}^{N\times 3}/\mathbb{Z}^{N\times 3}$ induced by the crystal periodicity.
  - Add noise sampled from Wrapped Normal (WN) distribution to X.
  - Score Matching Denosing Networks.
- **Diffusion on (L)**
  - Denoising Diffusion Probabilistic Model (DDPM)

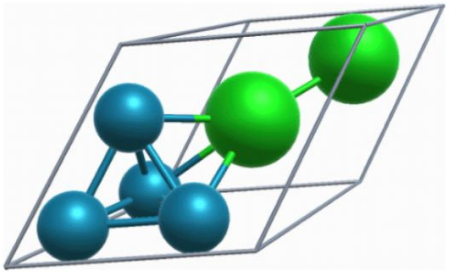
Textual Data

BaPd2 is Cubic structured and crystallizes in the cubic Fd-3m space group. Ba(1) is bonded in a 12-coordinate geometry to twelve equivalent Pd(1) atoms. All Ba(1)-Pd(1) bond lengths are 3.37 Ã. Pd(1) is bonded to six equivalent Ba(1) and six equivalent Pd(1) atoms to form a mixture of face, edge, and corner-sharing cuboctahedra. All Pd(1)-Pd(1) bond lengths are 2.88 Ã. Its formation energy per atom is -0.578, band gap is 0.0, energy above hull is 0.0. Generate the material

Detailed Description by Robocrystallographer

Below is a description of a bulk material. The chemical formula is BaPd2. The elements are Ba, Pd. The formation energy per atom is negative. The band gap is zero. The energy above the convex hull is zero. The space group number is 227. The crystal system is *cubic.*Generate the material

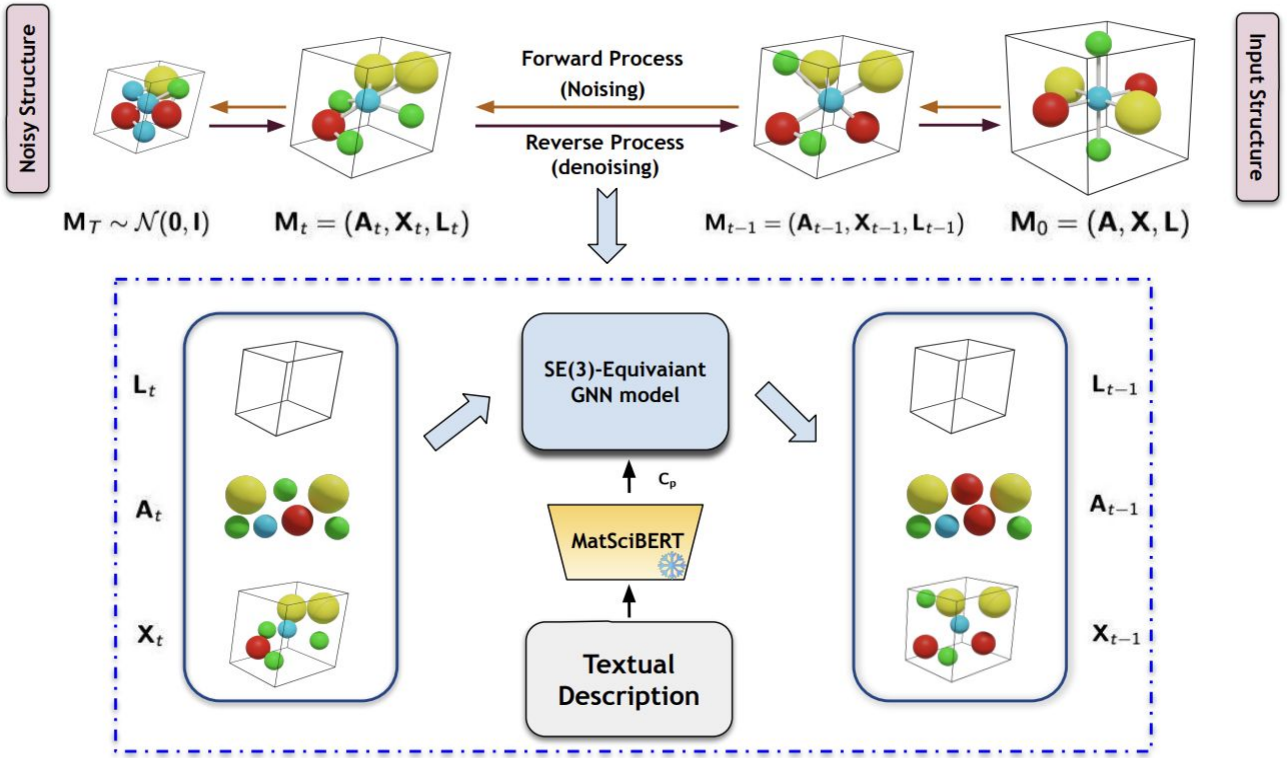
Short Prompt by Users



Unit Cell Structure

Figure 1: Detailed textual description generated by Robocrystallographer, less-detailed prompts by domain experts, and crystal unit cell structure of $\mathbf{BaPd_2}$.

TGDMat: Text-Guided Diffusion for Material



Results - Crystal Structure Prediction(CSP)

Method	# Samples	Perov-5		Carbon-24		MP-20	
		Match Rate ↑	RMSE ↓	Match Rate ↑	RMSE ↓	Match Rate ↑	RMSE ↓
P-cG-SchNet	1	48.22	0.4179	17.29	0.3846	15.39	0.3762
	20	97.94	0.3463	55.91	0.3551	32.64	0.3018
CDVAE	1	45.31	0.1138	17.09	0.2969	33.90	0.1045
	20	88.51	0.0464	88.37	0.2286	66.95	0.1026
DiffCSP	1	52.02	0.0760	17.54	0.2759	51.49	0.0631
	20	**98.60**	0.0128	88.47	0.2192	77.93	0.0492
TGDMat (Short)	1	56.54	0.0583	24.13	0.2424	52.22	0.0597
	20	98.25	0.0137	88.28	0.2252	80.97	0.0443
TGDMat (Long)	1	**90.46**	**0.0203**	**44.63**	**0.2266**	**55.15**	**0.0572**
	20	98.59	**0.0072**	**95.27**	**0.1534**	**82.02**	**0.0483**

Table 1: Summary of results on *CSP* task. We highlight the best and second-best performances in bold and underlined, respectively.

Results - Random Material Generation(Gen)

Dataset	Method	Validity ↑		Coverage ↑		Property Statistics (EMD) ↓		
		Compositional	Structural	COV-R	COV-P	# Element	ρ	$\mathcal{E}$
Perov-5	CDVAE	98.59	**100**	99.45	98.46	0.0628	0.1258	0.0264
	CDVAE+	98.45	99.8	99.53	99.09	0.0609	0.1276	0.0223
	SyMat	97.40	**100**	99.68	98.64	0.0177	0.1893	0.2364
	SyMat+	97.88	99.9	99.70	98.79	0.0172	0.1755	0.2566
	DiffCSP	**98.85**	**100**	99.74	98.27	0.0128	0.1110	0.0263
	DiffCSP+	98.44	**100**	99.85	98.53	0.0119	0.1070	0.0241
	TGDMat(Short)	98.28	**100**	99.7	99.24	0.0108	0.0947	0.0257
	TGDMat(Long)	98.63	**100**	**99.83**	**99.52**	**0.0090**	**0.0497**	**0.0187**
Carbon-24	CDVAE	-	**100**	99.8	83.08	-	0.1407	0.285
	CDVAE+	-	**100**	99.8	84.76	-	0.1377	0.266
	SyMat	-	**100**	**99.9**	97.59	-	0.1195	3.9576
	SyMat+	-	**100**	**99.9**	**97.63**	-	0.1171	3.862
	DiffCSP	-	**100**	**99.9**	97.27	-	0.0805	0.082
	DiffCSP+	-	**100**	**99.9**	97.33	-	0.0763	0.085
	TGDMat(Short)	-	**100**	99.8	91.77	-	0.0681	0.087
	TGDMat(Long)	-	**100**	**99.9**	92.43	-	**0.043**	**0.063**
MP-20	CDVAE	86.70	**100**	99.15	99.49	1.432	0.6875	0.2778
	CDVAE+	87.42	**100**	99.57	99.81	0.972	0.6388	0.2977
	SyMat	88.26	**100**	98.97	**99.97**	0.5067	0.3805	0.3506
	SyMat+	88.47	99.9	99.01	99.95	0.4865	0.3879	0.3489
	DiffCSP	83.25	**100**	99.71	99.76	0.3398	0.3502	0.1247
	DiffCSP+	85.07	**100**	99.8	99.89	0.3122	0.3799	0.1355
	TGDMat(Short)	86.60	**100**	99.79	99.88	0.3337	**0.3296**	**0.1154**
	TGDMat(Long)	**92.97**	**100**	**99.89**	99.95	**0.2890**	0.3382	0.1189

Table 2: Summary of results on *Gen* task, with the best and second-best performances in bold and underlined, respectively. The table contains ”-” values for metrics that don’t apply to certain datasets.

Conclusion

- **Text Guided Diffusion Model** will **bridge the gap** between **natural language understanding and material structure generation.**
- Given Condition using interpretable prompts, trained diffusion models will generate new novel and stable materials of different classes.
- Additional textual information will guide the diffusion process to **converge faster.**

Arxiv : https://arxiv.org/pdf/2503.00522
Github Repo for TGDMat : https://github.com/kdmsit/TGDMat