ICML
International Conference
On Machine Learning

NUS National University of Singapore | Institute for Functional Intelligent Materials

Wyckoff Transformer: Generation of Symmetric Crystals

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The space of possible materials is intractably vast

A rough estimate: 10^{160}

Even if quantum mechanical computation (DFT) is replaced with a 1000x faster algorithm we can't screen all

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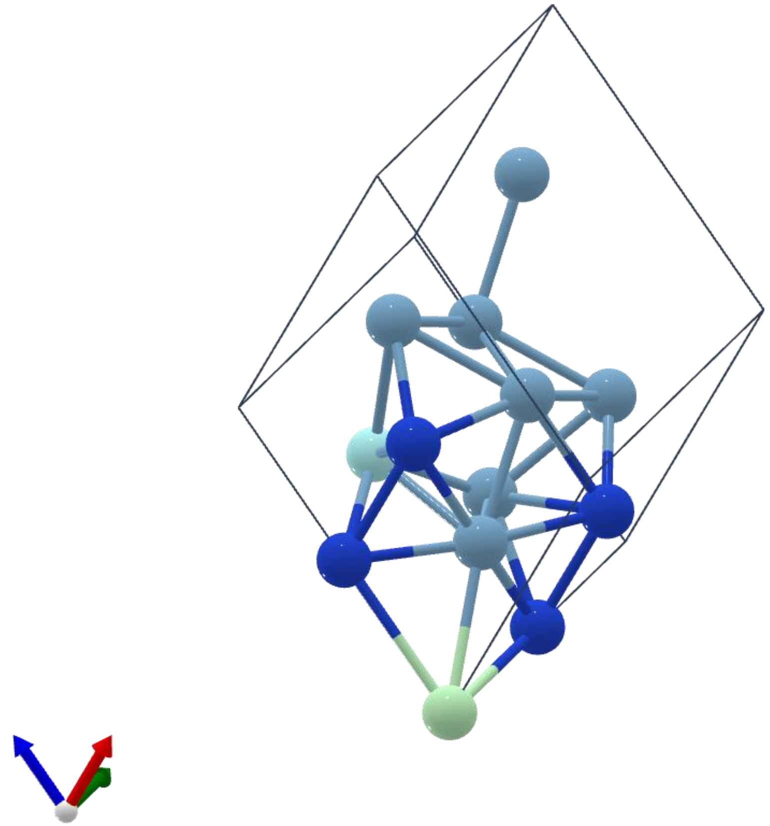
Material Generation Problem Statement



- A crystal consists of:
  - A 3D point cloud of atoms, including coordinates and chemical elements
  - Lattice parameters
- The goal is to generate crystals that are
  - Stable under normal conditions
  - Novel: not present in the training data

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ML Challenges

1. Atom types are discrete, coordinates are continuous
2. The number of atoms varies
3. Structures are permutation, rotation and translation invariant
4. **Lots of local energy minima**

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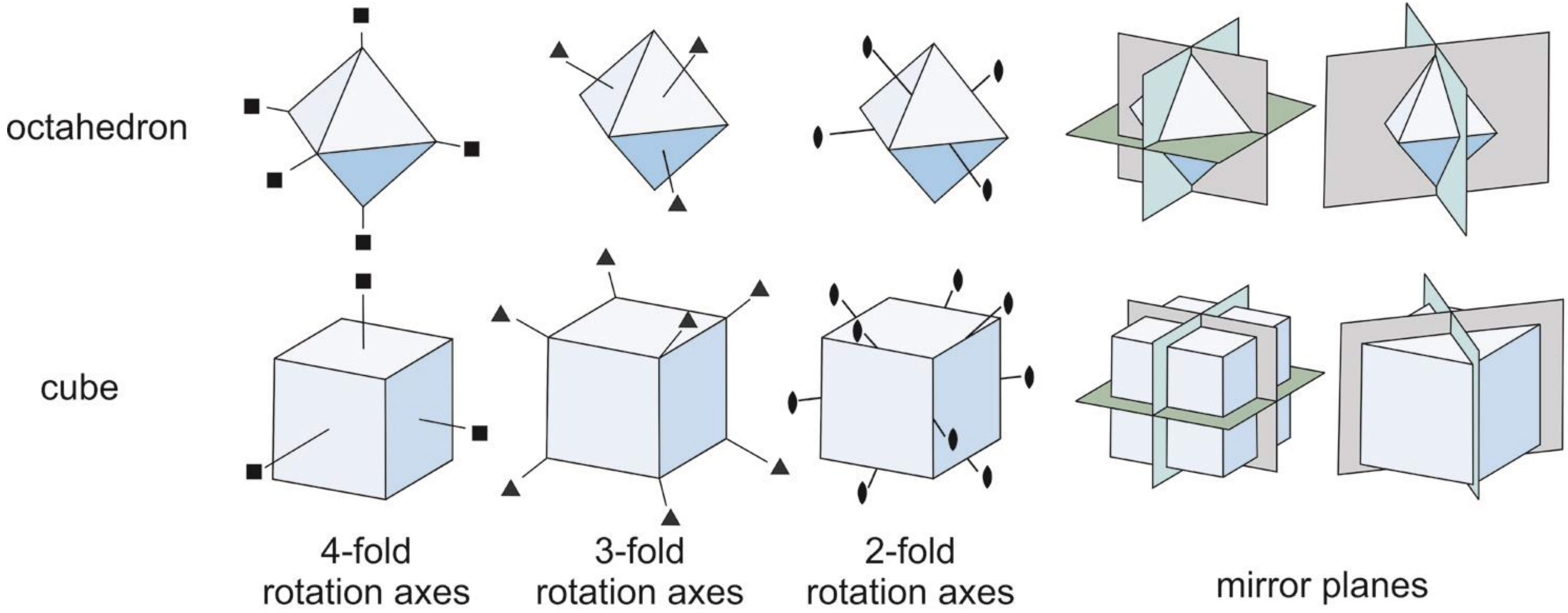
Symmetries in Crystals



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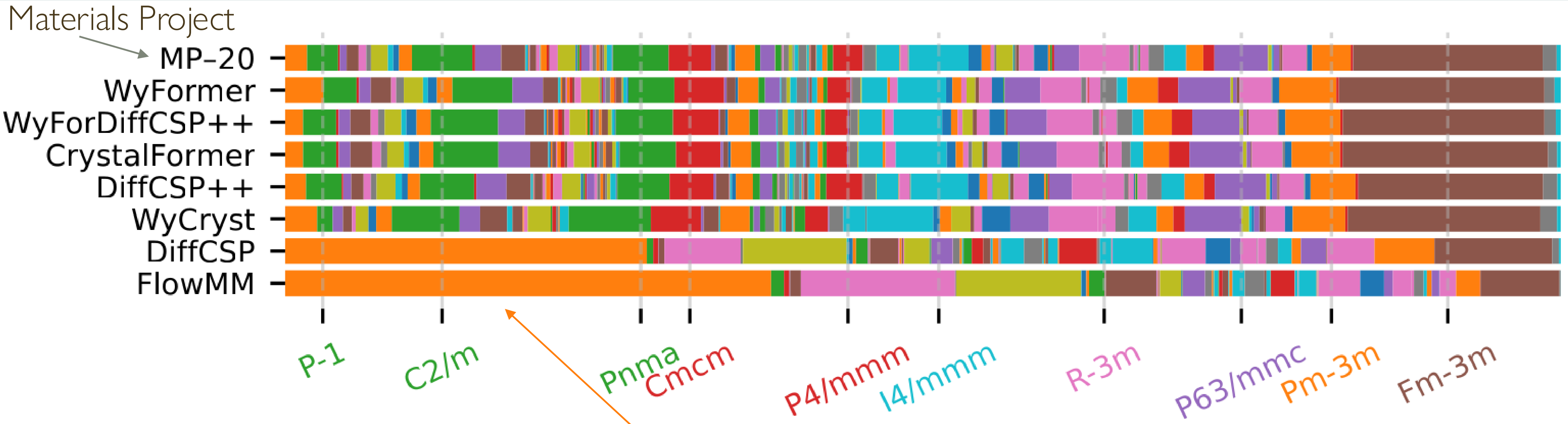
Not all of the symmetry elements are shown in these drawings

https://opengeology.org/Mineralogy/10-crystal-morphology-and-symmetry/

Most Real Crystals Have Internal Symmetry



Space group other than P1 indicates presence of symmetry beyond the lattice translation

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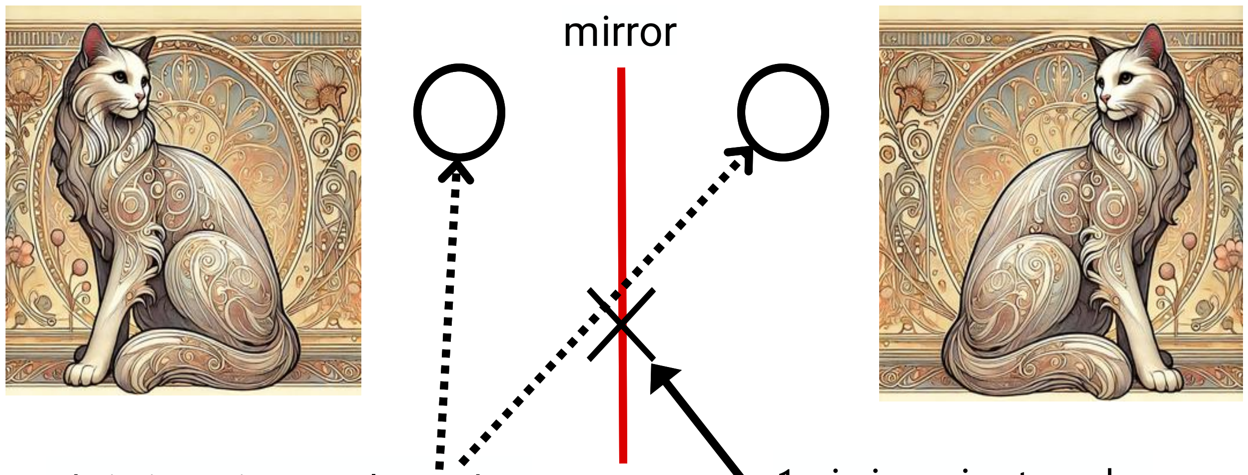
Wyckoff Positions



2b is invariant only under identity transformation. The two o's are just examples; almost whole plane is 2b

1a is invariant under mirror transformation. The two x are just examples; the whole line is 1a

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Wyckoff Positions for a Space Group

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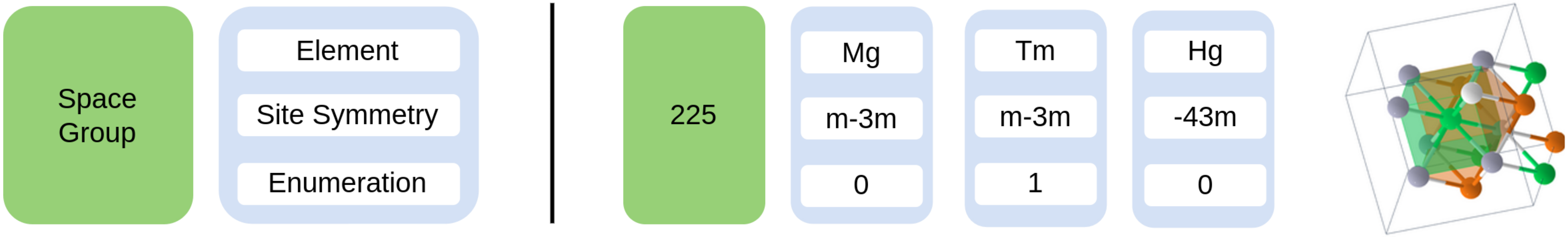
Wyckoff Positions of Group *I4/mmm* (No. 139)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates (0,0,0) + (1/2,1/2,1/2) +
32	o	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (-x,y,-z) (x,-y,-z) (y,x,-z) (-y,-x,-z) (-x,-y,-z) (x,y,-z) (y,-x,-z) (-y,x,-z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
16	n	.m.	(0,y,z) (0,-y,z) (-y,0,z) (y,0,z) (0,y,-z) (0,-y,-z) (y,0,-z) (-y,0,-z)
16	m	..m	(x,x,z) (-x,-x,z) (-x,x,z) (x,-x,z) (-x,x,-z) (x,-x,-z) (x,x,-z) (-x,-x,-z)
16	l	m..	(x,y,0) (-x,-y,0) (-y,x,0) (y,-x,0) (-x,y,0) (x,-y,0) (y,x,0) (-y,-x,0)
16	k	..2	(x,x+1/2,1/4) (-x,-x+1/2,1/4) (-x+1/2,x,1/4) (x+1/2,-x,1/4) (-x,-x+1/2,3/4) (x,x+1/2,3/4) (x+1/2,-x,3/4) (-x+1/2,x,3/4)
8	j	m2m .	(x,1/2,0) (-x,1/2,0) (1/2,x,0) (1/2,-x,0)
8	i	m2m .	(x,0,0) (-x,0,0) (0,x,0) (0,-x,0)
8	h	m.2 m	(x,x,0) (-x,-x,0) (-x,x,0) (x,-x,0)
8	g	2mm .	(0,1/2,z) (1/2,0,z) (0,1/2,-z) (1/2,0,-z)
8	f	..2/m	(1/4,1/4,1/4) (3/4,3/4,1/4) (3/4,1/4,1/4) (1/4,3/4,1/4)
4	e	4mm	(0,0,z) (0,0,-z)
4	d	-4m2	(0,1/2,1/4) (1/2,0,1/4)
4	c	mmm .	(0,1/2,0) (1/2,0,0)
2	b	4/mmm	(0,0,1/2)
2	a	4/mmm	(0,0,0)

Aroyo, et. al. Zeitschrift fuer Kristallographie (2006), 221, 1, 15-27.

Wyckoff Positions as Tokens



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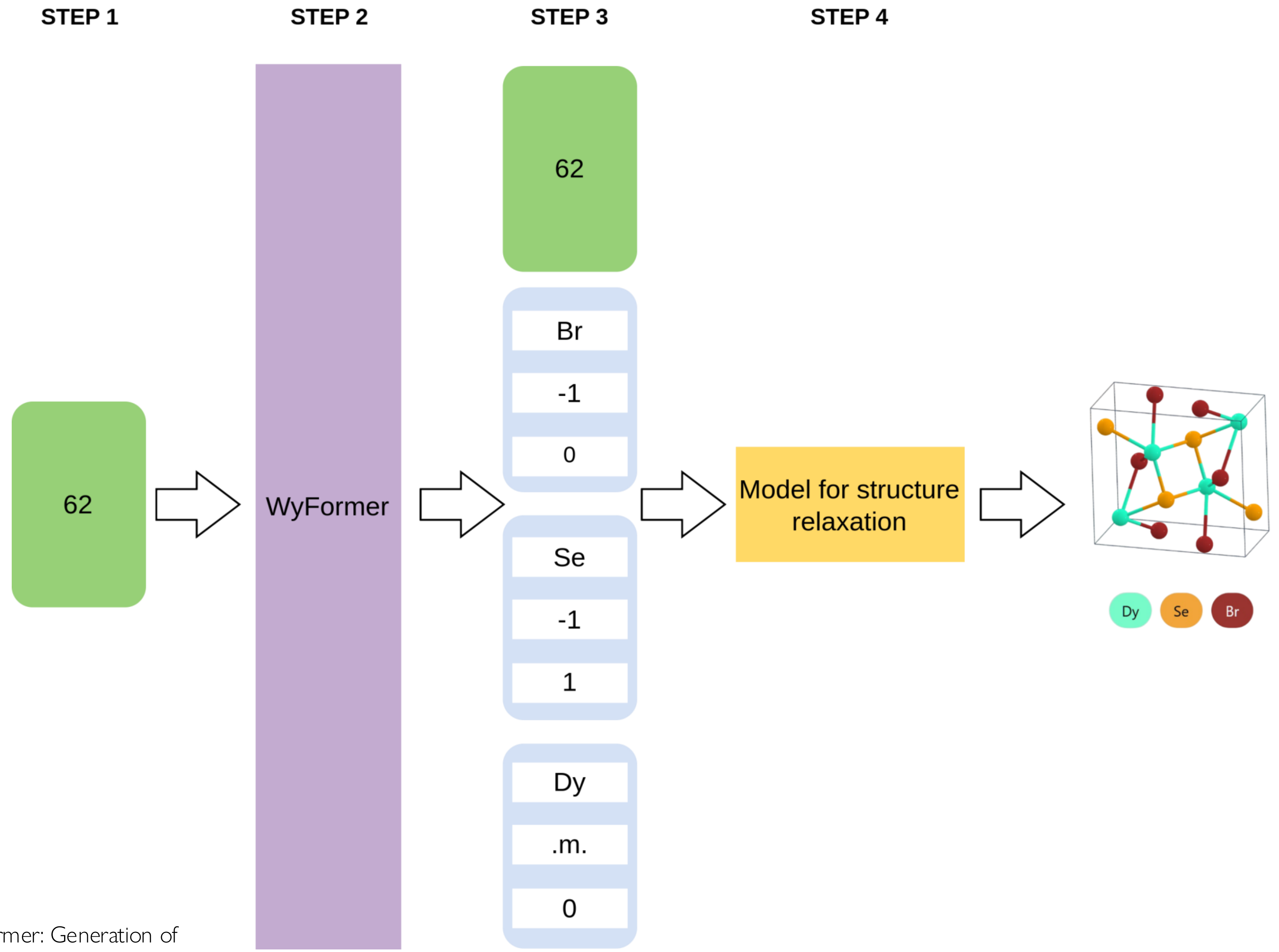

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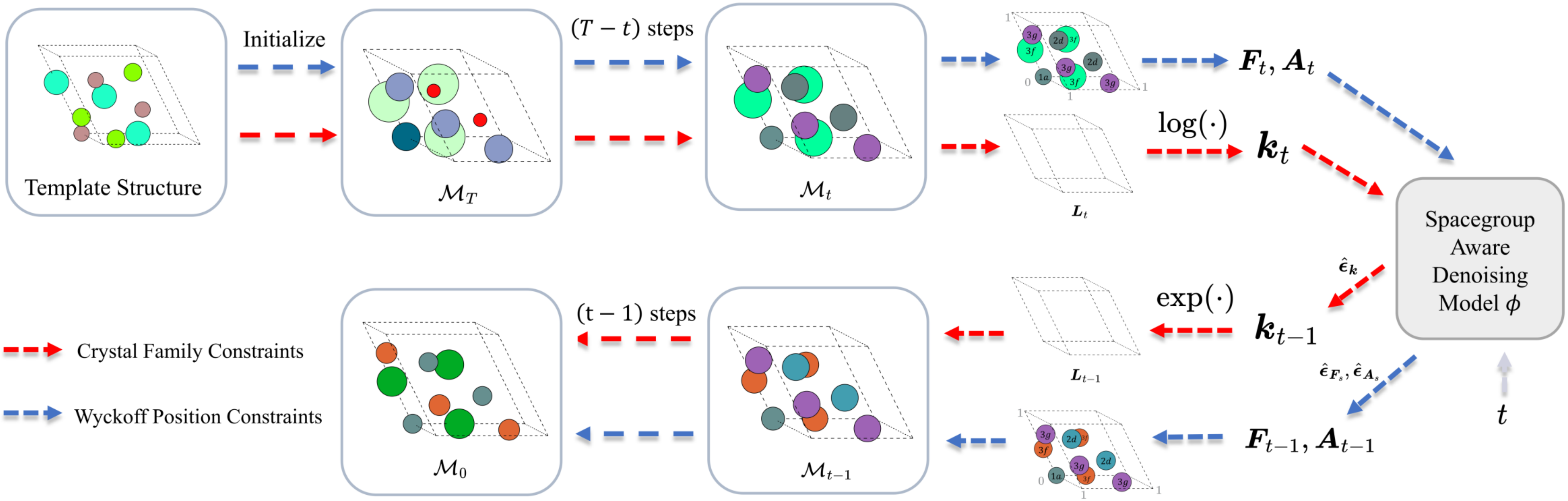
Relaxation: DiffCSP++



Jiao, Rui, et al. "Crystal structure prediction by joint equivariant diffusion." Advances in Neural Information Processing Systems 36 (2023): 17464-17497.

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Wyckoff Transformer

An autoregressive generative Transformer:

- Encoder-only
- Permutation-invariant: no positional encoding, shuffle token order
- Predict the probability for the next part of token

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Results

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Table 1. Evaluation. Symmetry metrics are computed only using novel structurally valid examples. Note that the 1000 and 105-example metrics are computed using MP-20 train and validation as reference datasets for novelty, while the 10 000-example S.U.N. only uses MP-20 train to remain compatible with the reported values. **Bold** indicates the values within $p = 0.1$ statistical significance threshold from the best. Values marked by * were computed by Miller et al. (2024), the rest by us; see note H.1 for an important caveat; in short, the values in (brackets) are less accurate, but are compatible with each other.

Method/Metric	**Novel Unique** Templates (#) ↑	**P1 (%)** ref = 1.7	**Space Group** χ^2 ↓	**S.U.N. % ↑** $E_{\text{hull}} < 80$ meV	**S.S.U.N. % ↑**	**S.U.N. % ↑** $E_{\text{hull}} < 0$ meV
Sample size	1000	1000	1000	105	105	10 000
Relaxation	CHGNet	CHGNet	CHGNet	DFT	DFT	DFT
WyFormerCHGNet	**180**	3.24	0.223	**23.1**	**22.3**	–
WyFormerDiffCSP++	**186**	**1.46**	**0.212**	**22.2**	**21.1**	**3.83 (4.14)**
DiffCSP++	*10*	2.57	0.255	14.4	**14.4**	–
CrystalFormer	74	**0.91**	0.276	**20.1**	**20.1**	–
SymmCD	101	**2.35**	0.24	**20.7**	**20.7**	–
WyCryst	**165**	4.79	0.710	5.5	5.5	–
DiffCSP	76	36.57	7.989	**22.2**	**20.6**	– (3.34*)
FlowMM	51	44.27	12.423	**17.8**	**16.9**	– (2.34*)
WyFormer *MPTS–52*	386	0	0.225	–	–	–

The nature is elegant, so is WyFormer

WyFormer

- Best-in-class symmetry-conditioned generation
- Relative 20% S.U.N. improvement
- Physics-motivated inductive bias
- Unparalleled inference speed

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