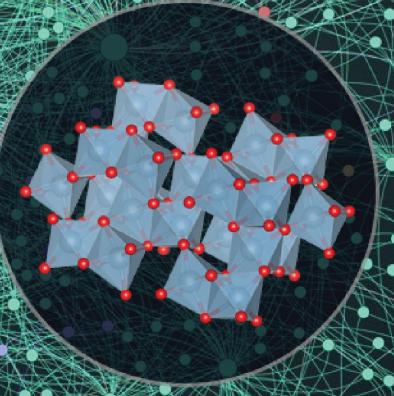
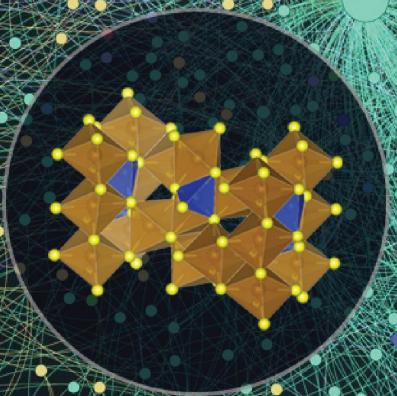


GAN use in Materials Science



GANs are being used regularly in materials science

Materials design (inverse design)

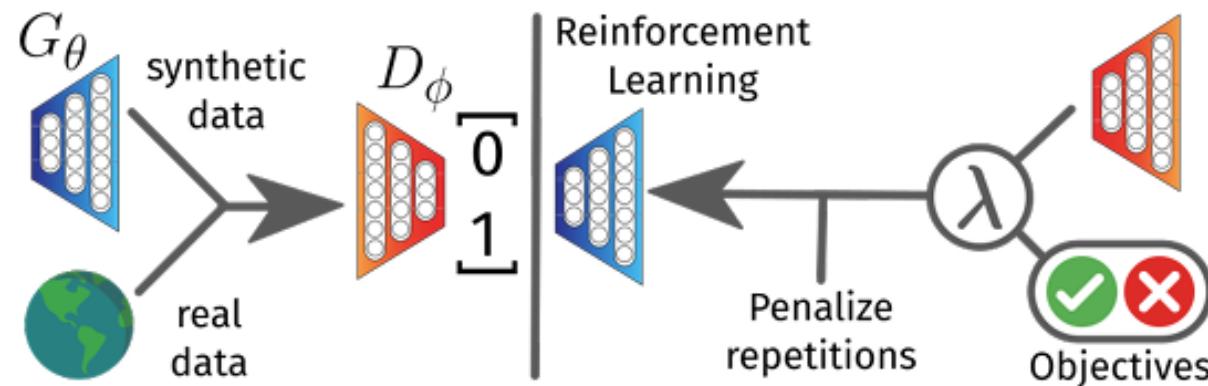
Data augmentation

Anomaly detection

ORGAN combined GAN with RL for guided discovery

Guimaraes et al. (2017) “ORGAN” for new molecules. GAN + RL

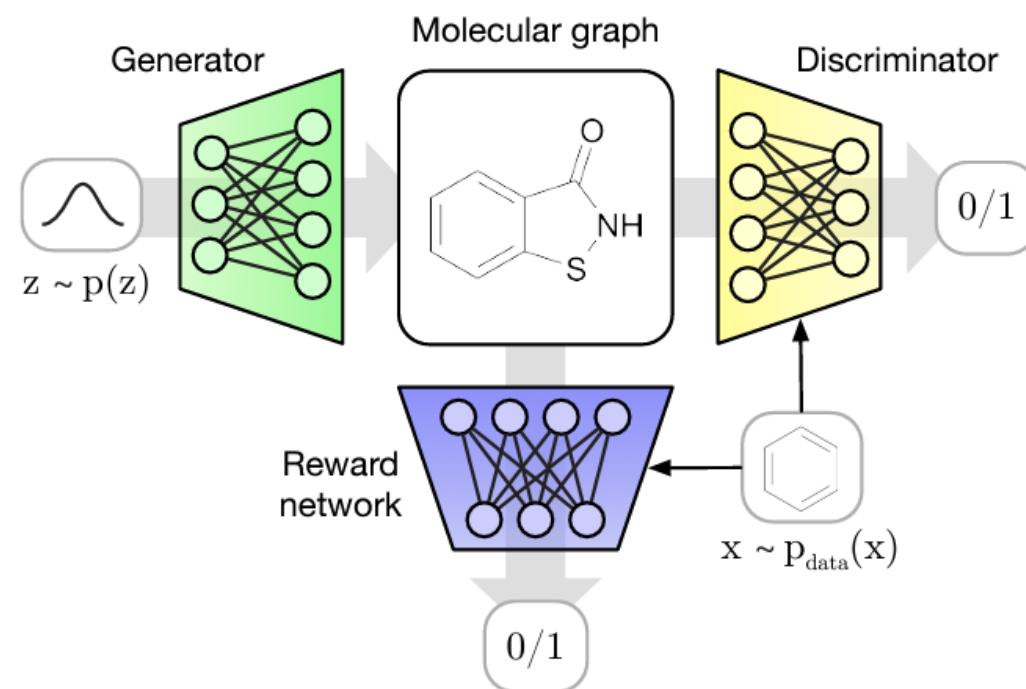
- Reinforcement learning following GAN
- Penalties for introducing nonunique generated sequences
- Generator had RNN architecture
- Discriminator had CNN architecture
- Data was 5000 molecules from ZINC database (drug and nondrugs)
- Objectives: solubility, synthesizability, drug-likeness



MolGAN improves this by working with graphs

Cao et al. (2018) “MolGAN” for new molecules.

- Generated molecule graphs directly
- By avoiding SMILES, it had nearly 100% valid molecule output
- GAN+RL to steer generation towards desired molecules
- Trained on QM9 dataset



Mol-CycleGAN lets us generate from other molecule templates

Maziarka et al. (2020) “Mol-CycleGAN” based on CycleGAN (Zhu 2017, 20k citations)

- Generated molecule based on input molecule (image to image)
- Structural similarity -> property similarity
- High Tanimoto similarity

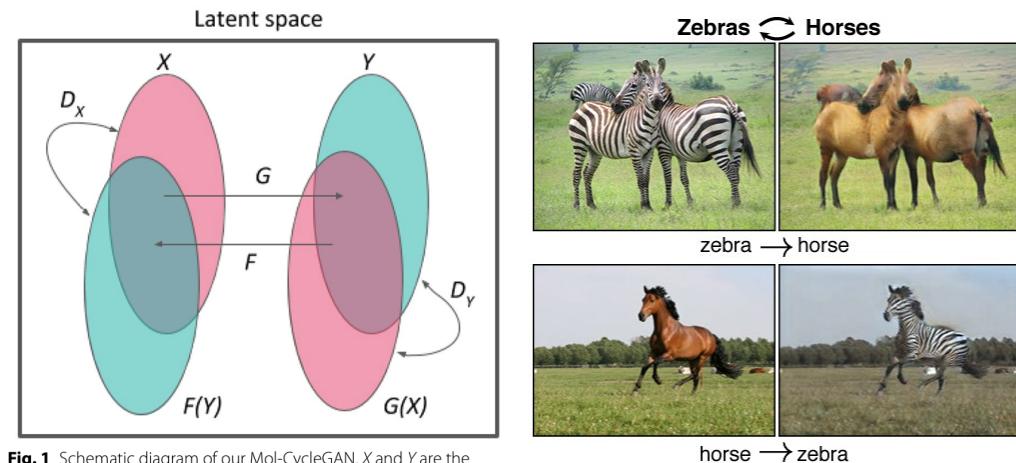


Fig. 1 Schematic diagram of our Mol-CycleGAN. X and Y are the sets of molecules with selected values of the molecular property (e.g. active/inactive or with high/low values of logP). G and F are the generators. D_X and D_Y are the discriminators

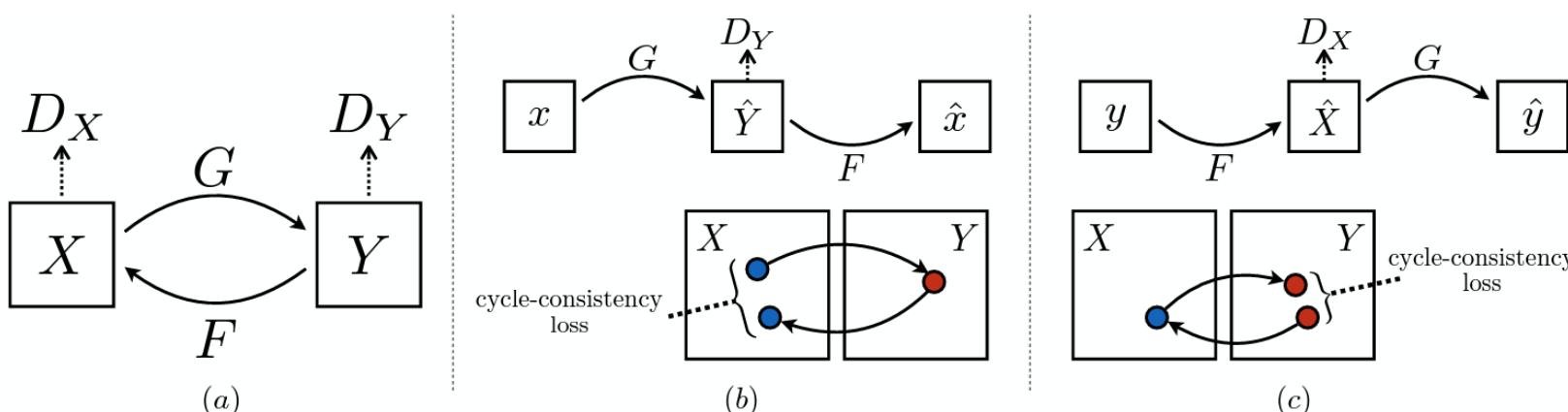


Figure 3: (a) Our model contains two mapping functions $G : X \rightarrow Y$ and $F : Y \rightarrow X$, and associated adversarial discriminators D_Y and D_X . D_Y encourages G to translate X into outputs indistinguishable from domain Y , and vice versa for D_X and F . To further regularize the mappings, we introduce two *cycle consistency losses* that capture the intuition that if we translate from one domain to the other and back again we should arrive at where we started: (b) forward cycle-consistency loss: $x \rightarrow G(x) \rightarrow F(G(x)) \approx x$, and (c) backward cycle-consistency loss: $y \rightarrow F(y) \rightarrow G(F(y)) \approx y$

MATGANIP uses a GAN to learn structure-property relationships in perovskites

Gao et al. (2019) “MATGANIP”

- Uses GAN to learn real vs fake property data to eventually “generate” labels that could be close to real

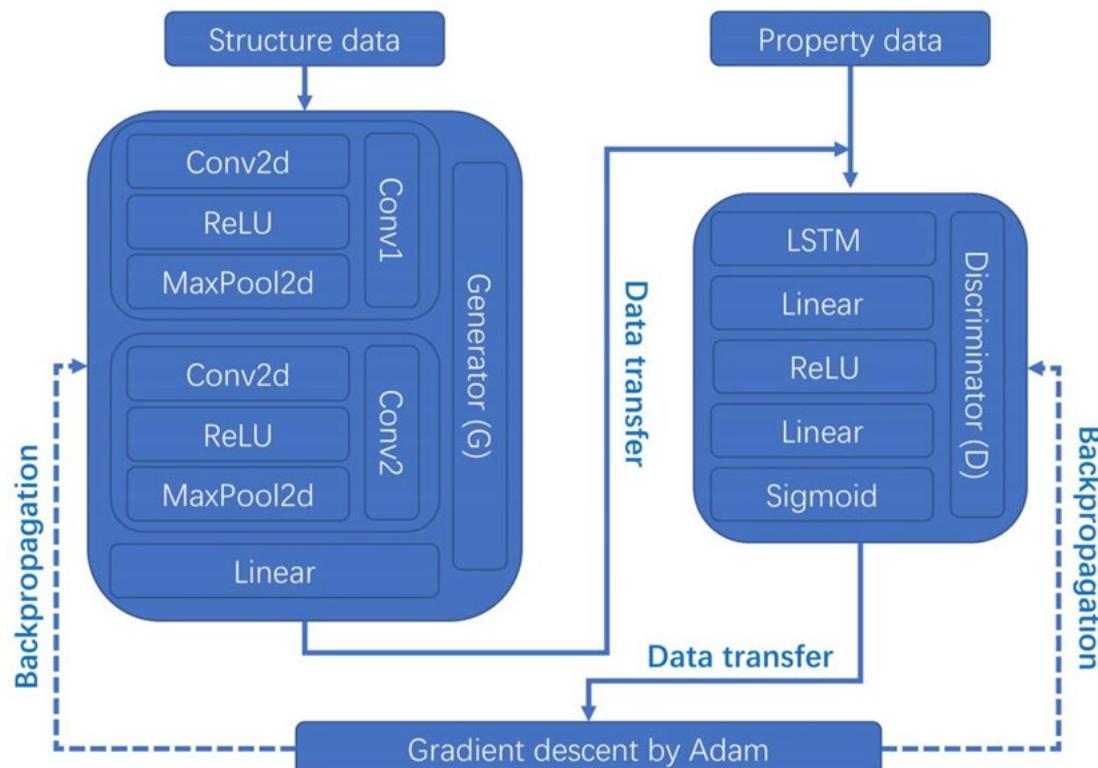


Figure 1: The schema diagram of MATGANIP. The structure data and property data are the input of the generator (G) and the discriminator (D) of the MATGANIP, respectively. In the inner of the G, there are the Conv1, Conv2, and Linear. Both of the Conv1 and Conv2 are the CNN layers, which contains the Conv2d, ReLU, and MaxPool2d layers. Linear is fully connected layers and provides a data-transfer from the G to the LSTM of the D. In the inner of the D. There are LSTM, Linear, ReLU, Linear, and Sigmoid. LSTM represents the long short term memory and enhances the ability to identify of the distribution of the input data. The sigmoid layer provides a Sigmoid function for the D and makes the output of the D to be a probability value. The other three layers, two Linear and ReLU, transform the data of LSTM into the Sigmoid. ReLU provides an active function. Based on the Adam, gradient descent calculation receives the data of the Sigmoid of the D and generates the backpropagation for the G and D of the MATGANIP.

CubicGAN generates cubic candidate structures

Zhao et al. (2021) “CubicGAN”

- Uses GAN to generate candidate cubic materials
- Trained on DFT data (OQMD)
- Rediscovered most of training data plus many new compounds
- 506 validated with phonon dispersion calcs

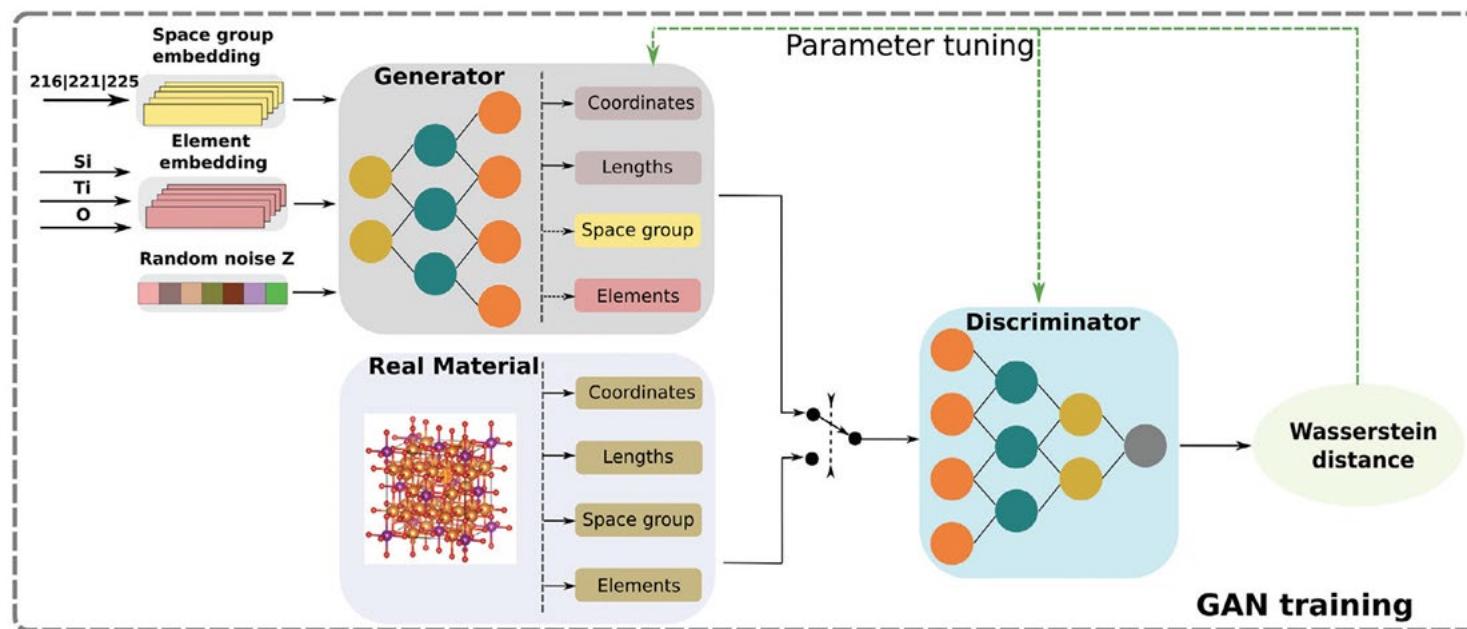


Figure 1. The workflow of our CubicGAN framework.

MatGAN generates compositions

Dan et al. (2020) “MatGAN”

- Uses GAN to generate compositions
- Unusual representation
- Inorganics trained on ICSD, MP, OQMD
- Show that compositional space could be big
- Screened output with SMACT and showed the generated compounds matched

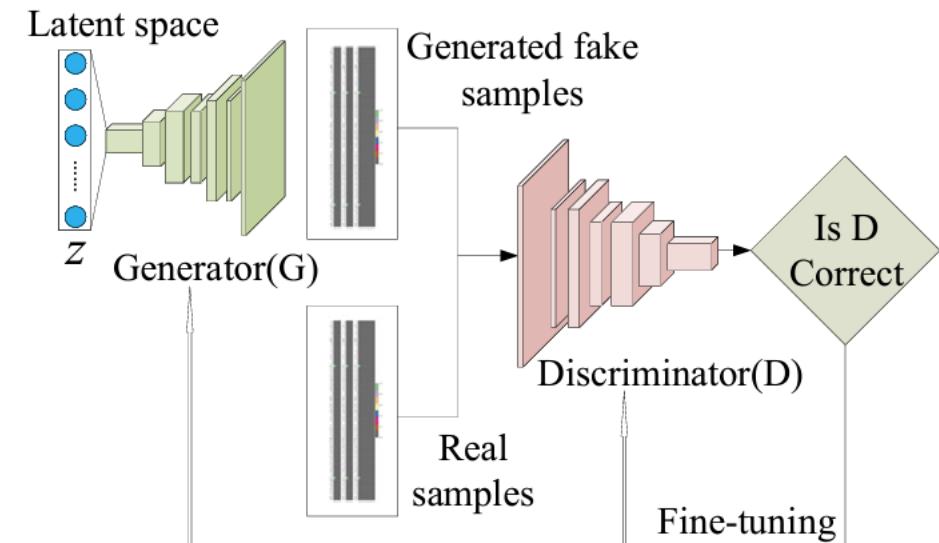
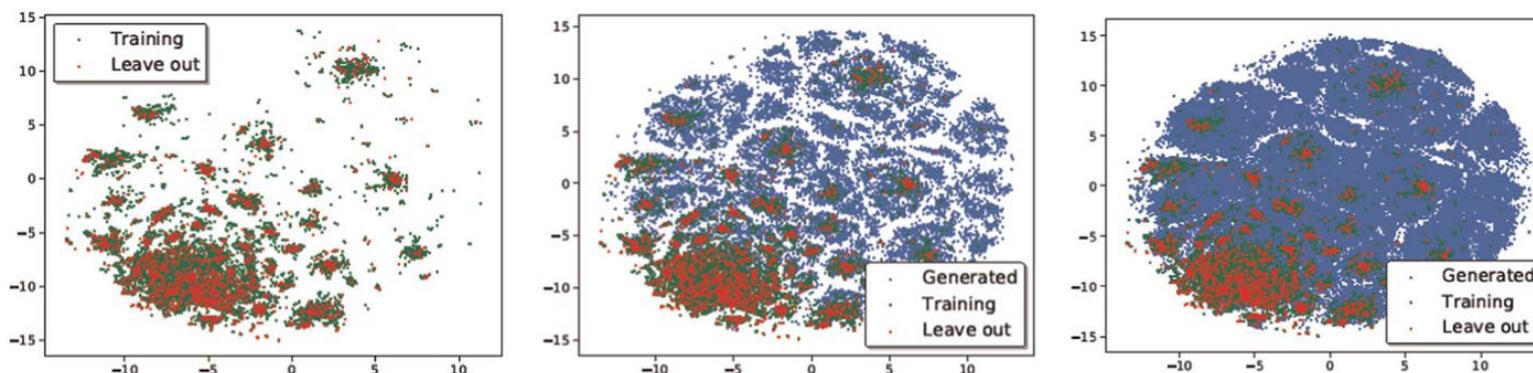


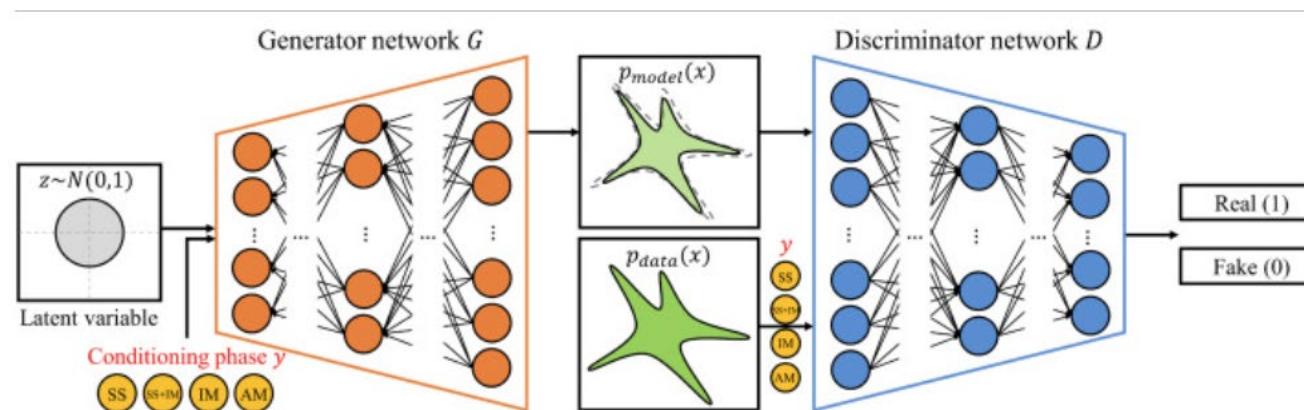
Fig. 1 Architecture of MatGAN for inorganic materials. It is composed of a generator, which maps random vectors into generated samples and a discriminator, which tries to differentiate real materials and generated ones. Detailed configuration parameters are listed in Supplementary Table 1 and Supplementary Fig. 1.



Conditional GANs have been used to augment data and predict properties

Lee et al. (2021)

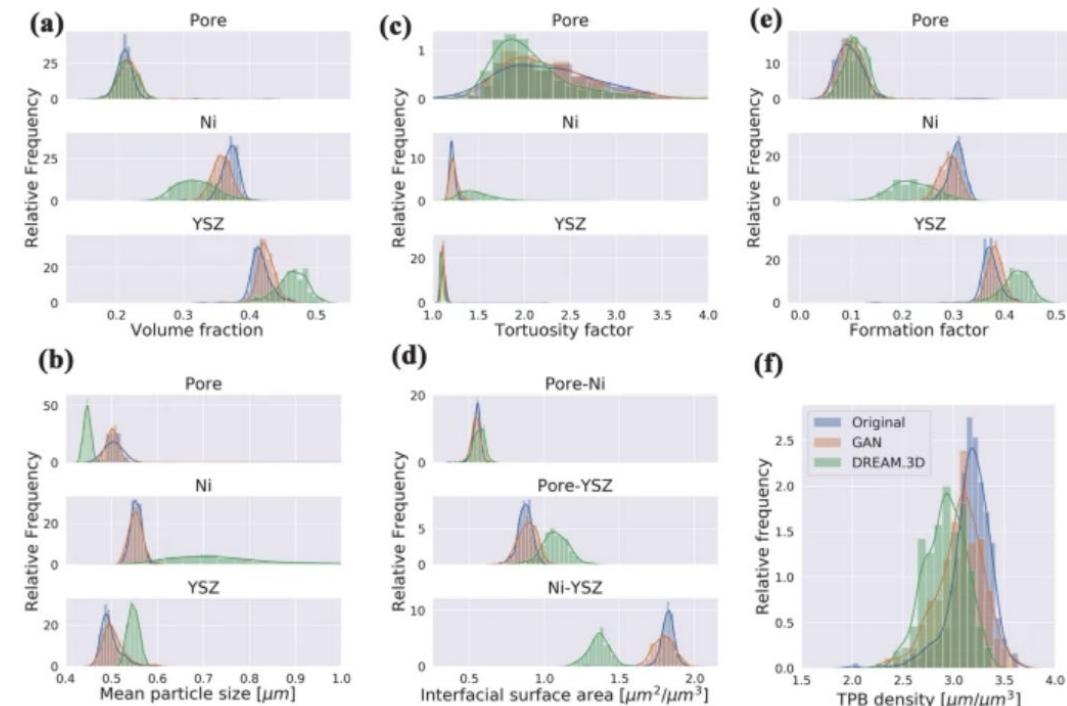
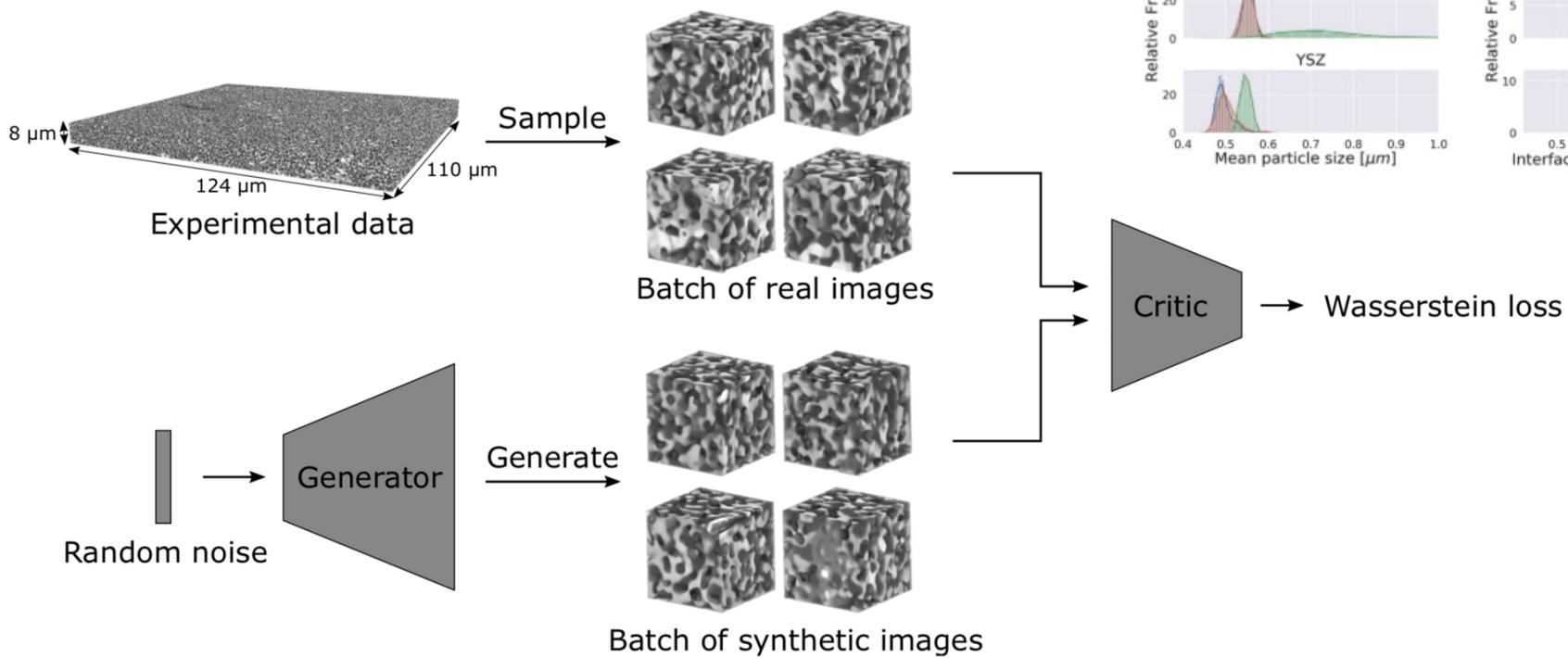
- Uses GAN to predict HEA phases compositions
- Phases get encoded alongside representation
- Used GAN for data augmentation resulting in improved test set performance



Wasserstein GANs have been used extensively to recreate synthetic microstructures

Hsu et al. (2021)

- Train on 3D microstructure data
- WGANs do a great job of matching real data
- DREAM.3D uses grain-based genetic algorithm does worse!



Can we use generative models to create full crystal structures?

Issue 1, 2024

Previous Article

Next Article



From the journal:
Digital Discovery

Generative adversarial networks and diffusion models in material discovery



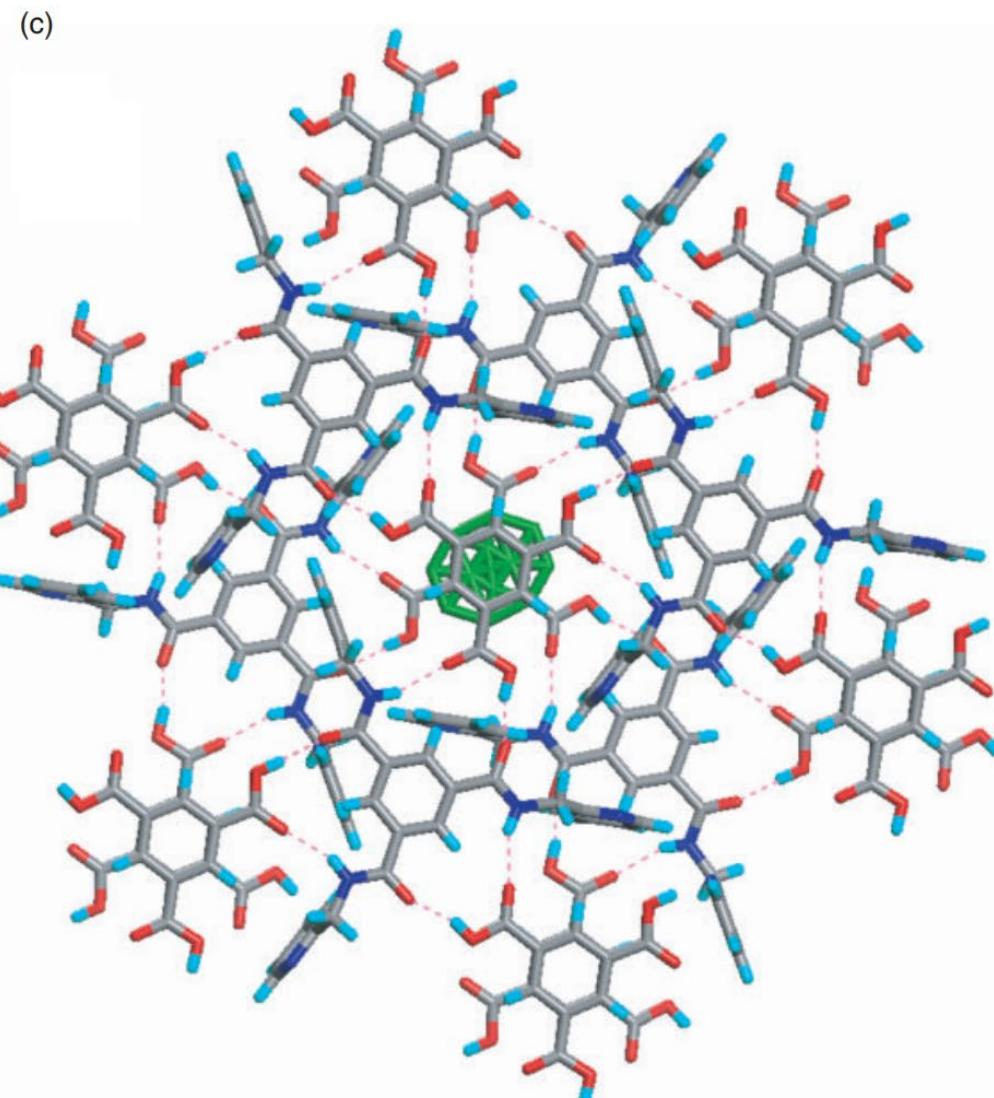
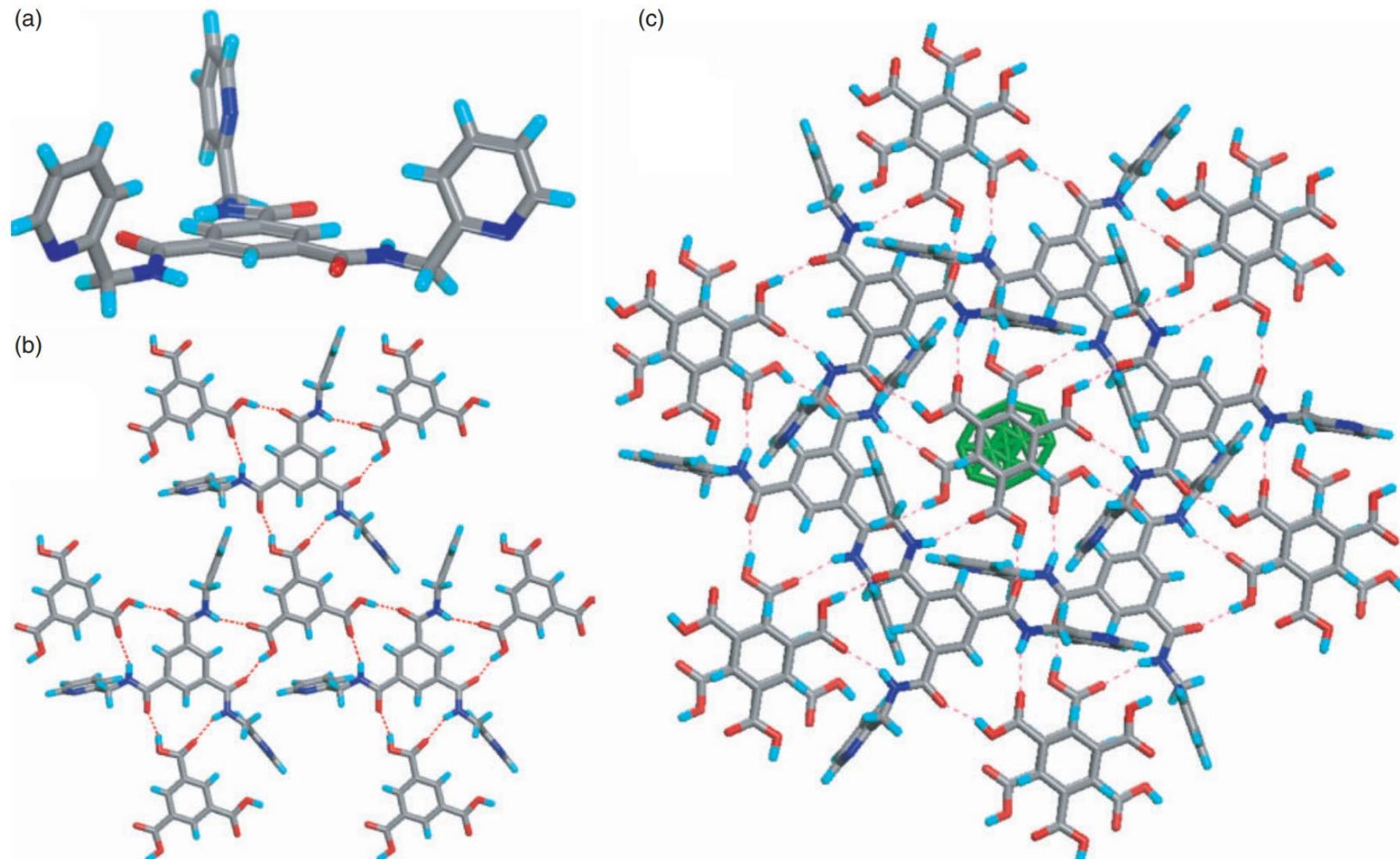
Michael Alverson, ^{*ac} Sterling G. Baird, ^a Ryan Murdock, ^a (Enoch) Sin-Hang Ho, ^b Jeremy Johnson, ^b and Taylor D. Sparks ^a

Author affiliations

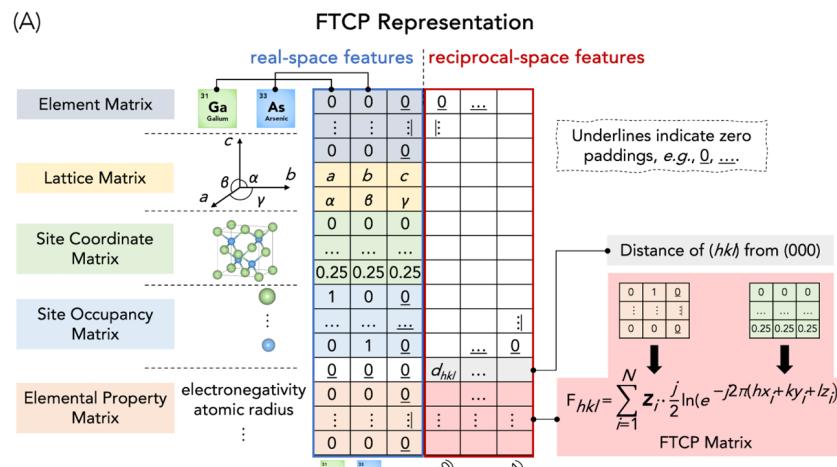
Abstract

The idea of materials discovery has excited and perplexed research scientists for centuries. Several different methods have been employed to find new types of materials, ranging from the arbitrary replacement of atoms in a crystal structure to advanced machine learning methods for predicting entirely new crystal structures. In this work, we pursue three primary objectives. (I) Introduce CrysTens, a crystal encoding that can be used in a wide variety of deep learning generative models. (II) Investigate and analyze the relative performance of Generative Adversarial Networks (GANs) and Diffusion Models to find an innovative and effective way of generating theoretical crystal structures that are synthesizable and stable. (III) Show that the models that have a better “understanding” of the structure of CrysTens produce more symmetrical and realistic crystals and exhibit a better apprehension of the dataset as a whole. We accomplish these objectives using over fifty thousand Crystallographic Information Files (CIFs) from Pearson’s Crystal Database.

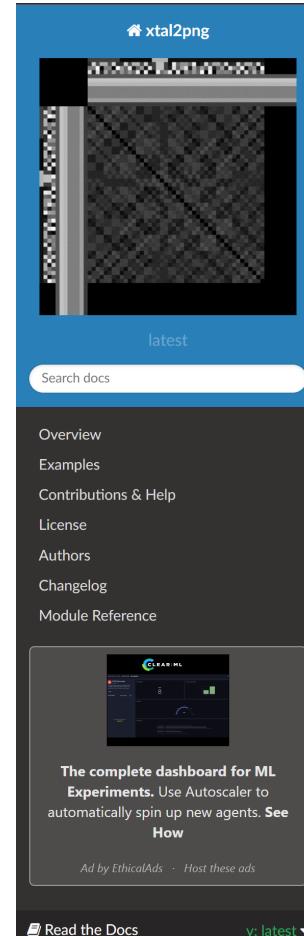
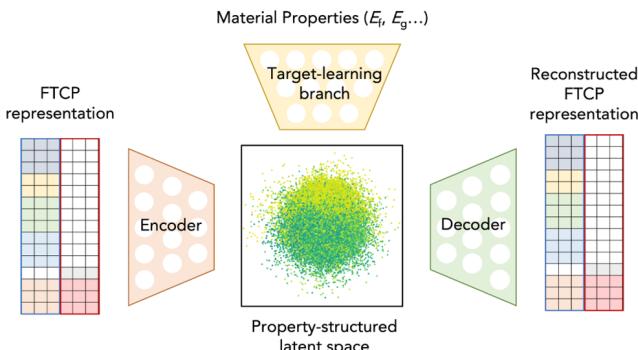
Solid-state chem has lagged organic chemistry here for years



Encoding cif info into representations has been key for crystalline materials



(B) VAE Model with Property-Structured Latent Space



xtal2png

Encode/decode a crystal structure to/from a grayscale PNG image for direct use with image-based machine learning models such as [Imagen](#), [DALLE2](#), or [Palette](#).¹

Open in Colab JOSS Under Review downloads: 422/month Conda Downloads 2.1k

Star 12 Follow @sgbaird 66 Issue 24 Discuss

The latest advances in machine learning are often in natural language such as with long short-term memory networks (LSTMs) and transformers or image processing such as with generative adversarial networks (GANs), variational autoencoders (VAEs), and guided diffusion models; however, transferring these advances to adjacent domains such as materials informatics often takes years. [xtal2png](#) encodes and decodes crystal structures via grayscale PNG images by writing and reading the necessary information for crystal reconstruction (unit cell, atomic elements, atomic coordinates) as a square matrix of numbers, respectively. This is akin to making/reading a QR code for crystal structures, where the [xtal2png](#) representation is invertible. The ability to feed these images directly into image-based pipelines allows you, as a materials informatics practitioner, to get streamlined results for new state-of-the-art image-based machine learning models applied to crystal structure.

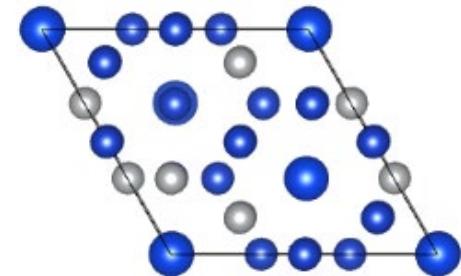
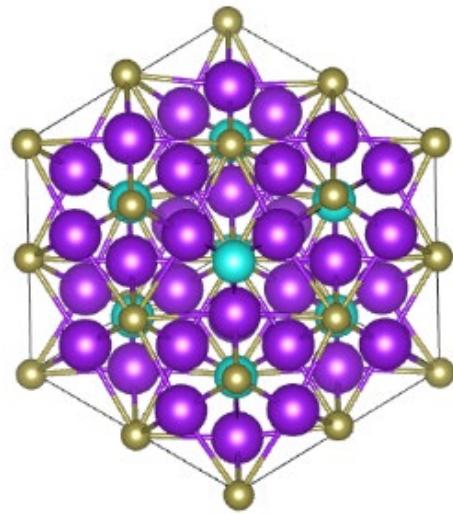
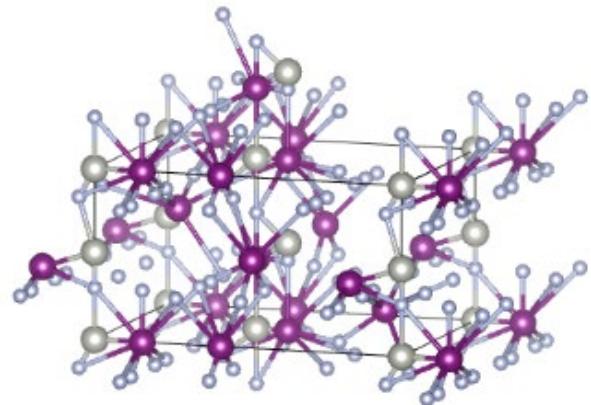
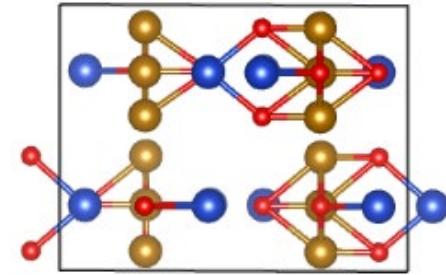
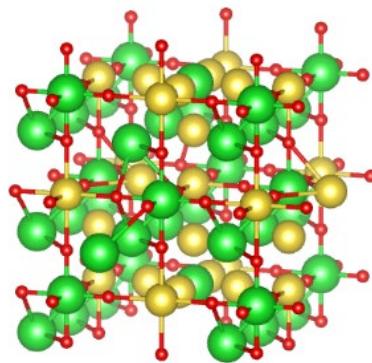
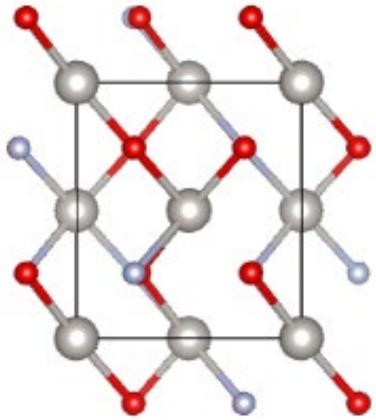
Results manuscript coming soon!

Contents

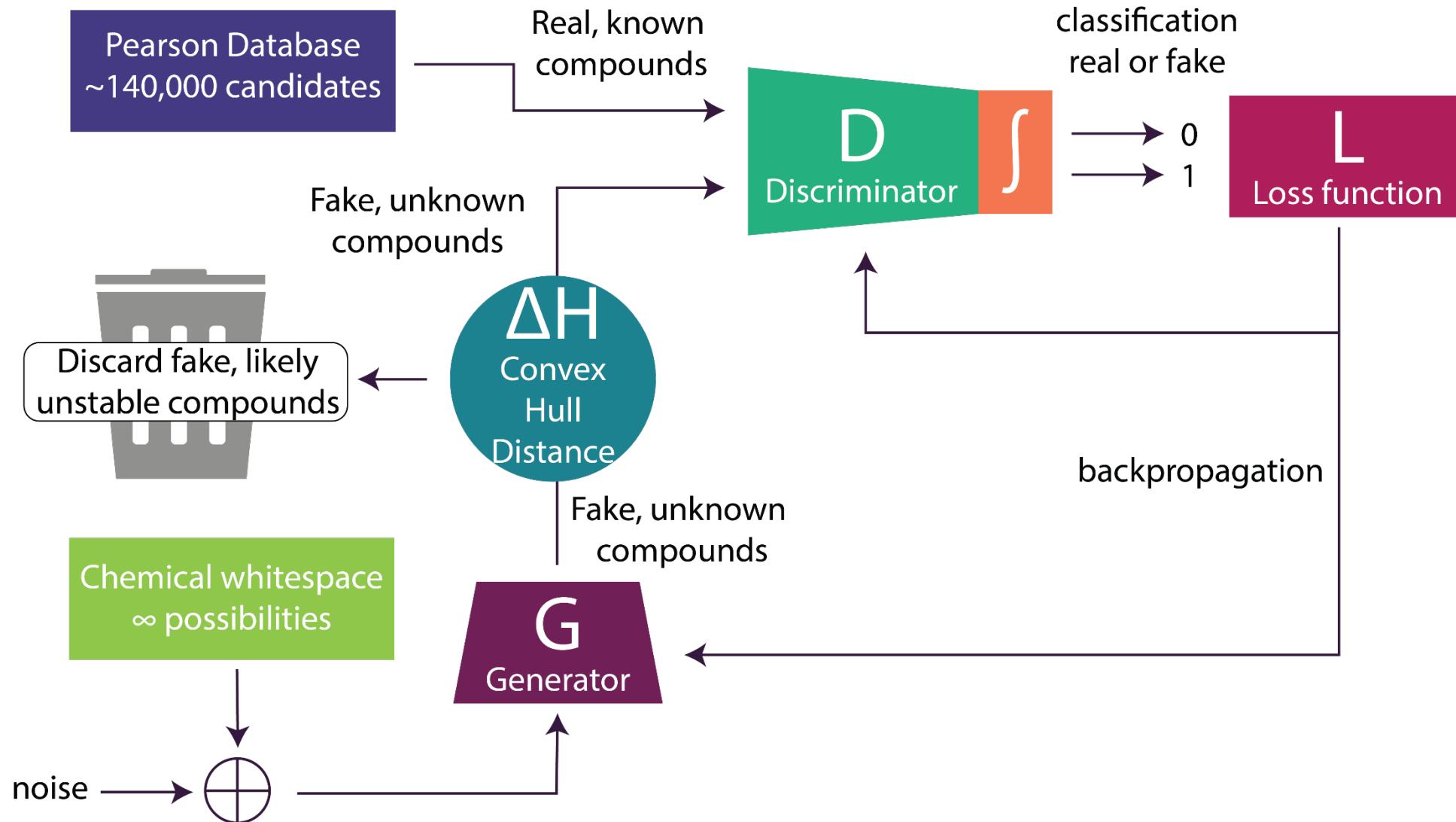
- Overview
 - Getting Started
 - Limitations and Design Considerations
 - Installation
 - Editable installation
 - Command Line Interface (CLI)

Ren et al, An invertible crystallographic representation for general inverse design of inorganic crystals with targeted properties, Matter 2022,
Baird et al, xtal2png: A Python package for representing crystal structure as PNG files, JOSS 2022

Generative models can now create increasingly convincing new structures



We initially used a modified GAN architecture

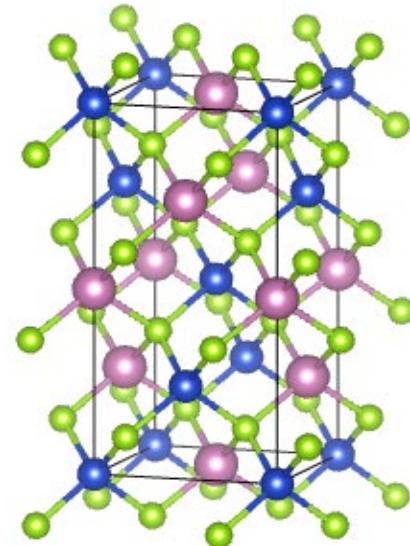
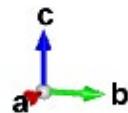


The necessary cif information is pretty simple

<code>_cell_length_a</code>	5.7828
<code>_cell_length_b</code>	5.7828
<code>_cell_length_c</code>	11.6207
<code>_cell_angle_alpha</code>	90
<code>_cell_angle_beta</code>	90
<code>_cell_angle_gamma</code>	90
<code>_cell_volume</code>	388.6
<code>_cell_formula_units_Z</code>	4
<code>space_group_IT_number</code>	122
<code>_space_group_name_H-M_alt</code>	'I -4 2 d'

Se Se 8 d 0.2344 0.25 0.125 1
In In 4 b 0 0 0.5 1
Cu Cu 4 a 0 0 0 1

VESTA



Tools like pymatgen make it easy to extract

```
Structure Summary
Lattice
    abc : 5.7828 5.7828 11.6207
    angles : 90.0 90.0 90.0
    volume : 388.605223803888
        A : 5.7828 0.0 3.540943755054657e-16
        B : 9.299451658550054e-16 5.7828 3.540943755054657e-16
        C : 0.0 0.0 11.6207
PeriodicSite: In (0.0000, 0.0000, 5.8103) [0.0000, 0.0000, 0.5000]
PeriodicSite: In (0.0000, 2.8914, 8.7155) [0.0000, 0.5000, 0.7500]
PeriodicSite: In (2.8914, 2.8914, 0.0000) [0.5000, 0.5000, 0.0000]
PeriodicSite: In (2.8914, 0.0000, 2.9052) [0.5000, 0.0000, 0.2500]
PeriodicSite: Cu (0.0000, 0.0000, 0.0000) [0.0000, 0.0000, 0.0000]
PeriodicSite: Cu (0.0000, 2.8914, 2.9052) [0.0000, 0.5000, 0.2500]
PeriodicSite: Cu (2.8914, 2.8914, 5.8103) [0.5000, 0.5000, 0.5000]
PeriodicSite: Cu (2.8914, 0.0000, 8.7155) [0.5000, 0.0000, 0.7500]
PeriodicSite: Se (1.3555, 1.4457, 1.4526) [0.2344, 0.2500, 0.1250]
PeriodicSite: Se (4.4273, 4.3371, 1.4526) [0.7656, 0.7500, 0.1250]
PeriodicSite: Se (4.3371, 1.5359, 4.3578) [0.7500, 0.2656, 0.3750]
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PeriodicSite: Se (1.5359, 1.4457, 7.2629) [0.2656, 0.2500, 0.6250]
```

Some data cleaning was necessary



About Pearson's CD

Data Information...

Software Functions...

Features...

Brochure (PDF)...

References...

Get Pearson's CD

Order Now

Demo Version

A **free-of-charge** demo

version with a few

thousand datasets can be

downloaded. [More...](#)

Quickstart

A quickstart manual is

also available in Spanish.

[More...](#)

Support

Updates...

Known Bugs...

HowTo...

Frequently Asked

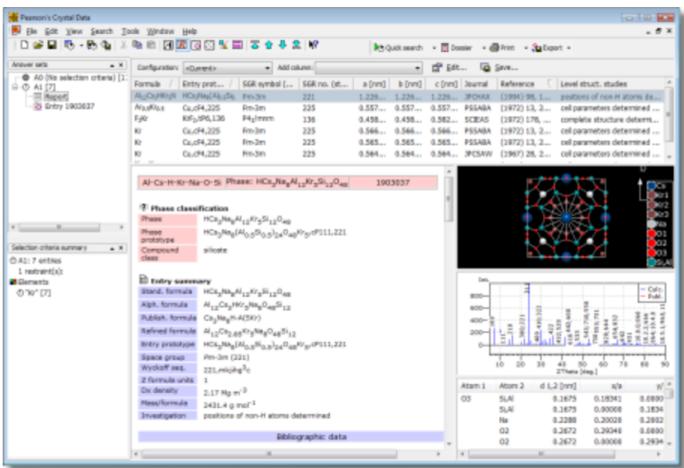
Questions...

User Group...

Pearson's Crystal Data

Crystal Structure Database for Inorganic Compounds

Pearson's Crystal Data is a crystallographic database published by [ASM International](#) (Materials Park, Ohio, USA), edited by Pierre Villars and Karin Cenzual. It has its roots in the well-known [PAULING FILE project](#) and contains crystal structures of a large variety of inorganic materials and compounds. The "PCD" (as it is typically abbreviated) is a collaboration between ASM International and [Material Phases Data System](#), Vitznau, Switzerland (MPDS), aiming to create and maintain the world's largest critically evaluated "Non-organic database".



The current release 2020/21 contains about 350,000 structural data sets (including atom coordinates and displacement parameters, when determined) for about 195,000 different chemical formulas, roughly 20,500 experimental powder diffraction patterns and about 297,000 calculated patterns (interplanar spacings, intensities, Miller indices). In addition over 53,000 figure descriptions for such as cell parameters as a function of temperature, pressure or concentration are given. To reach this result, scientific editors have critically analyzed and processed over 112,500 original publications.

The database comes with an innovative retrieval software for Windows PCs developed by Crystal Impact. It offers a large variety of new [elaborate new features](#) which make retrieval of the desired information extremely easy and comfortable.

Pearson's CD News

[October 15, 2020](#)

The new **Release 2020/21 of Pearson's Crystal Data** has just become available, with a total entry count of about **350,000**.
[More...](#)

[September 30, 2010](#)

Release 2019/20 of Pearson's Crystal Data has just become available, with a total entry count of about **335,000**.
[More...](#)

[July 31, 2019](#)

Another software **update** is available for both **release 2017/18** and **release 2018/19 of Pearson's Crystal Data**.
[More...](#)

[April 1, 2019](#)

Another software **update** is available for both **release 2017/18** and **release 2018/19 of Pearson's Crystal Data**.
[More...](#)

[February 7, 2019](#)

A software **update** is available for both **release 2017/18** and **release 2018/19 of Pearson's Crystal Data**.
[More...](#)

[October 5, 2018](#)

Release 2018/19 of Pearson's Crystal Data has just become available, with a total entry count of about **319,000**.
[More...](#)

~300,000 CIFs in PCD

After cleaning there was
143892 entries retained

Our original data representation was very simple

Structural
information was
averaged over 7
generated entries

								Atom #1		Atom #2					
	a	b	c	α	β	γ	SG	O	He	H	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{a}	\bar{a}	\bar{a}	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{b}	\bar{b}	\bar{b}	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{c}	\bar{c}	\bar{c}	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{x}	\bar{x}	\bar{x}	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{y}	\bar{y}	\bar{y}	-1	\dots	-1		
	a	b	c	α	β	γ	SG	\bar{z}	\bar{z}	\bar{z}	-1	\dots	-1		

Some constraints were necessary to obey symmetry rules

$SG > 195$, structure is cubic

$$\alpha = \beta = \gamma = 90^\circ \text{ and } a = b = c$$

$168 < SG < 194$, structure is hexagonal

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ \text{ and } a = b \neq c$$

Etc...

a, b, c were averaged over 7 generated entries.

Some angles were rounded to required values.

Obeying Pauling's 5th rule, parsimony, required clustering

13.4425125

12.922896

11.164495

15.148039

22.145111

20.458208

20.795254

19.797886

14.355895

12.193807

14.700731

13.9915695

11.117646

8.640331

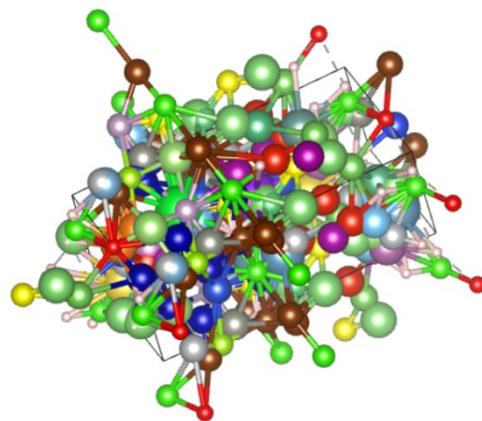
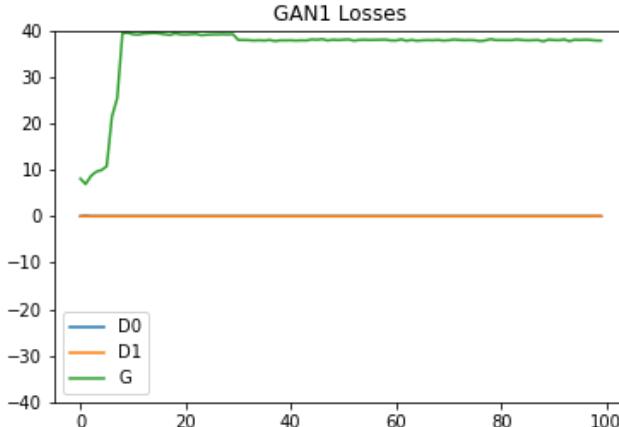
11.288832

Obeying Pauling's 5th rule, parsimony, required clustering

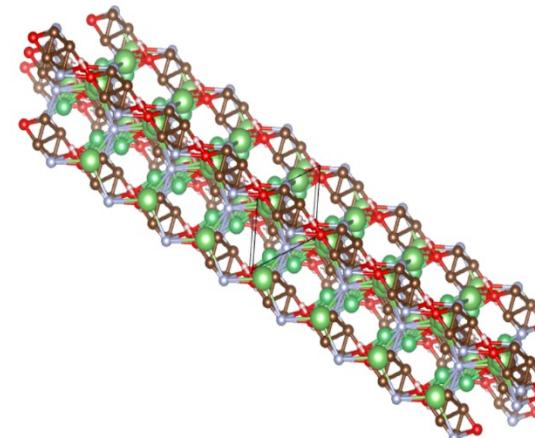
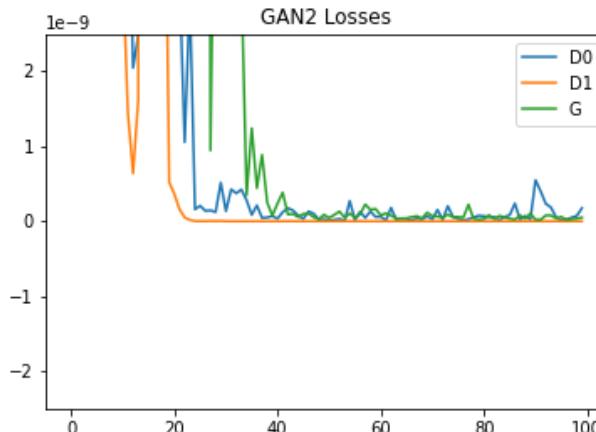
13.4425125	12.633341	Aluminium	Aluminium
12.922896	12.633341	Aluminium	Aluminium
11.164495	12.633341	Sodium	Aluminium
15.148039	12.633341	Phosphorus	Aluminium
22.145111	20.799114	Titanium	Scandium
20.458208	20.799114	Calcium	Scandium
20.795254	20.799114	Scandium	Scandium
19.797886	20.799114	Calcium	Scandium
14.355895	12.633341	Silicon	Aluminium
12.193807	12.633341	Magnesium	Aluminium
14.700731	12.633341	Phosphorus	Aluminium
13.9915695	12.633341	Silicon	Aluminium
11.117646	12.633341	Sodium	Aluminium
8.640331	12.633341	Fluorine	Aluminium
11.288832	12.633341	Sodium	Aluminium

Traditional GANS did not perform well

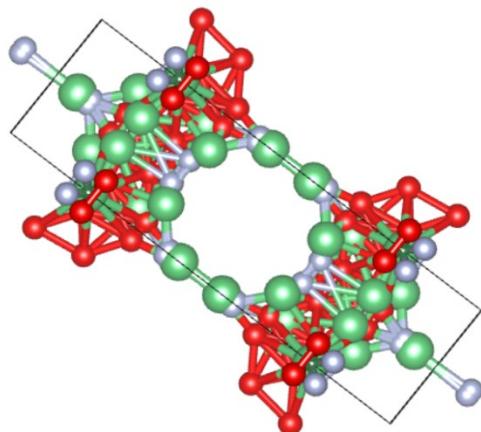
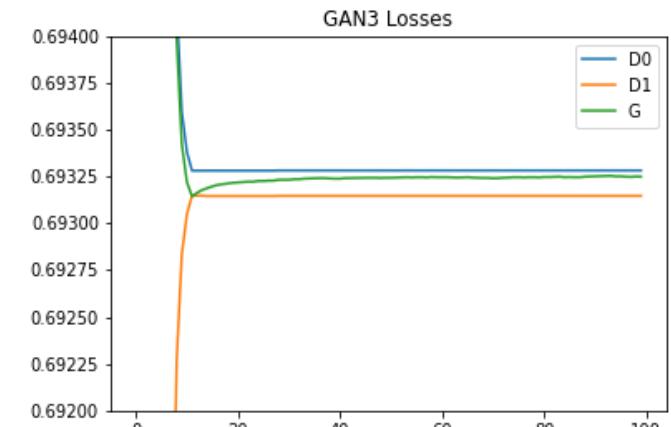
GAN1: Baseline Performance,
only convolutions, no
normalizations



GAN2: Batch normalization,
only convolutions



GAN3: Added LSTM layers



Symmetry only representations aren't going to cut it



2014



2015



2016



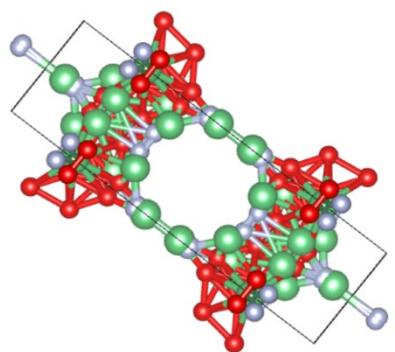
2017



2018

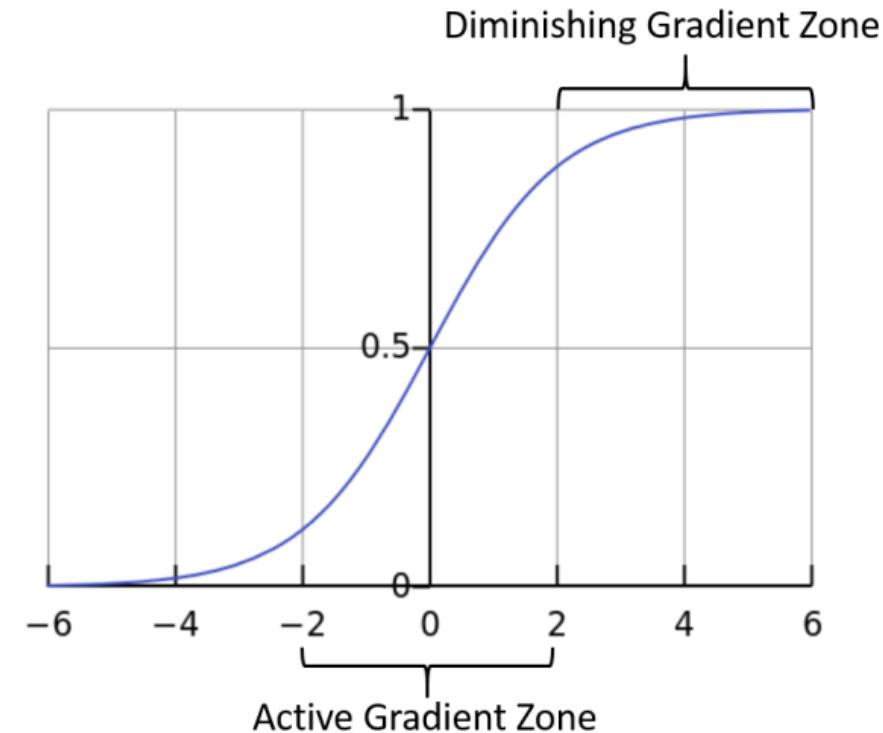


2021

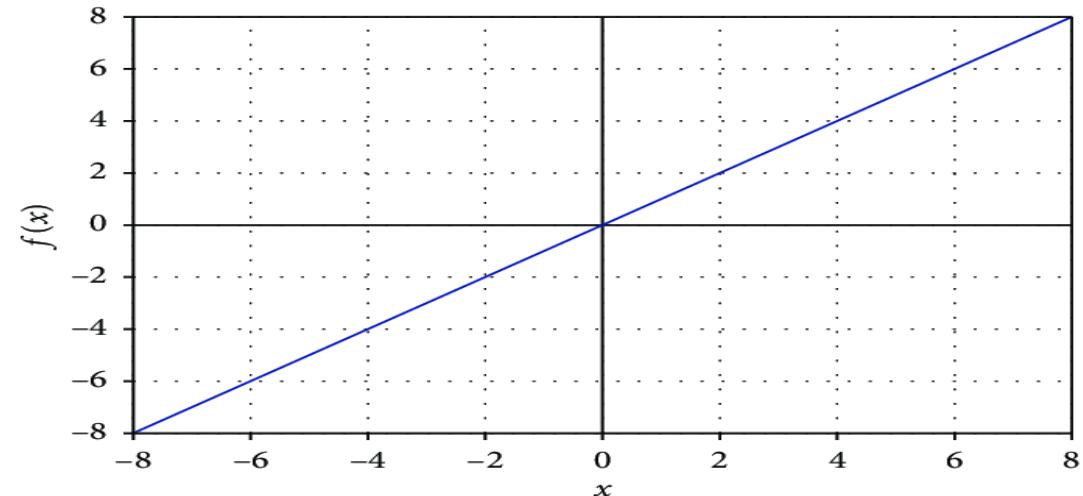
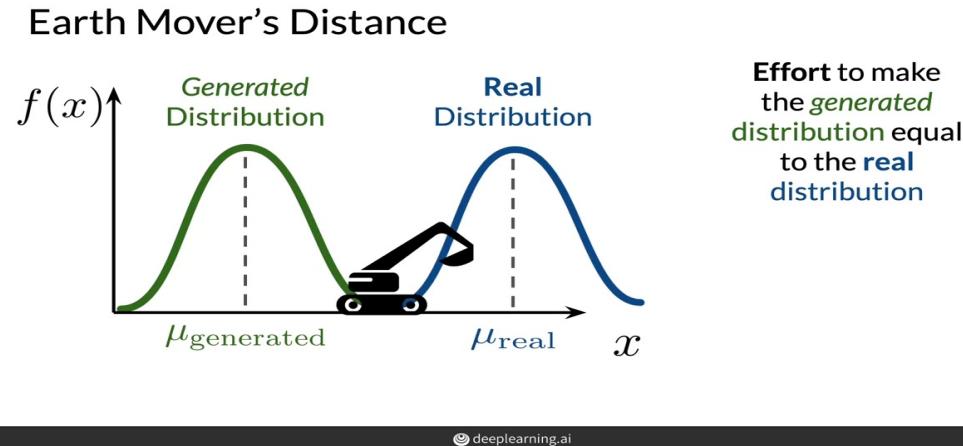


Traditional GANs have some training limitations

$$A = \frac{1}{1+e^{-x}}$$

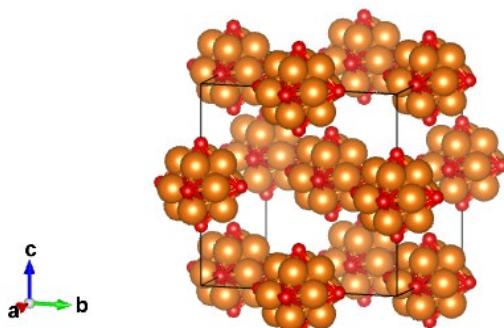


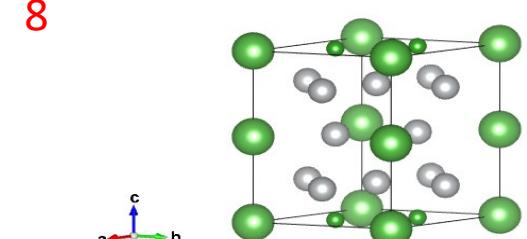
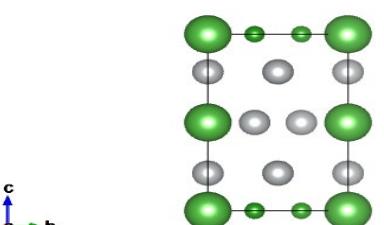
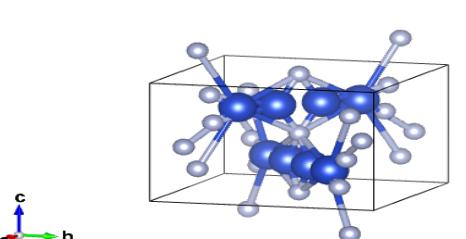
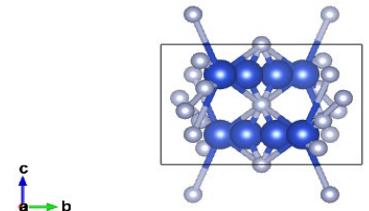
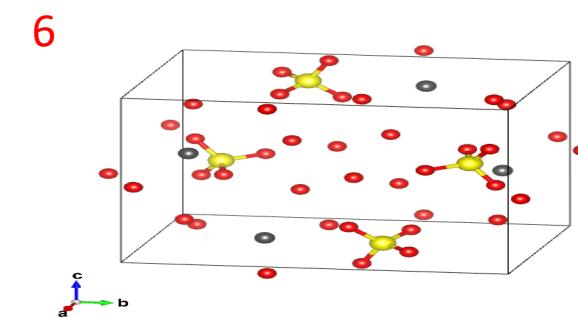
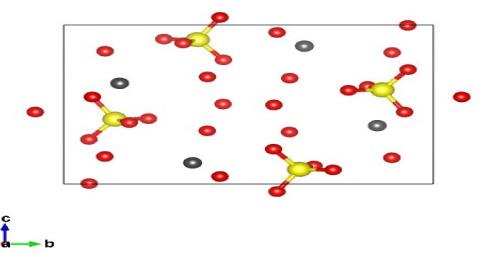
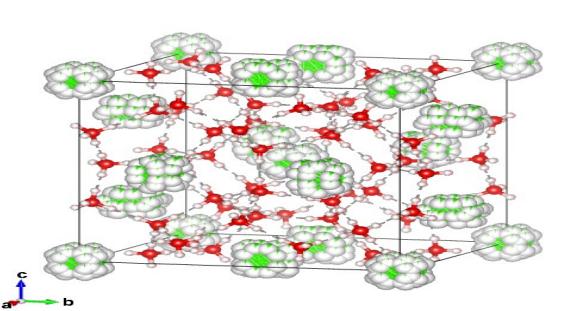
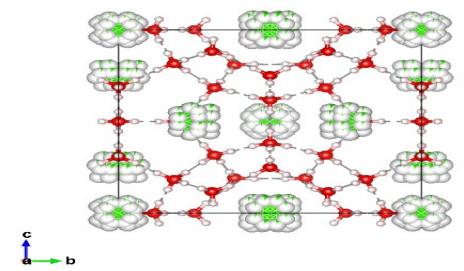
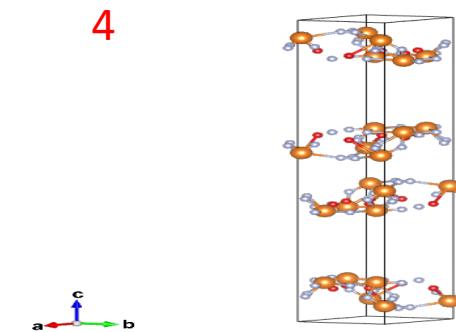
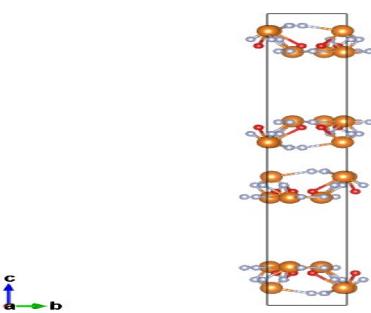
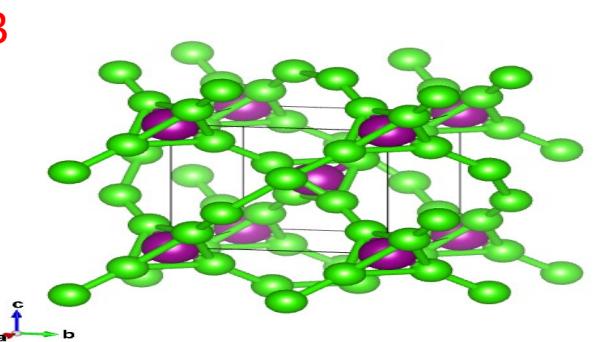
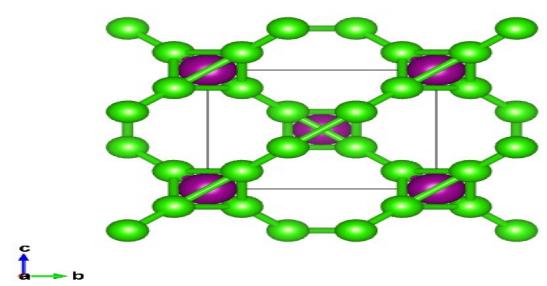
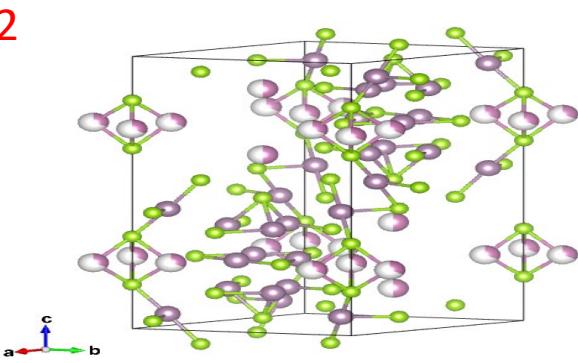
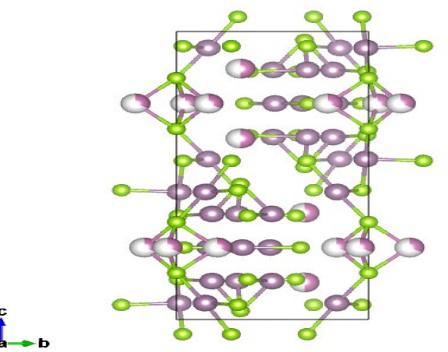
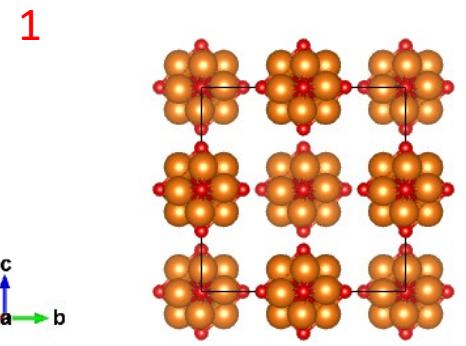
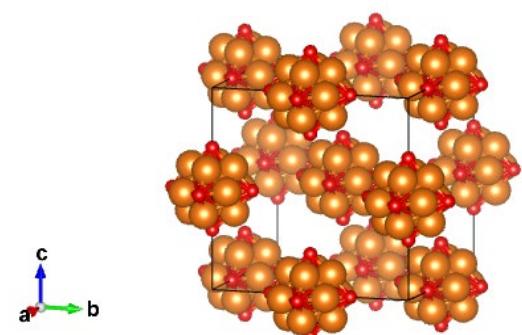
Wasserstein GANs offer some solutions

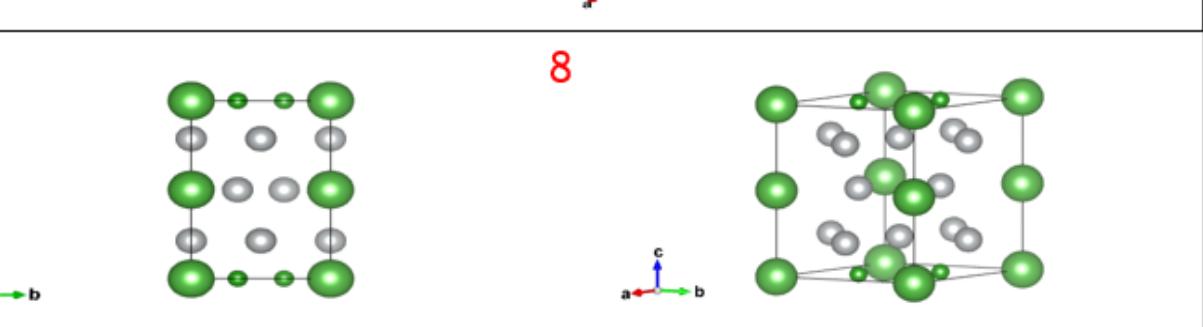
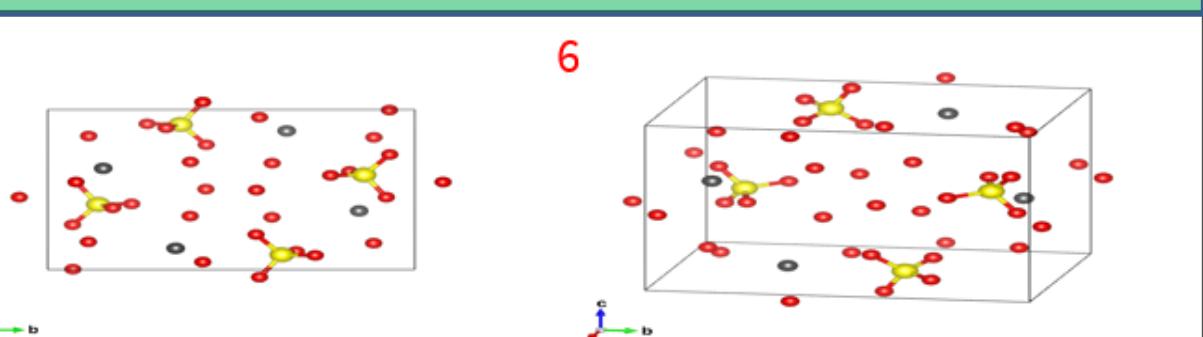
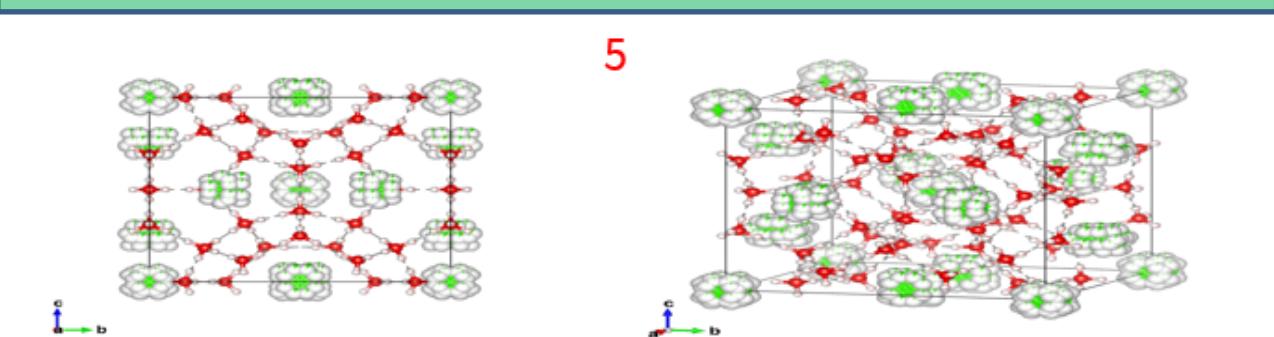
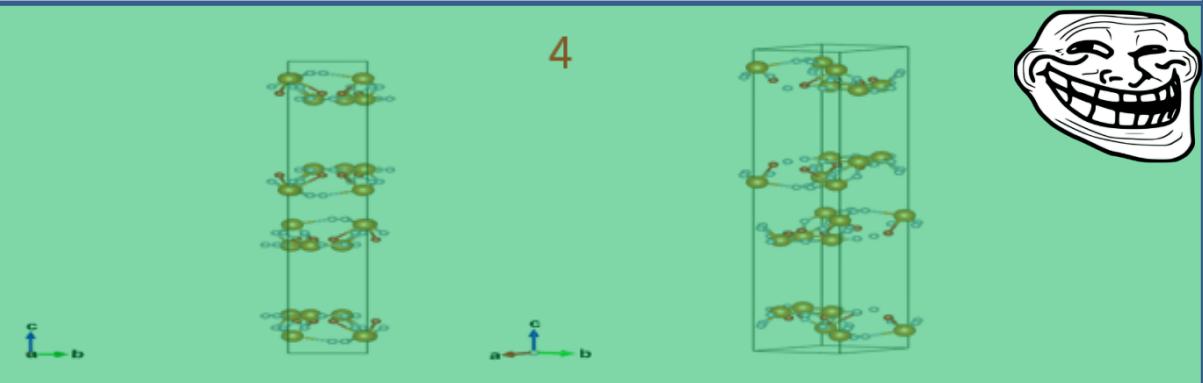
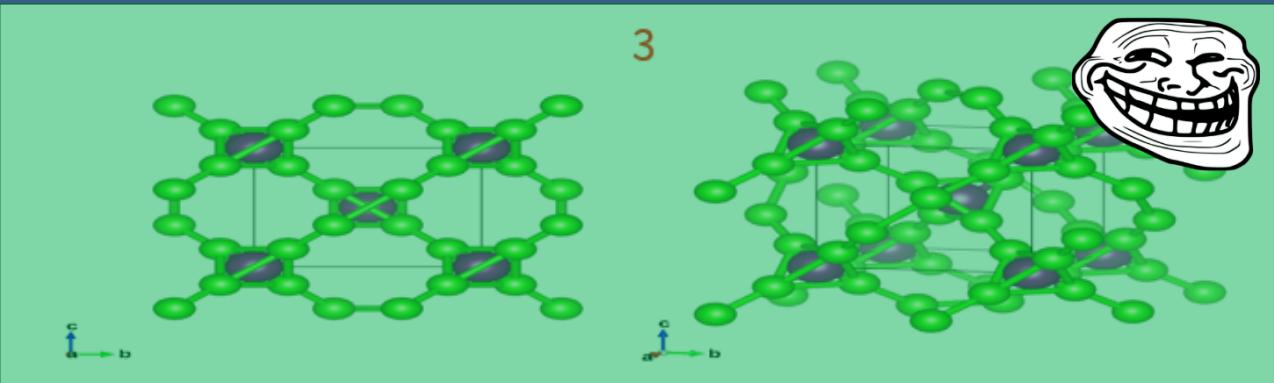
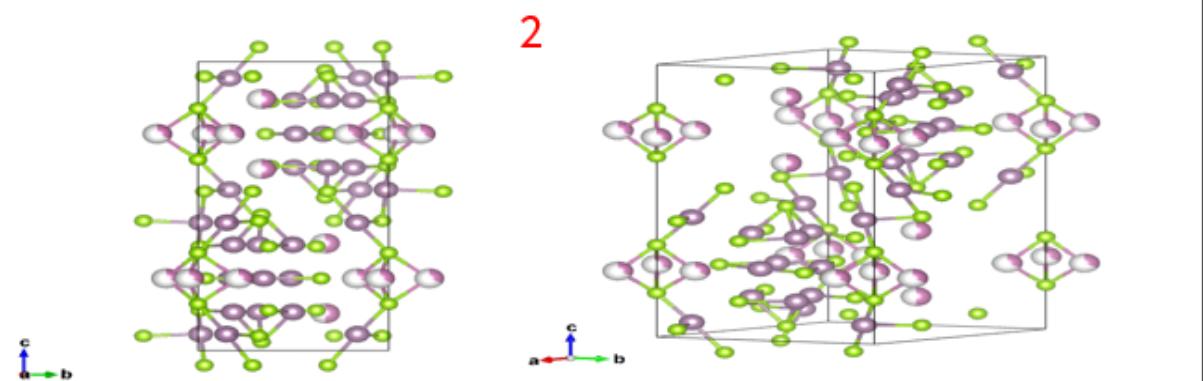
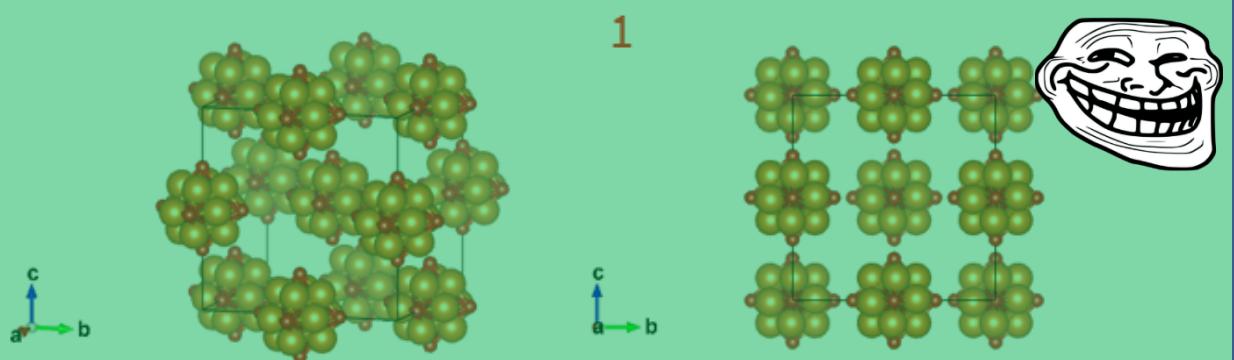


Lipschitz continuity: weight clipping vs gradient penalty

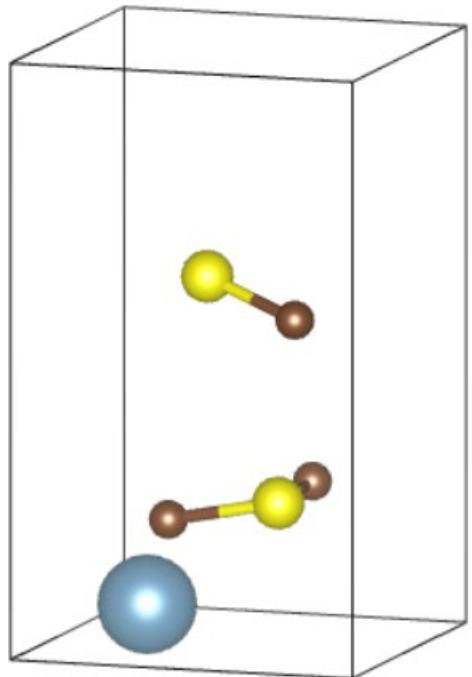
Normalization: batch normalization vs
layer normalization vs
spectral normalization



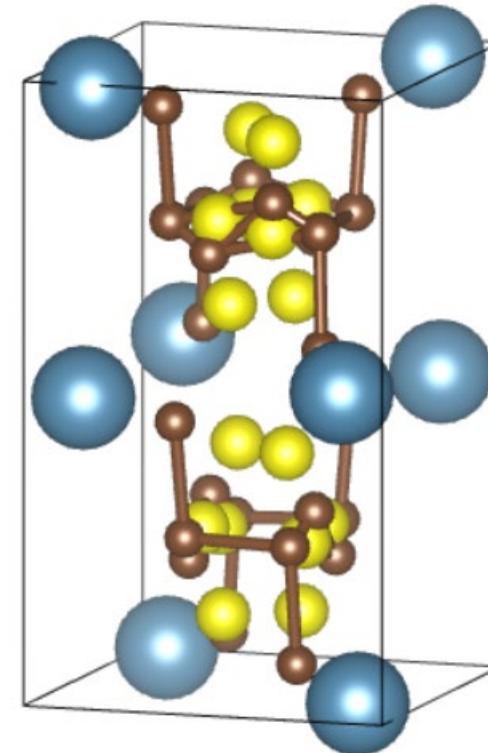




We are still not learning basics of chemistry like bond distances

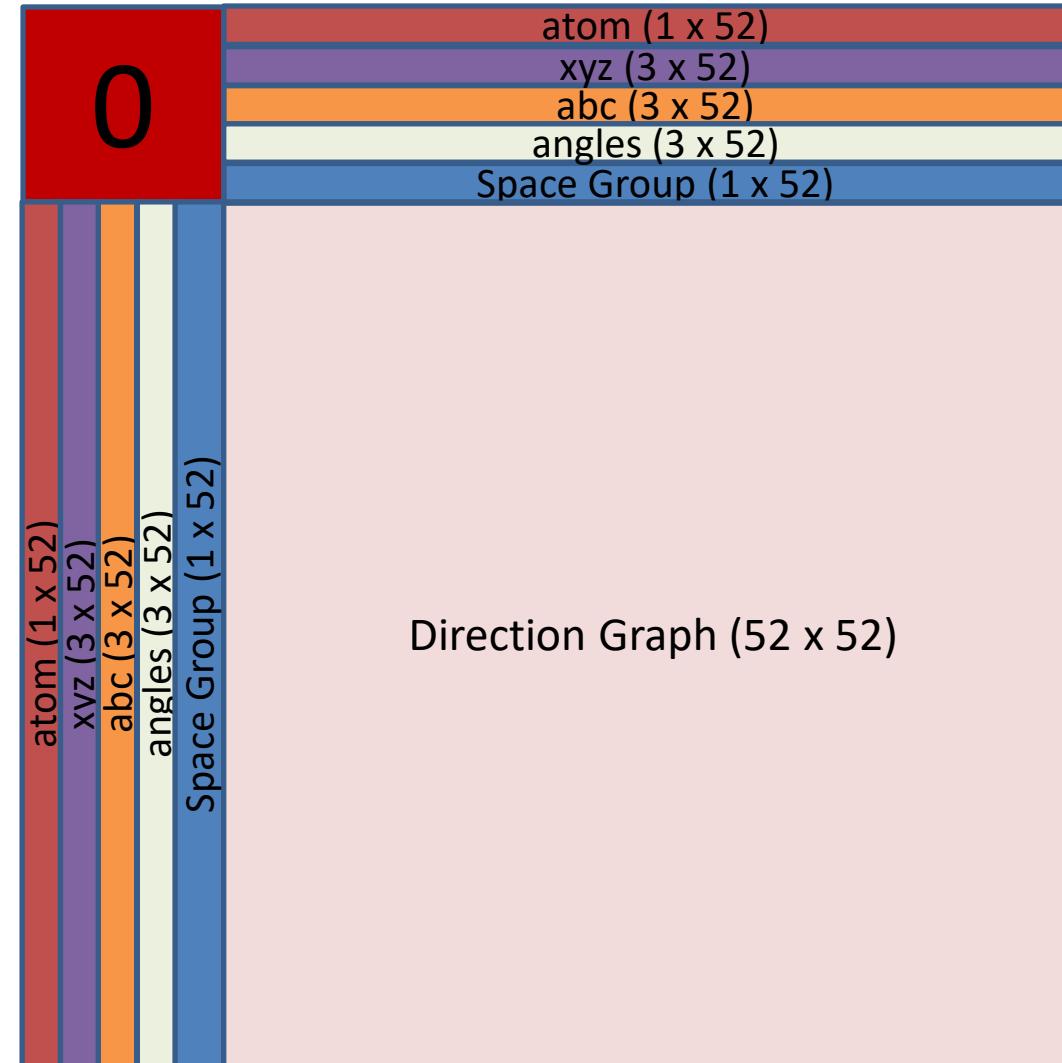


Pymatgen symmetry



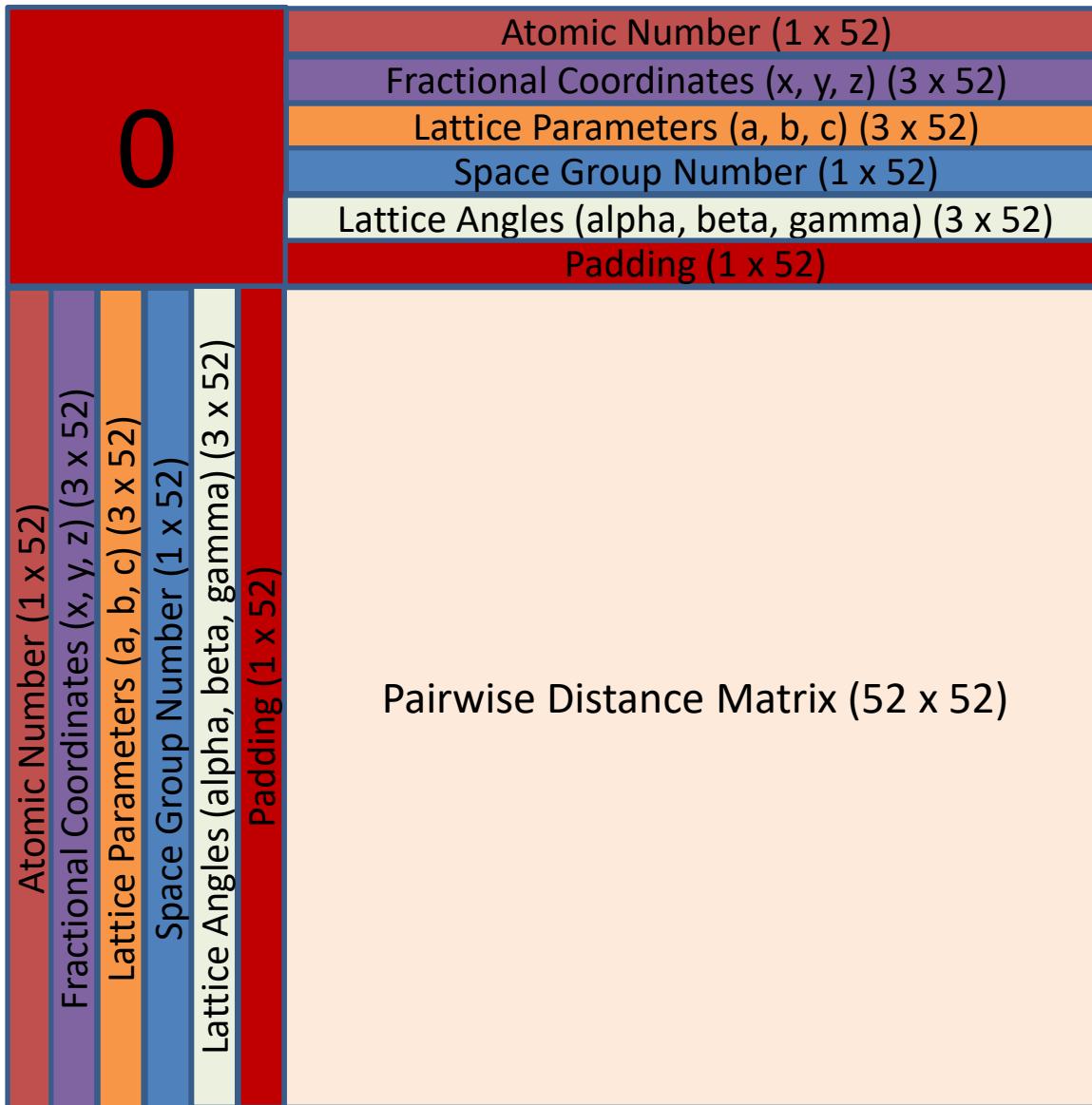
We need to encode chemical information into our representation

Graph tensor
representation is
needed

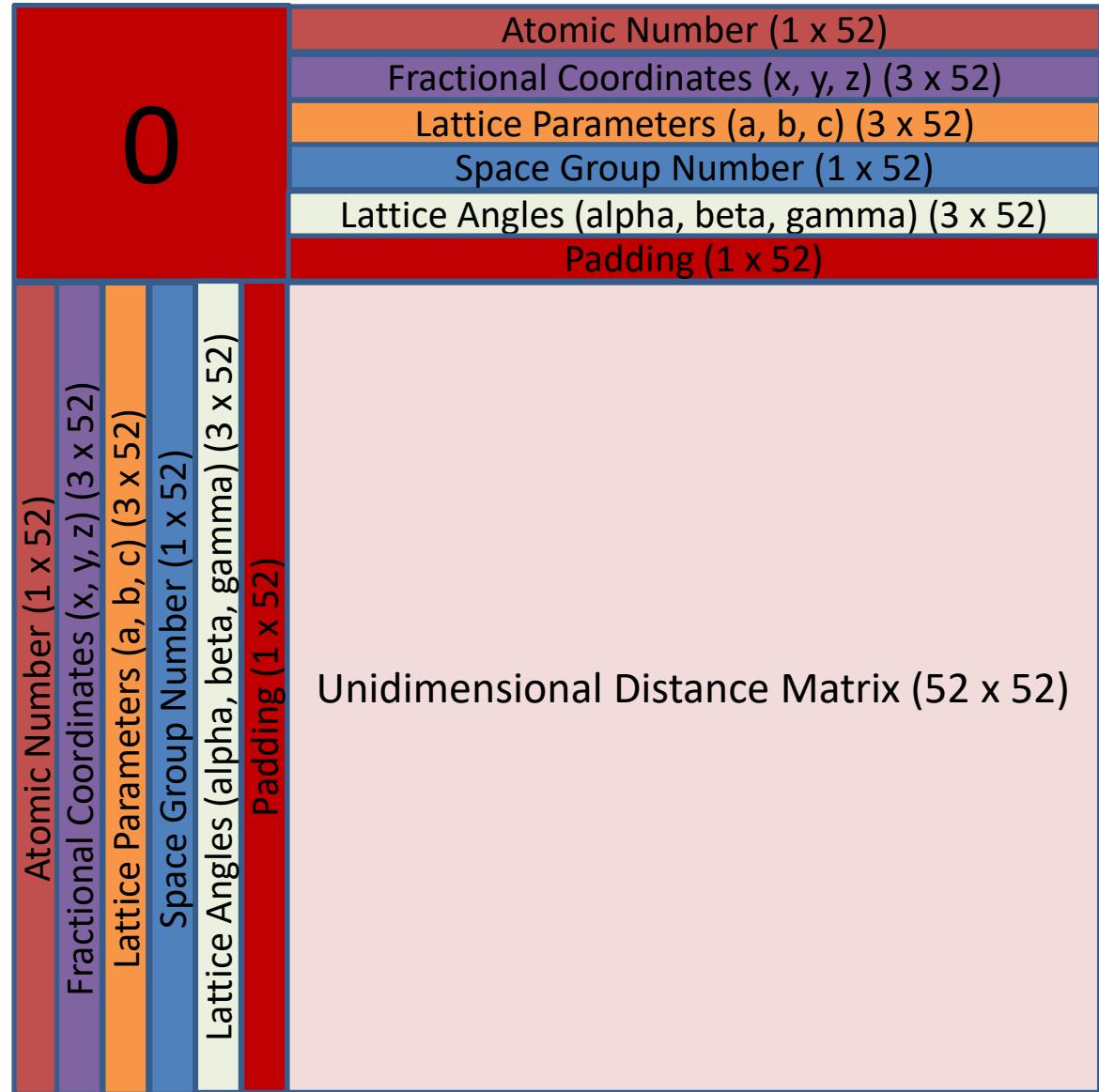


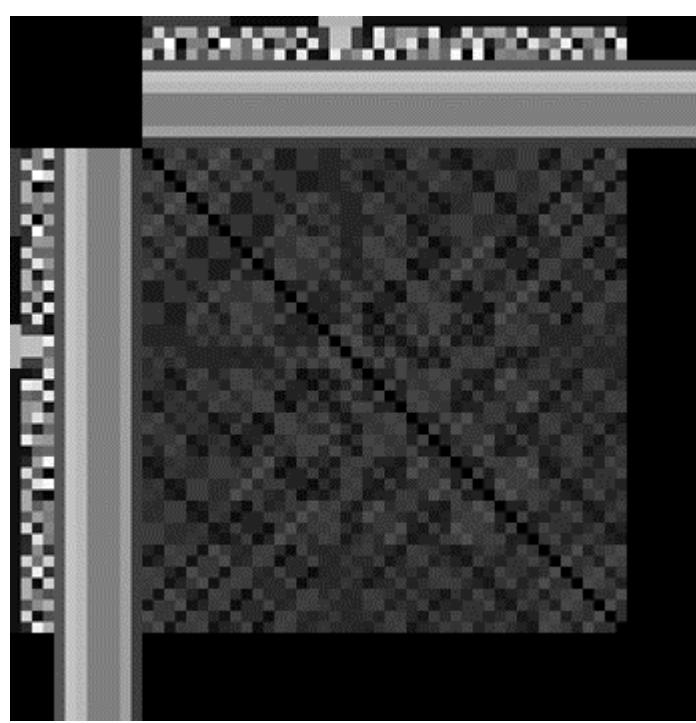
We need to encode chemical information into our representation

Layer 1

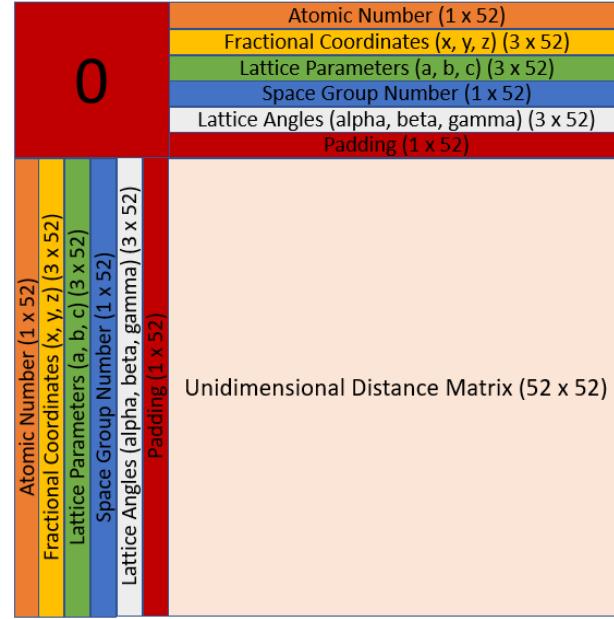
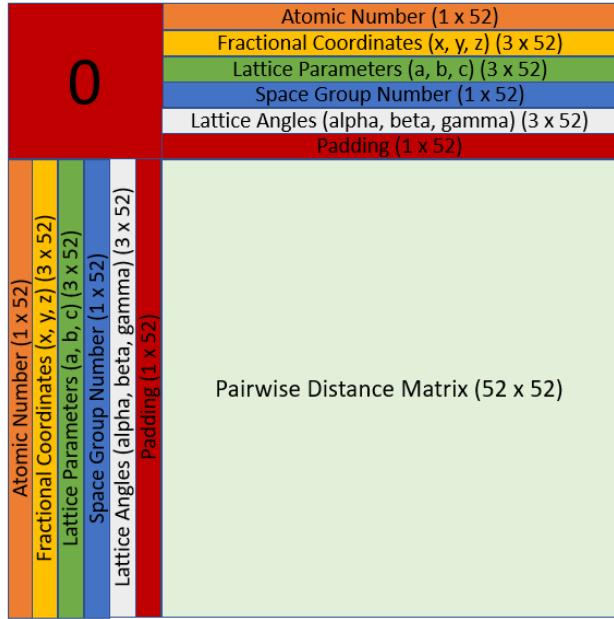


Layers 2-4

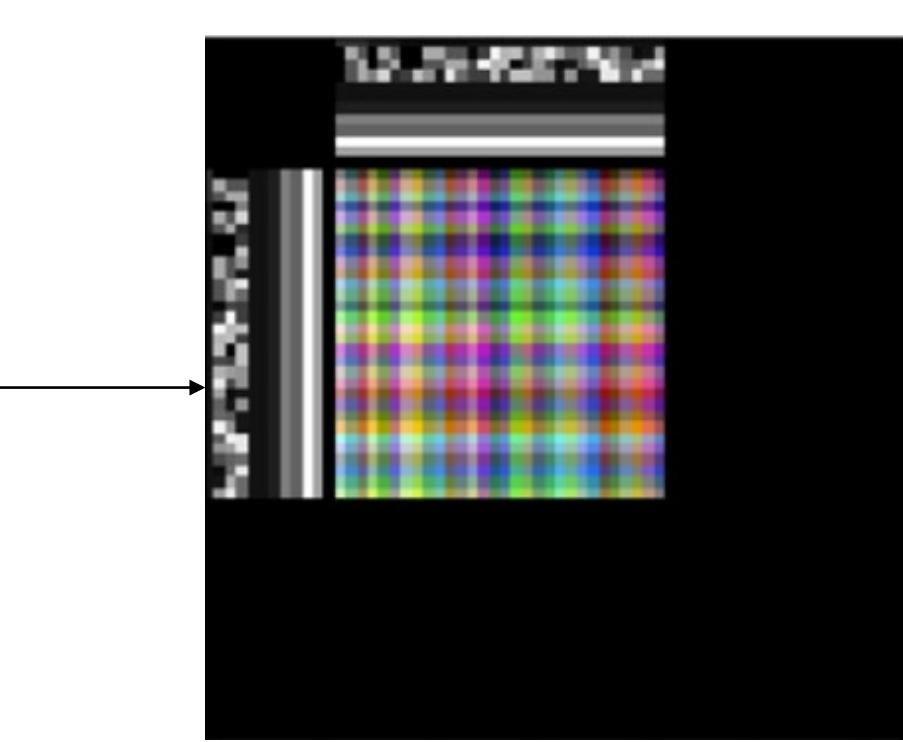


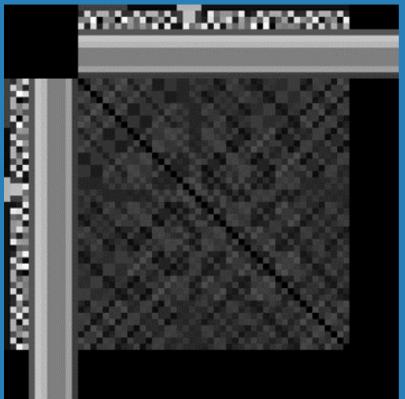


Pairwise Distance Matrix (52 x 52)



Unidimensional Distance Matrix (52 x 52)





latest

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xtal2png

Encode/decode a crystal structure to/from a grayscale PNG image for direct use with image-based machine learning models such as [Imagen](#), [DALLE2](#), or [Palette](#).¹

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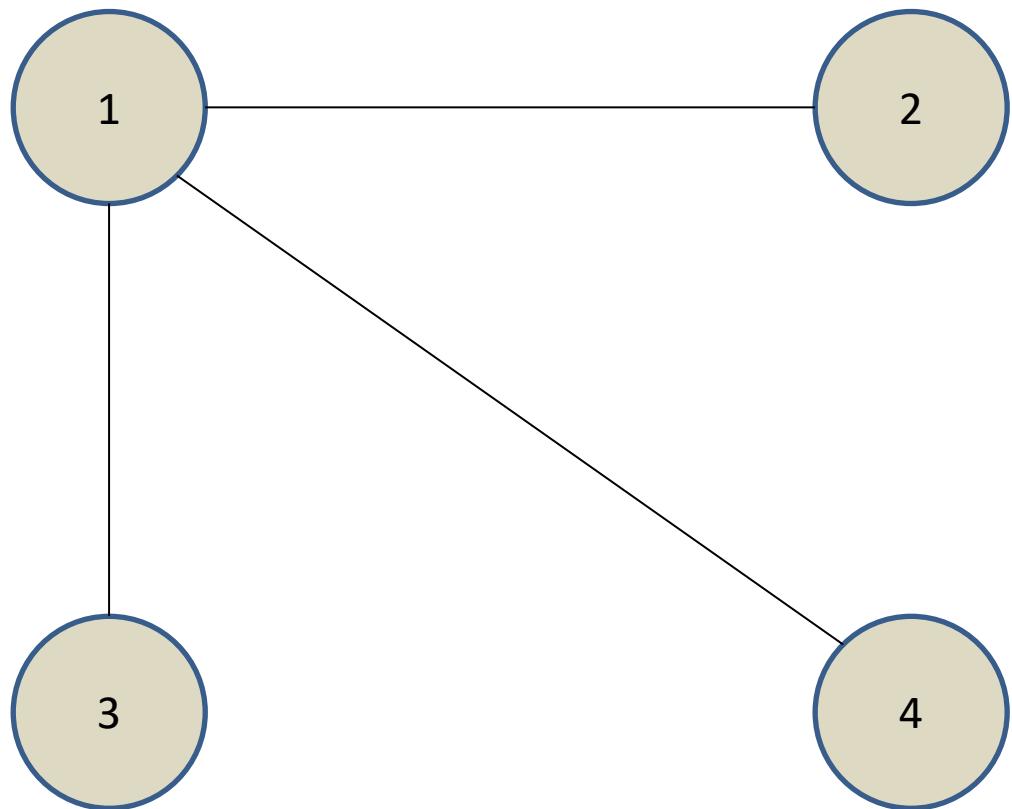
The latest advances in machine learning are often in natural language such as with long short-term memory networks (LSTMs) and transformers or image processing such as with generative adversarial networks (GANs), variational autoencoders (VAEs), and guided diffusion models; however, transferring these advances to adjacent domains such as materials informatics often takes years. `xtal2png` encodes and decodes crystal structures via grayscale PNG images by writing and reading the necessary information for crystal reconstruction (unit cell, atomic elements, atomic coordinates) as a square matrix of numbers, respectively. This is akin to making/reading a QR code for crystal structures, where the `xtal2png` representation is invertible. The ability to feed these images directly into image-based pipelines allows you, as a materials informatics practitioner, to get streamlined results for new state-of-the-art image-based machine learning models applied to crystal structure.

Results manuscript coming soon!

Contents

- [Overview](#)
 - [Getting Started](#)
 - [Limitations and Design Considerations](#)
 - [Installation](#)
 - [Editable installation](#)
 - [Command Line Interface \(CLI\)](#)

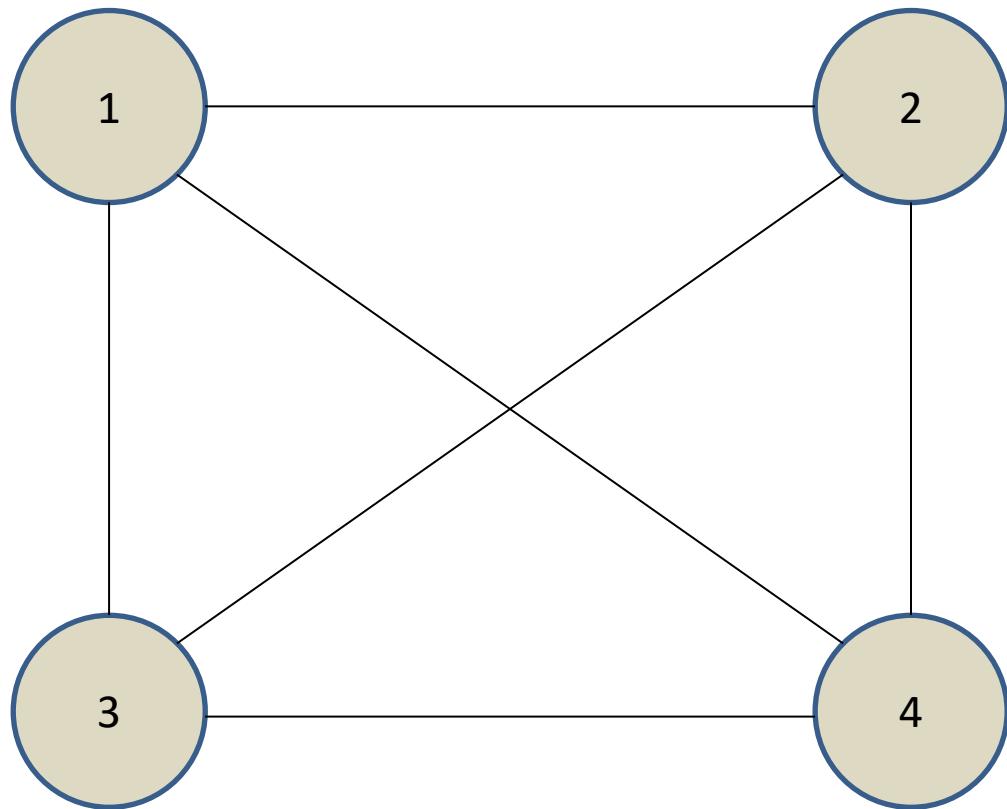
Direction graphs can be constructed in x, y, z directions



1	2	3	4	
1	0	s	0	s
2	-s	0		
3	0		0	
4	-s			0

X direction matrix

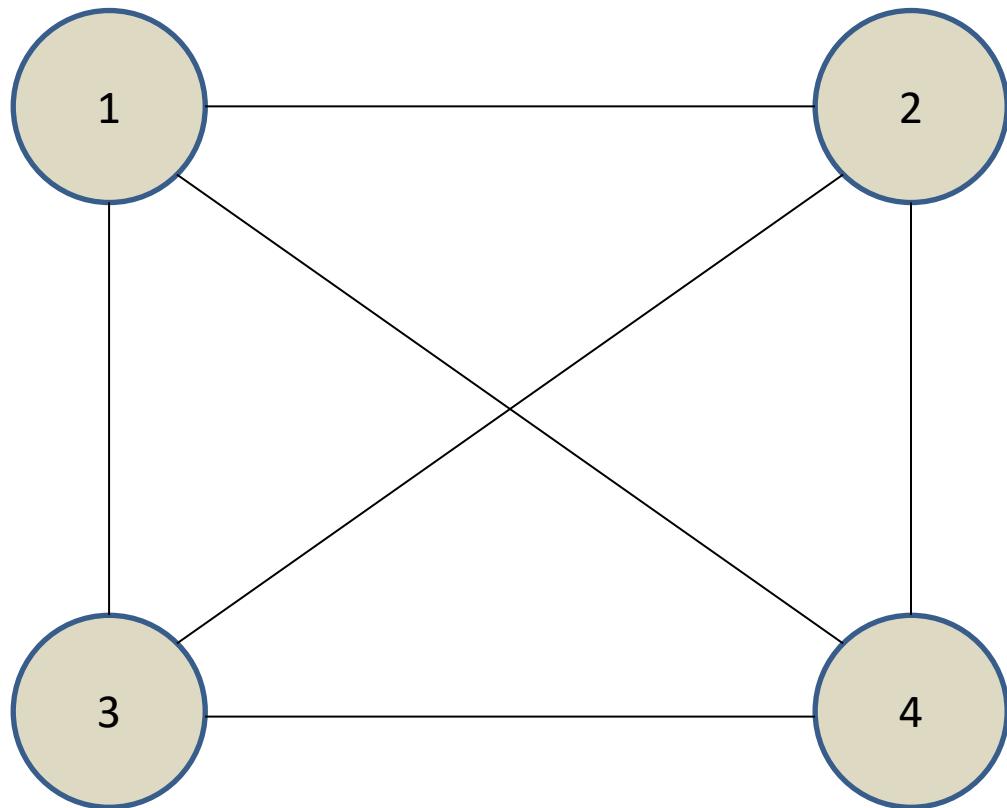
Direction graphs can be constructed in x, y, z directions



1	2	3	4
0	s	0	s
$-s$	0	$-s$	0
0	s	0	s
$-s$	0	$-s$	0

X direction matrix

Direction graphs can be constructed in x, y, z directions

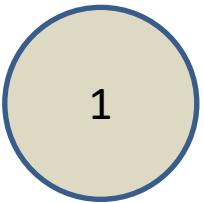


1	2	3	4	
1	0	0	s	s
2	0	0	s	s
3	$-s$	$-s$	0	0
4	$-s$	$-s$	0	0

$\text{Y direction matrix}$

Each atom has a map to where every other atom is

Atom 1
X = 0.0
Y = 0.0

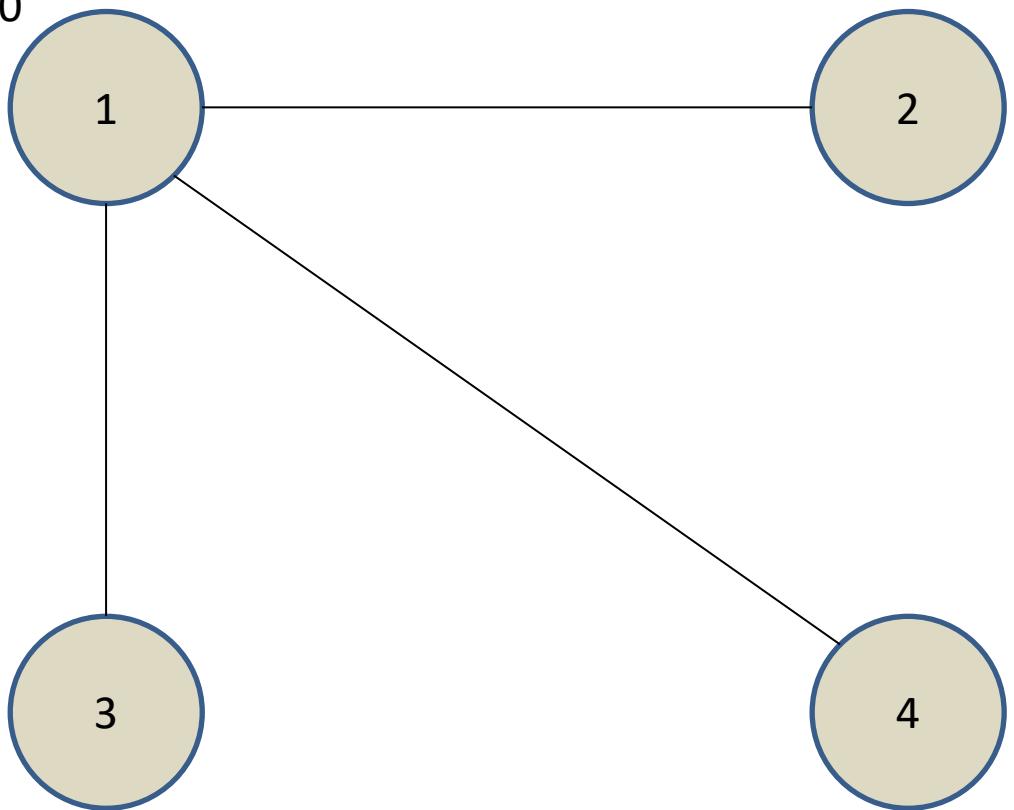


	1	2	3	4
1	0	s	0	s
2	-s	0	-s	0
3	0	s	0	s
4	-s	0	-s	0

	1	2	3	4
1	0	0	s	s
2	0	0	s	s
3	-s	-s	0	0
4	-s	-s	0	0

Each atom has a map to where every other atom is

Atom 1
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Y = 0.0



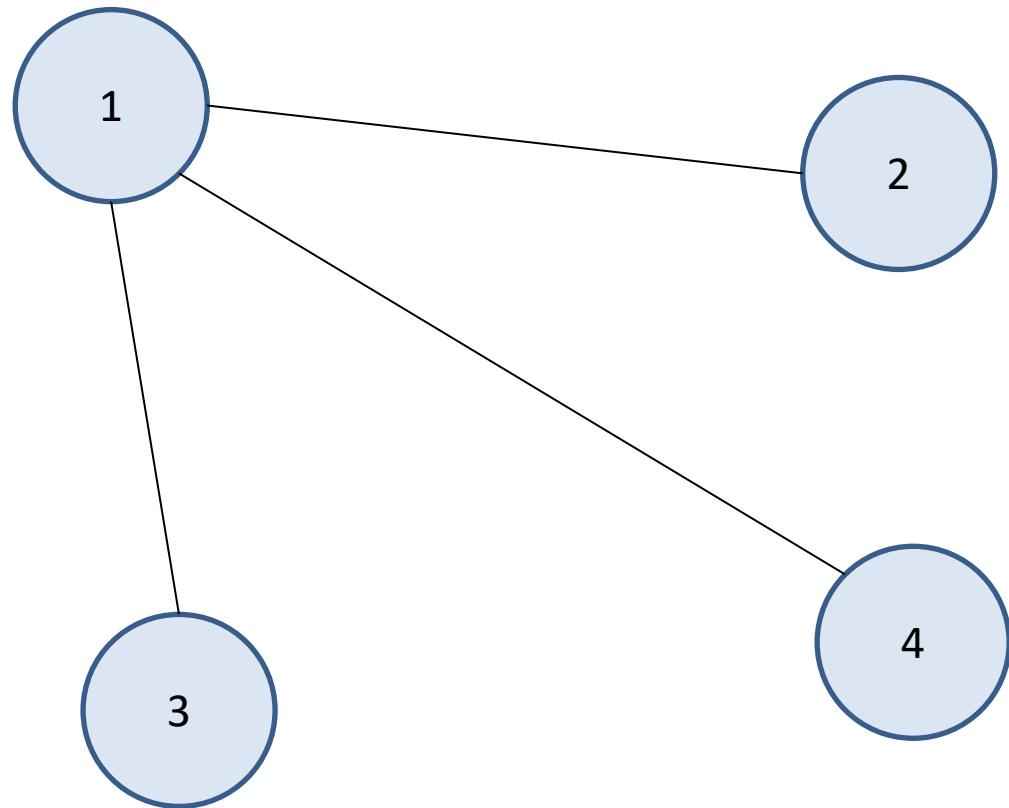
1	2	3	4
0	s	0	s
-s	0	-s	0
0	s	0	s
-s	0	-s	0

1	2	3	4
0	0	s	s
0	0	s	s
-s	-s	0	0
-s	-s	0	0

Every atom must learn where every other atom is

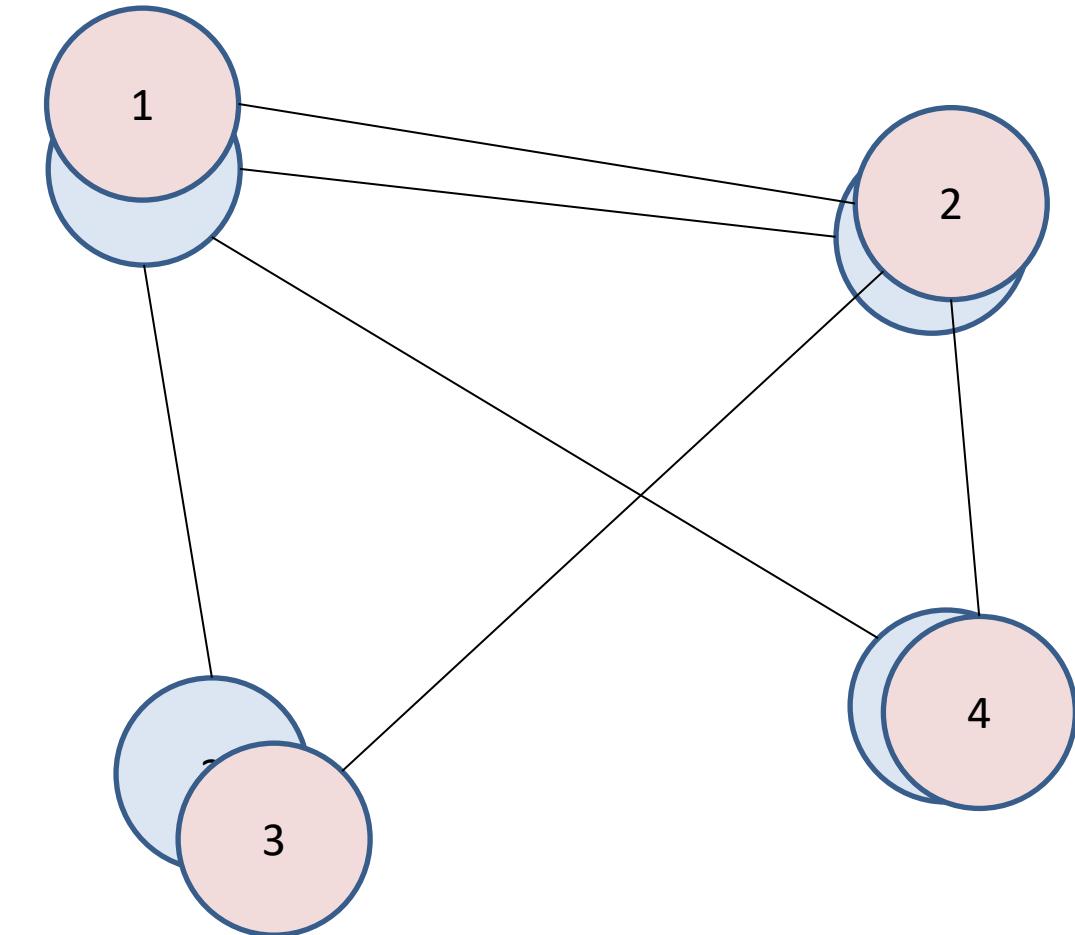
Iteration 1

Atom 1 guesses where 2, 3, and 4 are relative to itself



Iteration 2

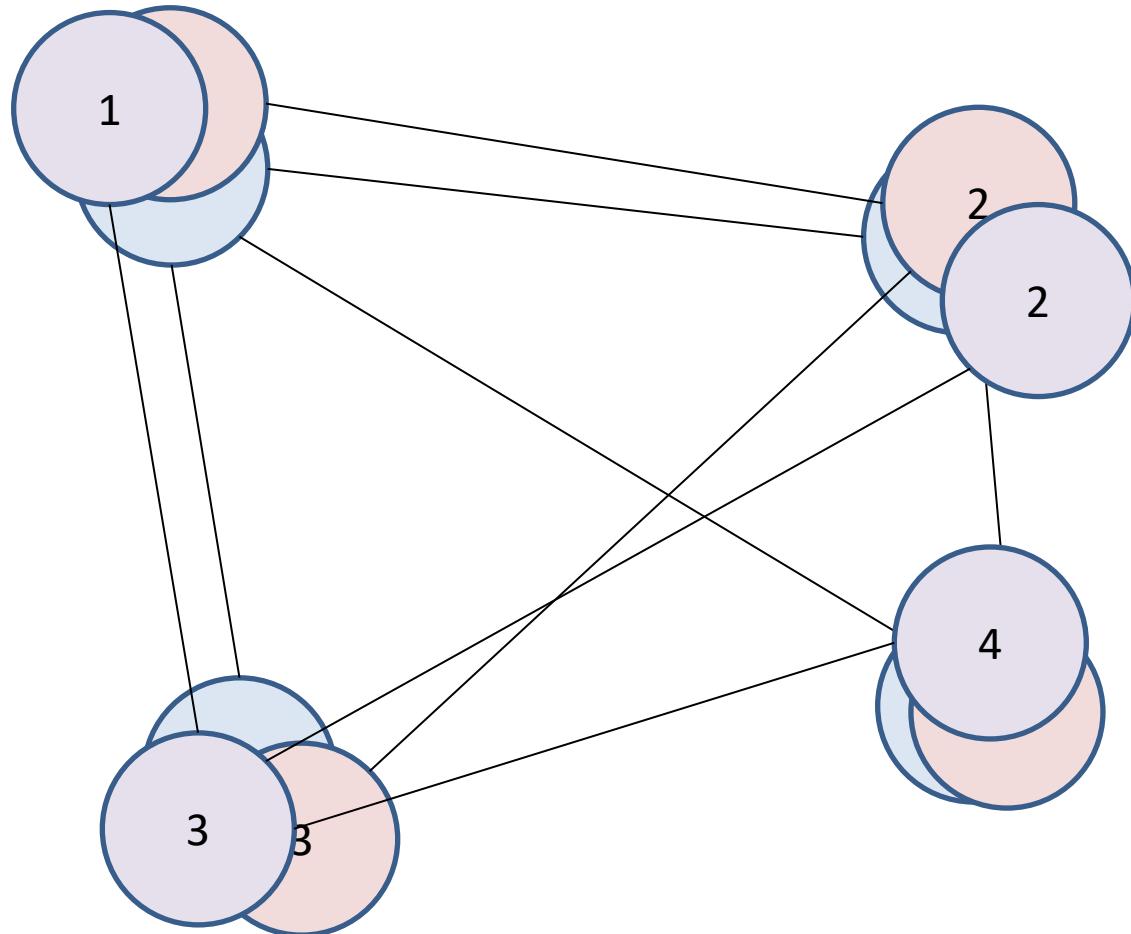
Atom 2 guesses where 1, 3, and 4 are relative to itself



Every atom must learn where every other atom is

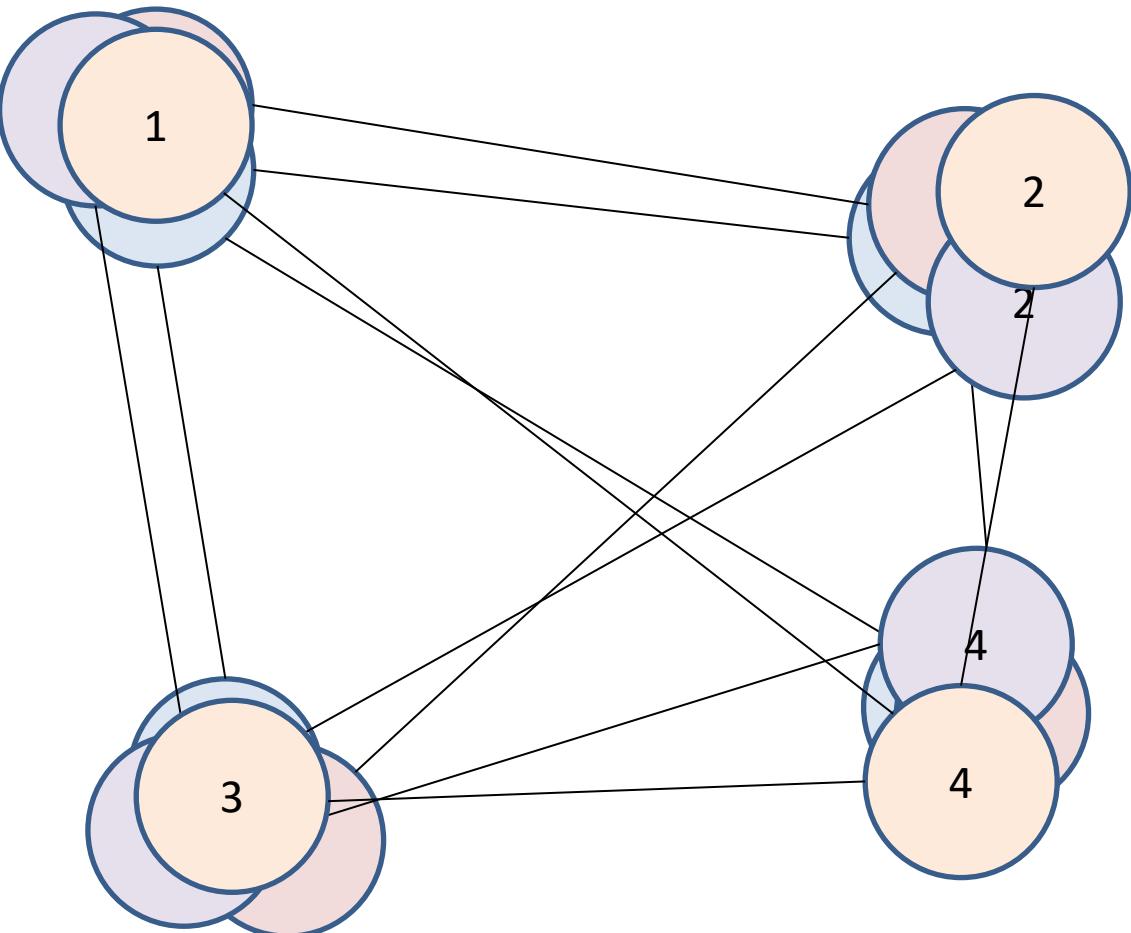
Iteration 3

Atom 3 guesses where 1, 2, and 4 are relative to itself

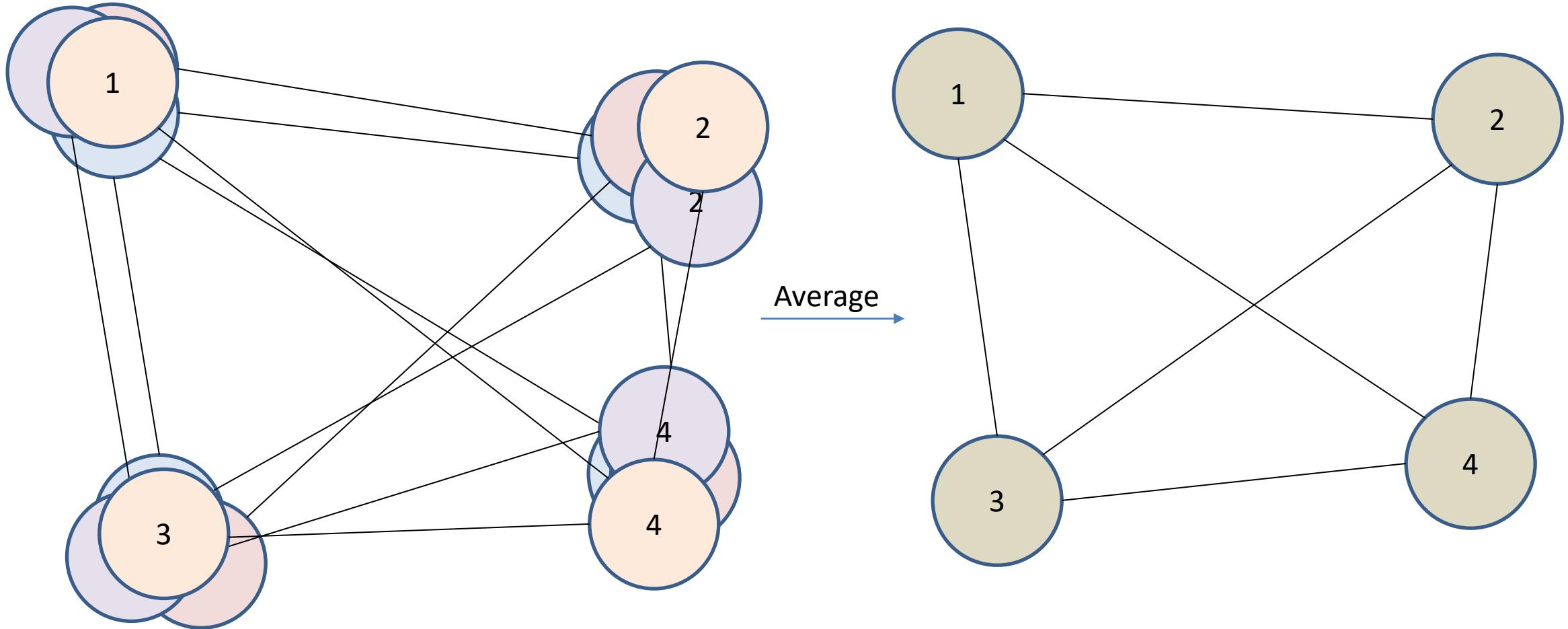


Iteration 4

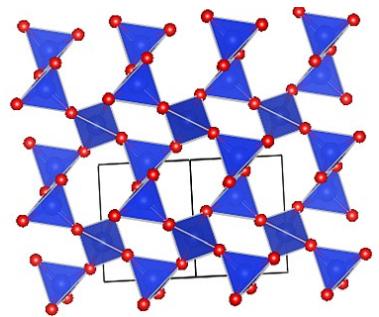
Atom 4 guesses where 1, 2, and 3 are relative to itself



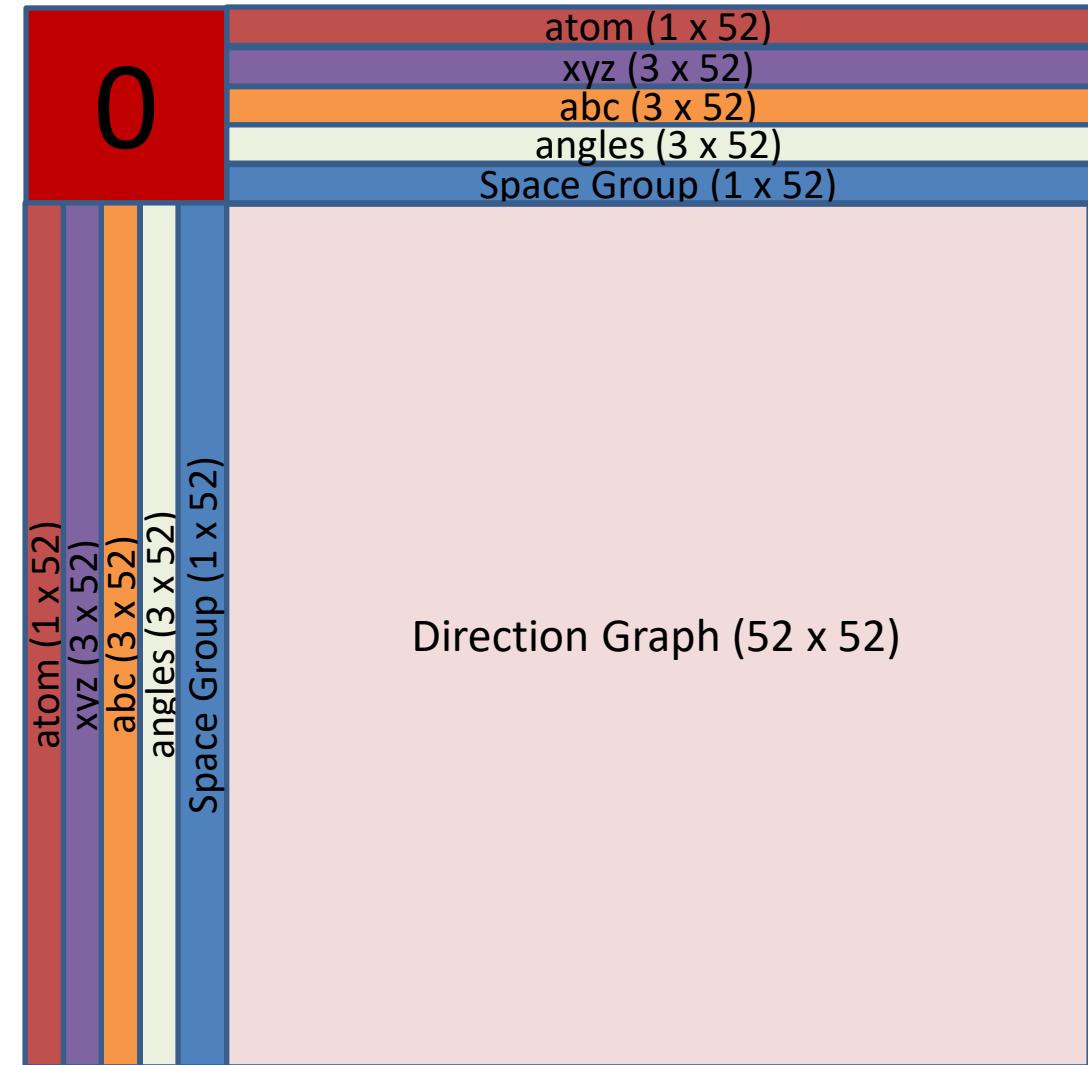
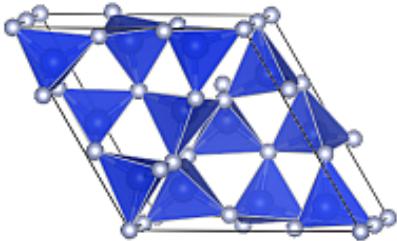
Positions can be averaged across all learned positions



Ultimately... How do we know how good these models are?



vs



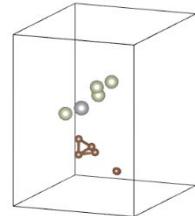
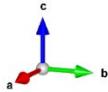
Diffusion models are the top performers by most metrics

Model	$\sigma^2_{parameter}$	σ^2_{angle}	$\sigma^2_{SpaceGroup}$	$\sigma^2_{x,y,z}$	$\sigma^2_{coordinate}$
GAN	8.34	41.90	2497	2.63e-2	4.77e-2
WGAN	4.56e-1	5.03e-1	37	2.25e-3	1.35e-2
Diffusion	5.33e-1	3.42e-1	6.1	3.72e-4	9.46e-4

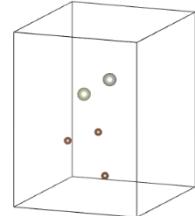
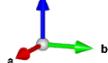
Vanilla GANs do awful

Obvious mode collapse + zero understanding of what crystals look like

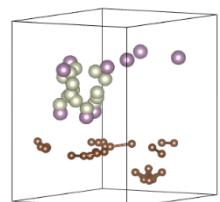
InRh_2C_3



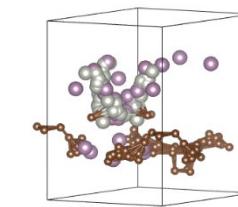
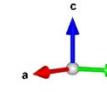
PdRhC



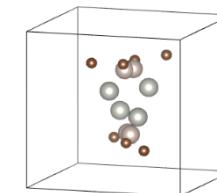
$\text{Mo}_5\text{Pd}_7\text{C}_{12}$



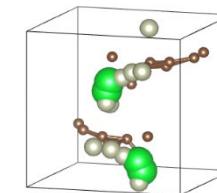
$\text{Mo}_5\text{Pd}_7\text{C}_{12}$



RuPdC_2

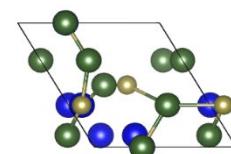
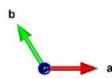
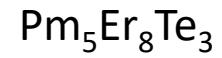
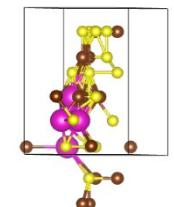
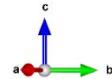
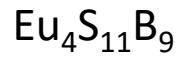
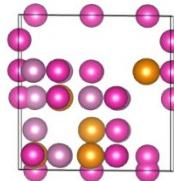
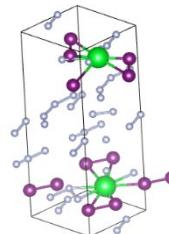
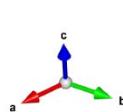
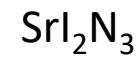
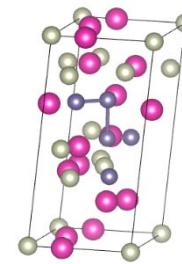
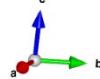
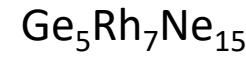
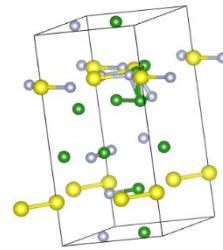
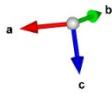
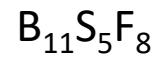


$\text{Sr}_2\text{Rh}_5\text{C}_8$



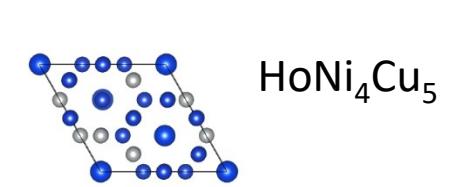
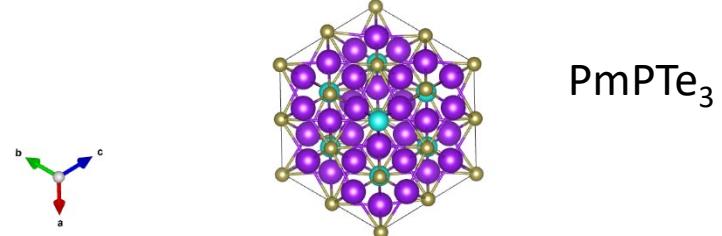
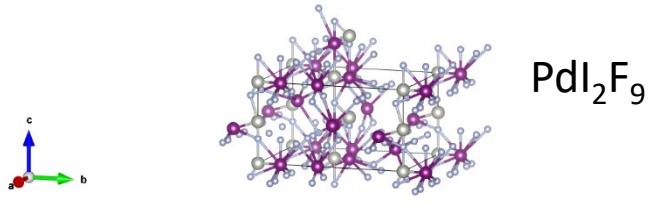
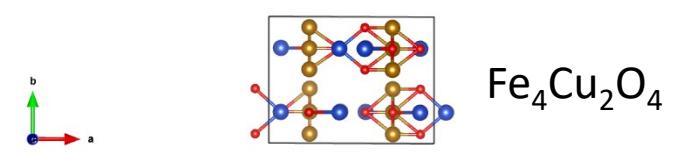
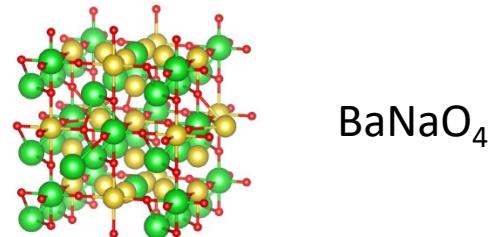
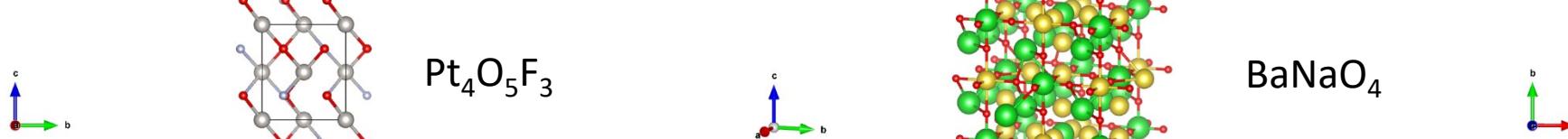
Wasserstein GANs do better

More variability of shapes and atoms, overall structures still not great



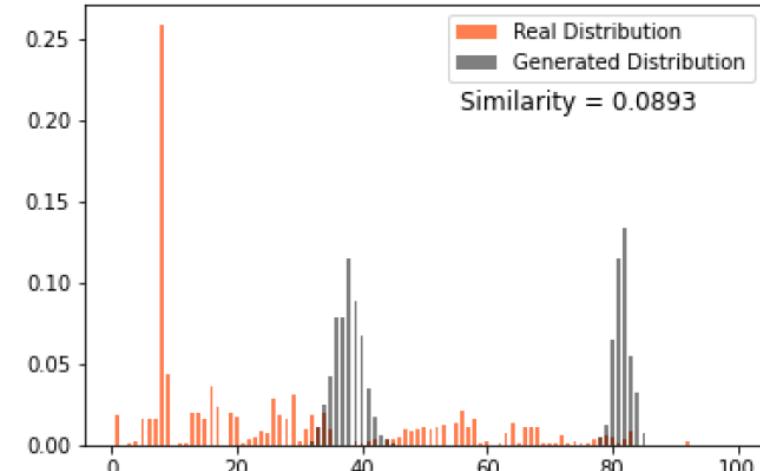
Diffusion models produce the most realistic crystals

Diverse symmetrical crystal structures

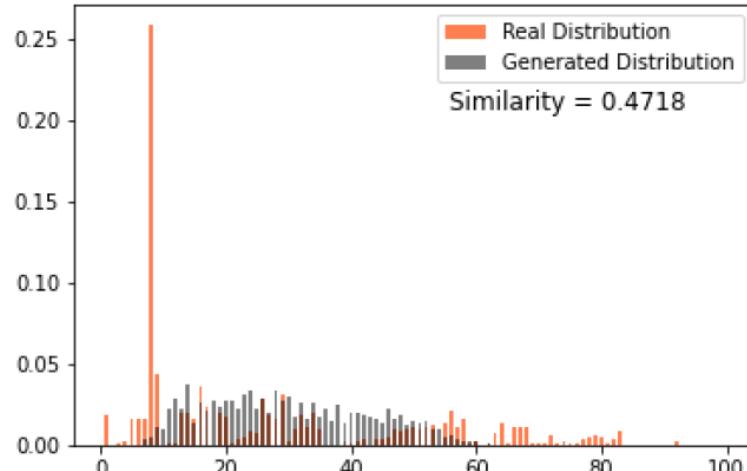


Advanced models seem to be capable of drawing from the breadth of training data

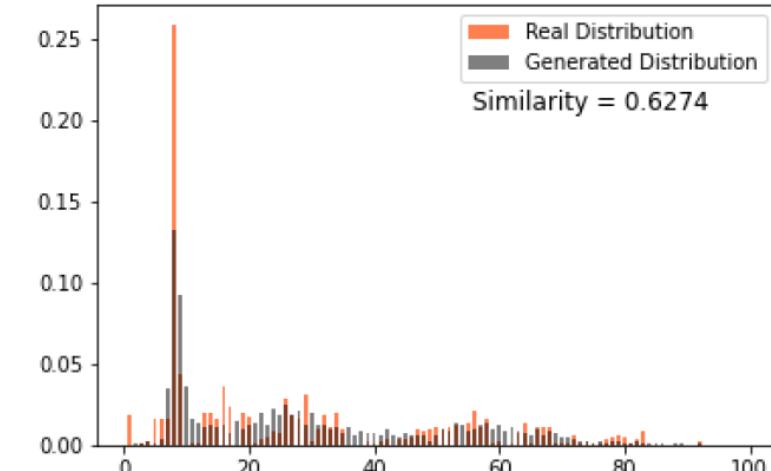
Vanilla Generative Adversarial Network
Proportion of atomic number values



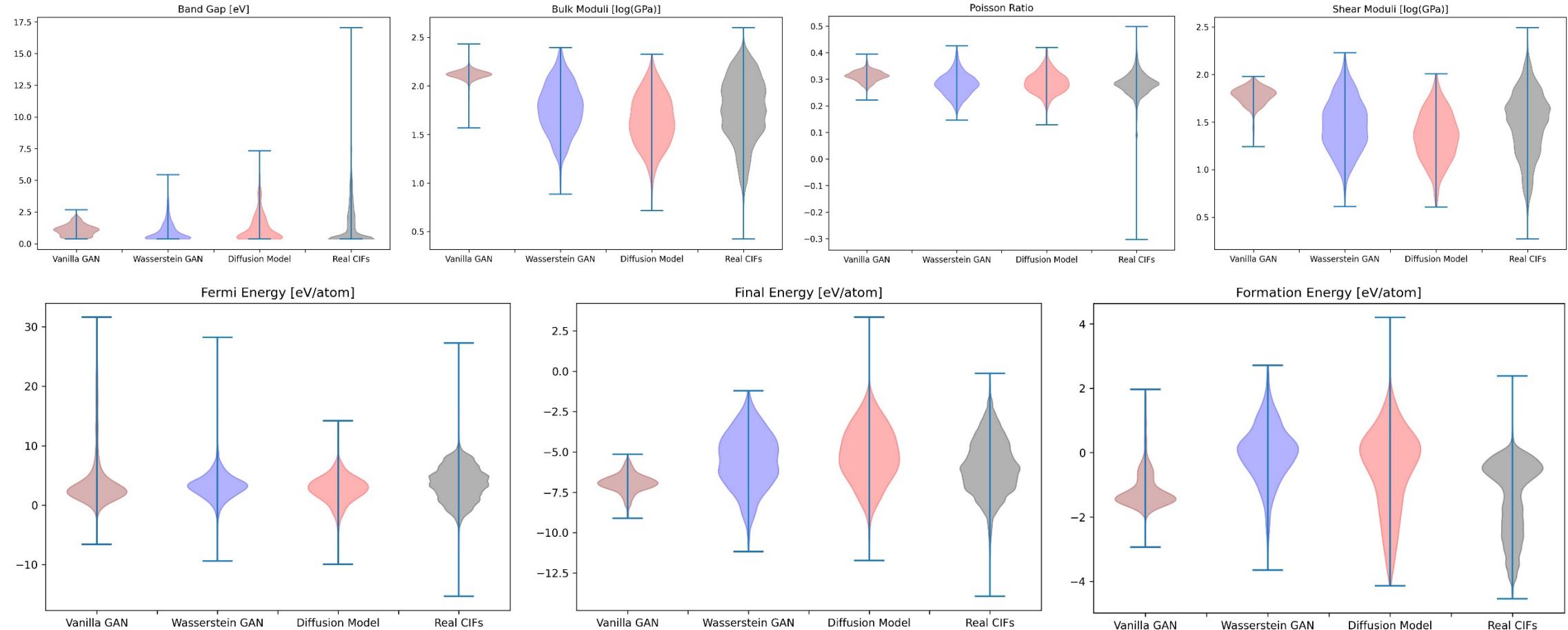
Wasserstein Generative Adversarial Network
Proportion of atomic number values



Diffusion Model
Proportion of atomic number values



Comparison to real properties also suggests good learning



We are approaching utility



2014



2015



2016



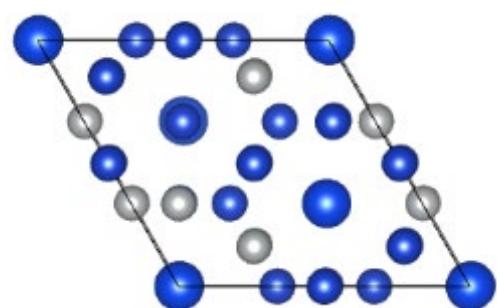
2017



2018



2021



variational autoencoders

