Q1D Study

Aiden Man

Introduction

Who is Aiden?

- Undergraduate from Foothill College studying Mechanical Engineering
- Transferring to UC Berkeley next week

Project Highlight: Q1D structures, working with Akash and Johnathan

Motivation

- 2D structures can be computationally difficult to relax/calculate
  - Heterobilayers at certain twist angles can create large systems
  - DFT calculation complexity scales cubic with the number of atoms
- Q1D structures can act as a proposed surrogate for training and validating MLIPs (Machine-Learned Interatomic Potentials)
  - Want the MLIPs to capture length-scale moire effects and physics at varying twist angles while significantly reducing system size
  - More efficient production of datasets with smaller systems
  - Q1D can sample high energy and low energy stacking configurations
- Further investigation into use of disregistry analysis
  - How it indicates sampling different energy environments

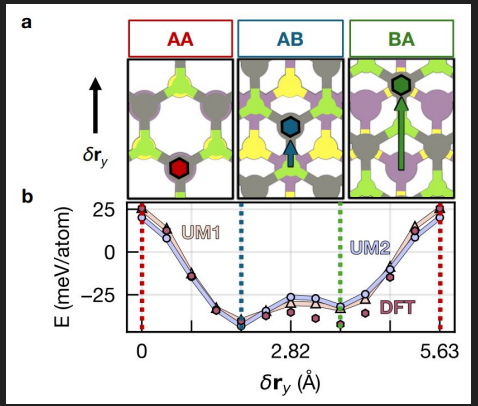


Figure 3a and 3b from Johnathan and Akash's paper:

https://arxiv.org/pdf/2503.15432

Project Question

How can Q1D structures sample 2D?

How can these structures validate MLIPs?

Approach Overview

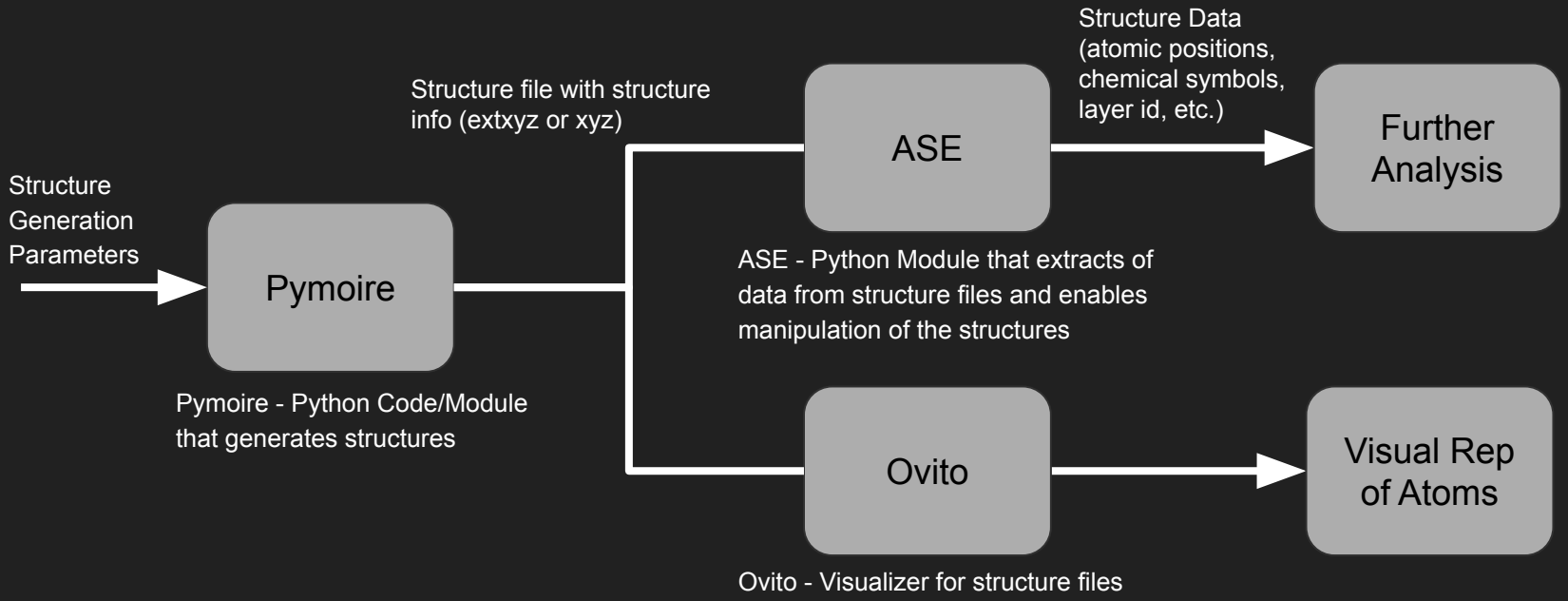
Goal: Compare Q1D disregistry vectors against 2D counterparts

=> Compare structures of MoS2/WSe2 from 0 to 60 degrees (Q1D vs. 2D)

=> Relax those structures and compare (Q1D vs. 2D, Relaxed vs. Unrelaxed)

How?

Construct and Analyze structures using Pymoire, ASE, and Ovito



Structure Construction Approach

Wrote code to run Pymoire for various twist angles

Algorithmically adjusted Rmax and max strain to achieve construction

- Assigned initial Rmax of 16, max strain 0.02 (goal atom count ~100, <200)
- Increased max strain up to a certain point before raising Rmax and reverting max strain

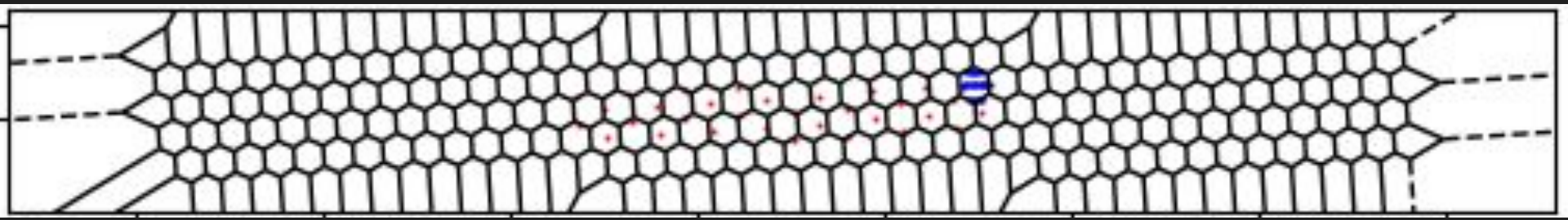
```python
def run_pymoire(pymoire_config: PymoireConfig):
    # Set environment variable in Python for Pymoire
    os.environ["PYTHONPATH"] = r"C:\Users\aiden\Documents\Jornada Group - Moire\pymoire"
    print("Running Pymoire")
    orig_max_strain = pymoire_config.max_strain
    orig_Rmax = pymoire_config.Rmax_max_search

    while not os.path.isfile(pymoire_config.out_struc_name):
        """Run the Pymoire script with the specified parameters."""
        output = "python main_script.py "
        if pymoire_config.struc_dir:
            output += f"--structures-dir {pymoire_config.struc_dir} "
        if pymoire_config.struc_files:
            output += f"--structure-files {pymoire_config.struc_files} "
        if pymoire_config.struc_file_format:
            output += f"--structures-file-format {pymoire_config.struc_file_format} "
        if pymoire_config.out_struc_name:
            output += f"--output-struc-name {pymoire_config.out_struc_name} "
        if f"{pymoire_config.twist_min_search}":
            output += f"--twist-min-search {pymoire_config.twist_min_search} "
        if f"{pymoire_config.twist_max_search}":
            output += f"--twist-max-search {pymoire_config.twist_max_search} "
        if pymoire_config.desired_strain:
            output += f"--desired-strain {pymoire_config.desired_strain} "
        if pymoire_config.max_strain:
            output += f"--max-permissible-strain {pymoire_config.max_strain} "
        if pymoire_config.is_1D_dir_1:
            output += "--is-1D-dir-1 "
        if pymoire_config.is_1D_dir_2:
            output += "--is-1D-dir-2 "
        if pymoire_config.Rmax_max_search:
            output += f"--Rmax-max-search {pymoire_config.Rmax_max_search} "
        if pymoire_config.max_iter_twist_search:
            output += f"--max-iter-twist-search {pymoire_config.max_iter_twist_search} "
        if pymoire_config.output_plot_name:
            output += f"--output-plot-name {pymoire_config.output_plot_name} "

        print(output)
        result = subprocess.run(output, shell=True, capture_output=True, text=True)

        # Alter parameters if structure not found
        if not os.path.isfile(pymoire_config.out_struc_name):
            pymoire_config.max_strain += 0.005
            if pymoire_config.Rmax_max_search > orig_Rmax * 2:
```

Voronoi Analysis

Used scipy modules to extract disregistry vectors from the structures

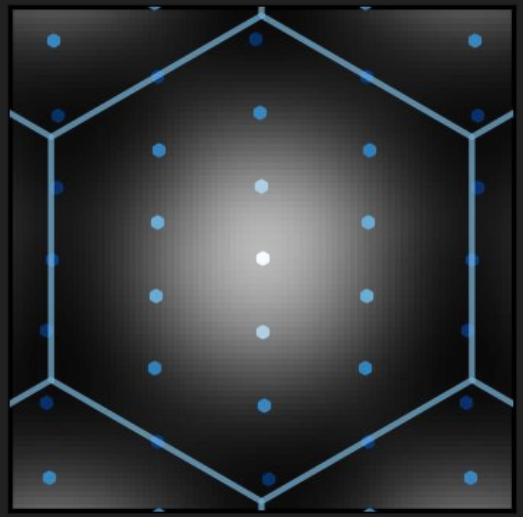
Constructed Voronoi cells around padded bottom layer transition metals (Mo)

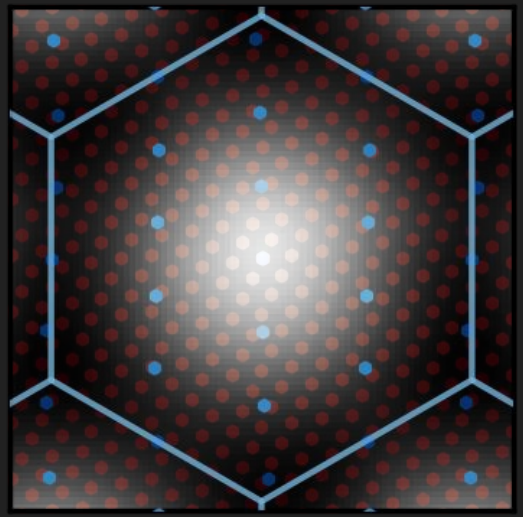
Top layer transition metals (W) (red points) => single voronoi cell (blue)

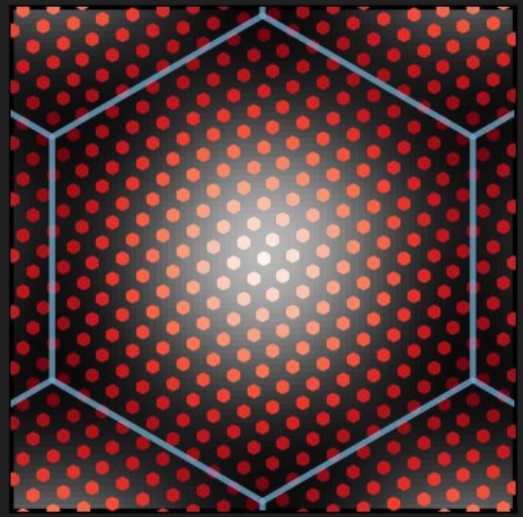


Johnathan's Code

Initially visualized the generated structures in disregistry space using Johnathan’s code







Q1D (Left, Blue) vs 2D (Right, Red) at ~10 degree twist angle

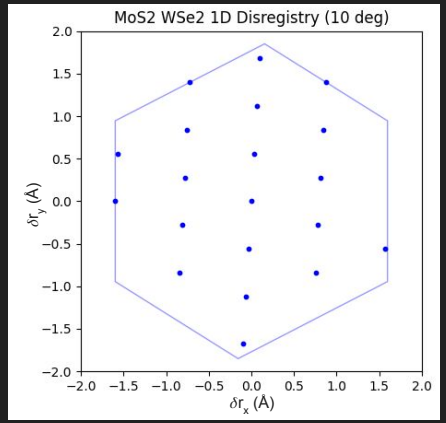
My Code

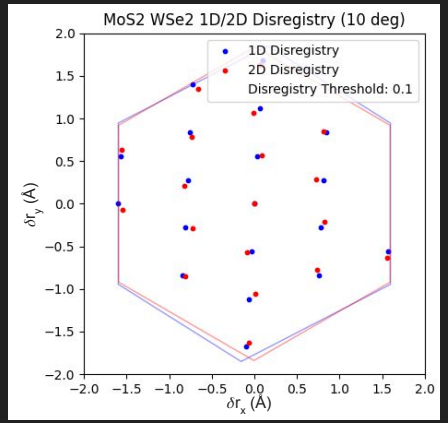
Wrote my own code to measure and visualize the disregistry points

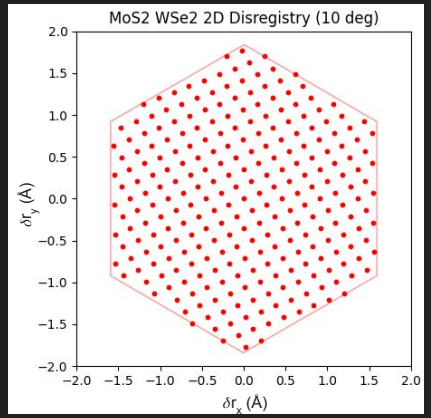
Display of captured points within an arbitrary threshold of 0.1 Å

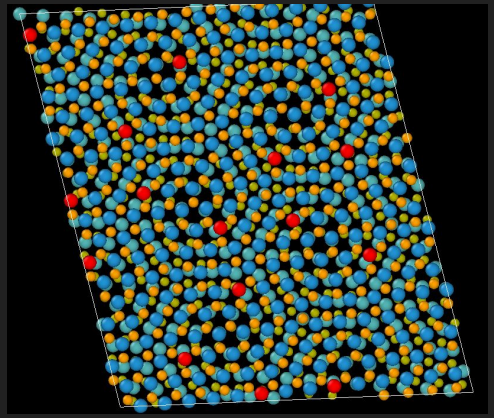
- Mapped each Q1D disregistry point to closest 2D disregistry point

Potential use of interpolation to normalize voronoi cells (used by JDG, but not me)



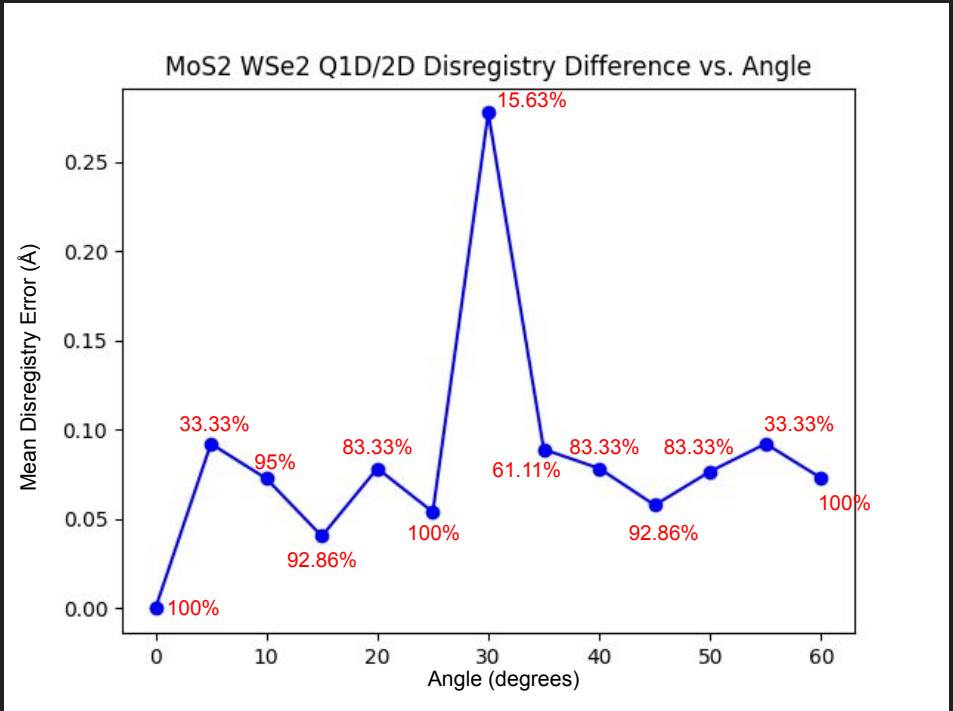






My Code Cont.

Plotted Mean Disregistry Error between Q1D and 2D against varying twist angles



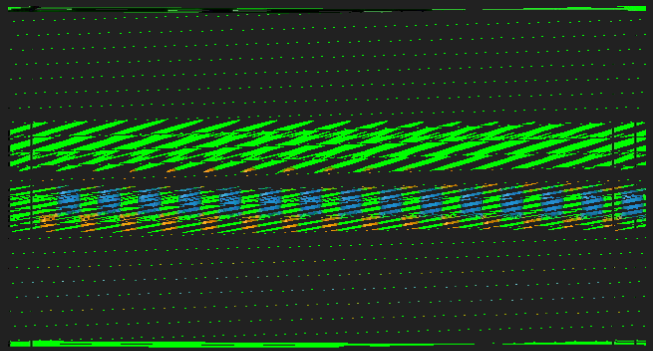
Ratios of Disregistry Errors captured by the 0.1 Å threshold

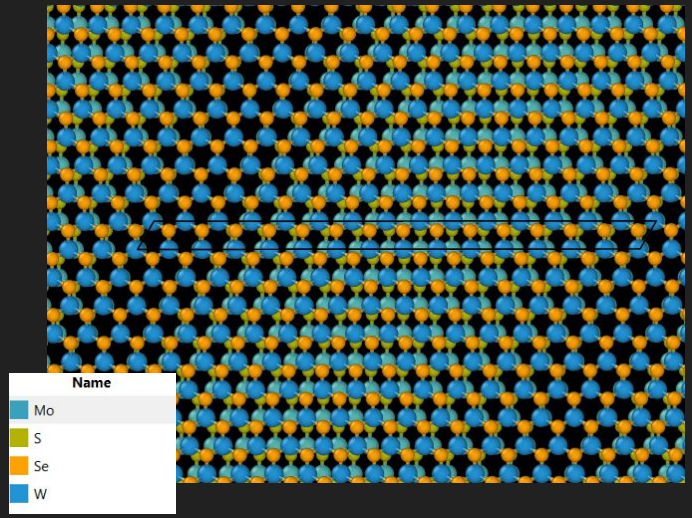
Relaxations

Ran relaxations using Akash's code, MLIP relaxation using a version of MACE (until Fmax < 1e-4 eV/Å)

Visualized relaxations in Ovito

Applied same analysis methods from before on the relaxed structures

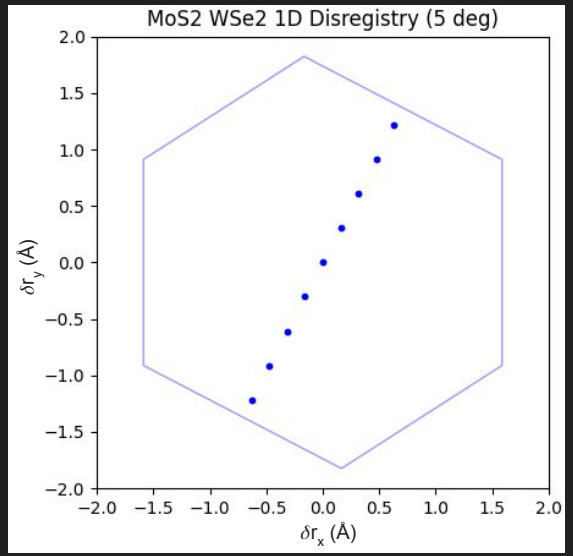


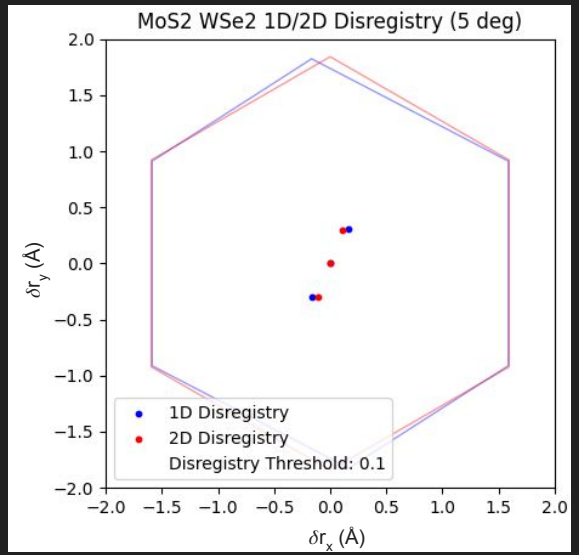


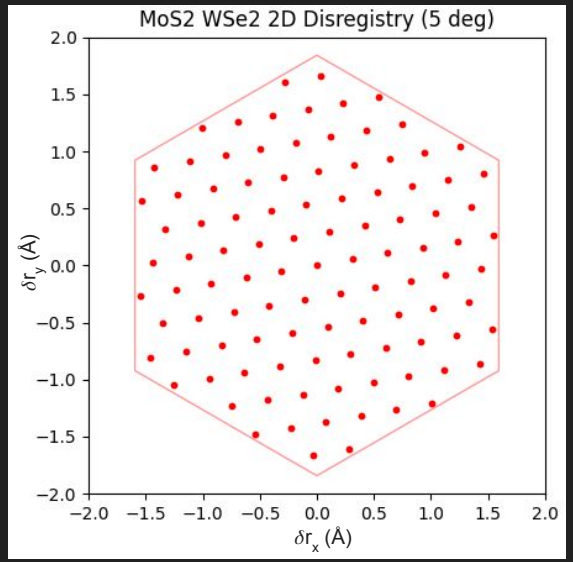
Relaxation of 0 degree twist angle, Q1D structure

Pre Relaxation Disregistry (5 degrees)

Q1D structure shows line of disregistry points in high energy region prior to relaxation

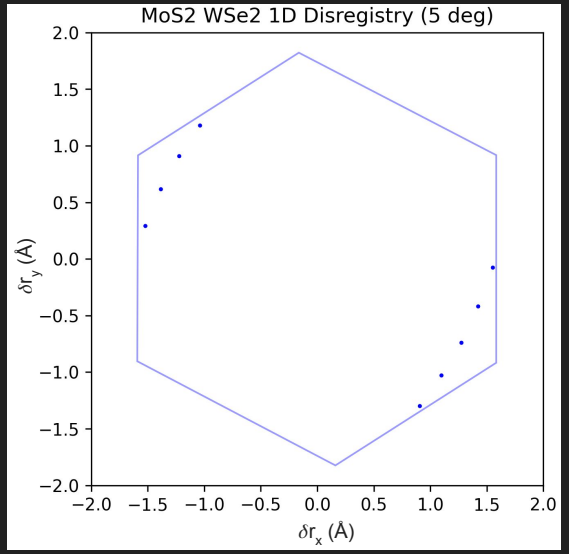


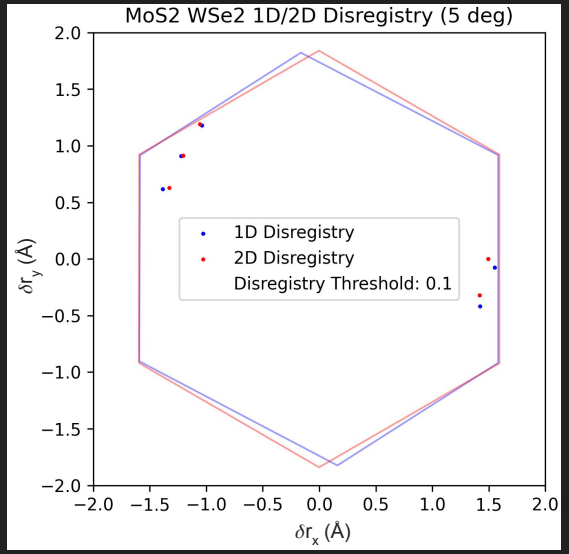


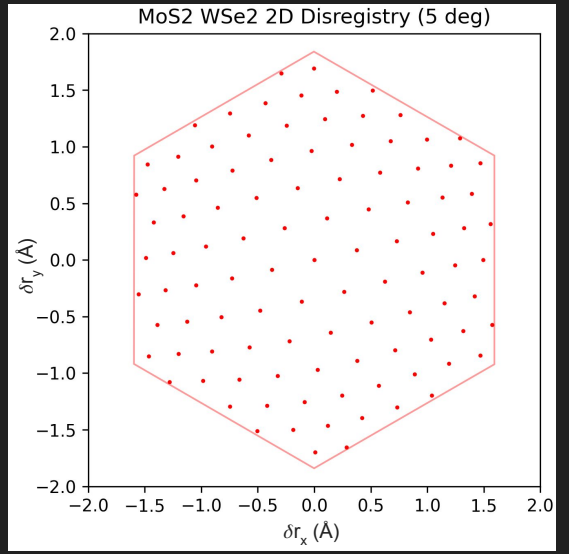


Post Relaxation Disregistry (5 degrees)

Q1D structure after relaxation shows shift toward lower energy regions

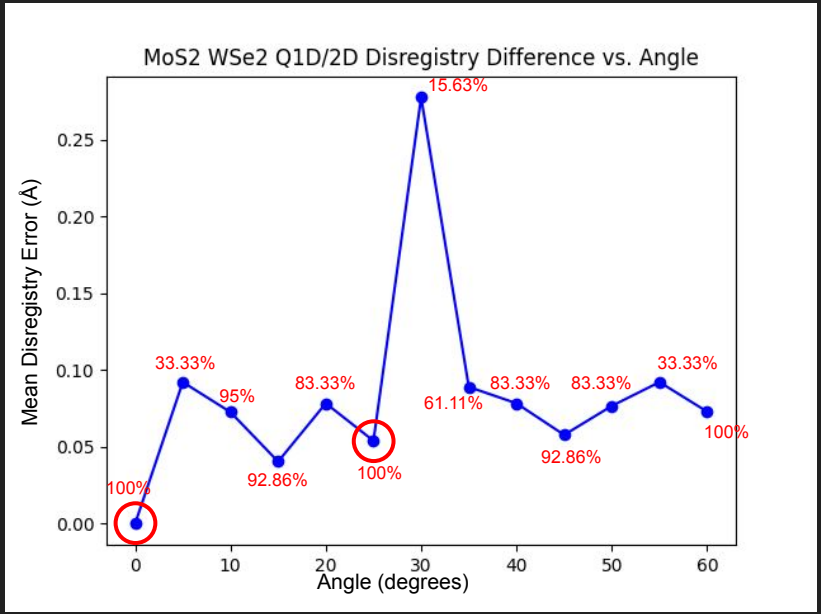


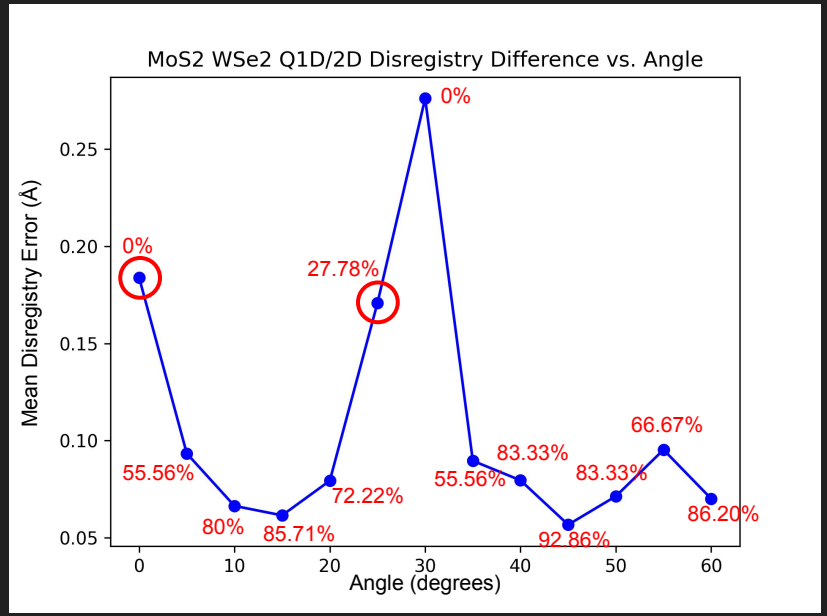




Unrelaxed vs. Relaxed

Generally, both follow similar MDE trends (aside from the circled points)





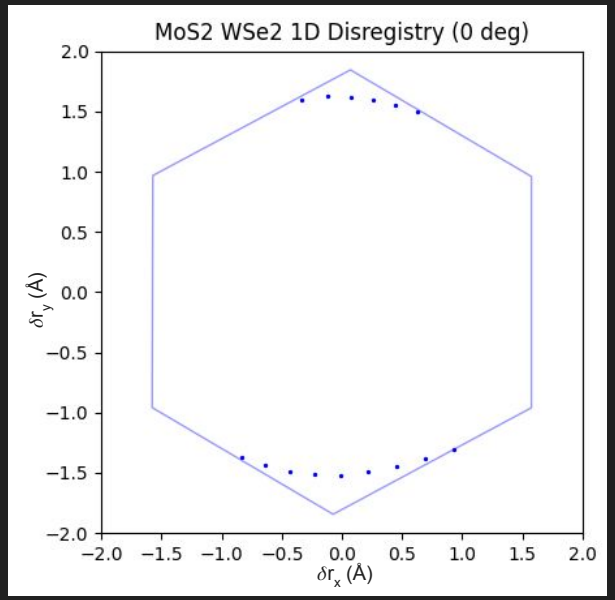
Pre Relaxation (Left) vs. Post Relaxation (Right) Mean Disregistry Error between Q1D and 2D

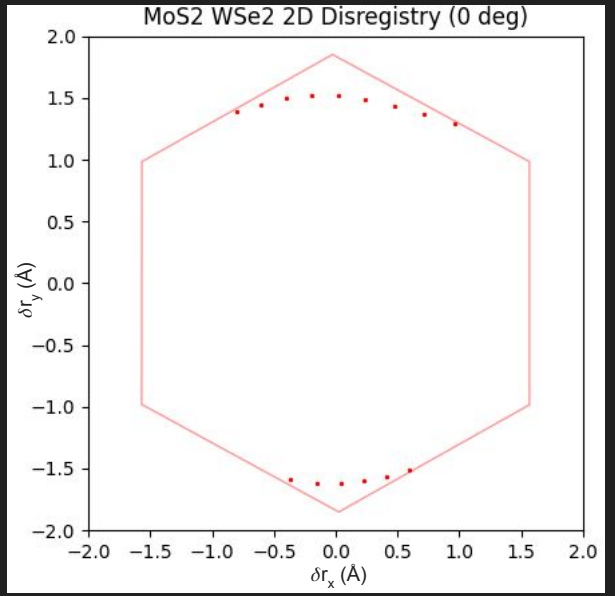
Ratios of Disregistry Errors captured by the 0.1 Å threshold

Pitfalls of My Analysis

Differences in voronoi cell alignment not accounted for

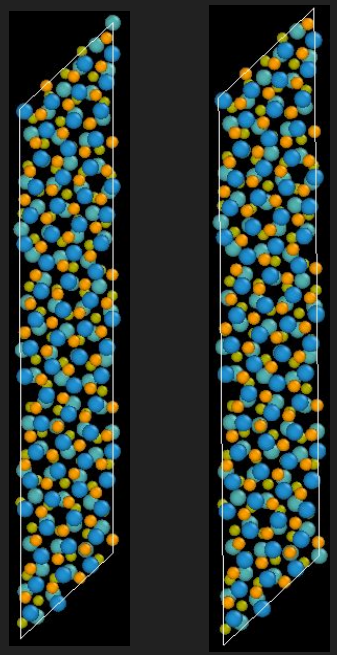
Post relaxation disregistry plots of 0 degree Q1D and 2D seem mirrored to each other

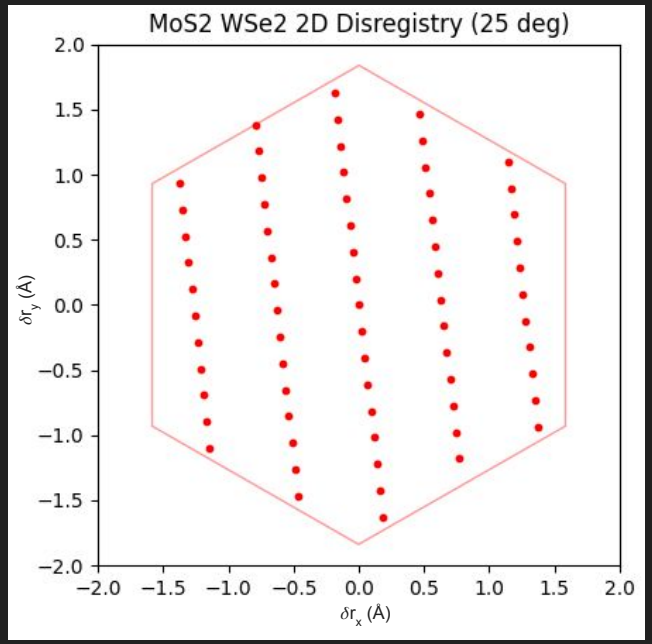


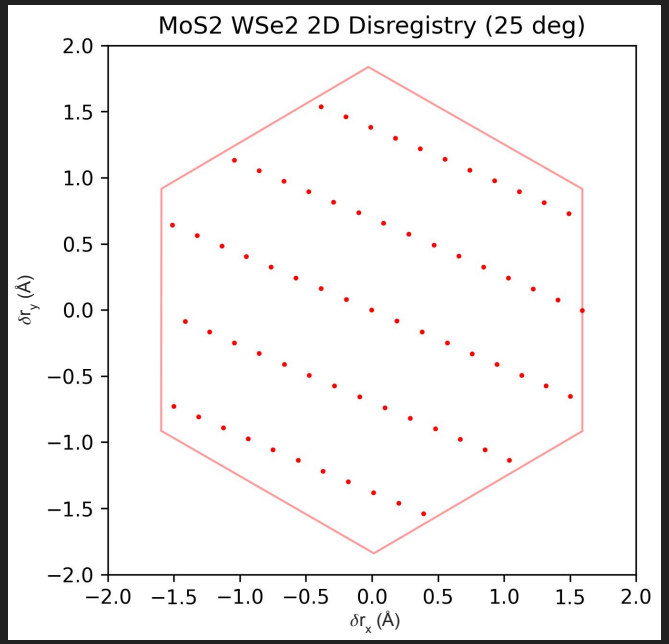


Pitfalls Cont.

Minimal positional changes observed in reconstruction of 2D structure at 25-degree twist, but voronoi cell alignment seems offset by 60 degrees

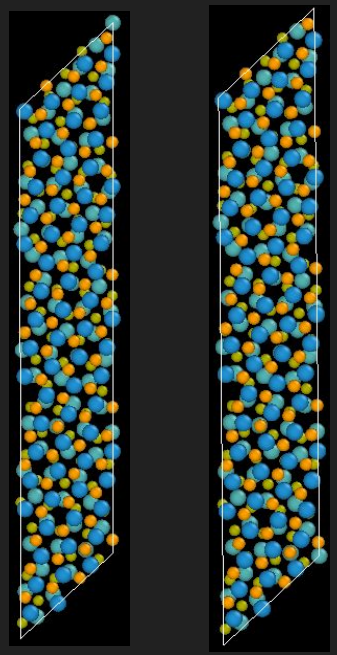


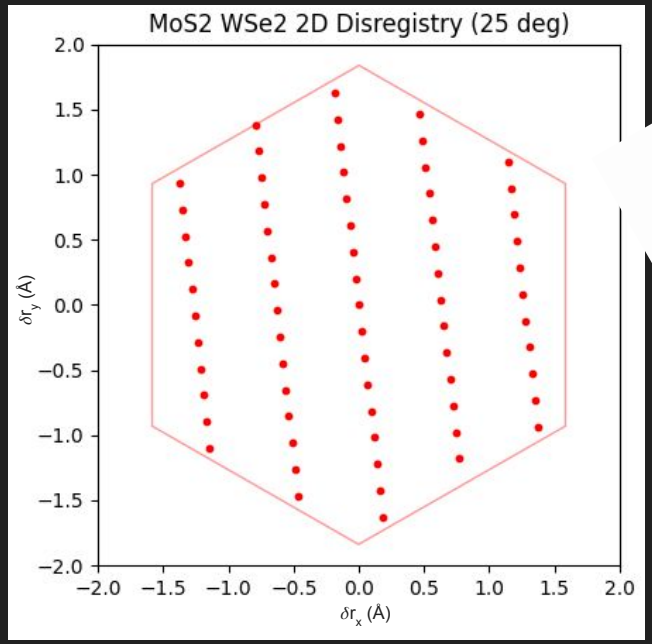


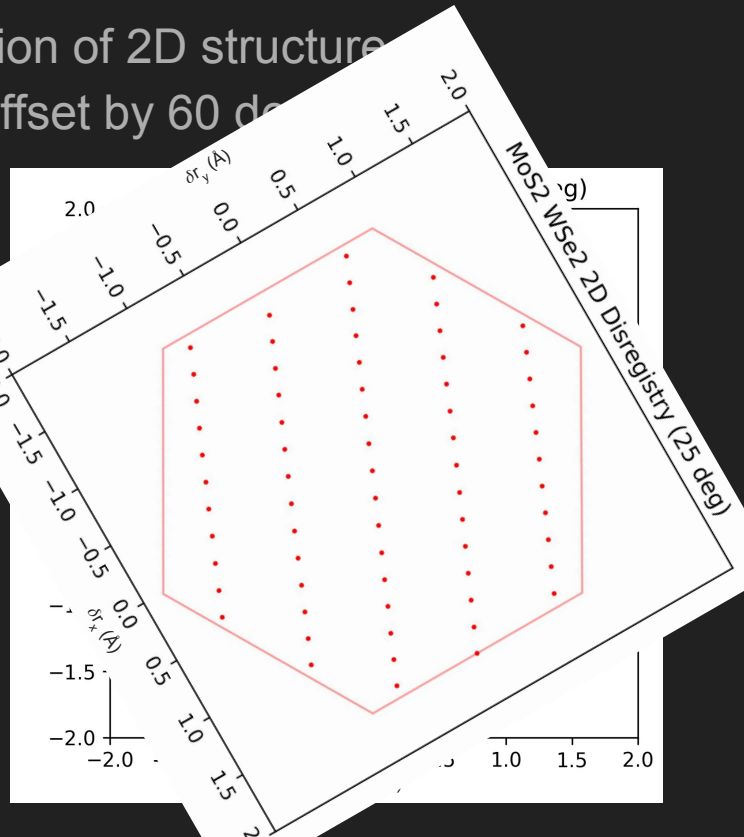


Pitfalls Cont.

Minimal positional changes observed in reconstruction of 2D structure
25-degree twist, but voronoi cell alignment seems offset by 60 d







Conclusion

Main observations:

- Relaxation only shows significant reconstruction for angles close to 0, 30, 60 degrees
- MDE between Q1D/2D generally seems consistent before and after relaxation

Main pitfalls:

- Lack of account for voronoi cell alignment

What can be done to further answer the question: How can Q1D better sample 2D structures?

- RBF interpolator to normalize voronoi cells
- Run DFT driven relaxation to verify consistency MDE before/after relaxation
- Analyze smaller resolutions near 0, 30, 60 degrees
- Additional steps to modify Q1D structures to better replicate geometries in 2D counterparts
- Analyze different, non-TMD structures (BP, HfS)

Thank You!

Huge thanks to Akash and Johnathan for mentoring me and helping me through this project!

Pre-Relaxation

0 degree

twist_min_search = 0

twist_max_search = 0.1

max_strain = 0.2

is_1D_dir_1 = True

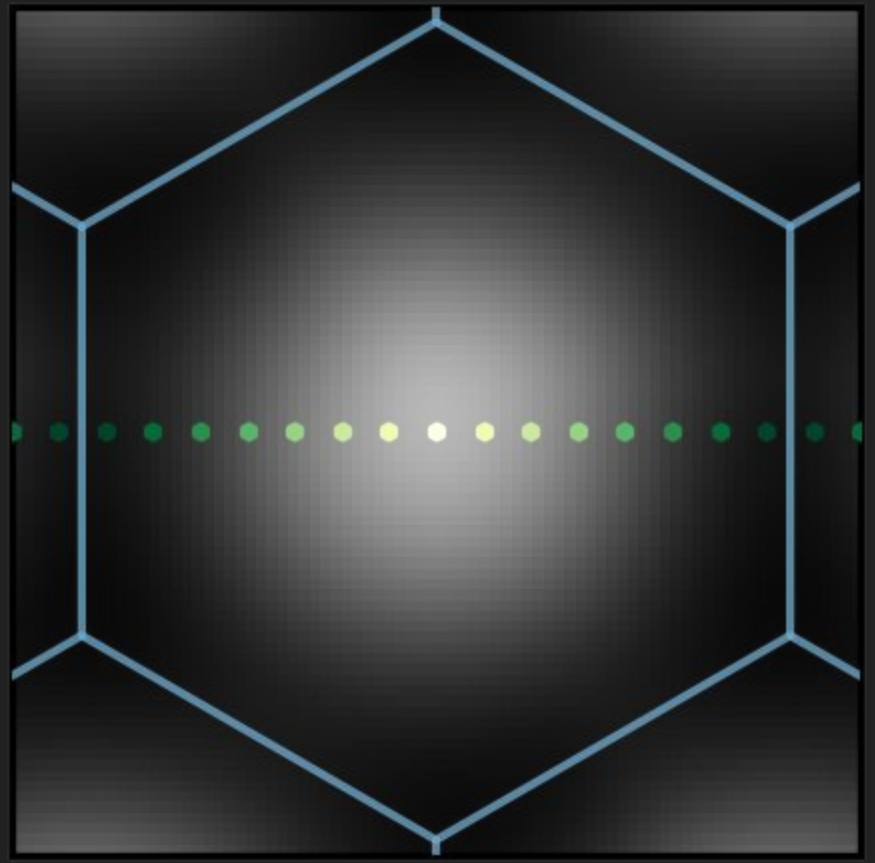
Rmax_max_search = 16

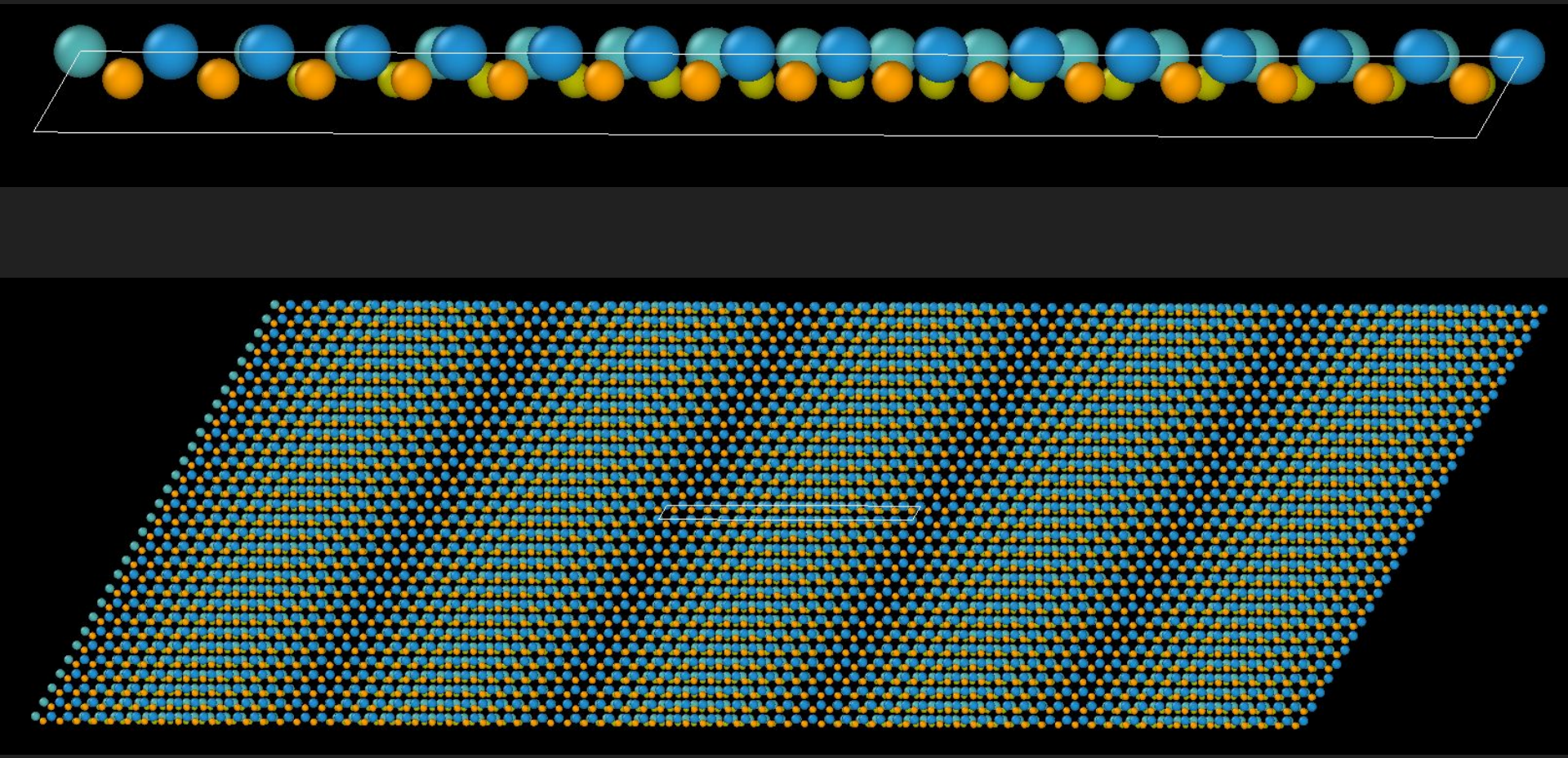
max_iter_twist_search = 5

Total atoms: 93

Mo count: 16

W count: 15





4 degree

twist_min_search = 4

twist_max_search = 4.1

max_strain = 0.1

is_1D_dir_1 = True

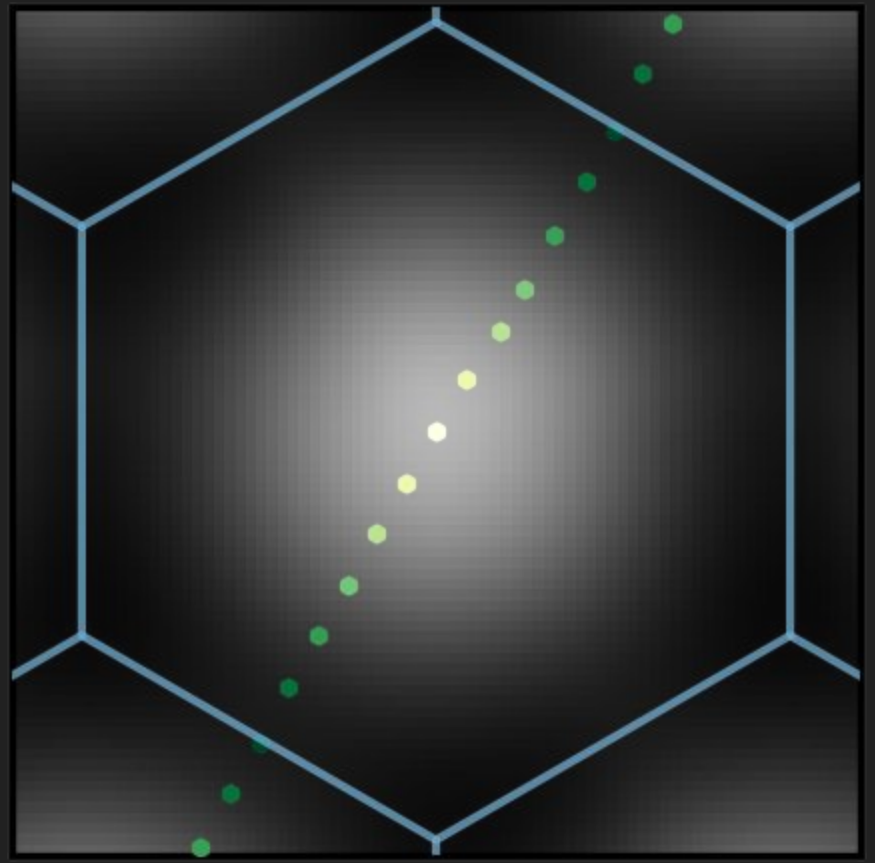
Rmax_max_search = 16

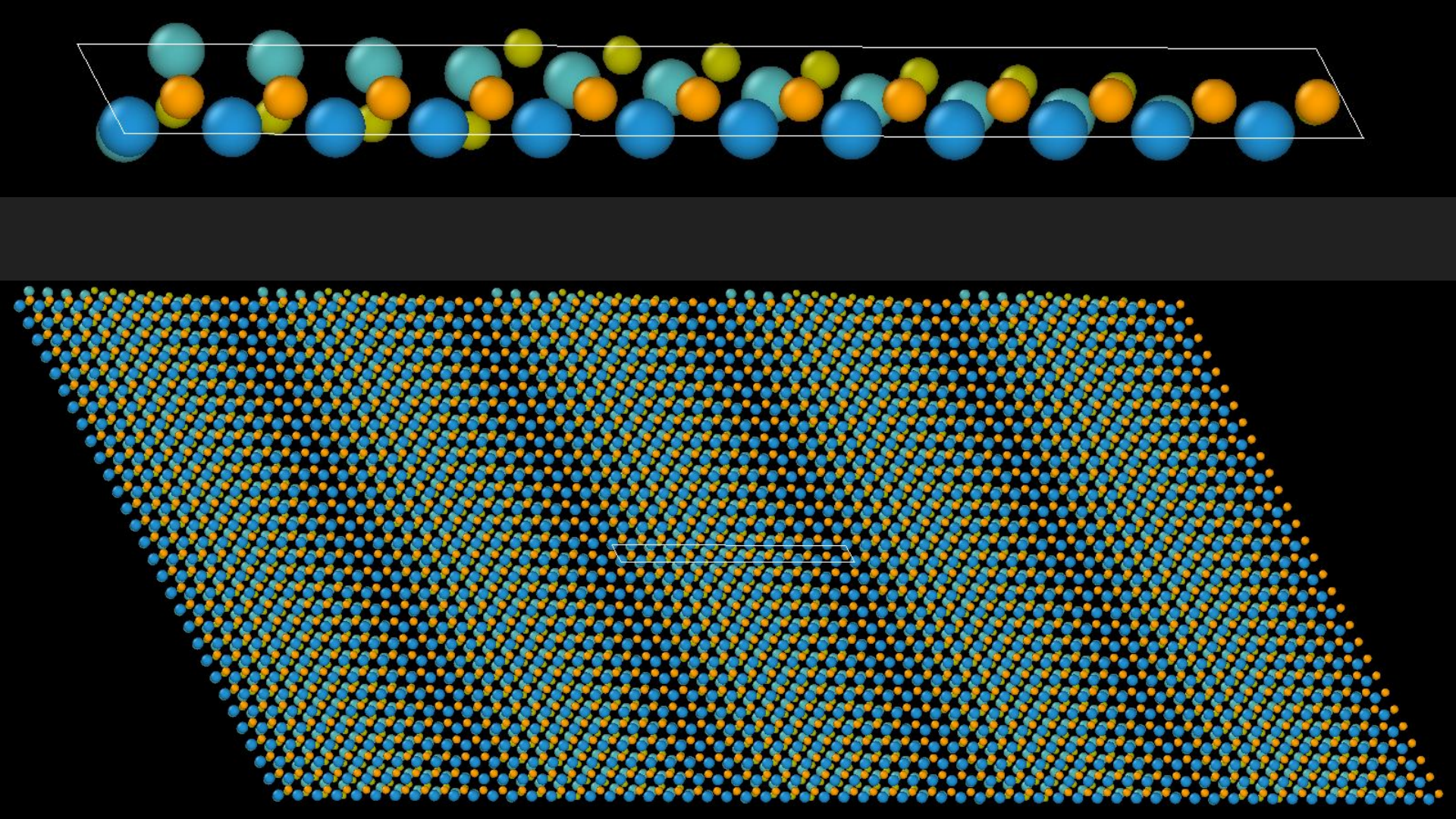
max_iter_twist_search = 5

Total atoms: 75

Mo count: 13

W count: 12





8 degree

twist_min_search = 8

twist_max_search = 8.1

max_strain = 0.02

is_1D_dir_1 = True

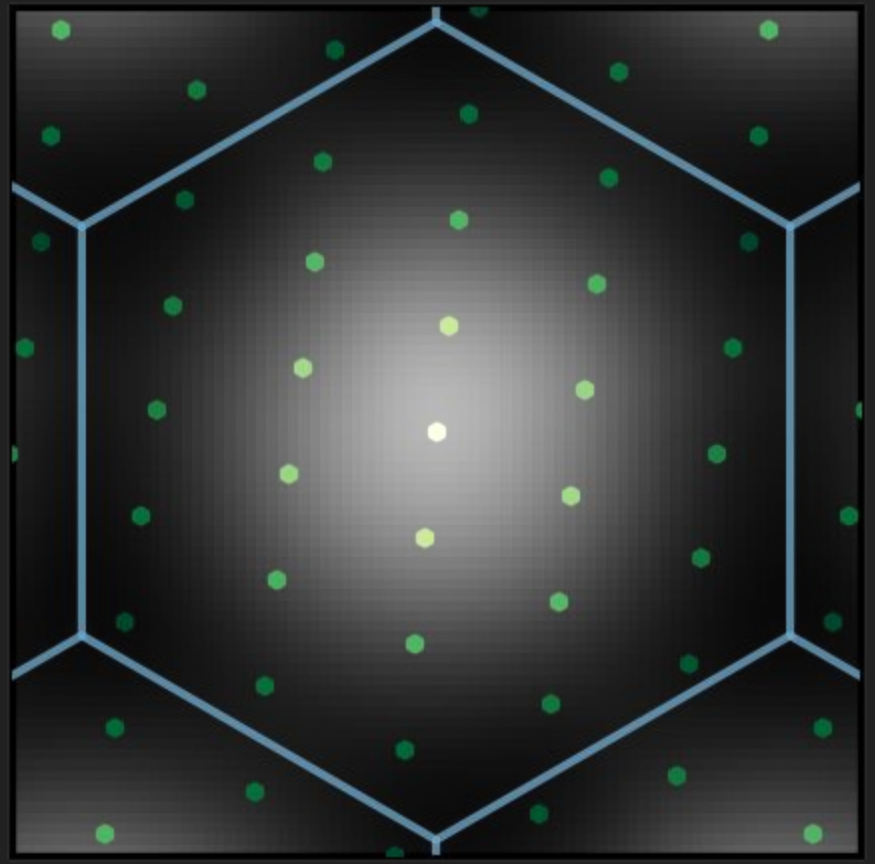
Rmax_max_search = 30

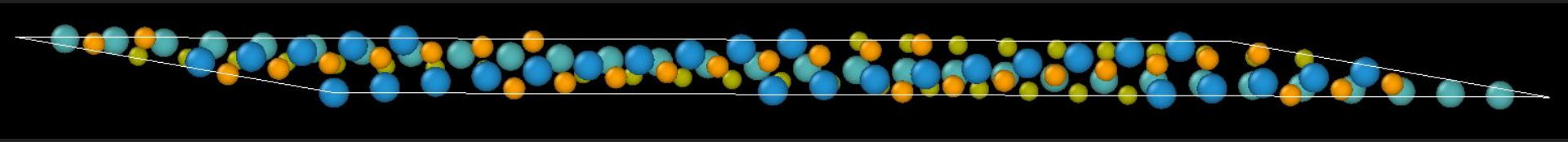
max_iter_twist_search = 5

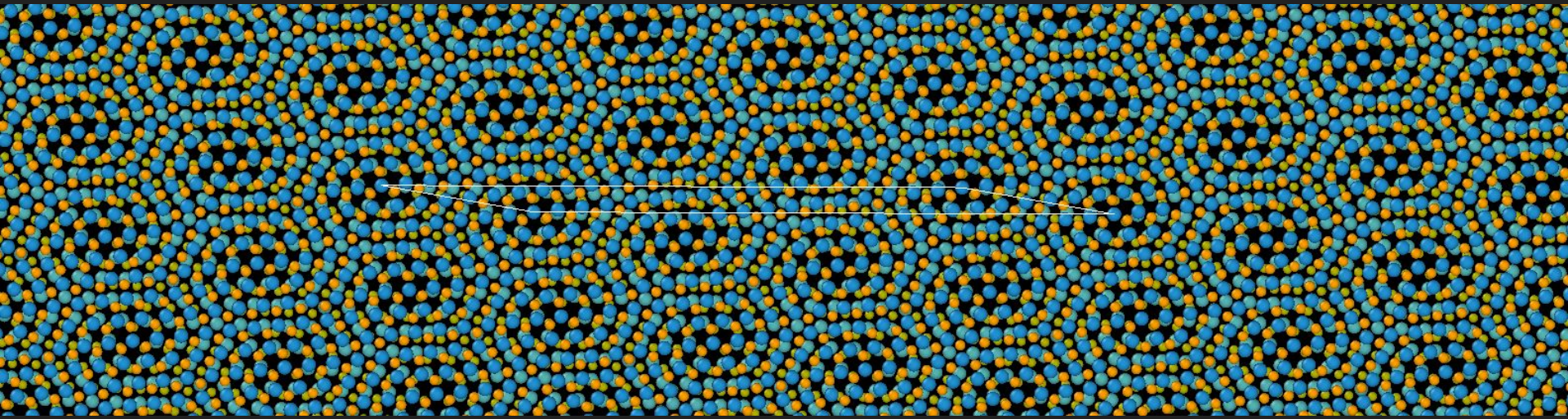
Total atoms: 180

Mo count: 31

W count: 29







12 degrees

twist_min_search = 12

twist_max_search = 12.1

max_strain = 0.02

is_1D_dir_1 = True

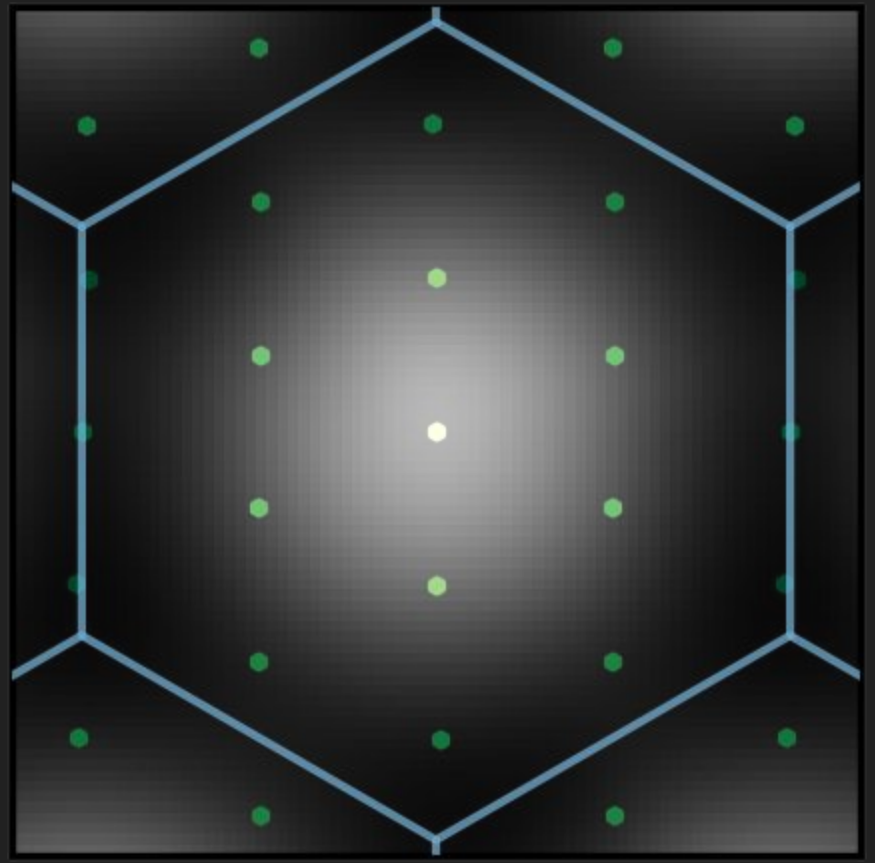
Rmax_max_search = 14

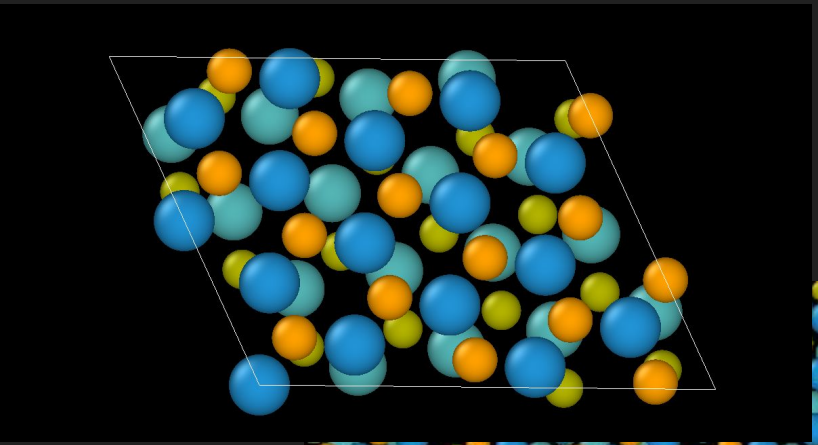
max_iter_twist_search = 5

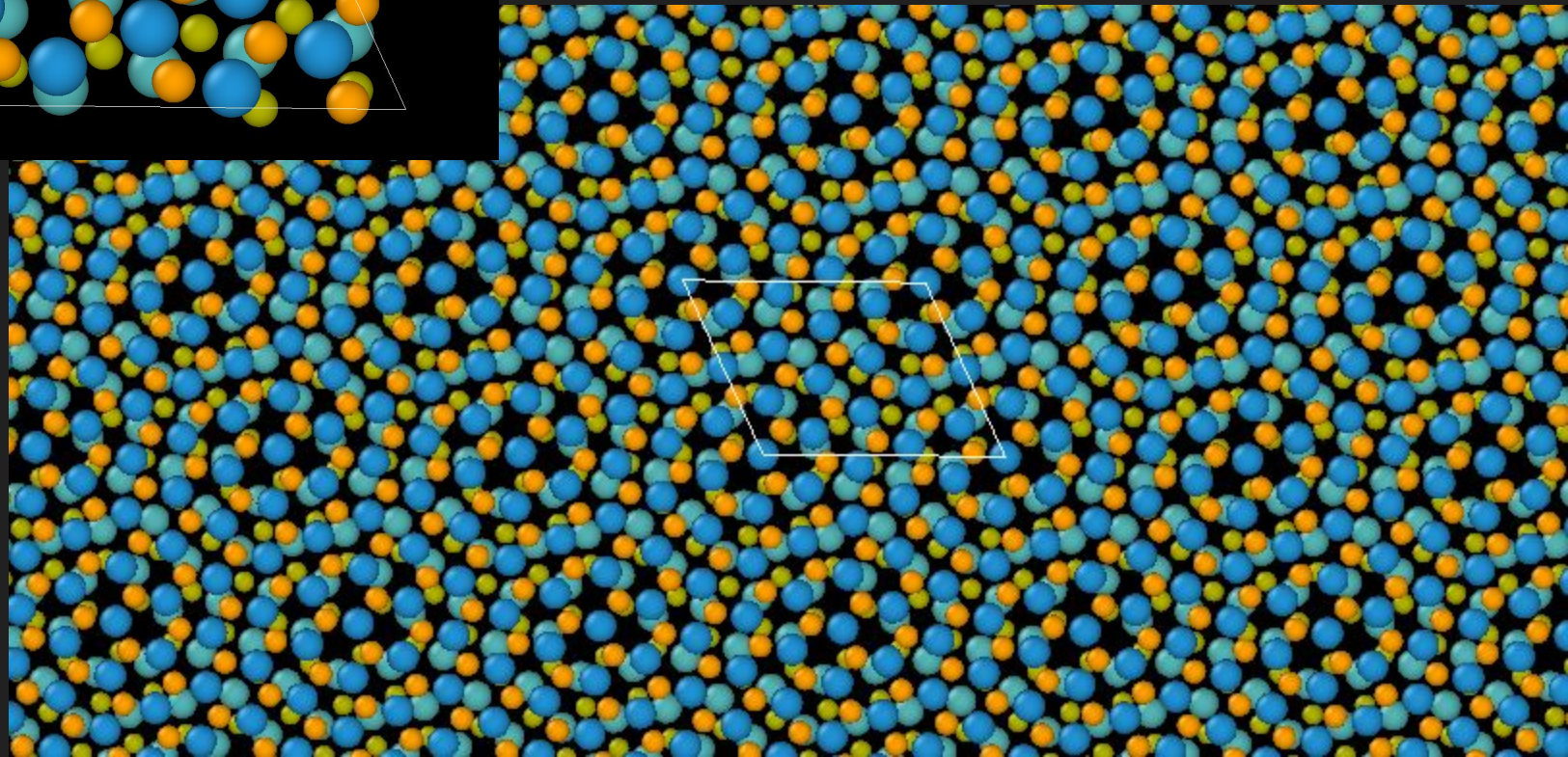
Total atoms: 99

Mo count: 17

W count: 16







16 degree

twist_min_search = 16

twist_max_search = 16.1

max_strain = 0.1

is_1D_dir_1 = True

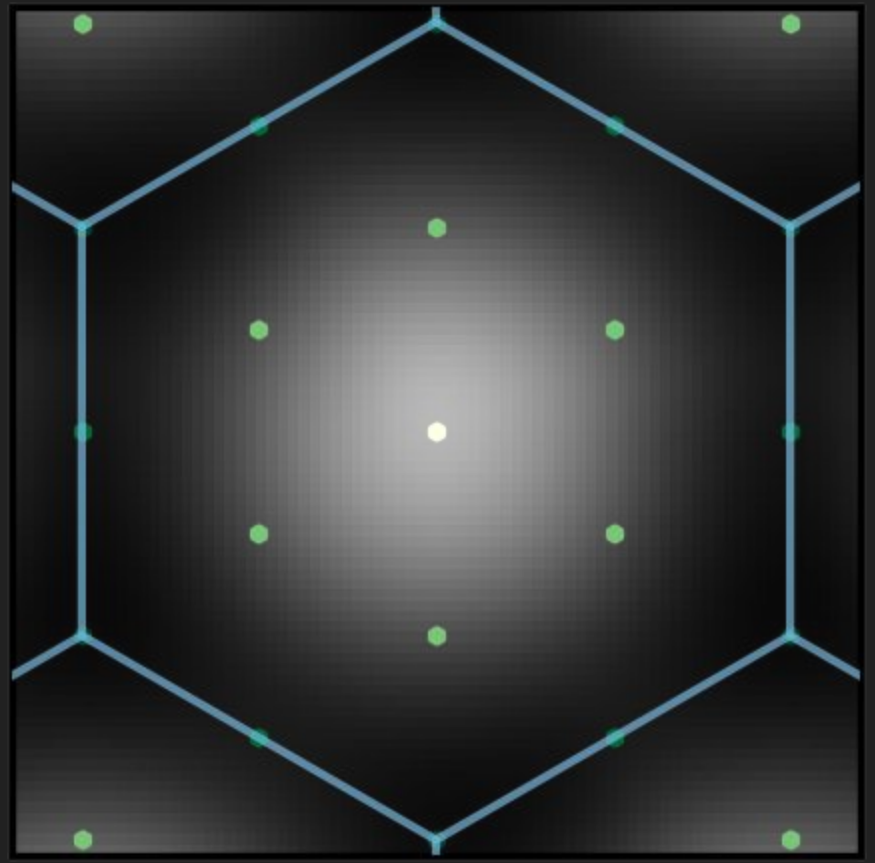
Rmax_max_search = 16

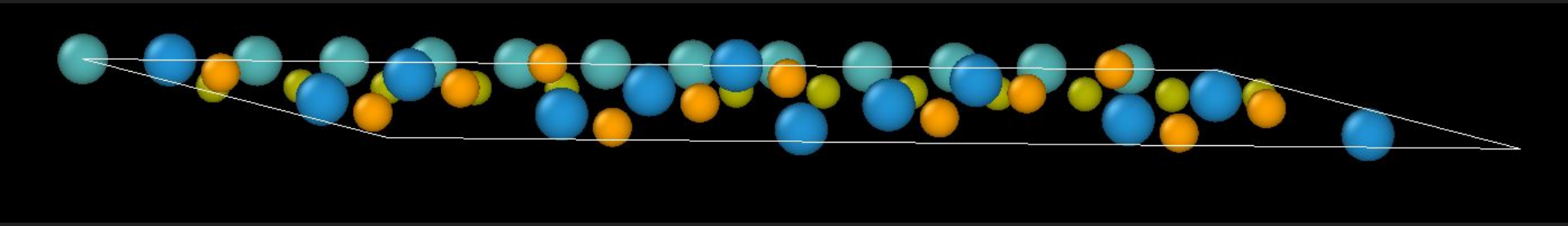
max_iter_twist_search = 5

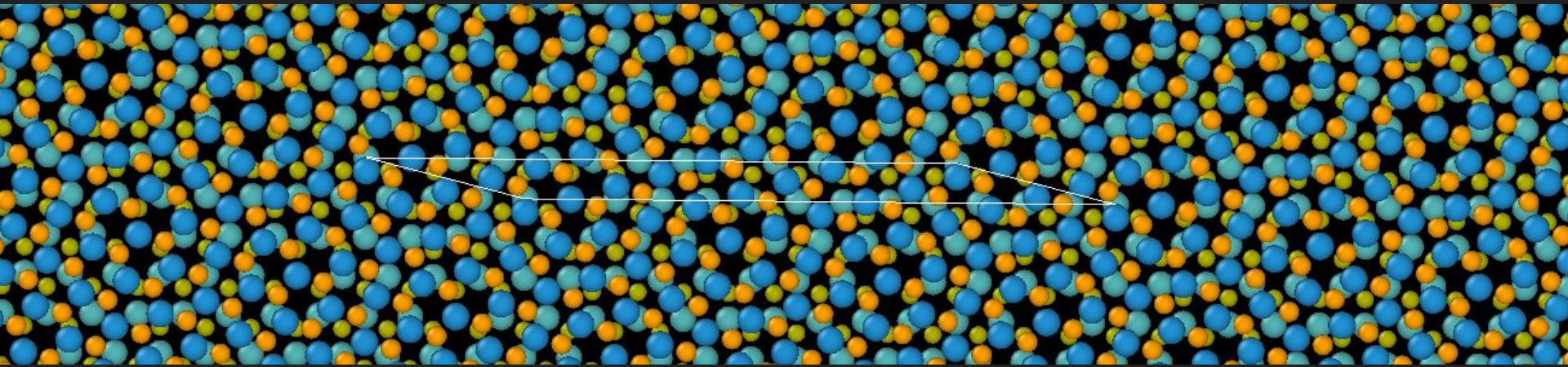
Total atoms: 75

Mo count: 13

W count: 12







20 degree

twist_min_search = 20

twist_max_search = 20.1

max_strain = 0.1

is_1D_dir_1 = True

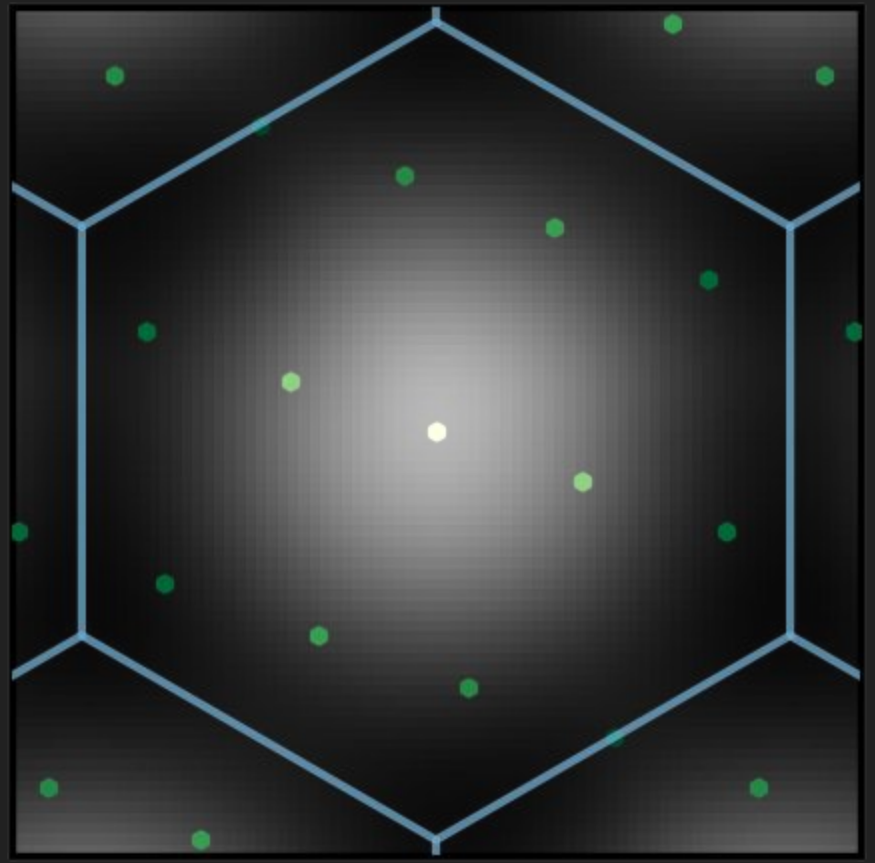
Rmax_max_search = 16

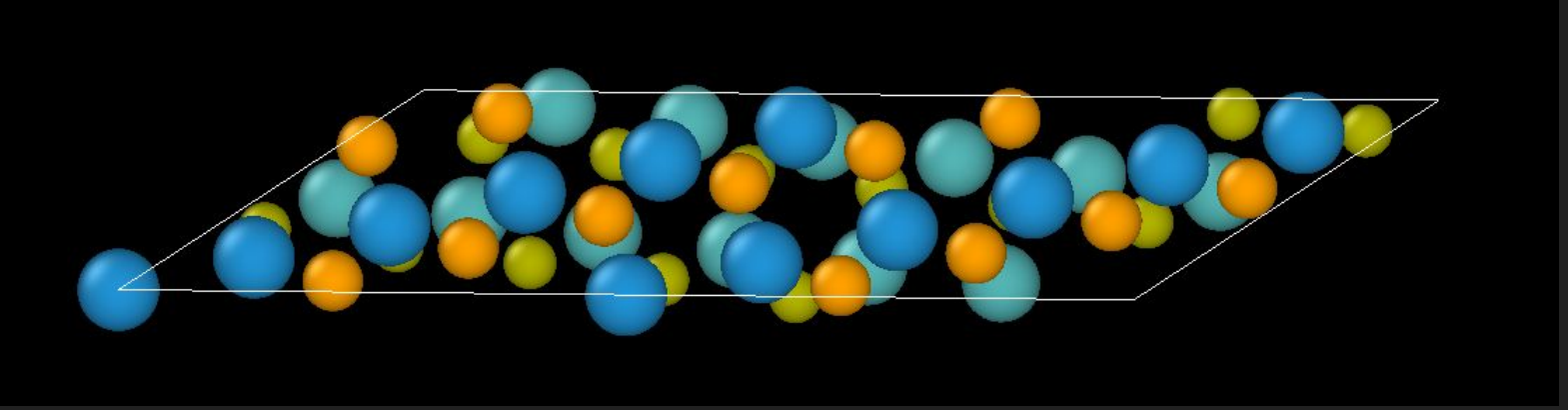
max_iter_twist_search = 5

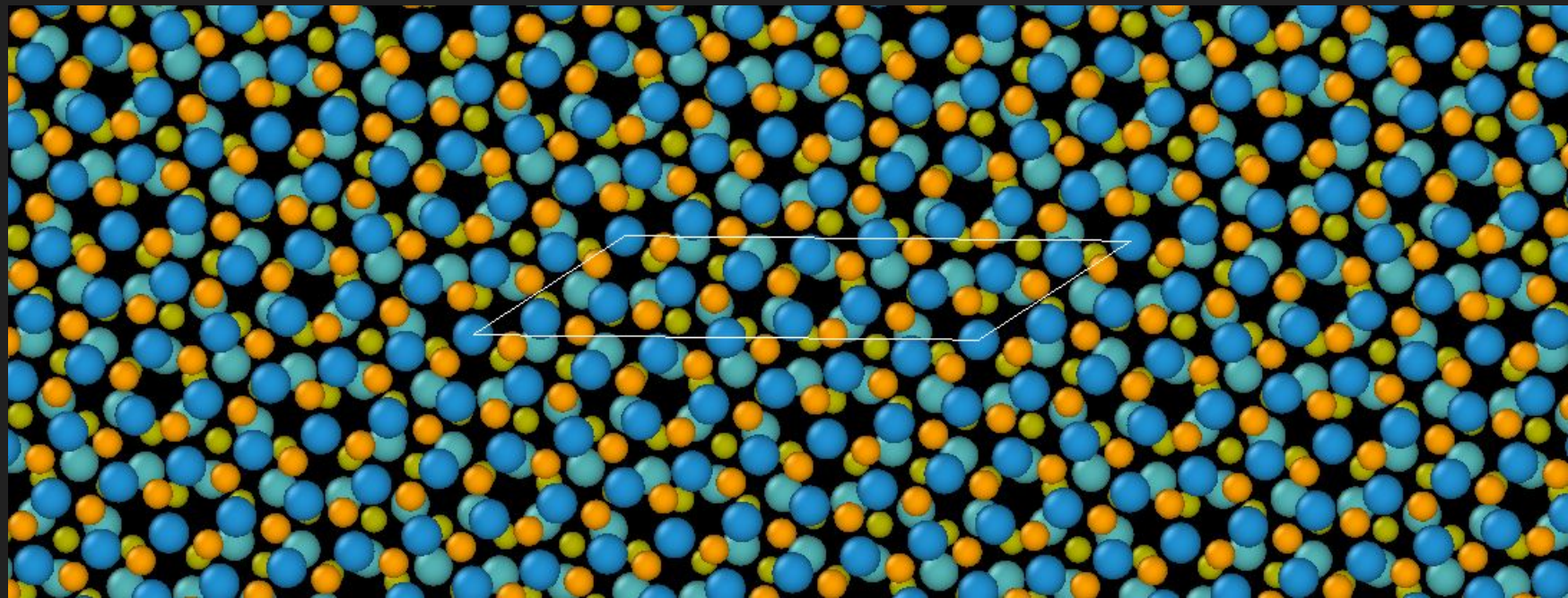
Total atoms: 75

Mo count: 13

W count: 12







24 degree

twist_min_search = 24

twist_max_search = 24.1

max_strain = 0.02

is_1D_dir_1 = True

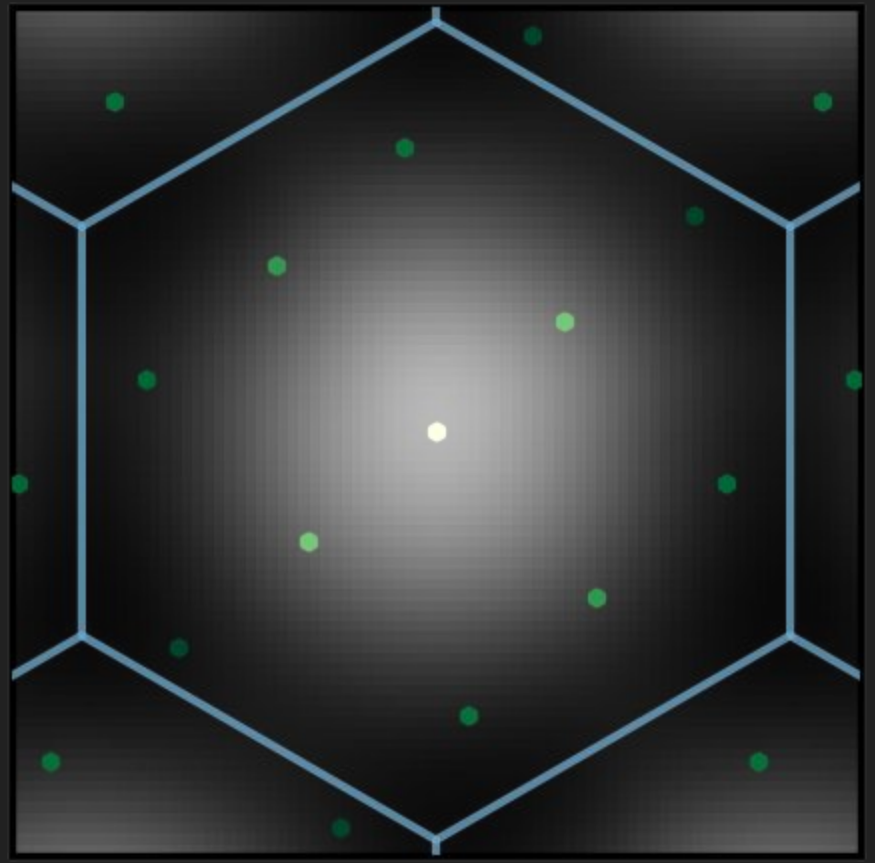
Rmax_max_search = 14

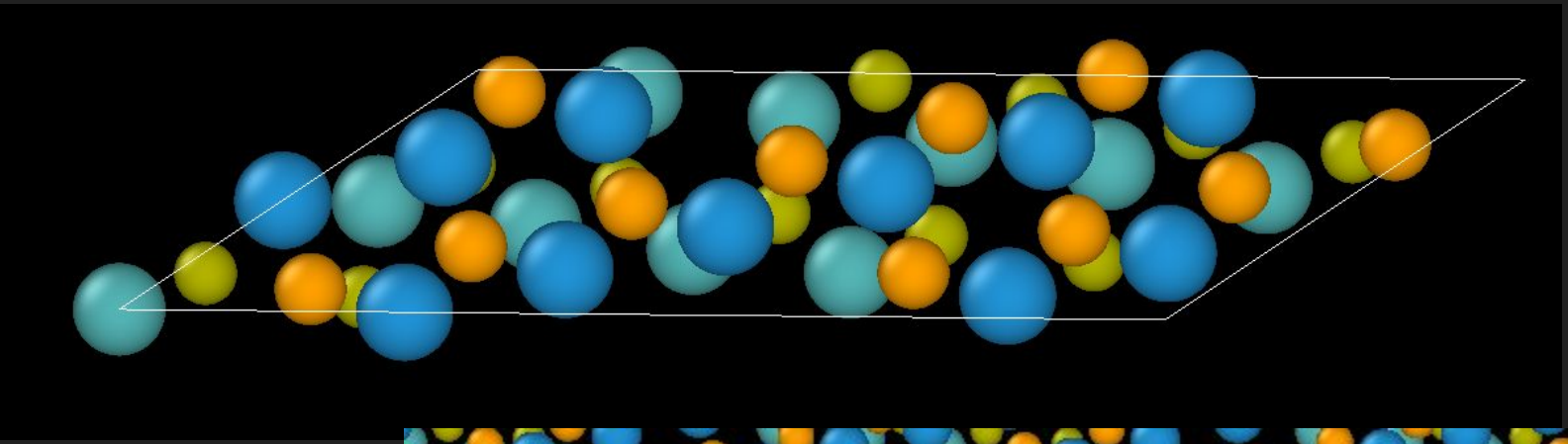
max_iter_twist_search = 5

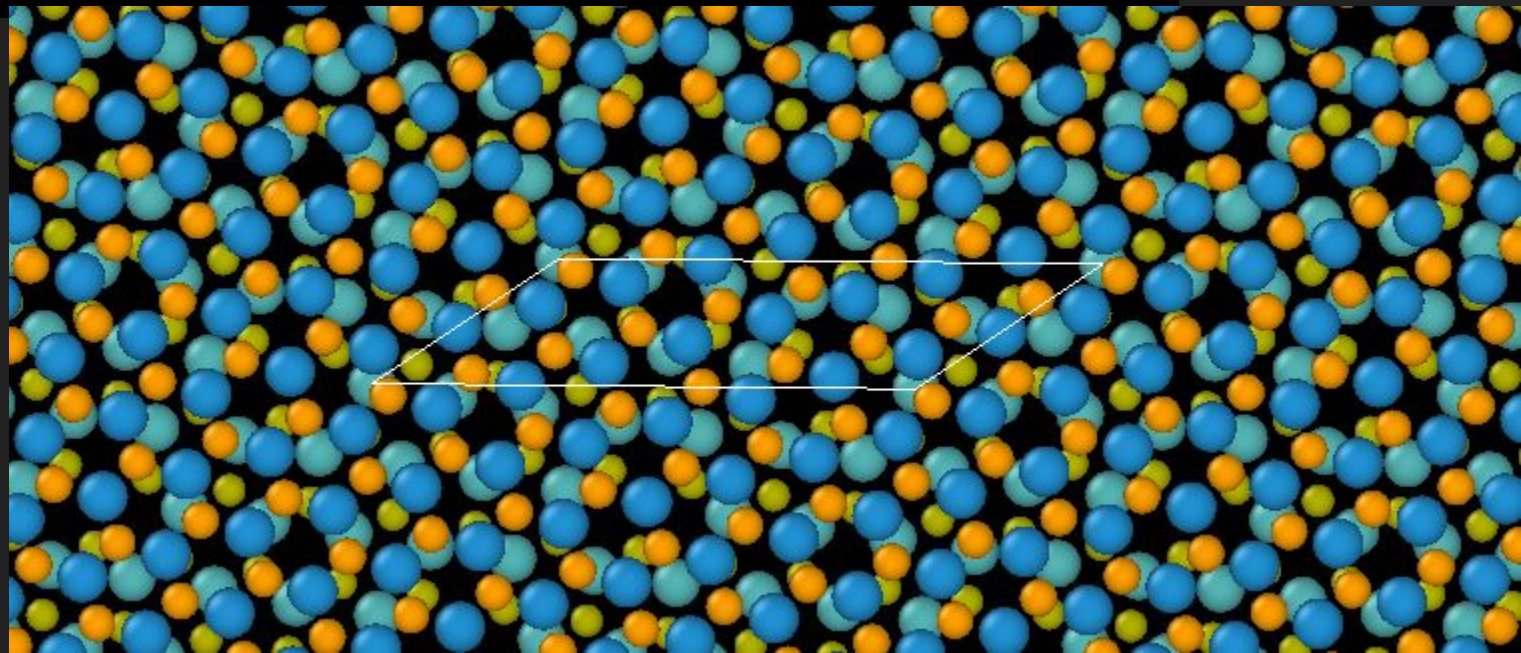
Total atoms: 66

Mo count: 11

W count: 11







28 degree

twist_min_search = 28

twist_max_search = 28.02

max_strain = 0.02

is_1D_dir_1 = True

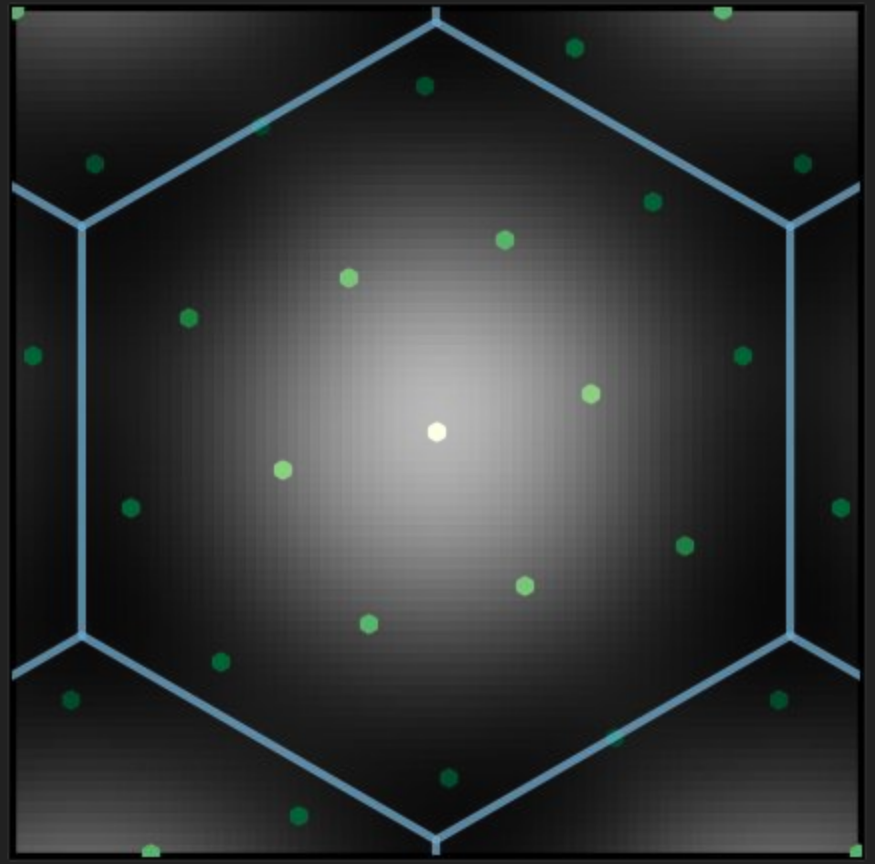
Rmax_max_search = 14

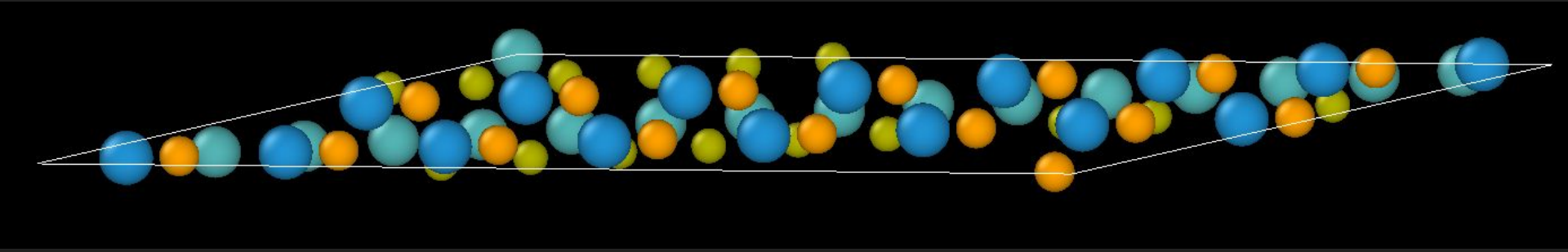
max_iter_twist_search = 5

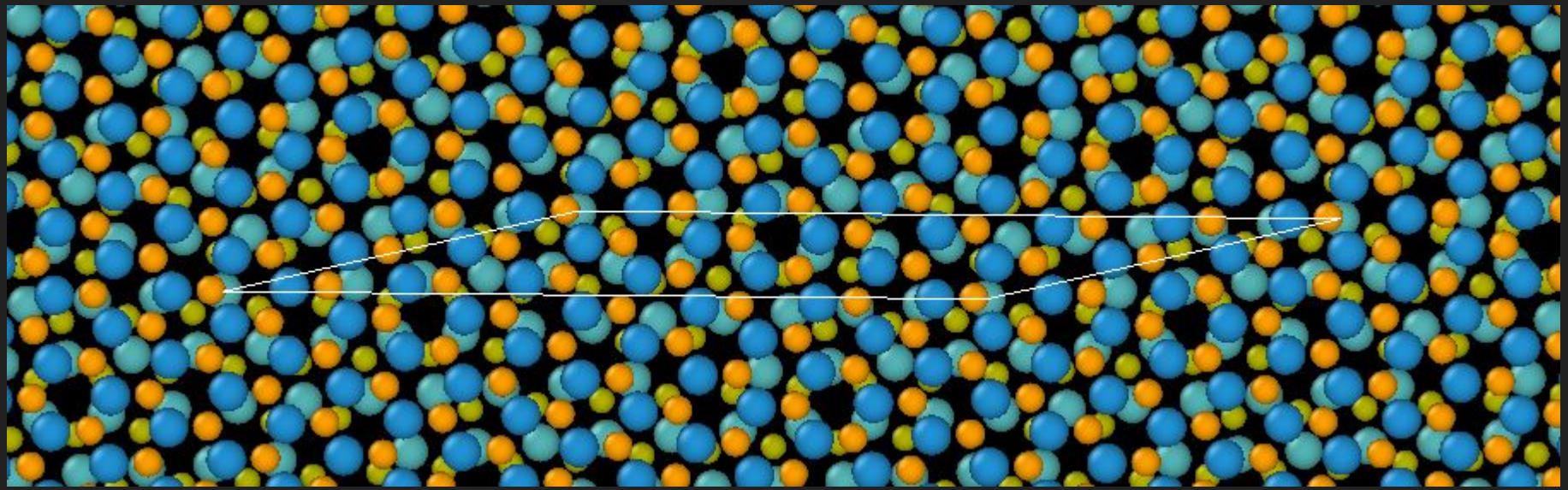
Total atoms: 99

Mo count: 17

W count: 16







30 degree

twist_min_search = 30

twist_max_search = 30.02

max_strain = 0.02

is_1D_dir_1 = True

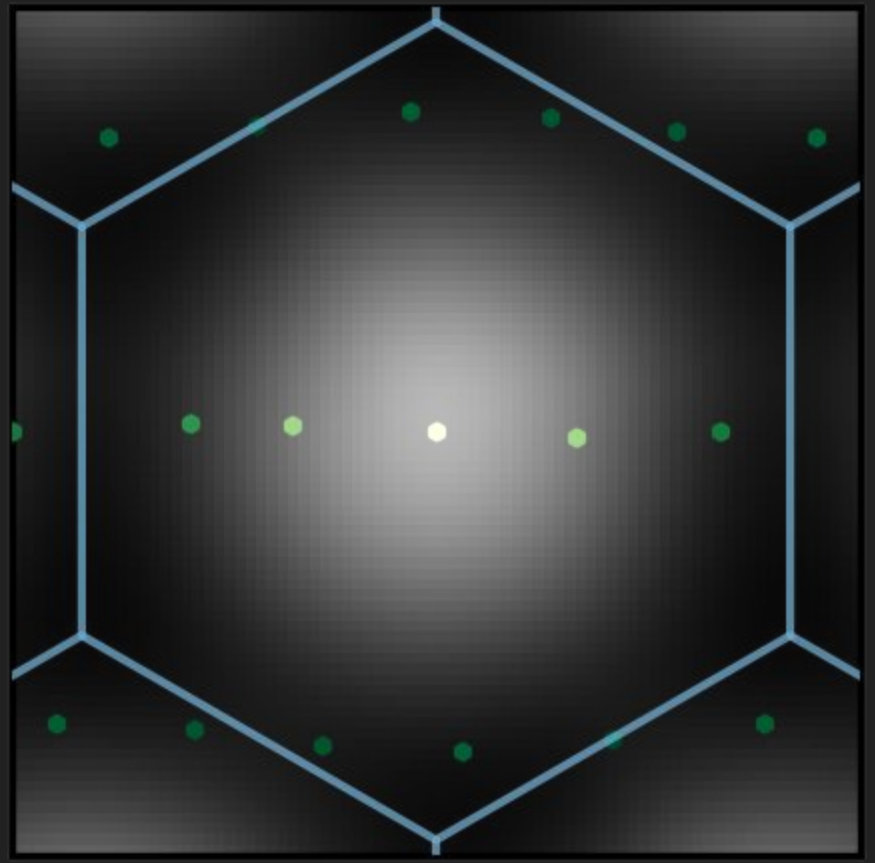
Rmax_max_search = 14

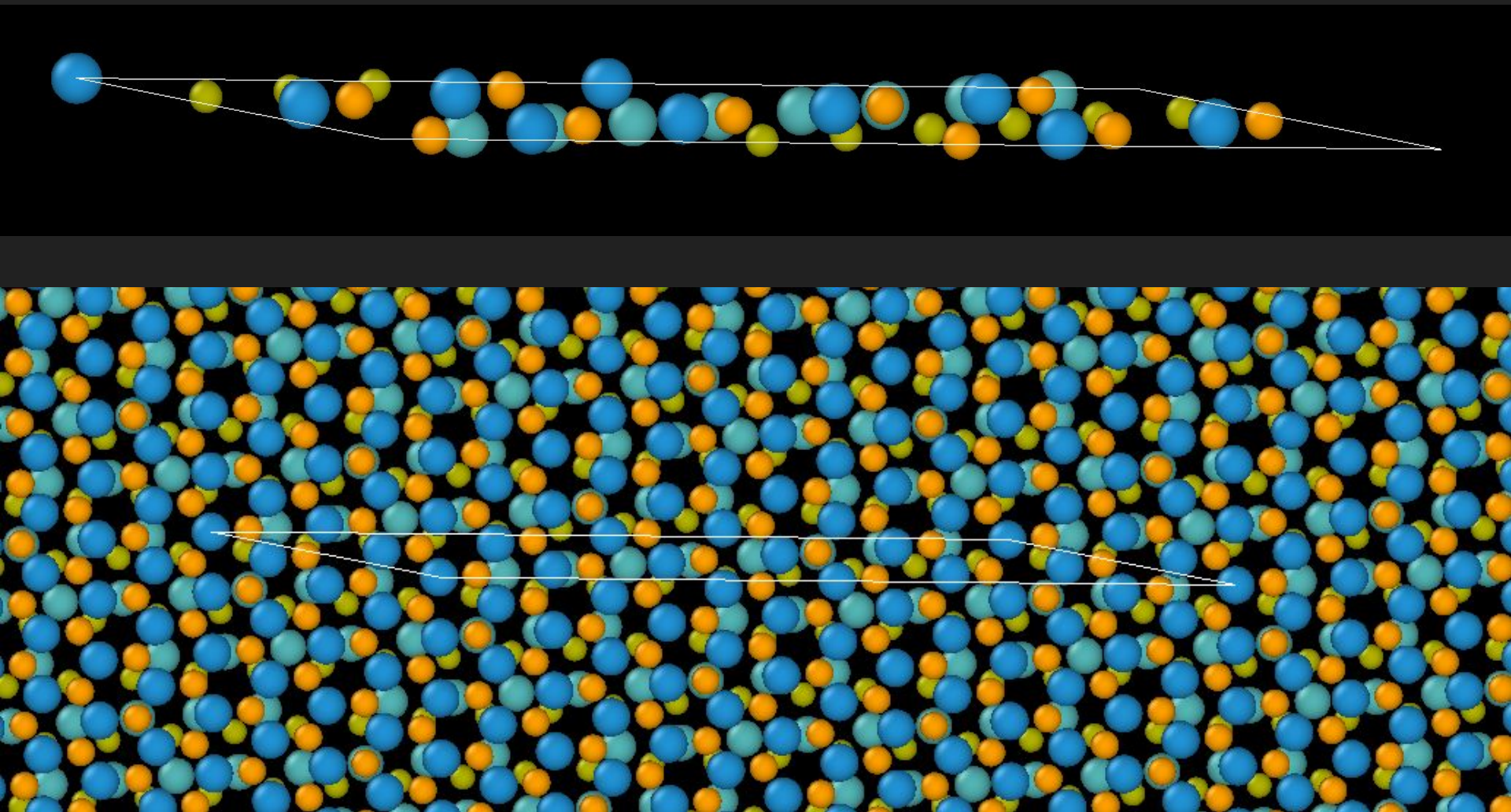
max_iter_twist_search = 5

Total atoms: 57

Mo count: 9

W count: 10





35 degree

twist_min_search = 35

twist_max_search = 35.02

max_strain = 0.02

is_1D_dir_1 = True

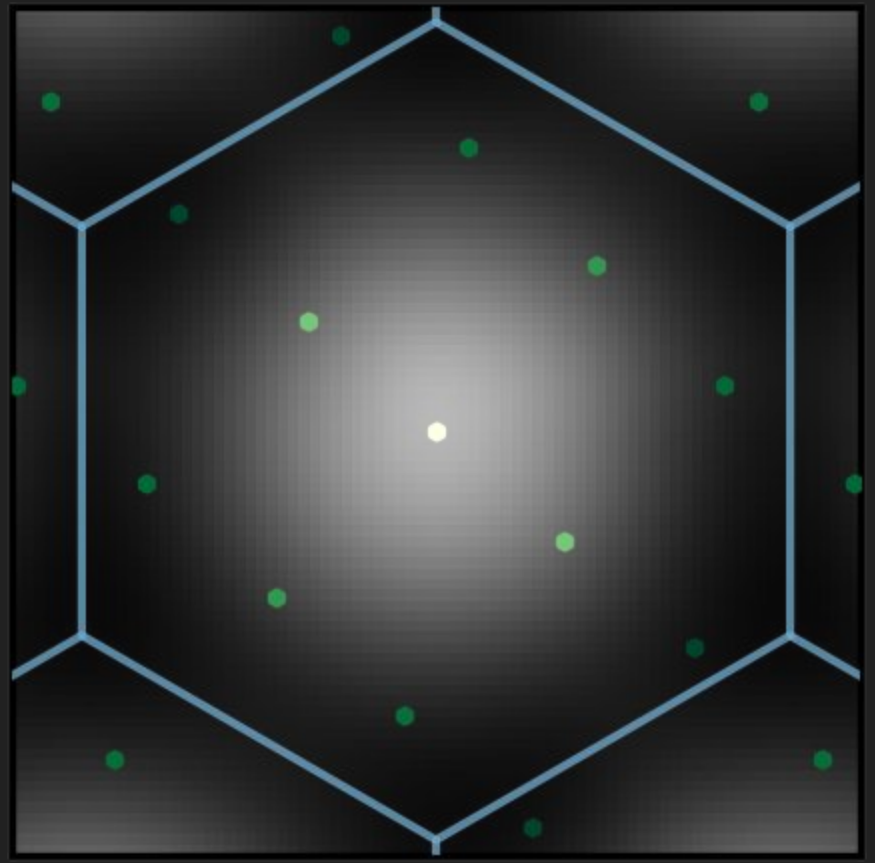
Rmax_max_search = 14

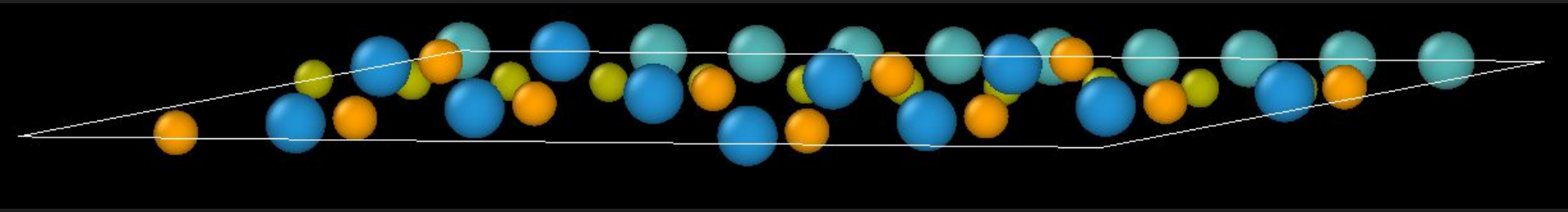
max_iter_twist_search = 5

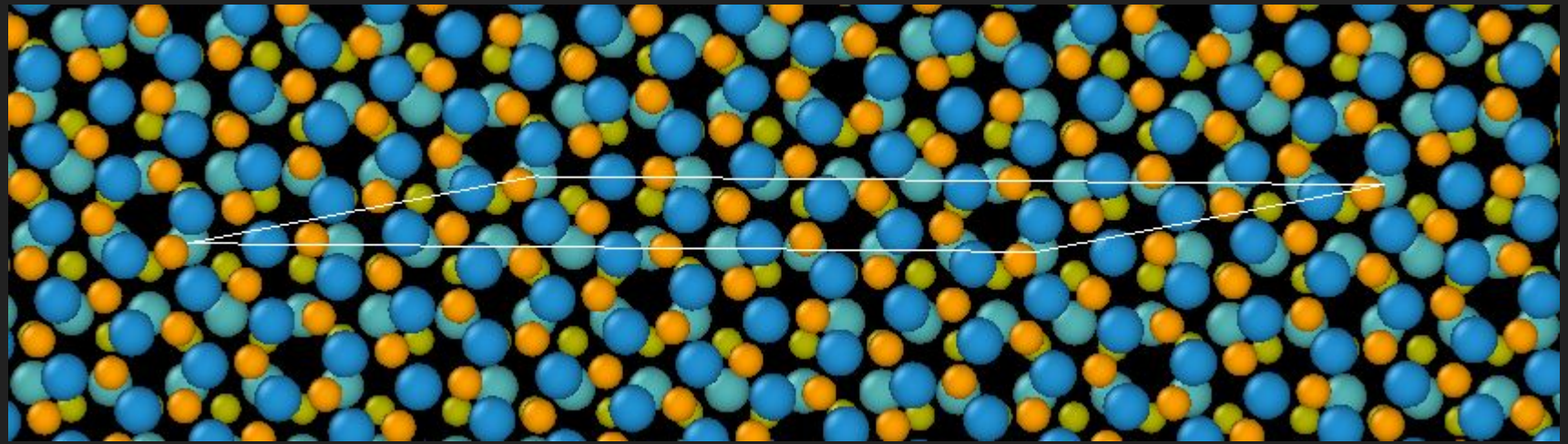
Total atoms: 66

Mo count: 11

W count: 11







40 degree

twist_min_search = 40

twist_max_search = 40.1

max_strain = 0.05

is_1D_dir_1 = True

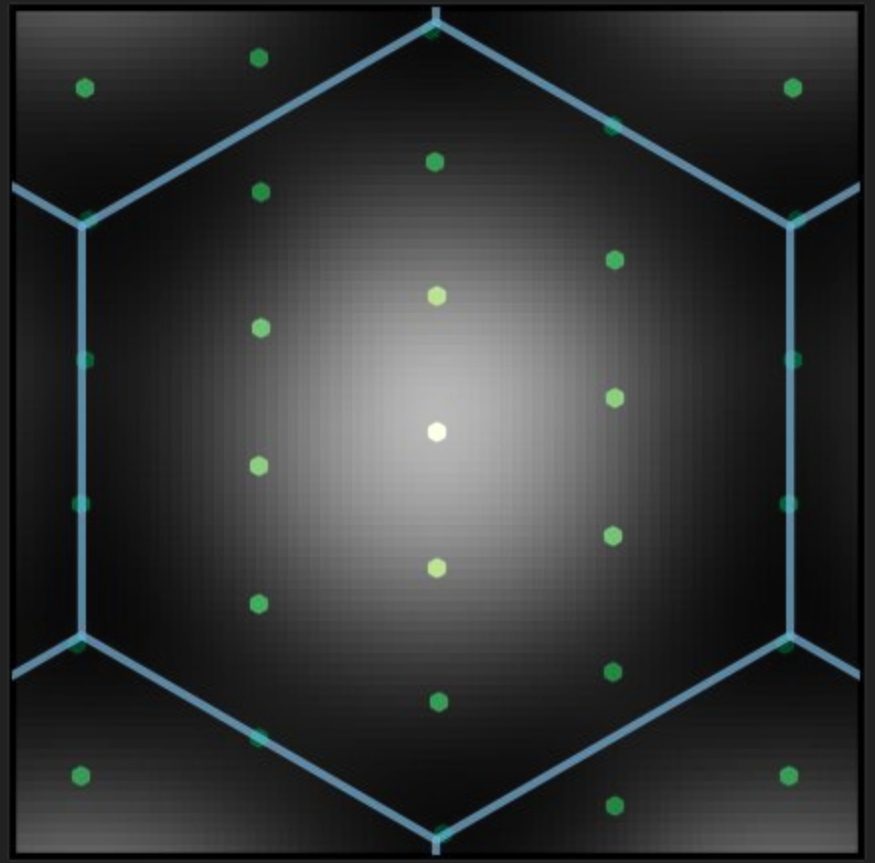
Rmax_max_search = 16

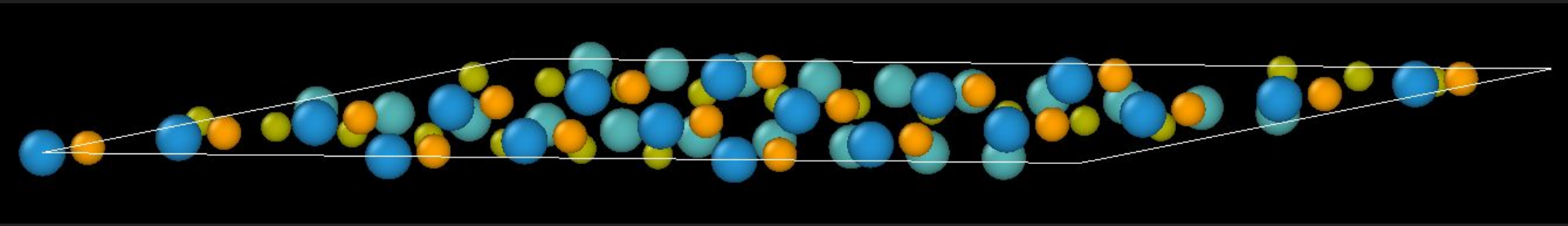
max_iter_twist_search = 5

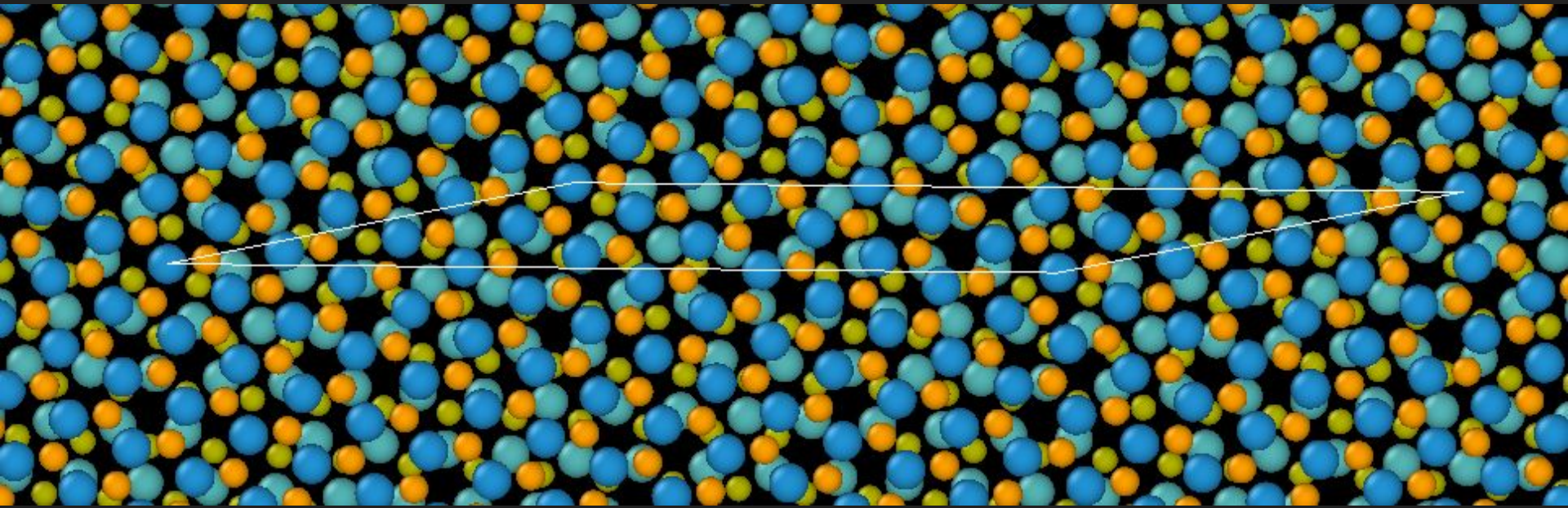
Total atoms: 117

Mo count: 21

W count: 18







45 degree

twist_min_search = 45

twist_max_search = 45.1

max_strain = 0.05

is_1D_dir_1 = True

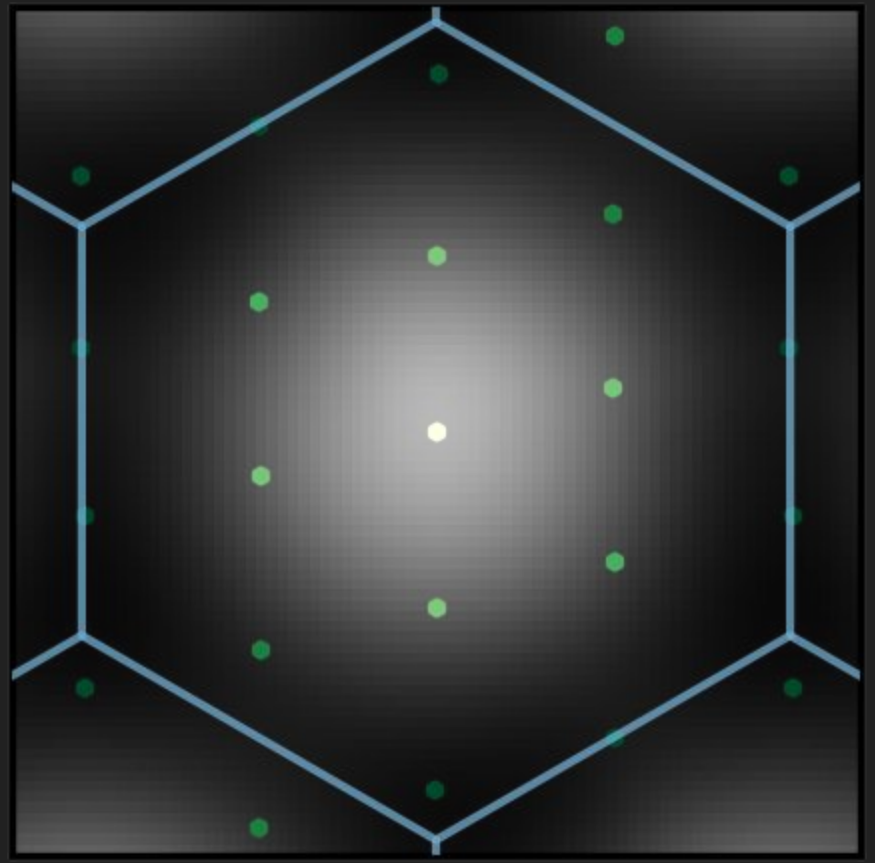
Rmax_max_search = 16

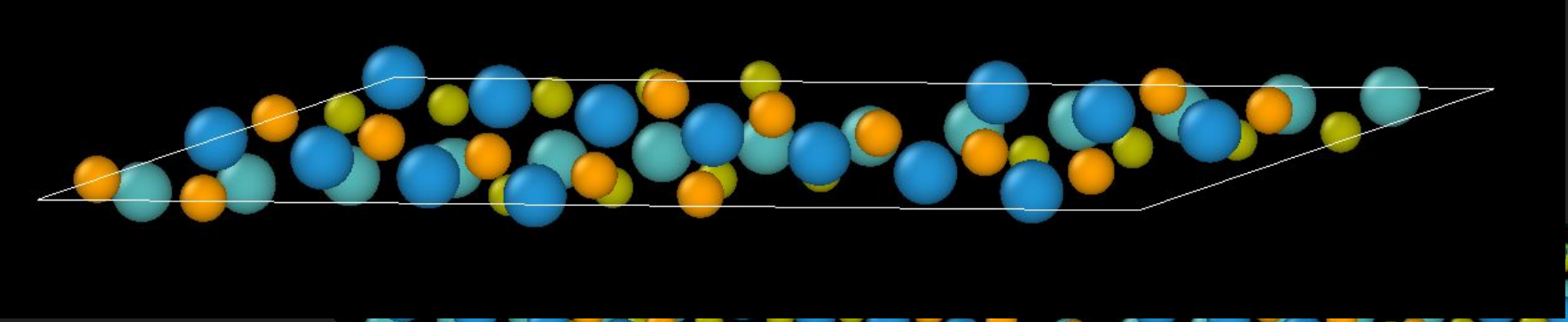
max_iter_twist_search = 5

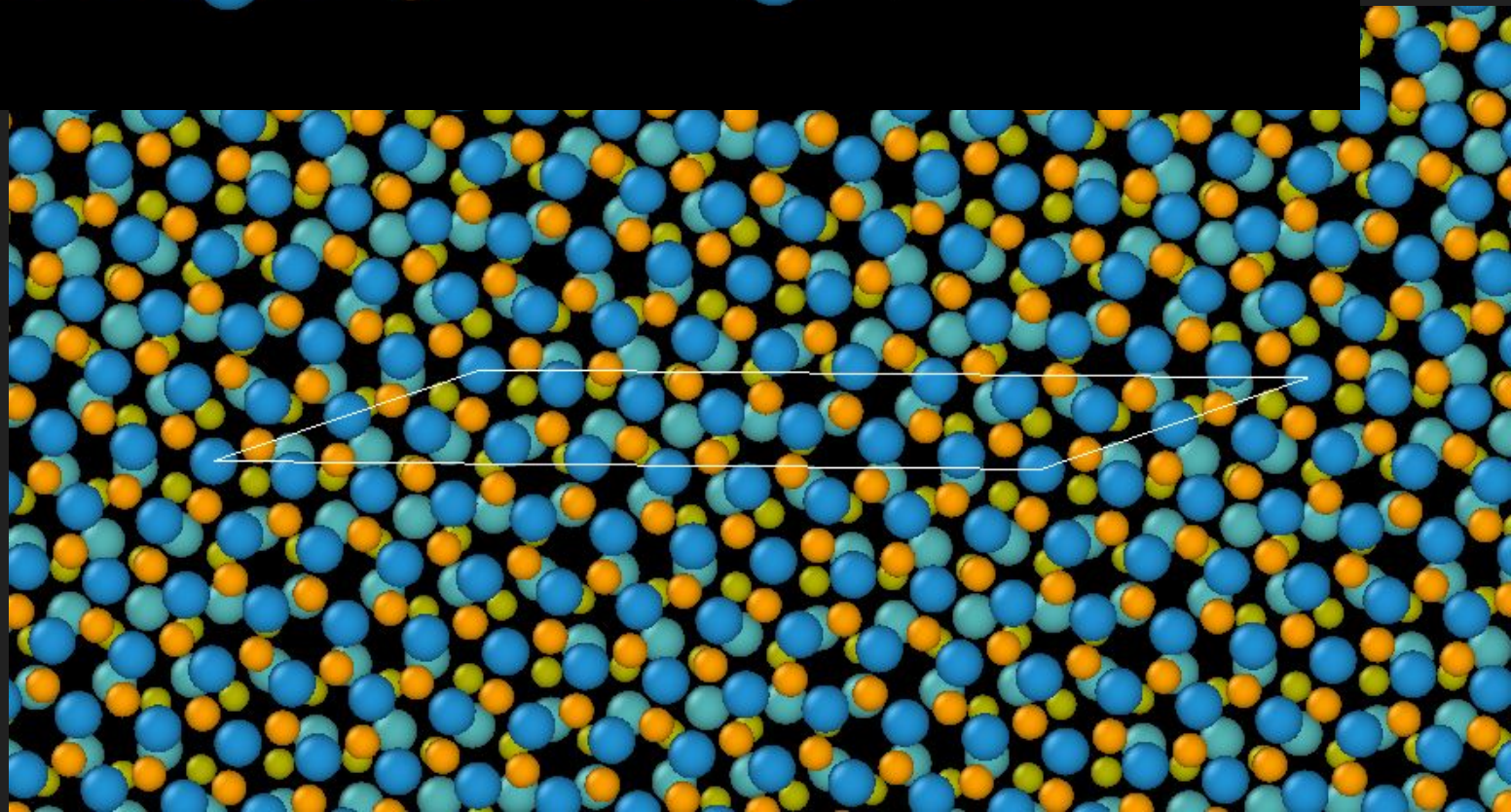
Total atoms: 84

Mo count: 14

W count: 14







50 degree

twist_min_search = 50

twist_max_search = 50.1

max_strain = 0.05

is_1D_dir_1 = True

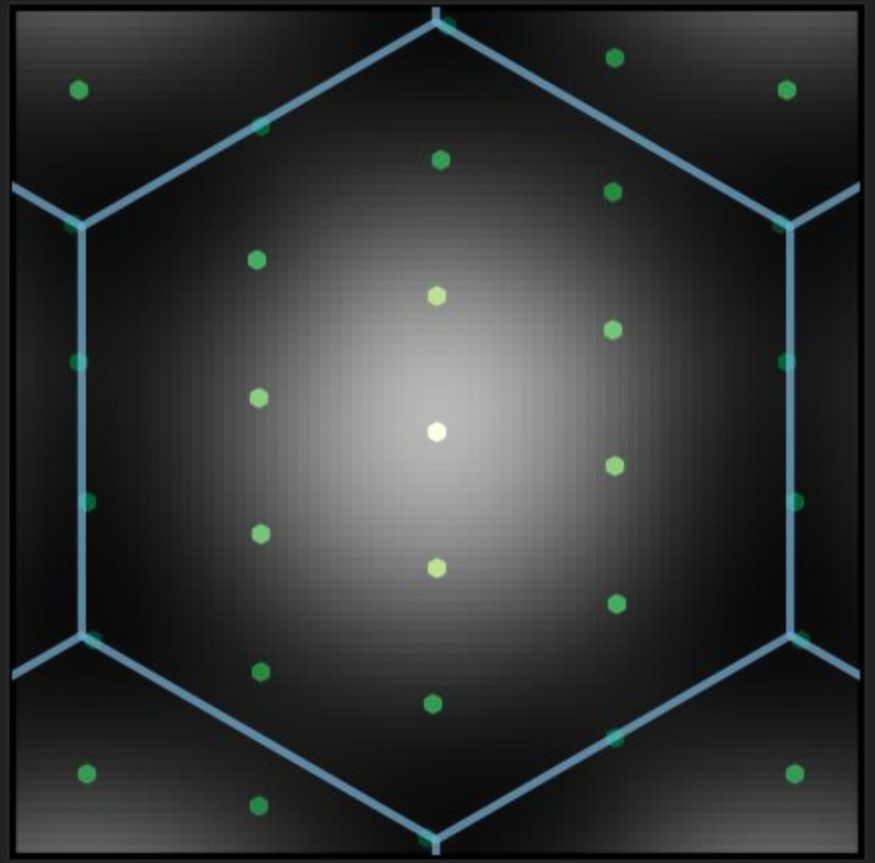
Rmax_max_search = 16

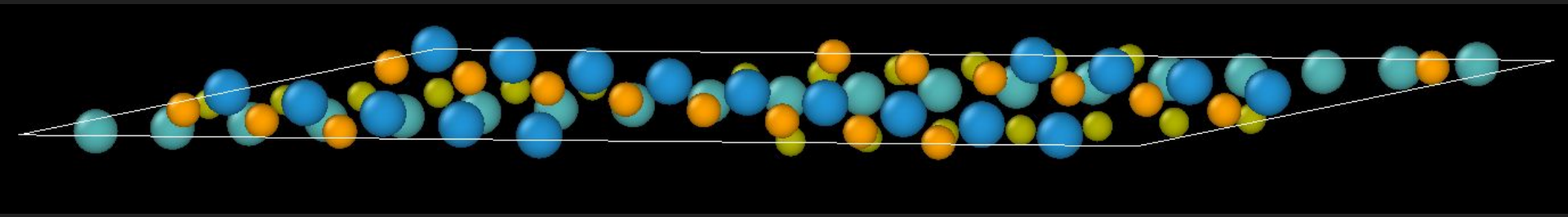
max_iter_twist_search = 5

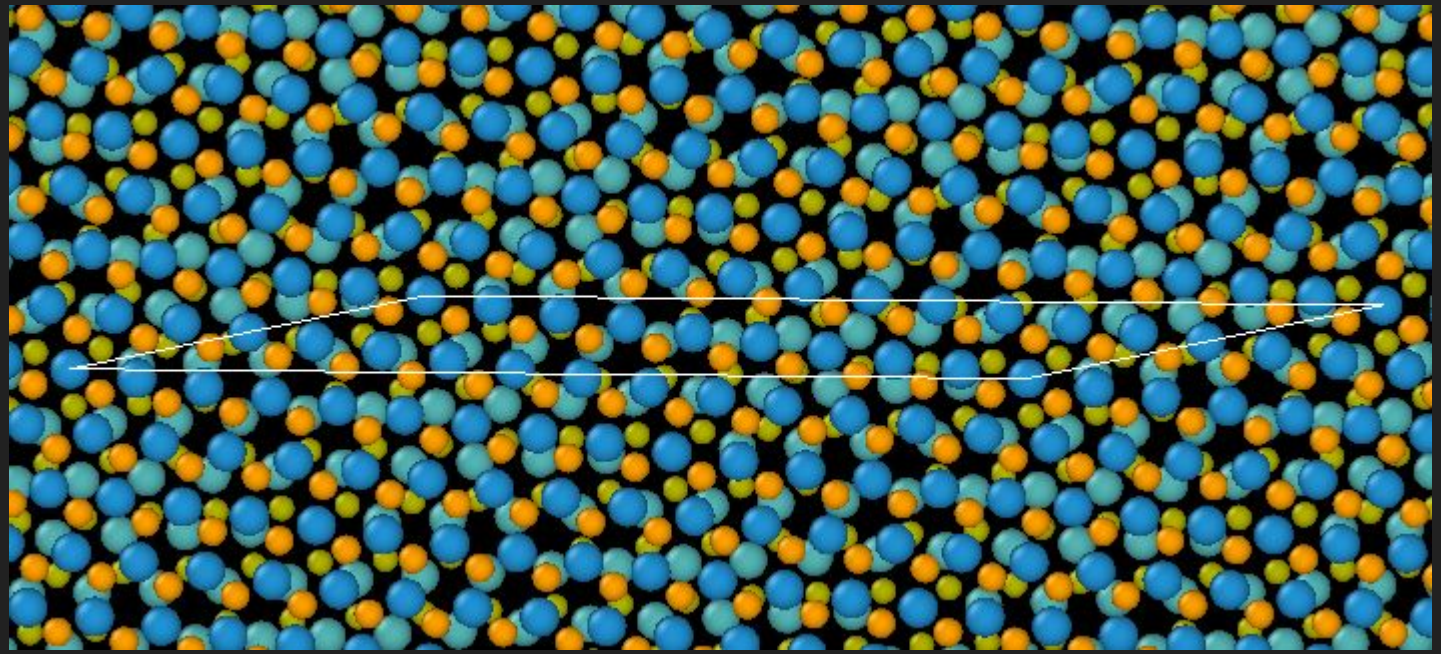
Total atoms: 114

Mo count: 20

W count: 18







55 degree

twist_min_search = 55

twist_max_search = 55.1

max_strain = 0.01

is_1D_dir_1 = True

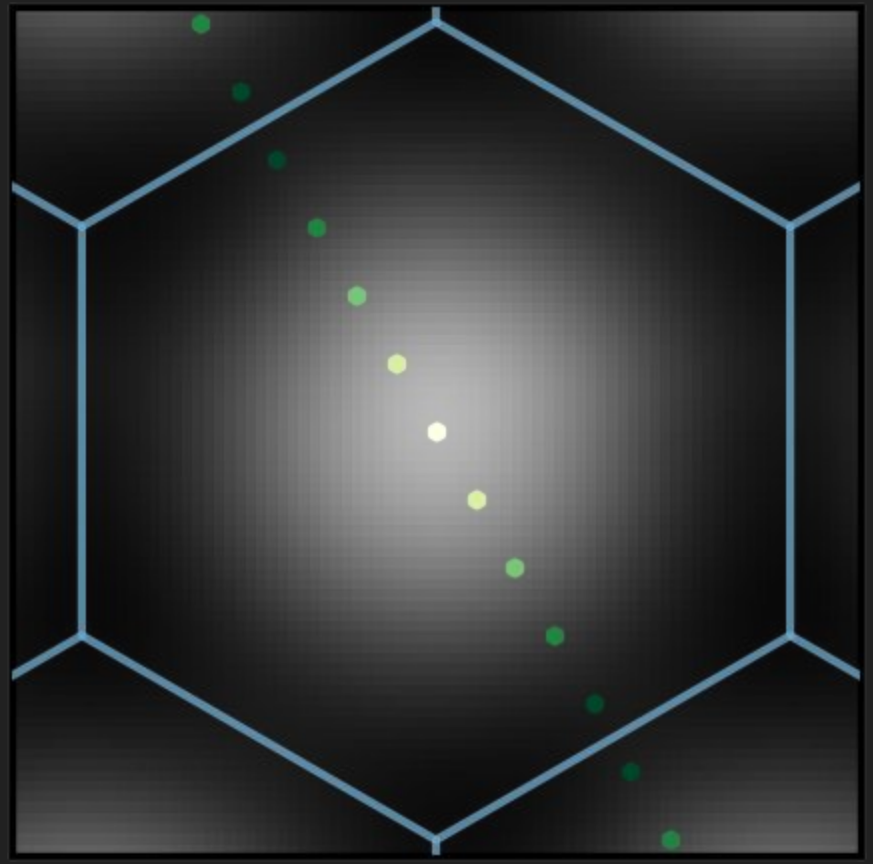
Rmax_max_search = 16

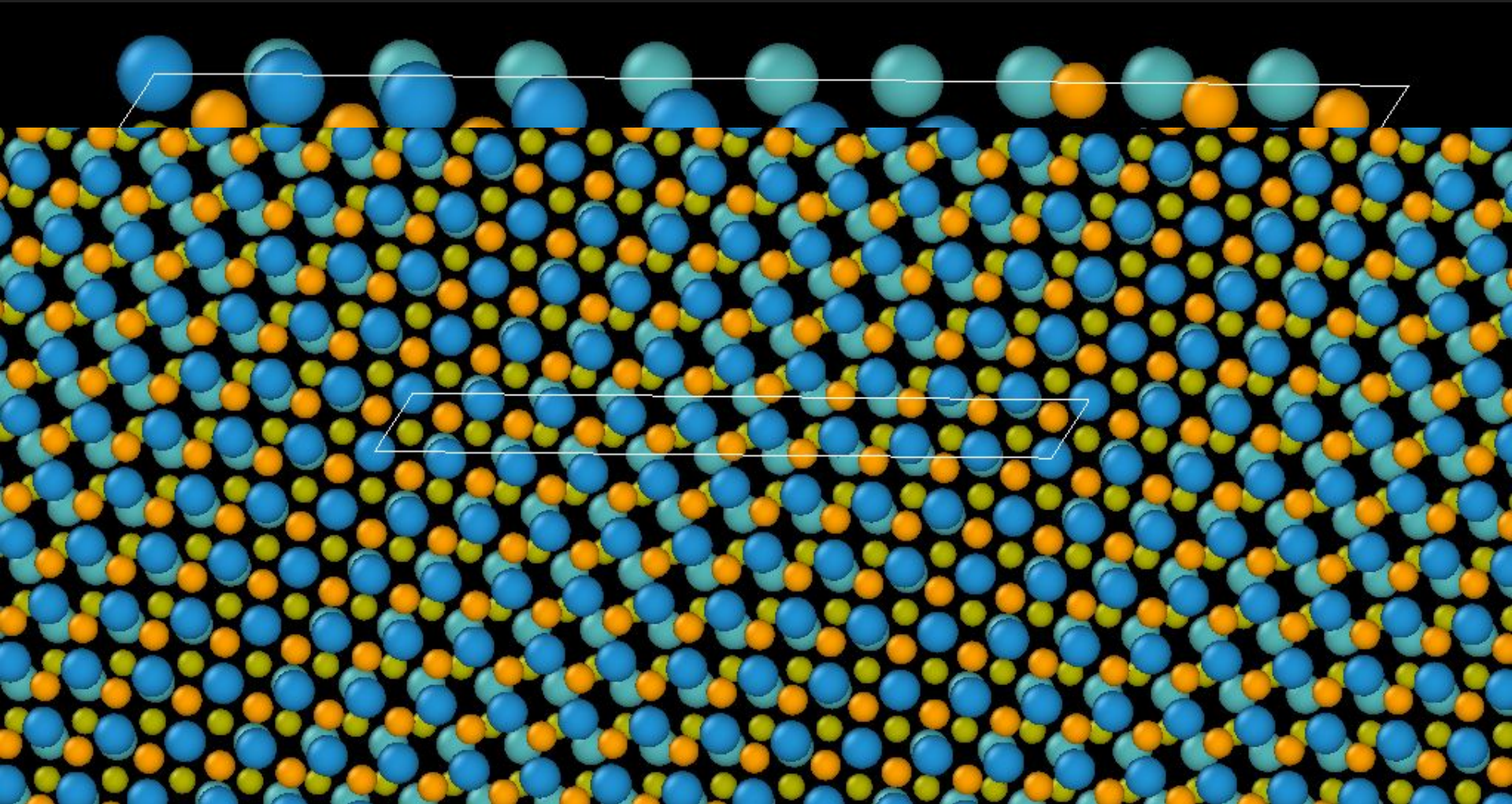
max_iter_twist_search = 5

Total atoms: 57

Mo count: 10

W count: 9





60 degree

twist_min_search = 60

twist_max_search = 60.1

max_strain = 0.05

is_1D_dir_1 = True

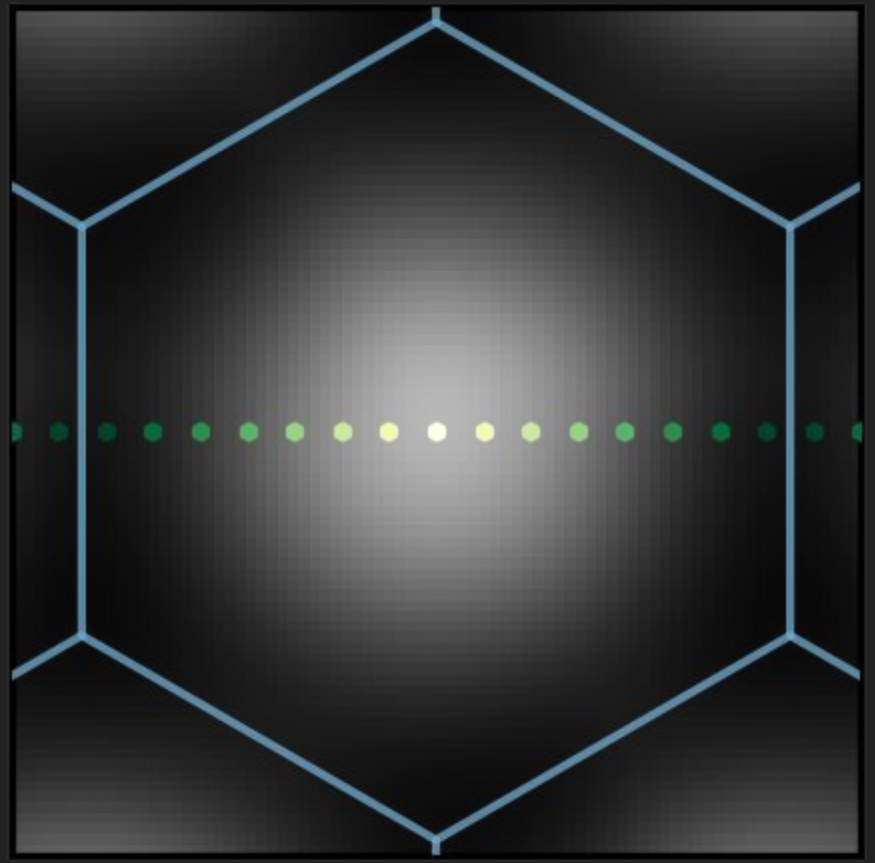
Rmax_max_search = 16

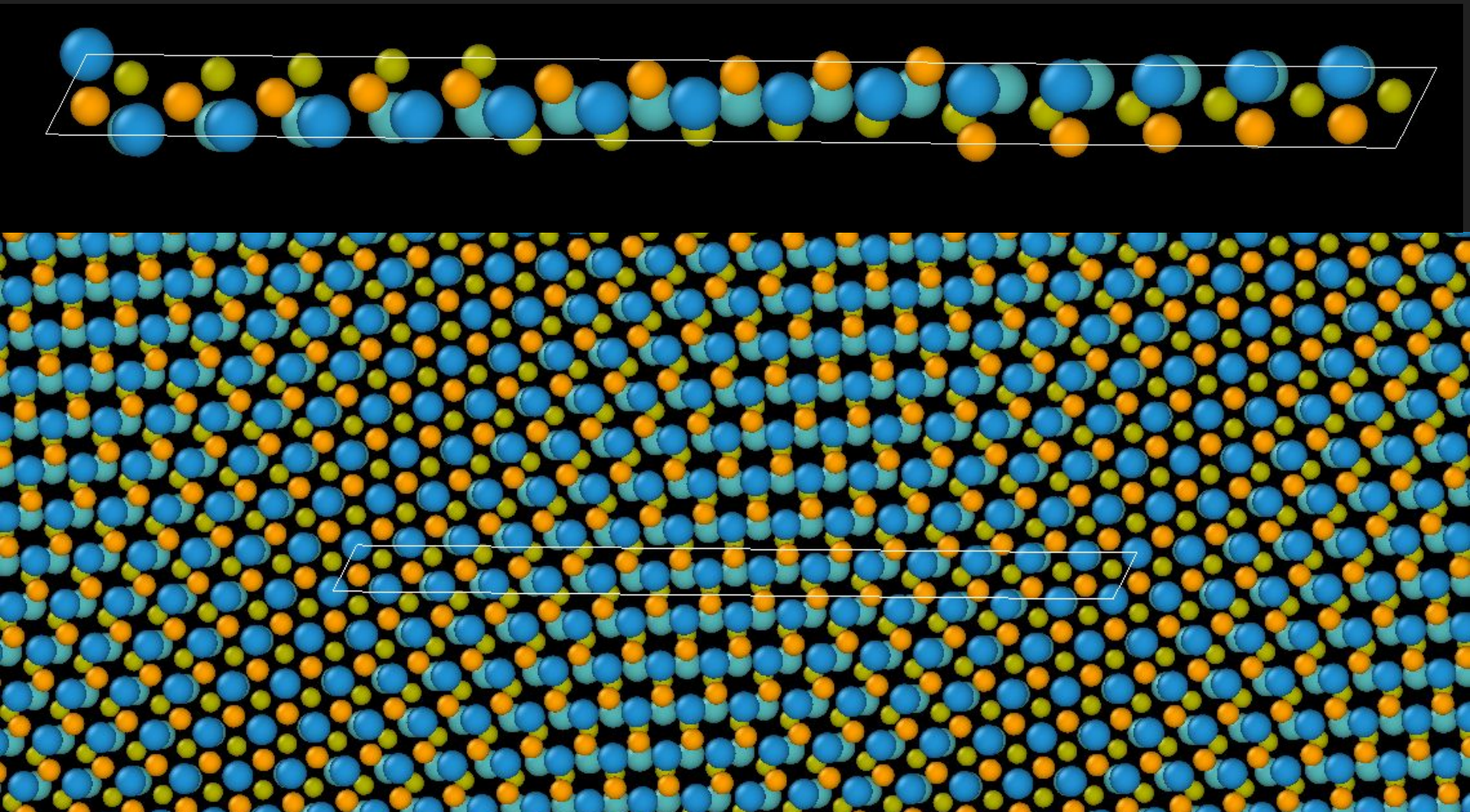
max_iter_twist_search = 5

Total atoms: 93

Mo count: 16

W count: 15





65 degree

twist_min_search = 65

twist_max_search = 65.1

max_strain = 0.02

is_1D_dir_1 = True

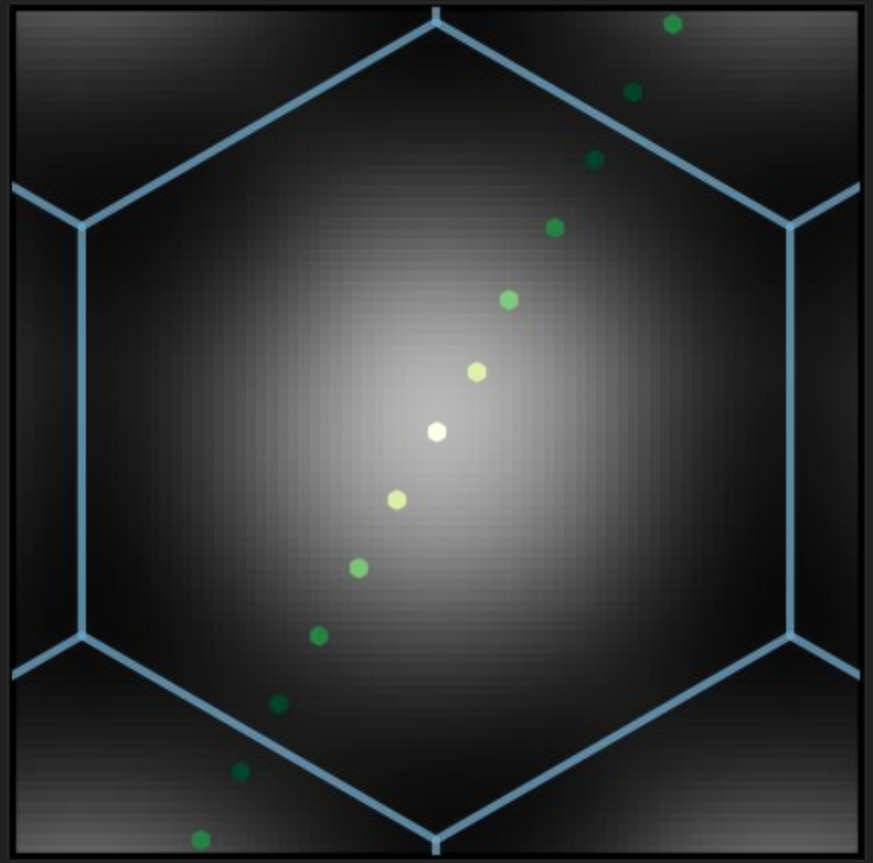
Rmax_max_search = 14

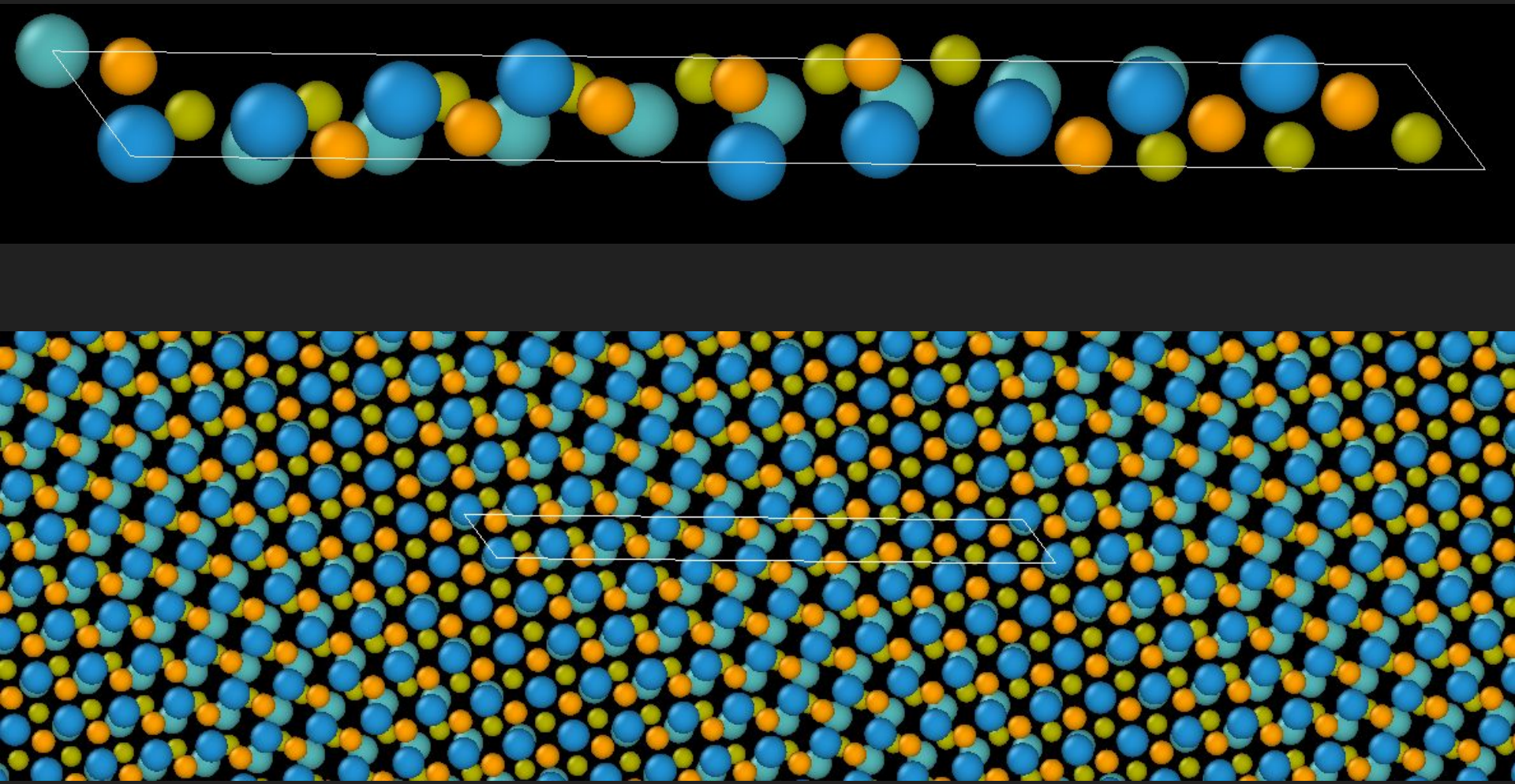
max_iter_twist_search = 5

Total atoms: 57

Mo count: 10

W count: 9





70 degree

twist_min_search = 70

twist_max_search = 70.1

max_strain = 0.02

is_1D_dir_1 = True

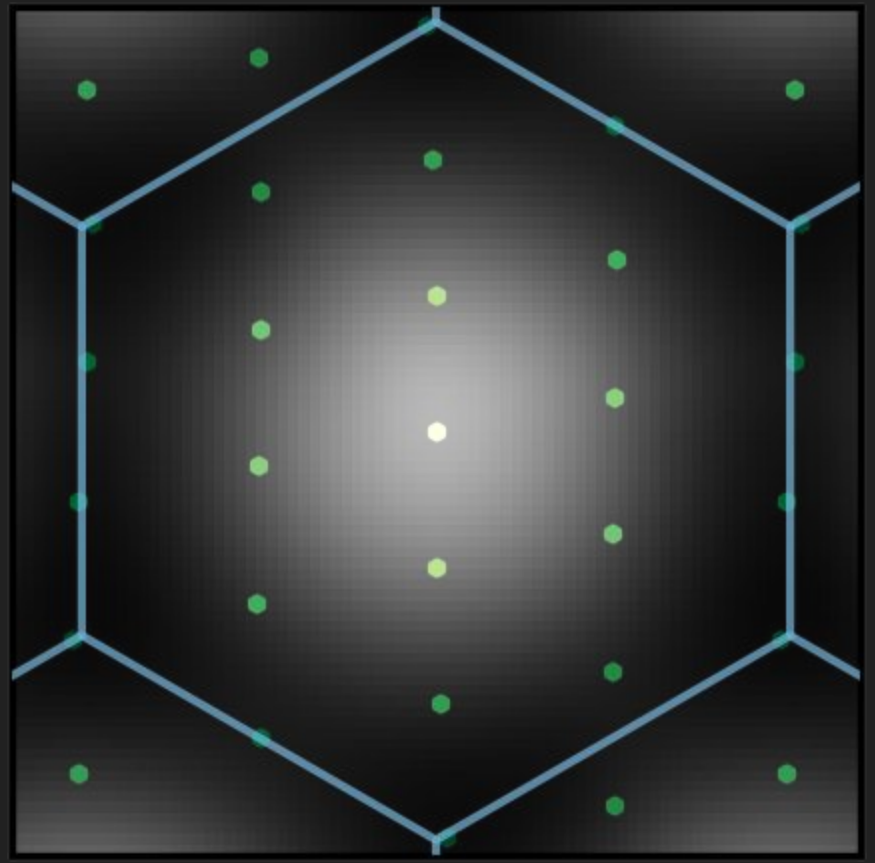
Rmax_max_search = 16

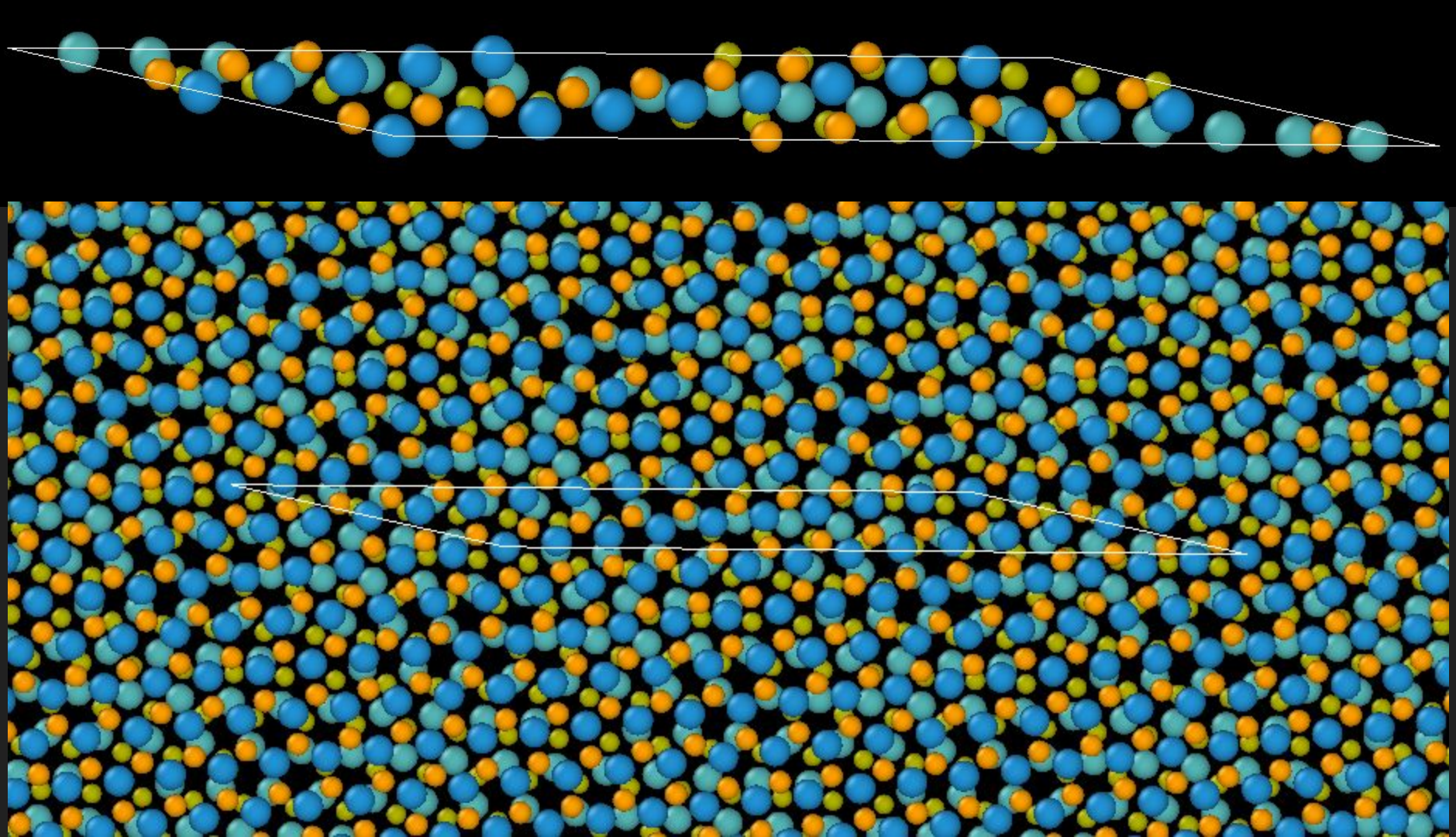
max_iter_twist_search = 5

Total atoms: 114

Mo count: 20

W count: 18





75 degree

twist_min_search = 75

twist_max_search = 75.1

max_strain = 0.02

is_1D_dir_1 = True

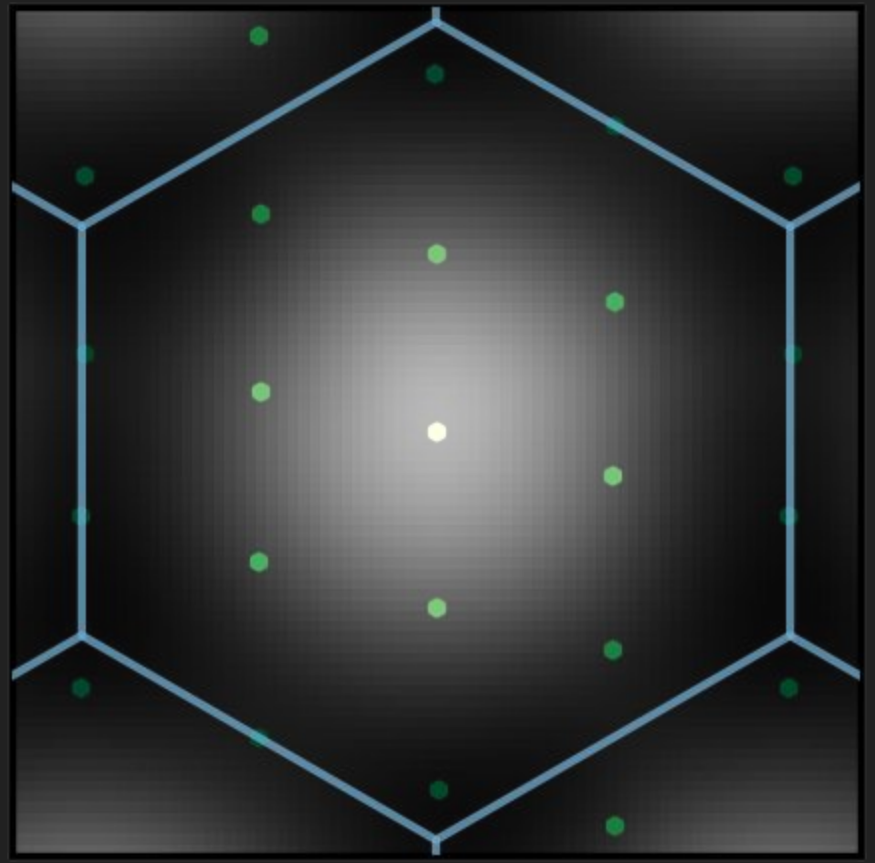
Rmax_max_search = 16

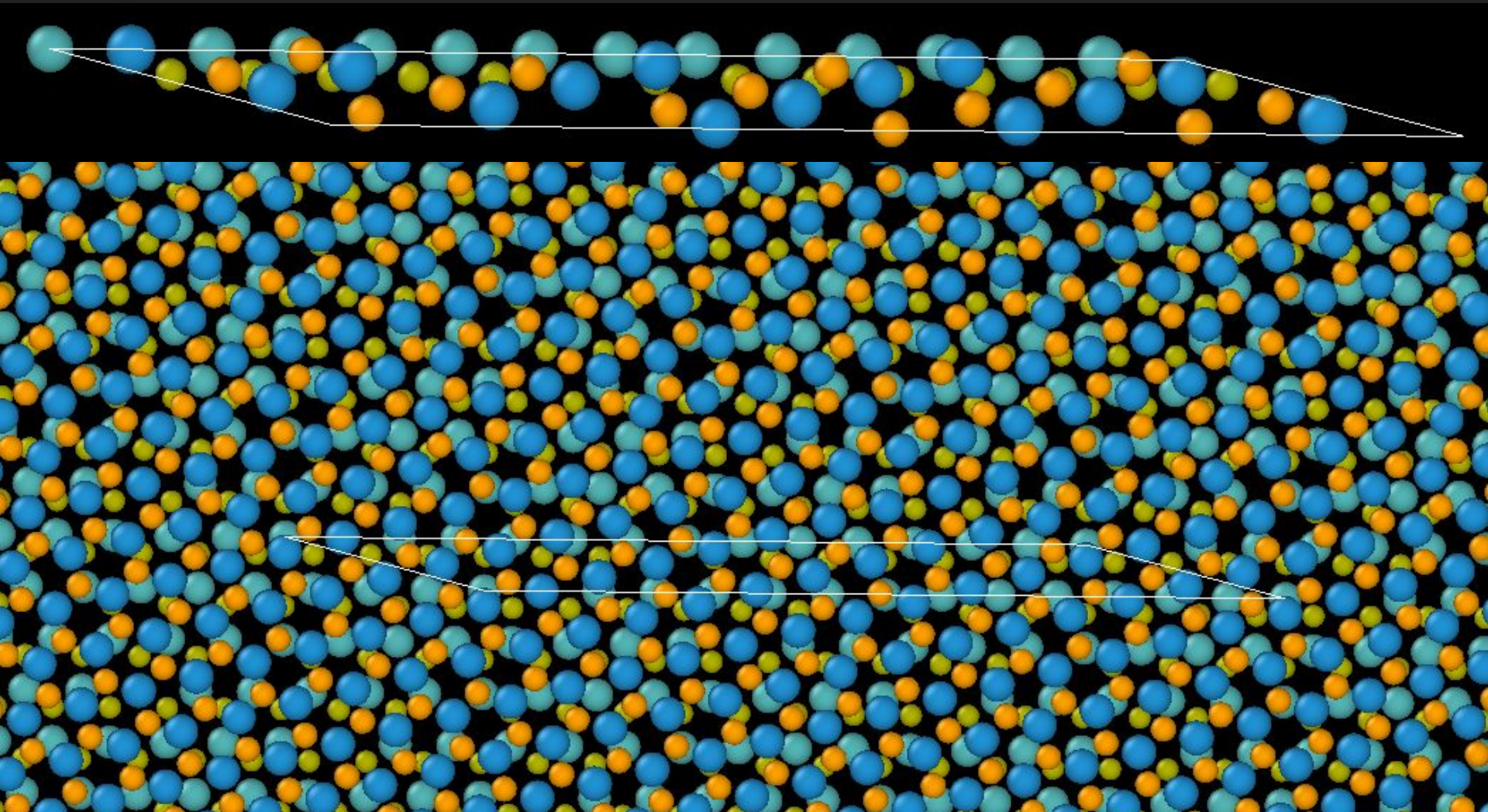
max_iter_twist_search = 5

Total atoms: 84

Mo count: 14

W count: 14





80 degree

twist_min_search = 80

twist_max_search = 80.1

max_strain = 0.01

is_1D_dir_1 = True

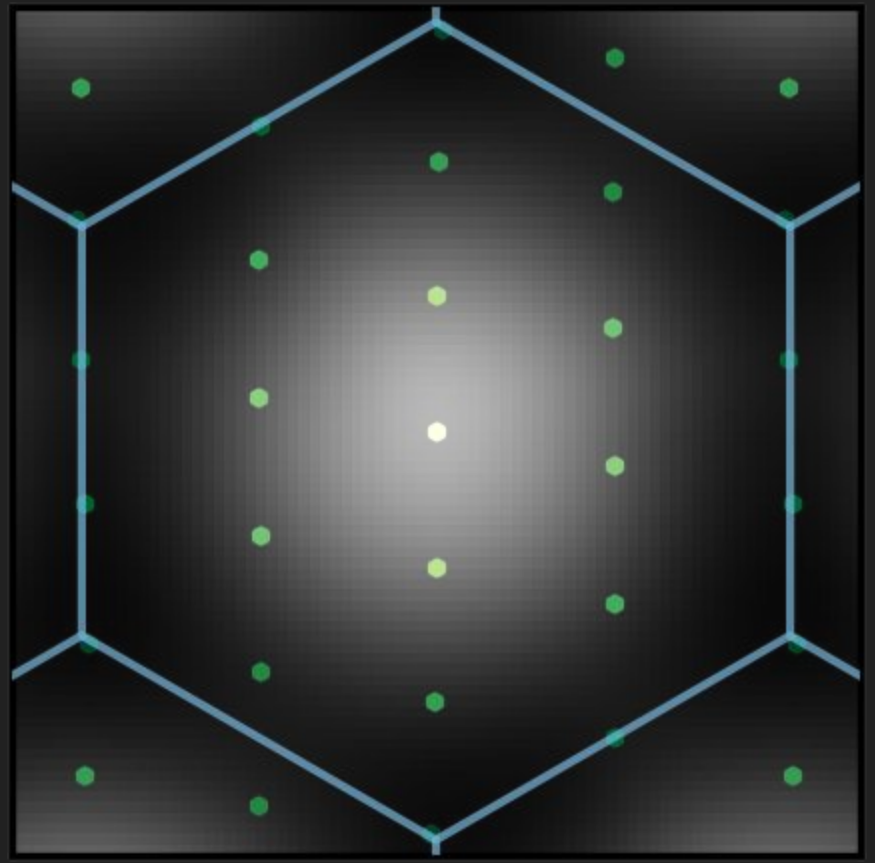
Rmax_max_search = 16

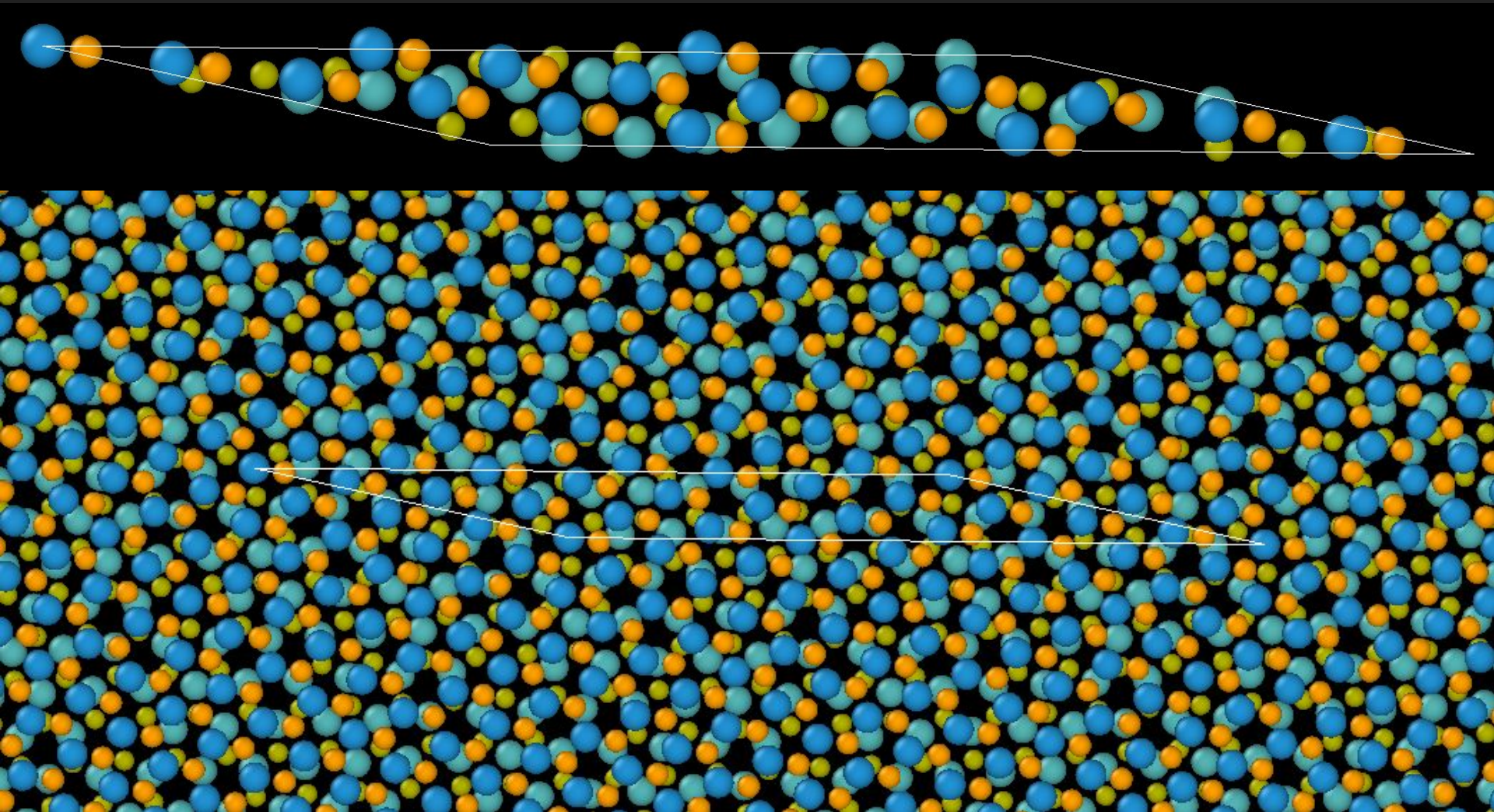
max_iter_twist_search = 5

Total atoms: 117

Mo count: 21

W count: 18





85 degree

twist_min_search = 85

twist_max_search = 85.1

max_strain = 0.02

is_1D_dir_1 = True

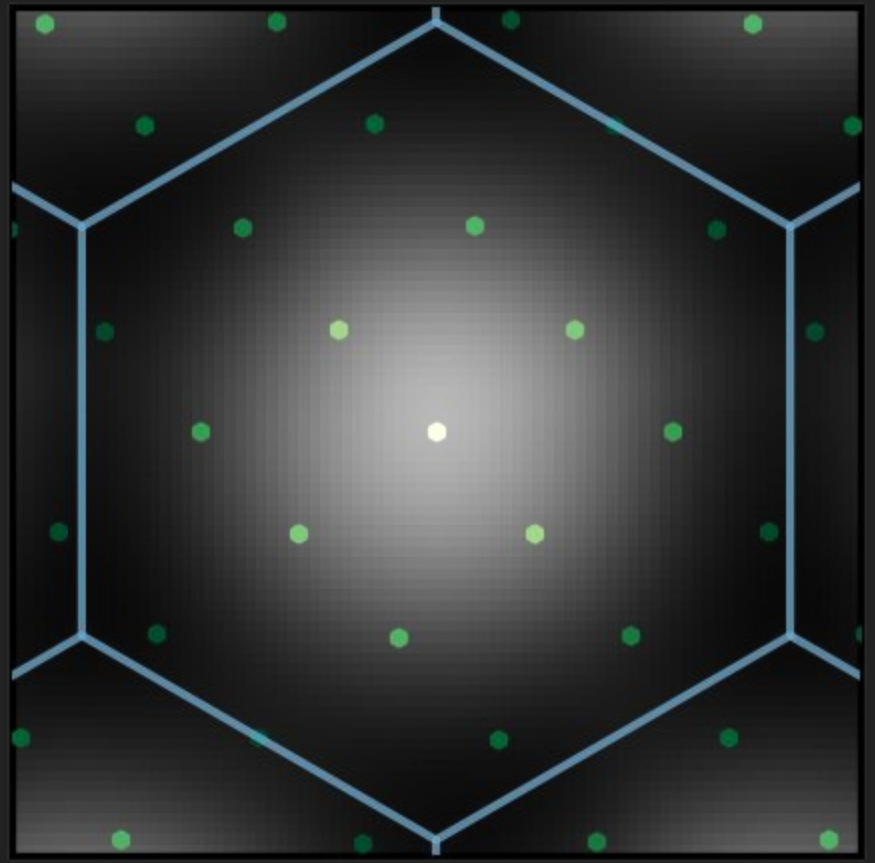
Rmax_max_search = 16

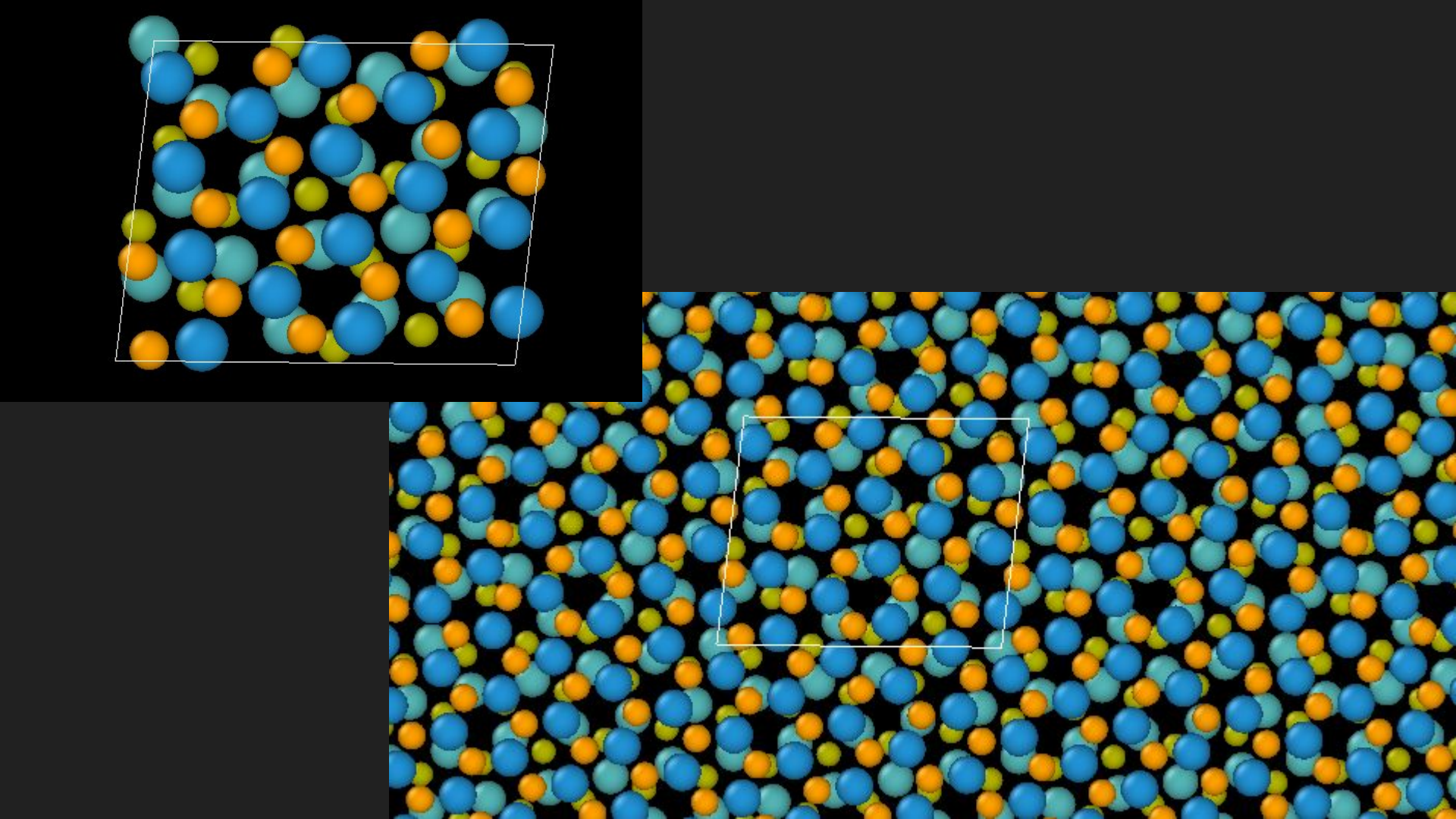
max_iter_twist_search = 5

Total atoms: 111

Mo count: 19

W count: 18





90 degree

twist_min_search = 90

twist_max_search = 90.1

max_strain = 0.02

is_1D_dir_1 = True

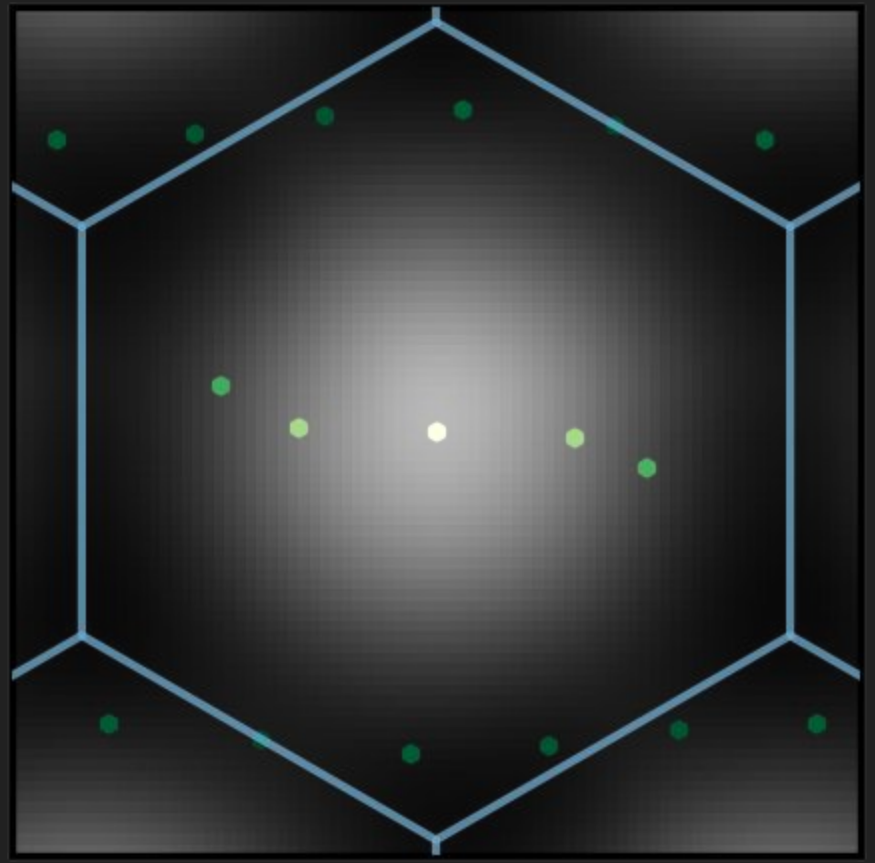
Rmax_max_search = 16

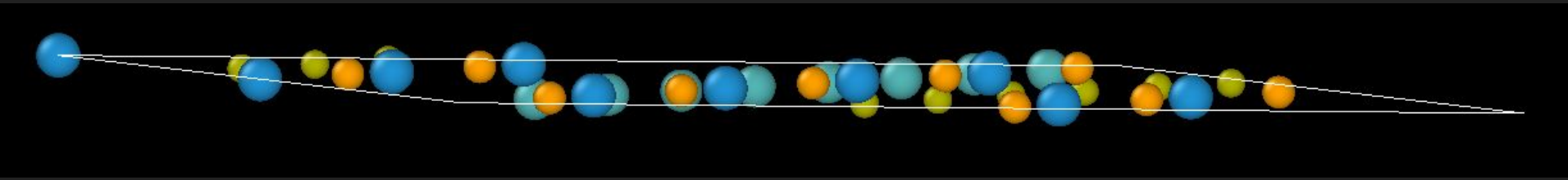
max_iter_twist_search = 5

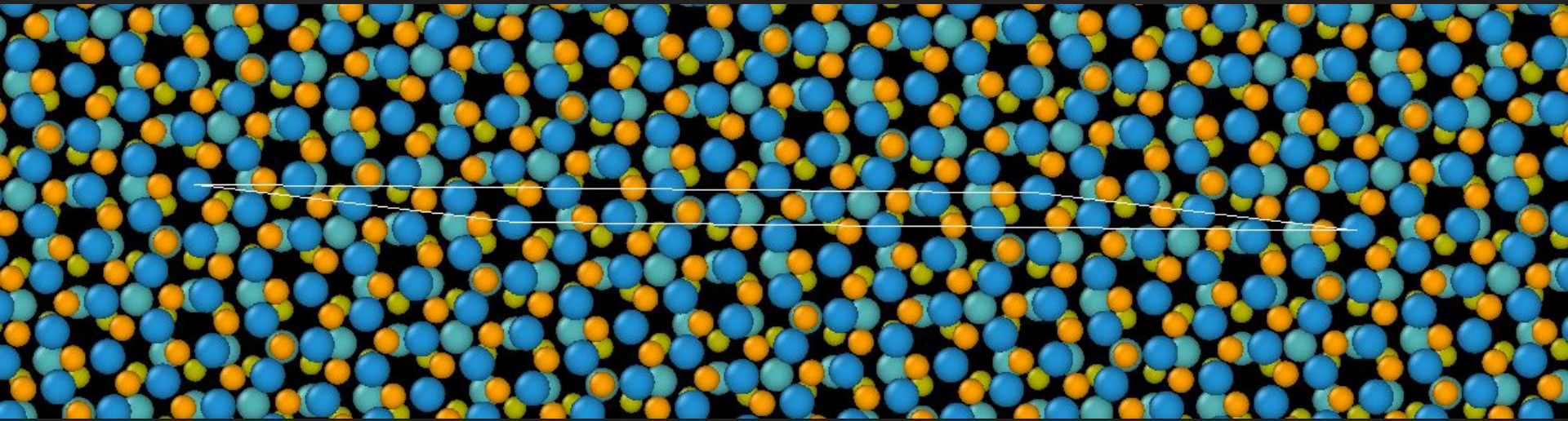
Total atoms: 57

Mo count: 9

W count: 10







95 degree

twist_min_search = 95

twist_max_search = 95.1

max_strain = 0.02

is_1D_dir_1 = True

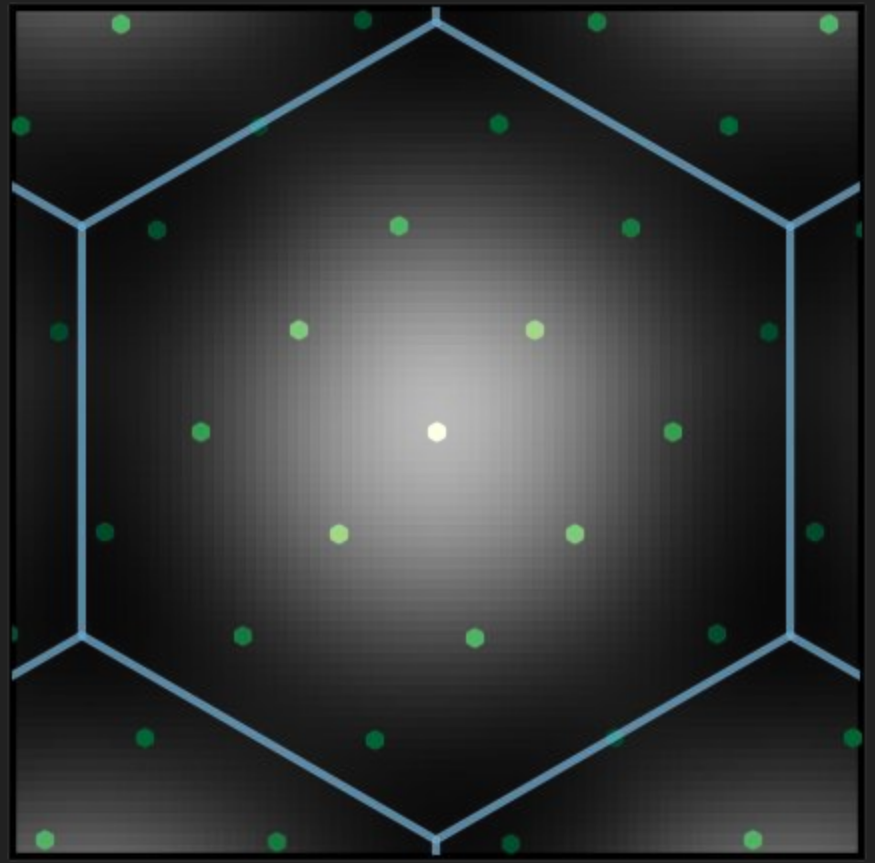
Rmax_max_search = 16

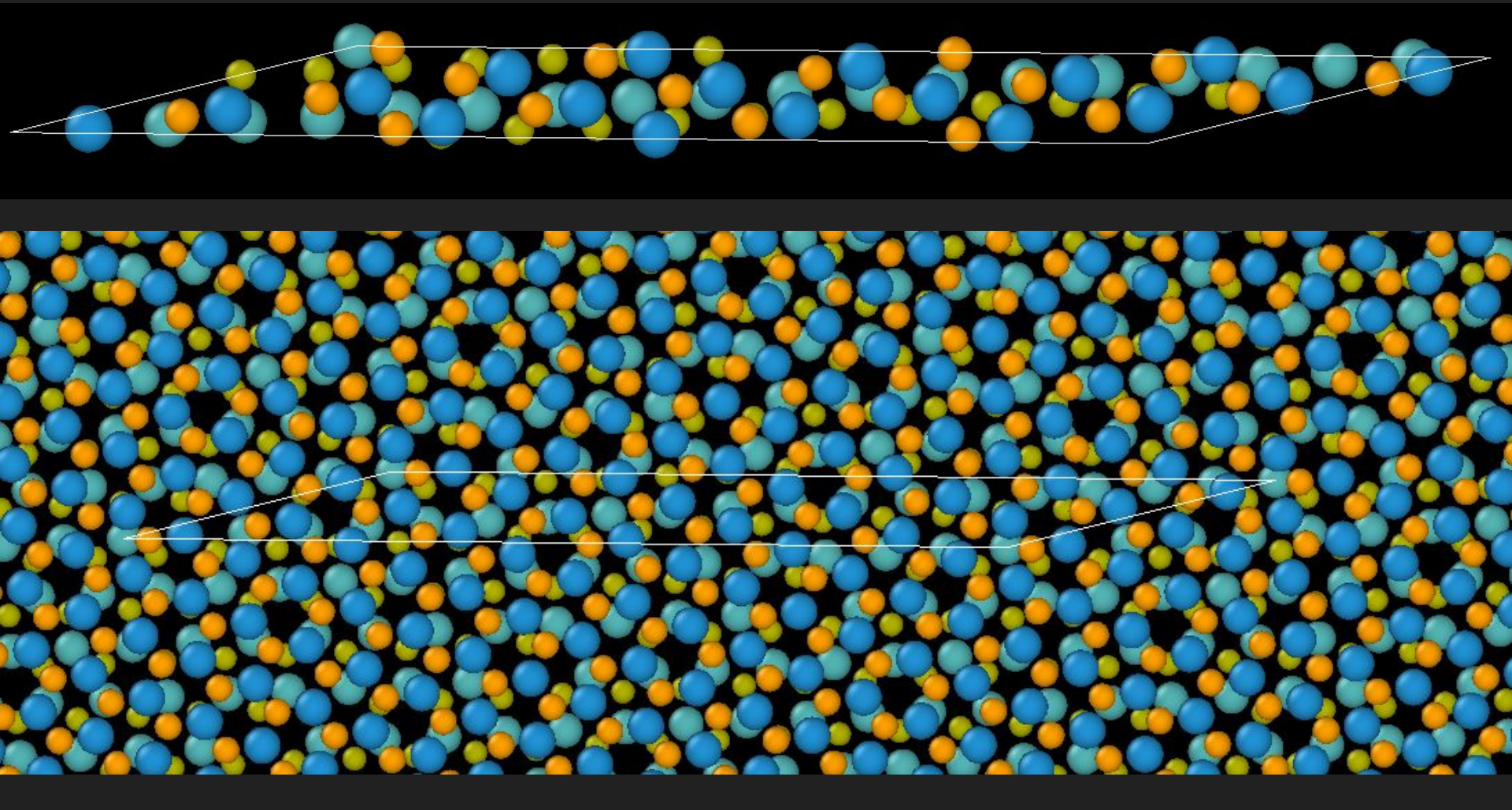
max_iter_twist_search = 5

Total atoms: 111

Mo count: 19

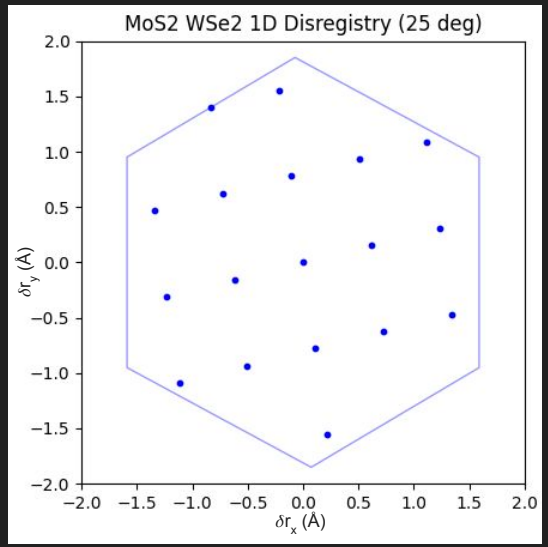
W count: 18

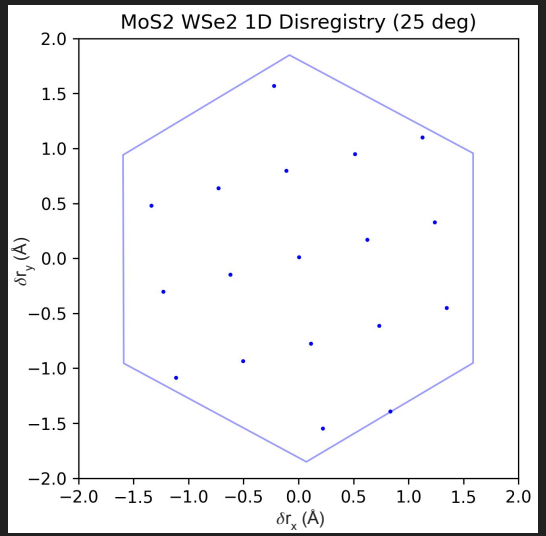




Pitfalls Cont.

Minimal positional changes observed in reconstruction of Q1D structure at 25-degree twist, but voronoi cell alignment seems to be offset by 180 degrees

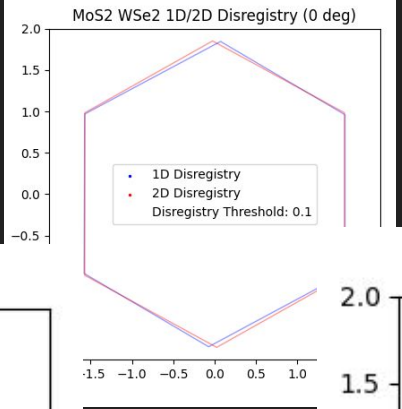


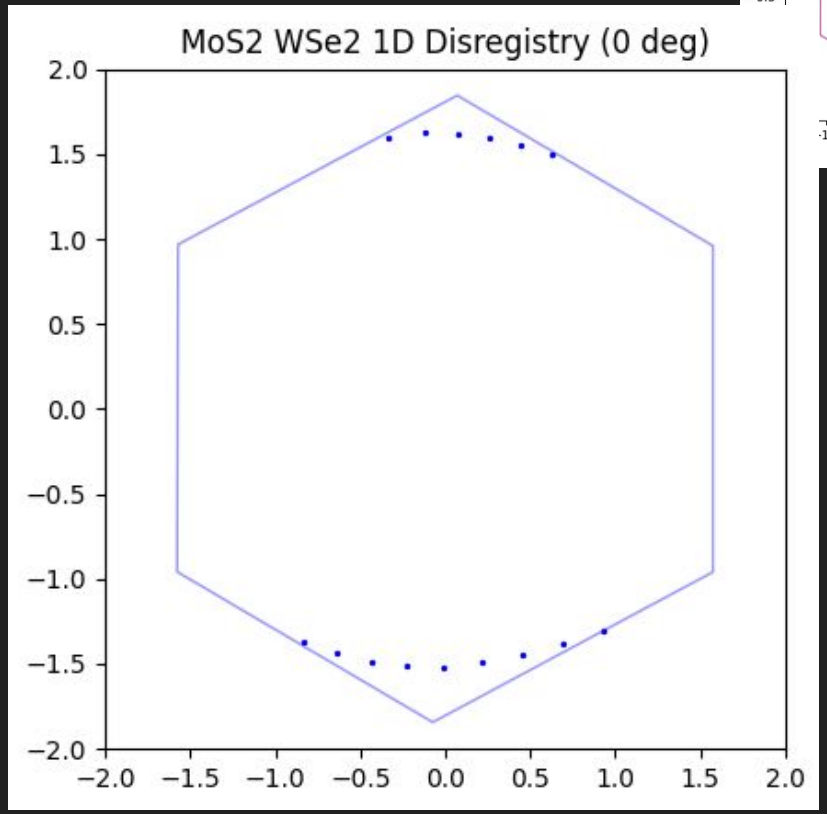


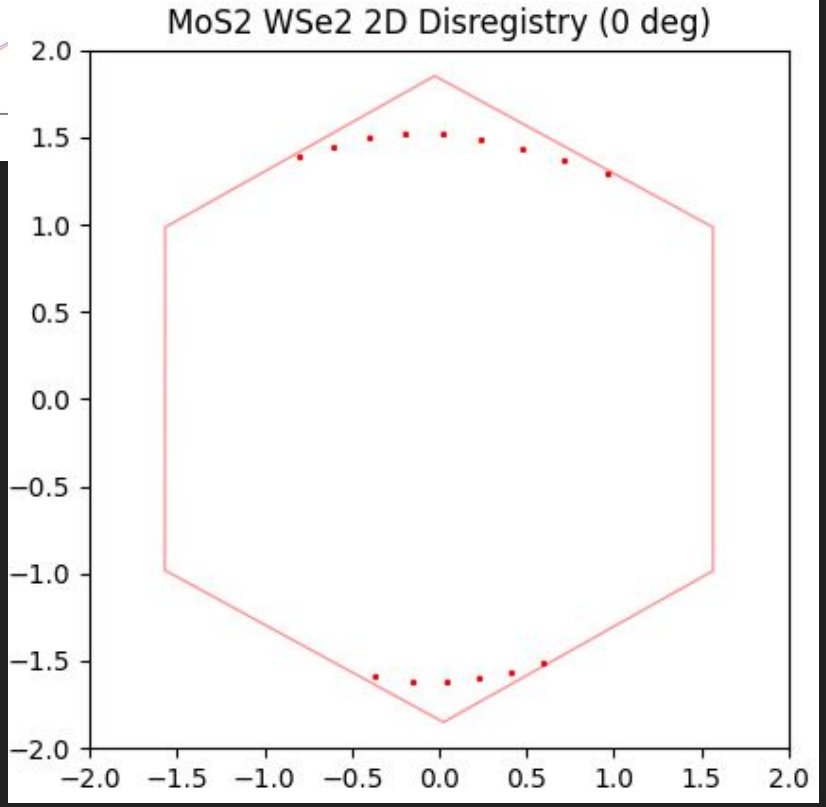
25 degree twist angle for Q1D Pre Relaxation vs. Post Relaxation

Post Relaxation

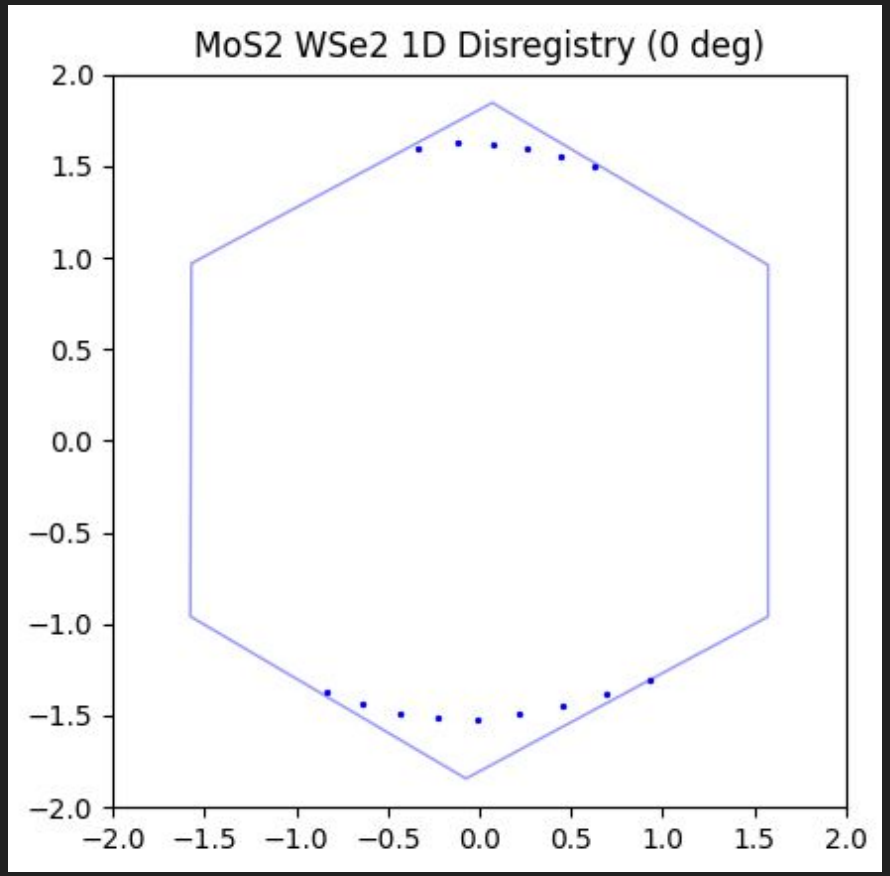
0 Degrees

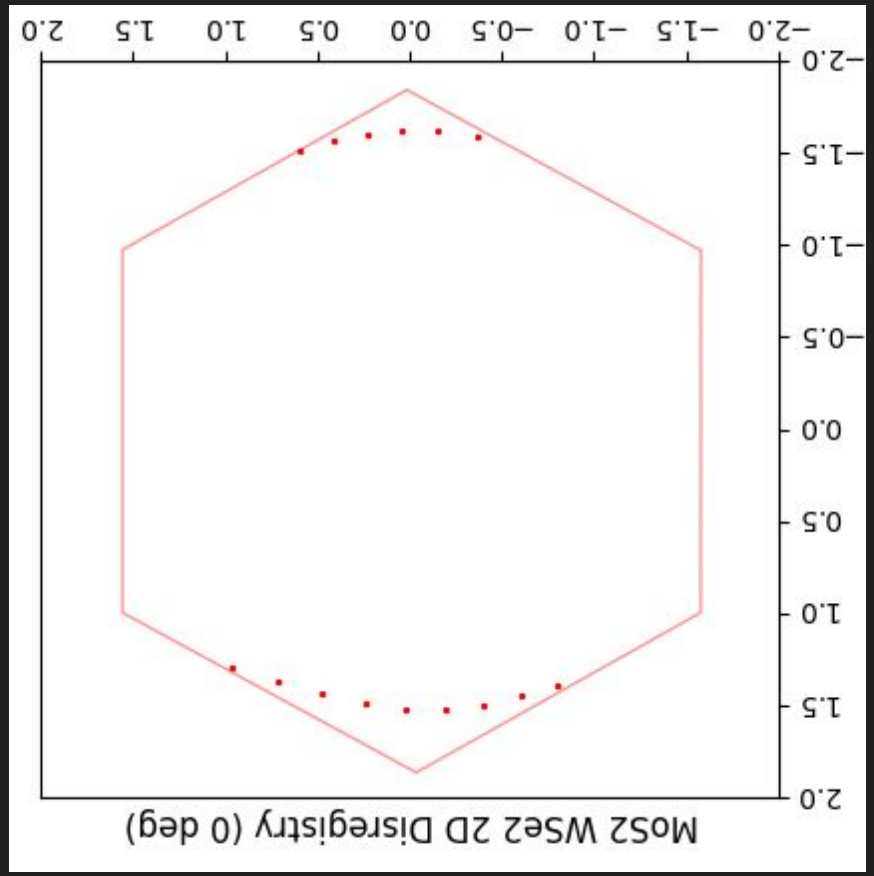

MoS2 WSe2 1D/2D Disregistry (0 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1


MoS2 WSe2 1D Disregistry (0 deg)

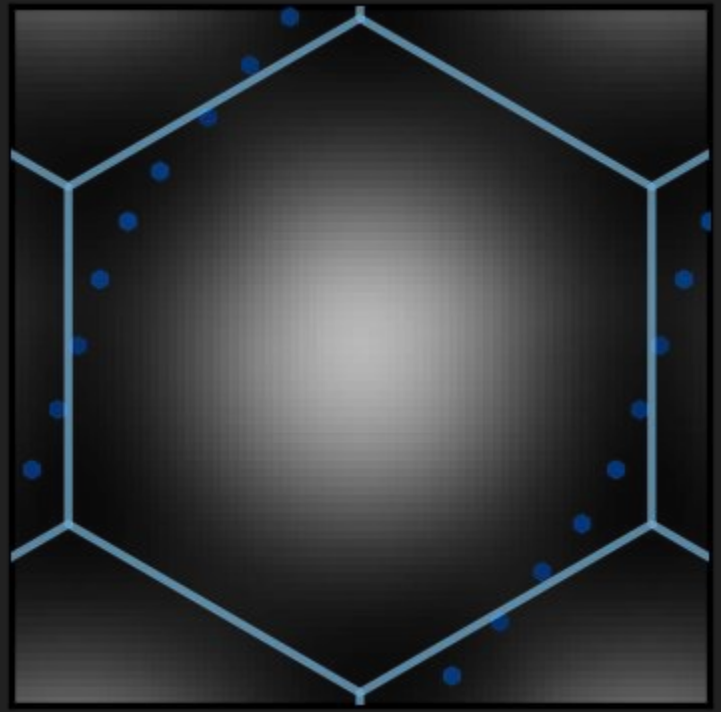

MoS2 WSe2 2D Disregistry (0 deg)

0 deg

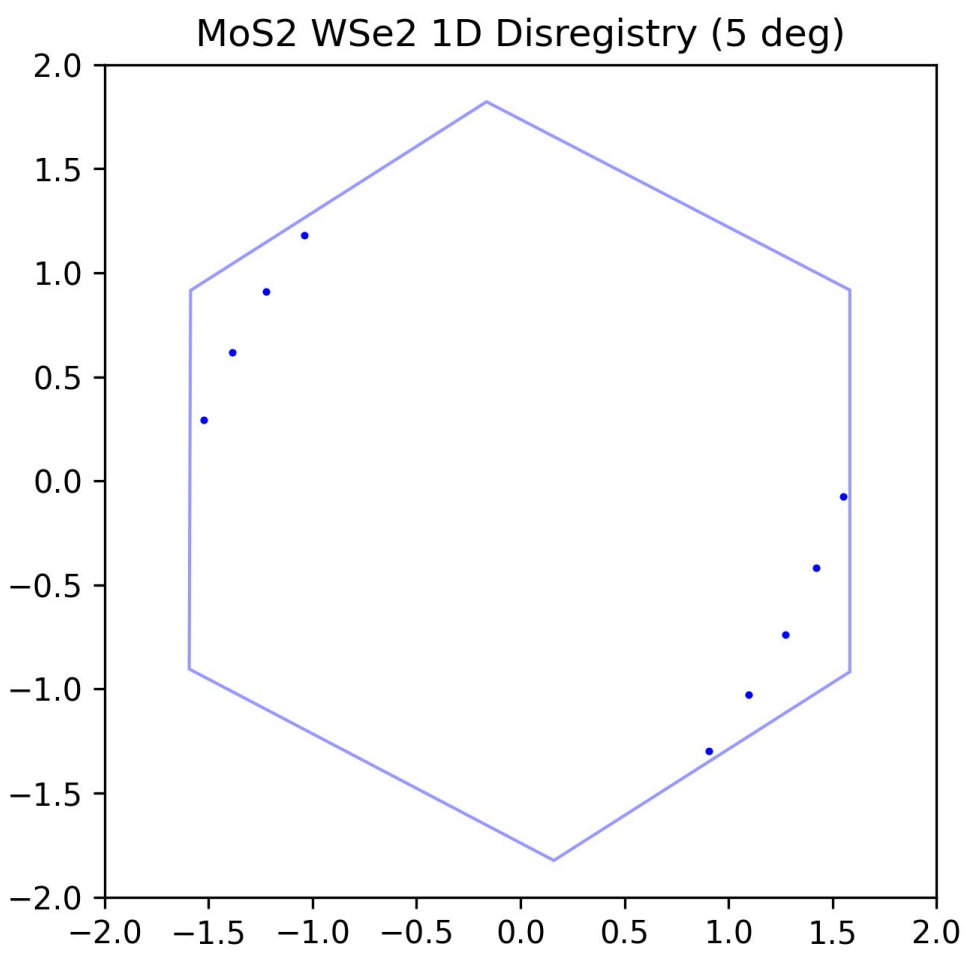

MoS2 WSe2 1D Disregistry (0 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

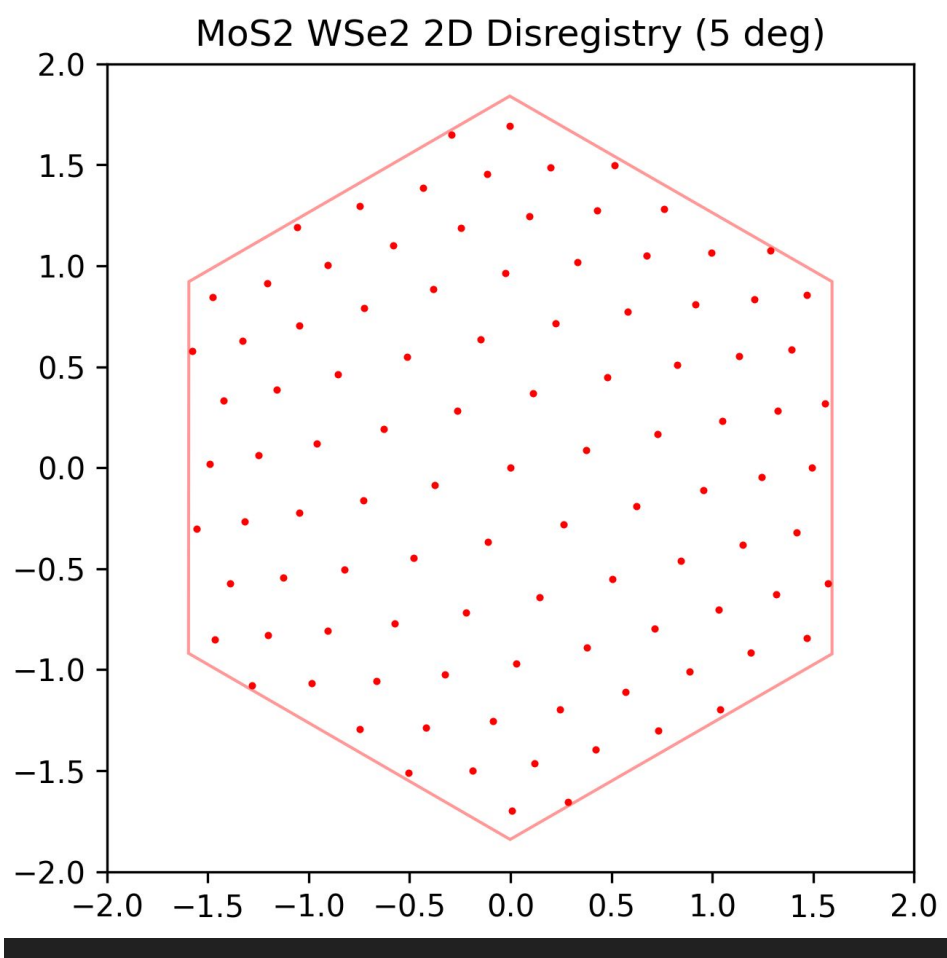

MoS2 WSe2 2D Disregistry (0 deg)

5 Degrees

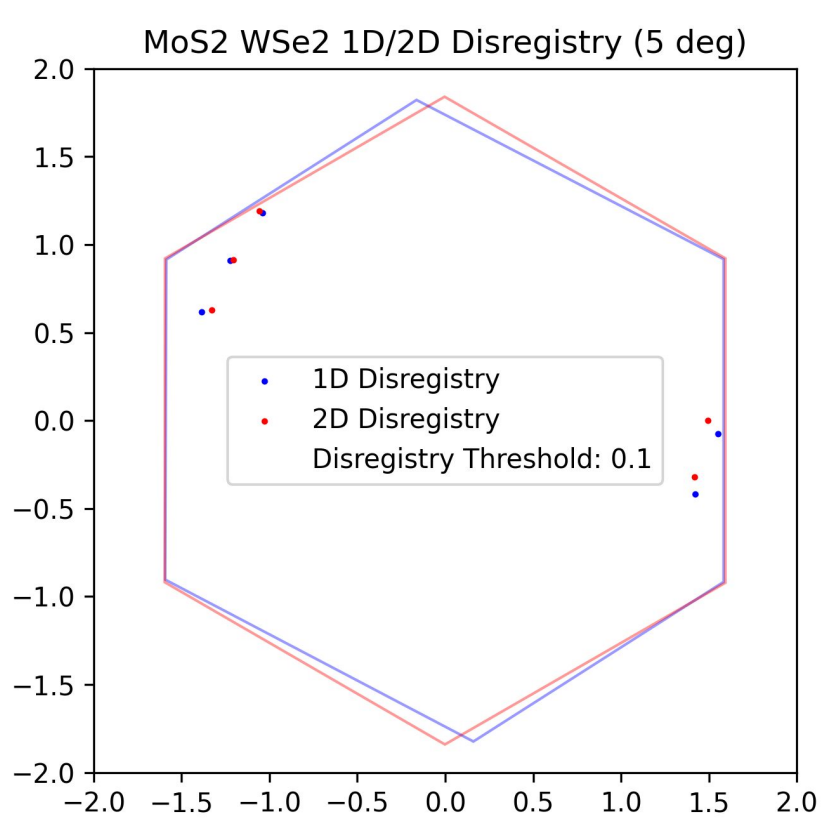


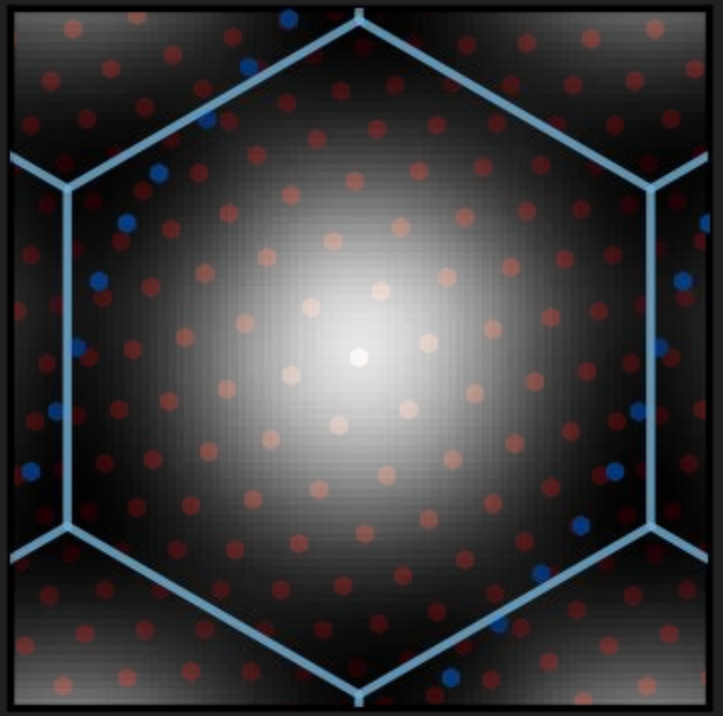
Actual Twist Angle: 4.97900323968
Total Atoms: 642
W Atoms (Top Layer): 103
Mo Atoms (Bottom Layer): 111


MoS2 WSe2 1D Disregistry (5 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

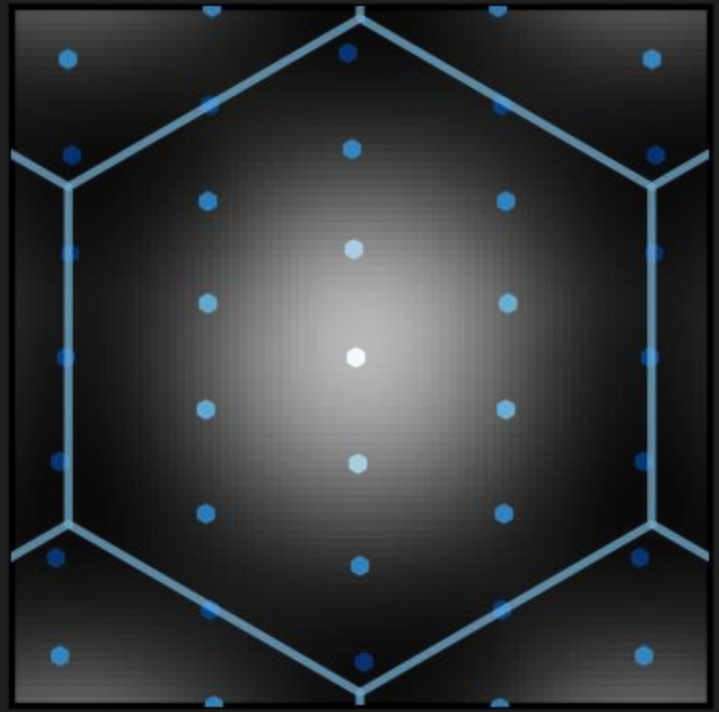

MoS2 WSe2 2D Disregistry (5 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

5 deg

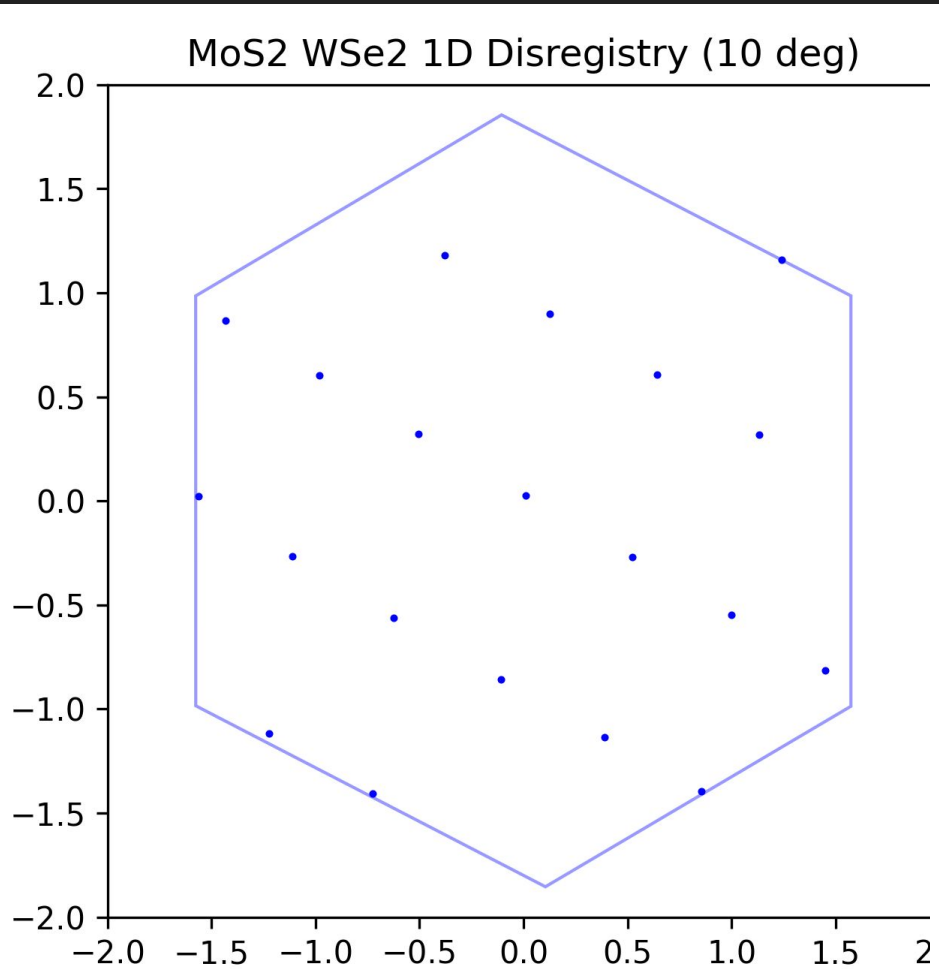

MoS2 WSe2 1D/2D Disregistry (5 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

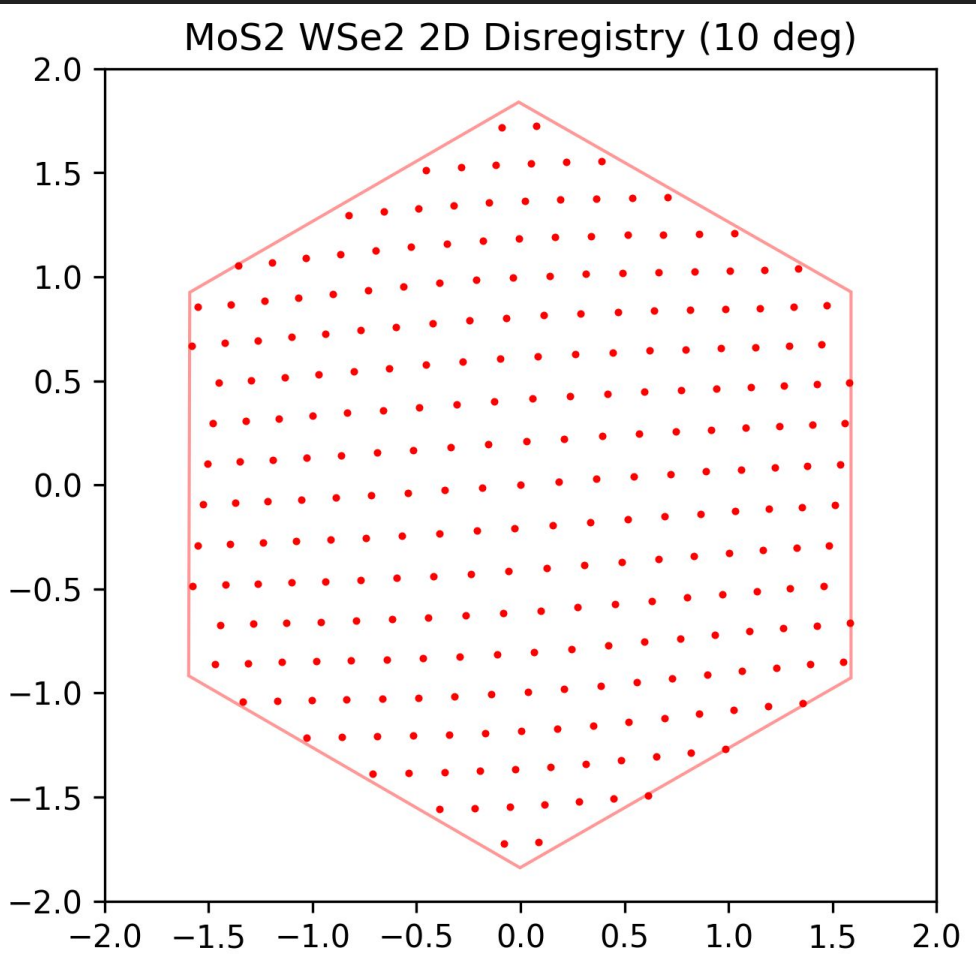


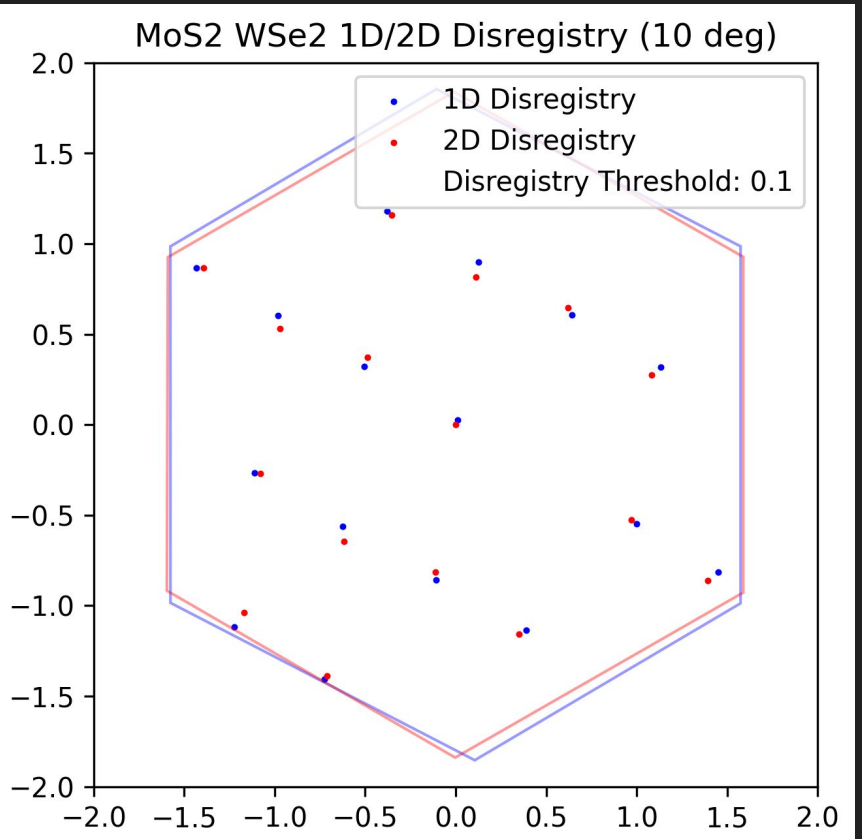
10 deg

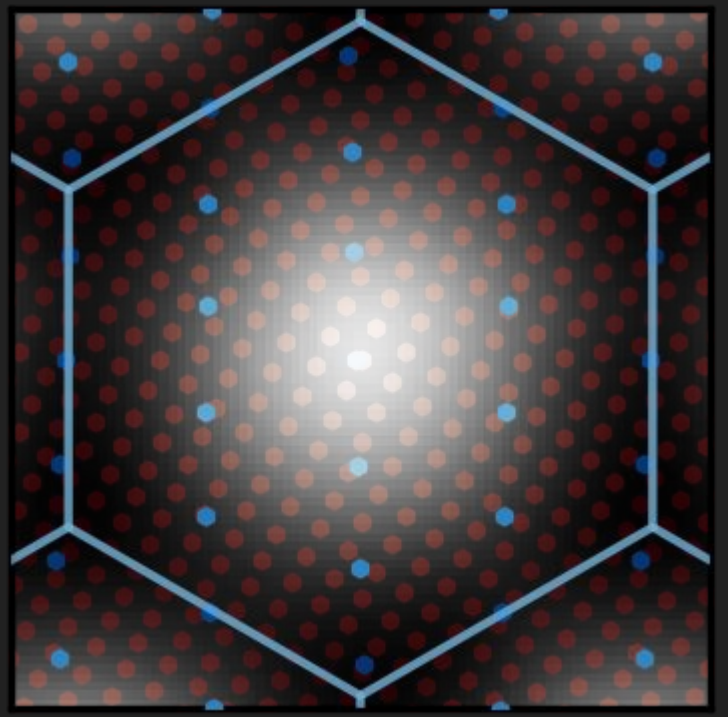


Actual Twist Angle: 9.998113525 03
Total Atoms: 1707
W Atoms (Top Layer): 273
Mo Atoms (Bottom Layer): 296

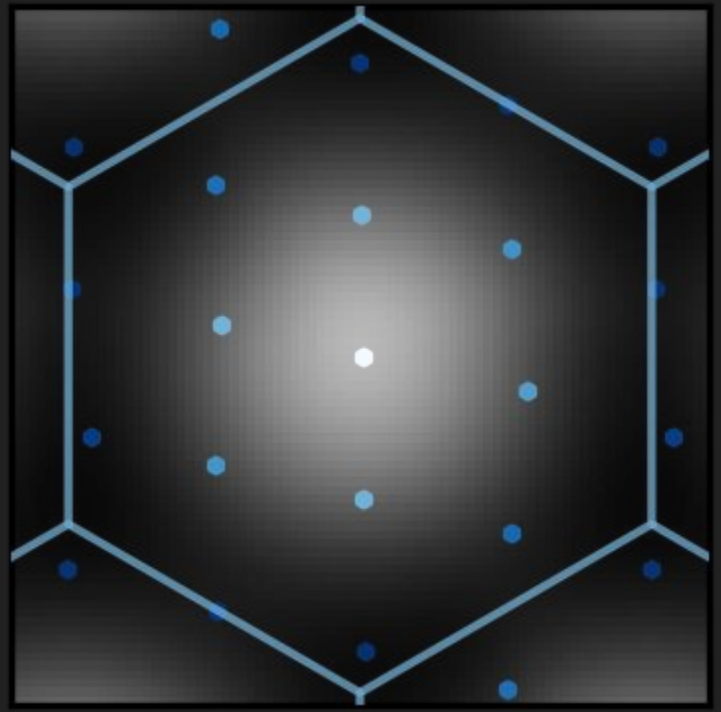

MoS2 WSe2 1D Disregistry (10 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2


MoS2 WSe2 2D Disregistry (10 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

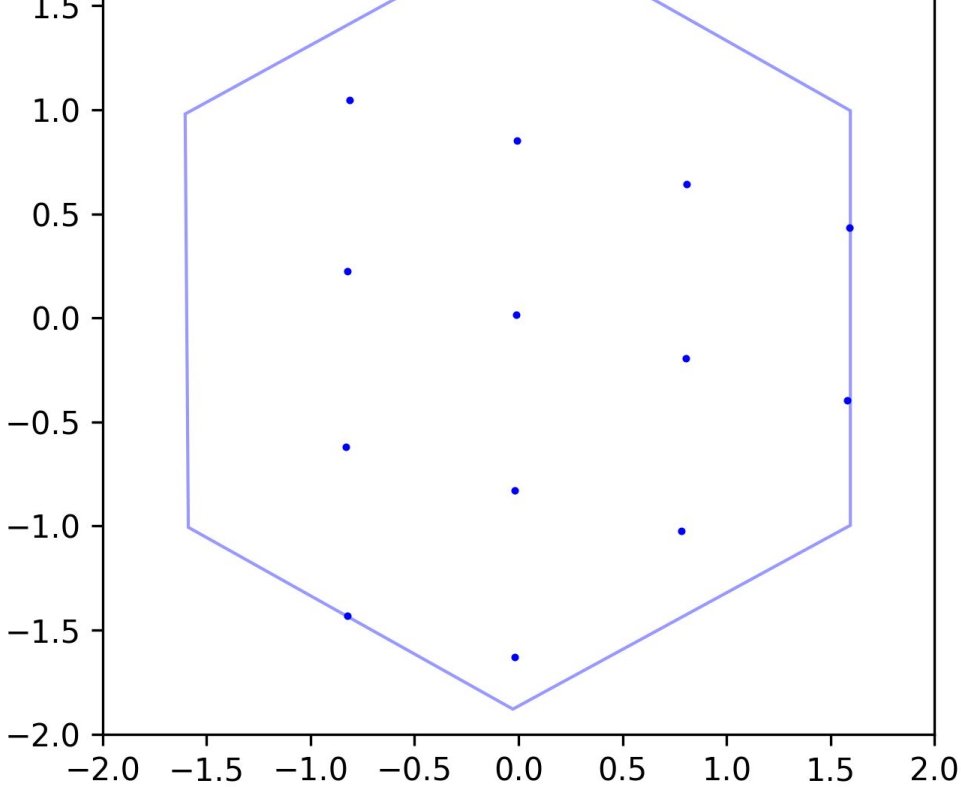

MoS2 WSe2 1D/2D Disregistry (10 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0



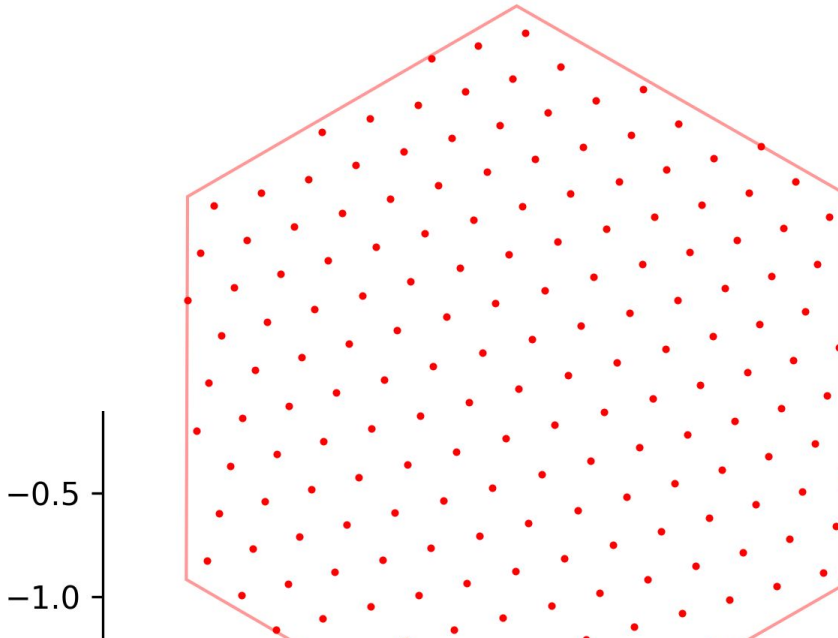
15 deg

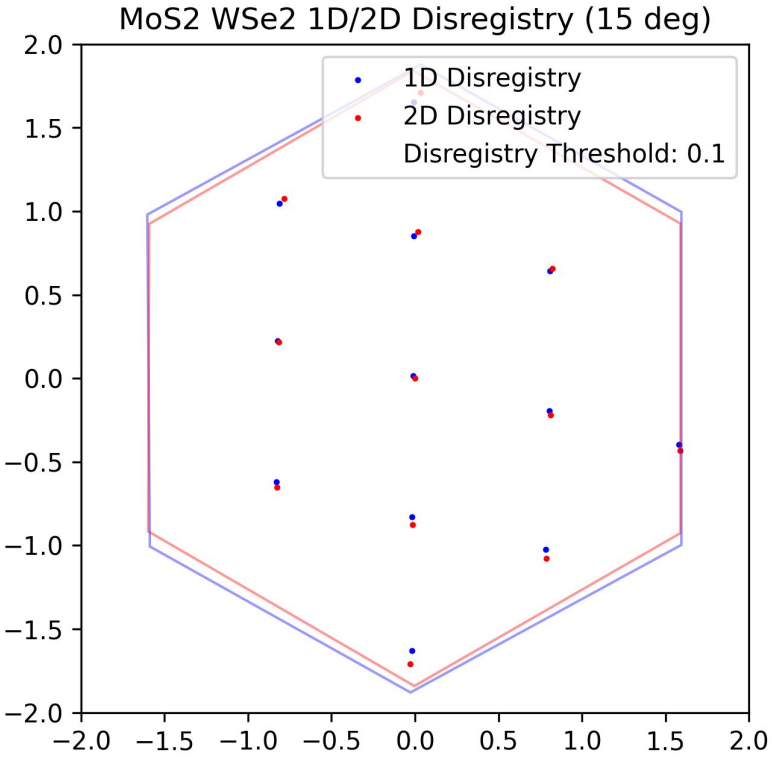


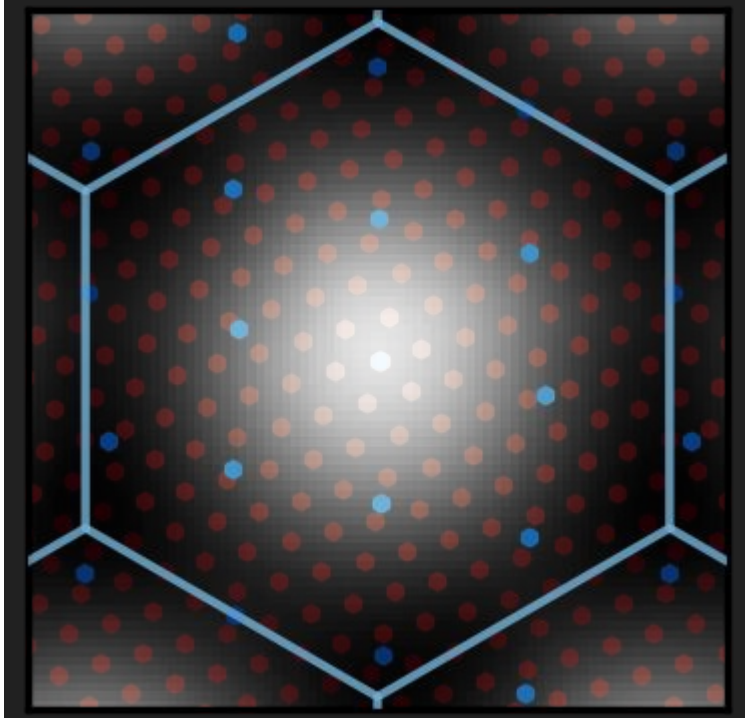
Actual Twist Angle: 15.0172238103
Total Atoms: 1131
W Atoms (Top Layer): 181
Mo Atoms (Bottom Layer): 196



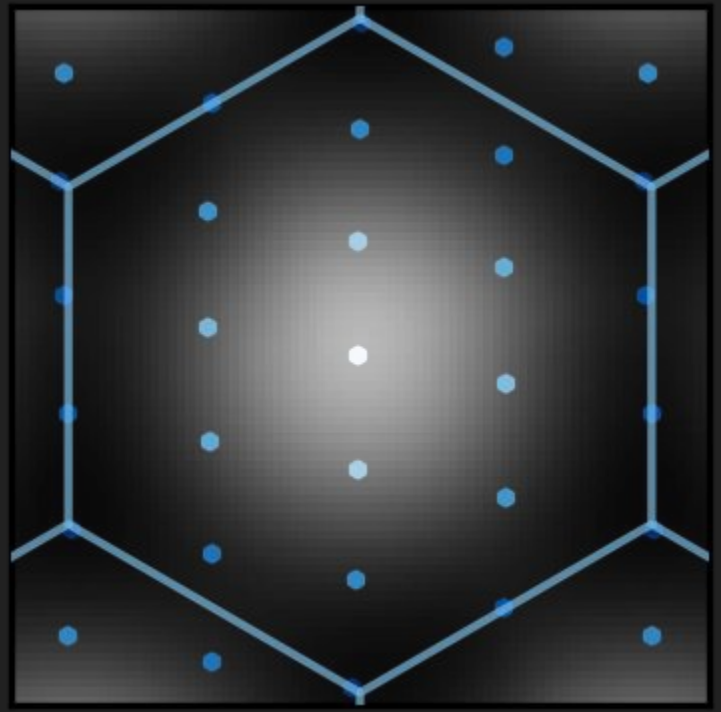
MoS2 WSe2 2D Disregistry (15 deg

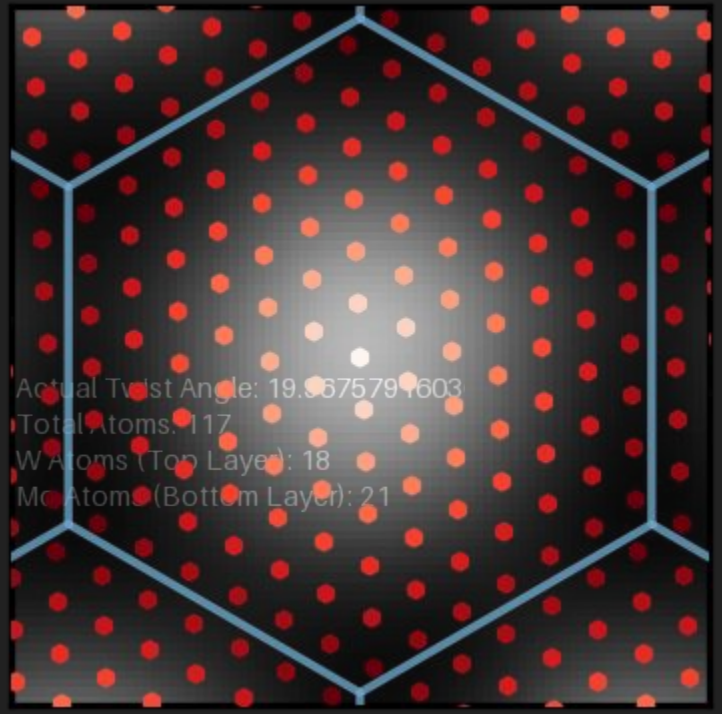



MoS2 WSe2 1D/2D Disregistry (15 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

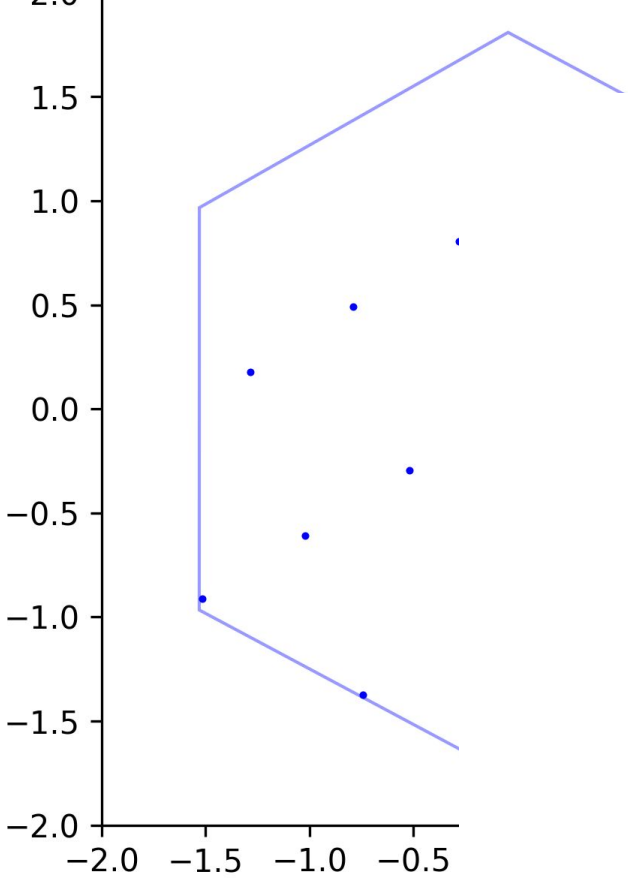


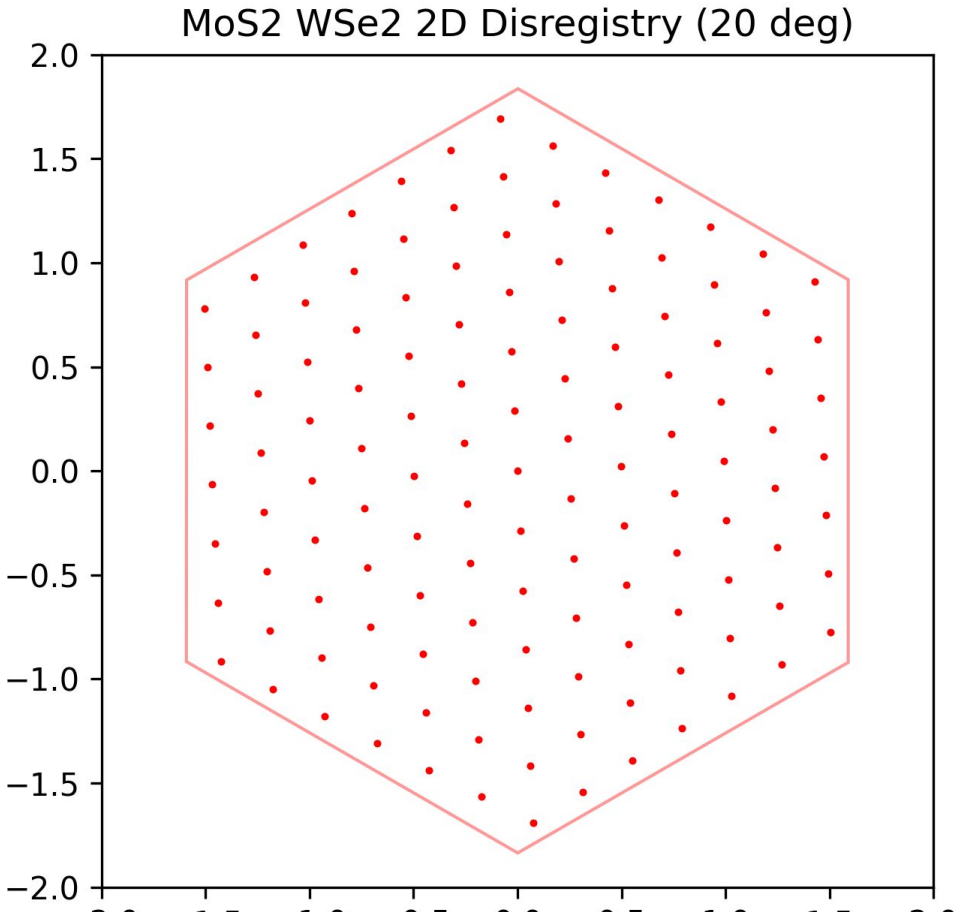
20 deg

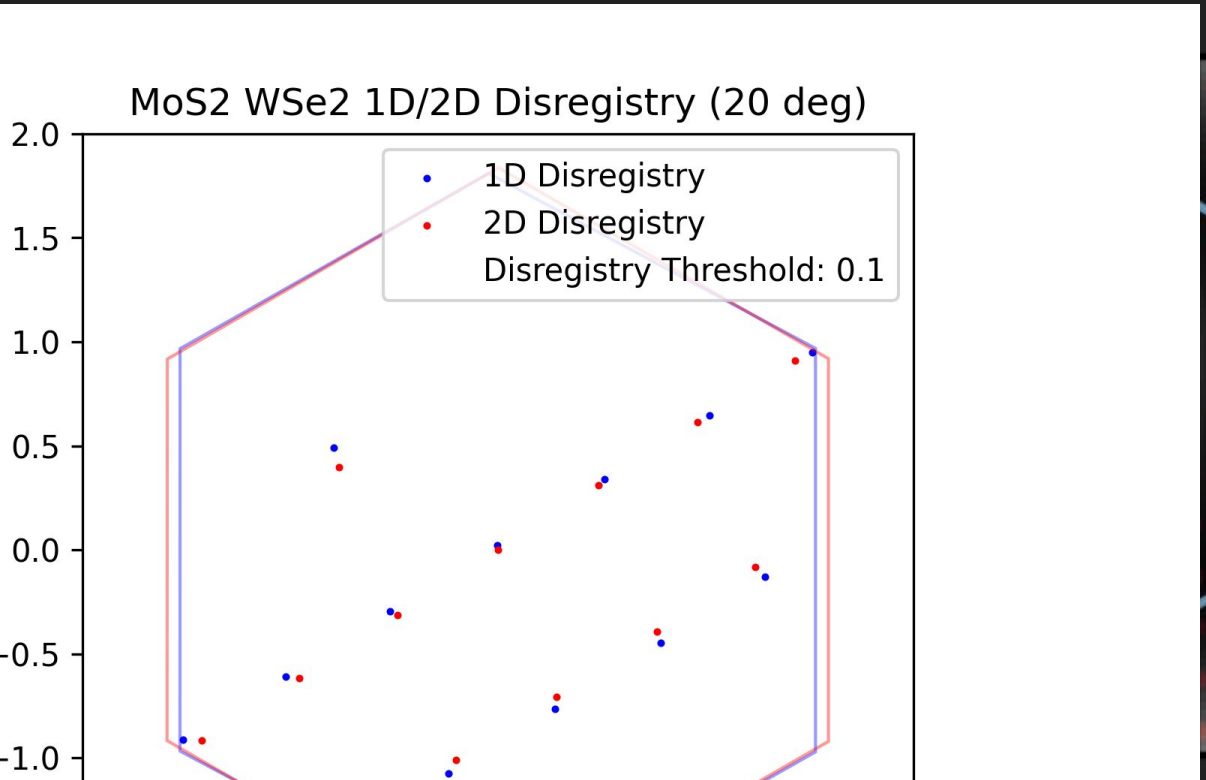


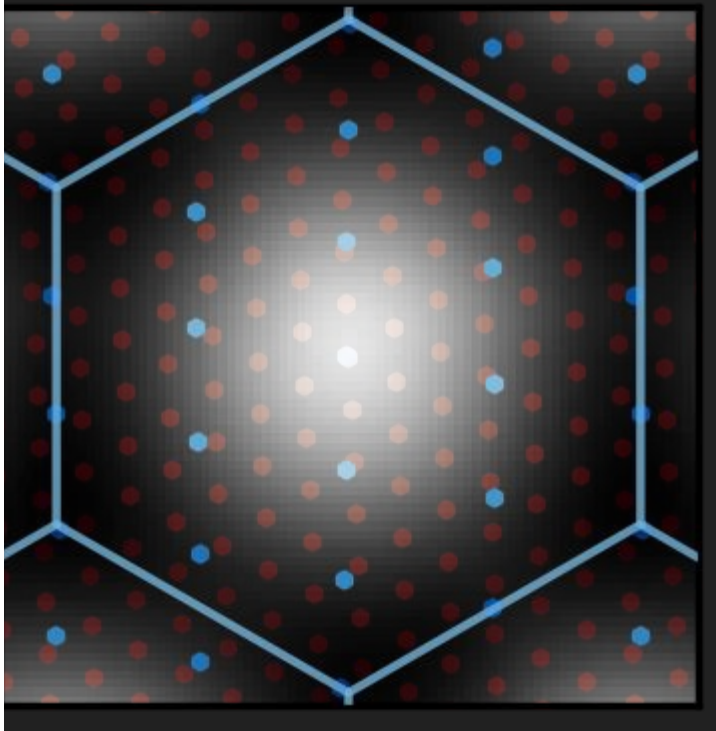


Actual Twist Angle: 19.9790383162
Total Atoms: 798
W Atoms (Top Layer): 127
Mo Atoms (Bottom Layer): 139

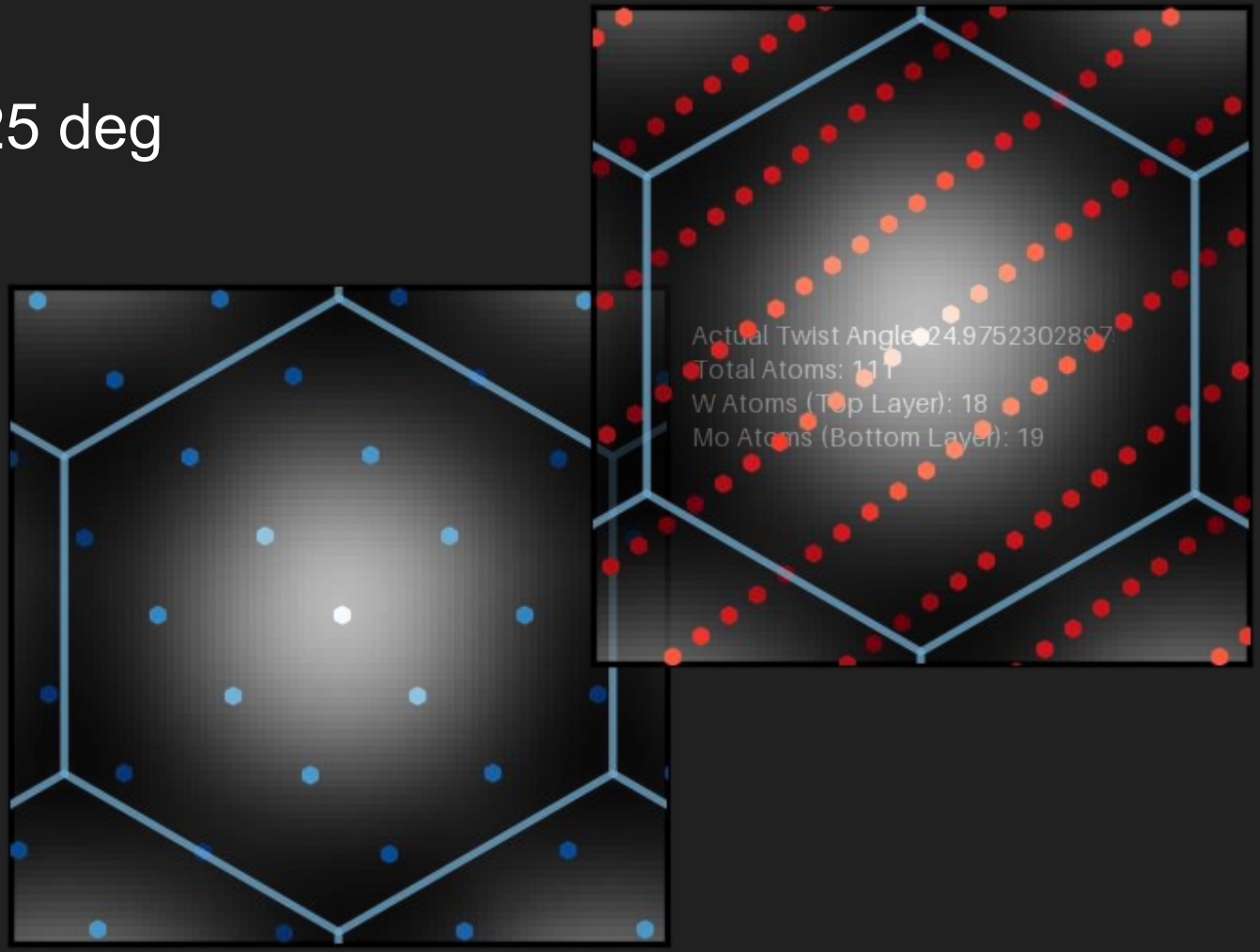

2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5

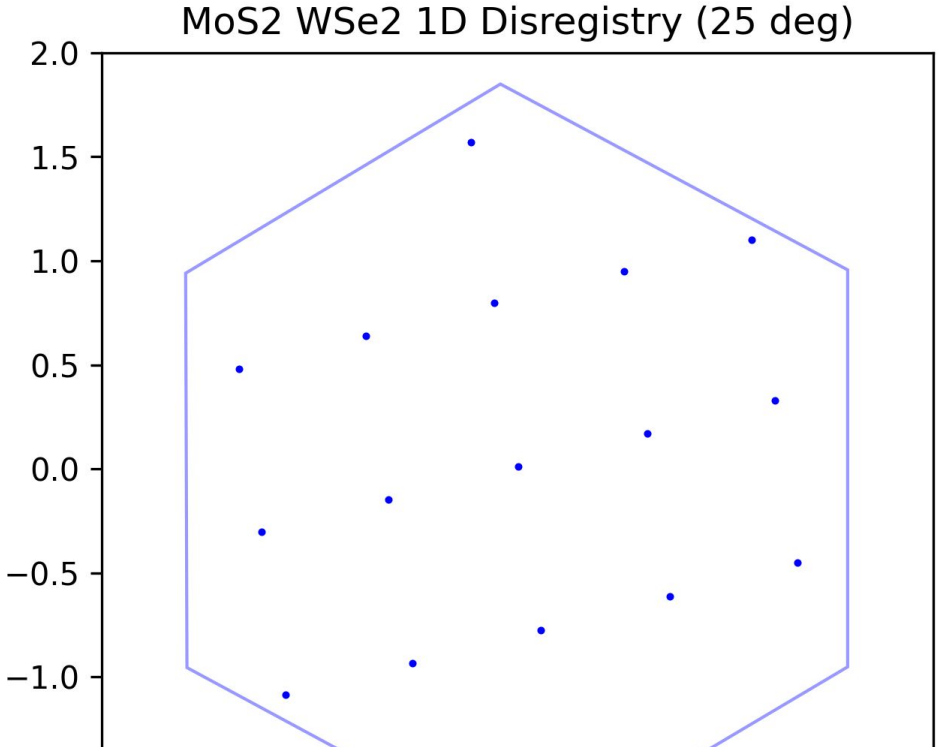

MoS2 WSe2 2D Disregistry (20 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

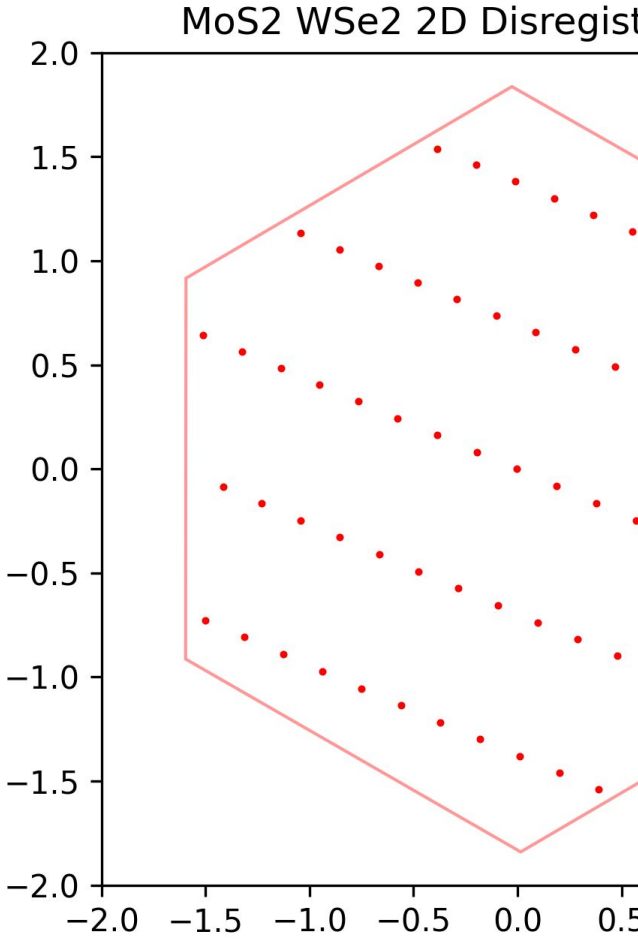

MoS2 WSe2 1D/2D Disregistry (20 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

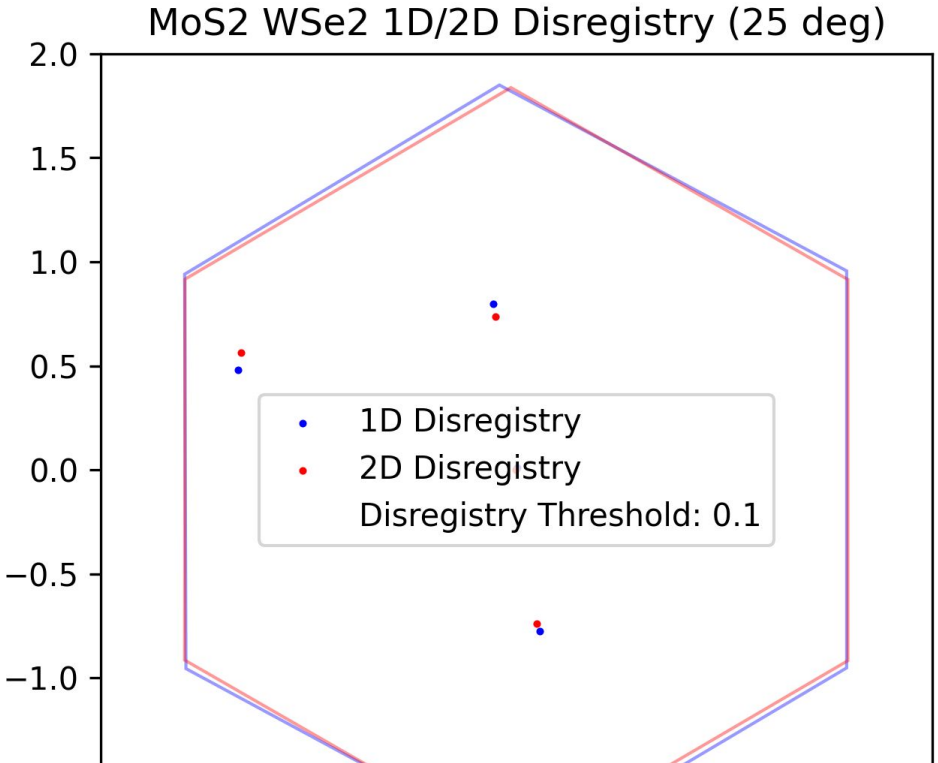


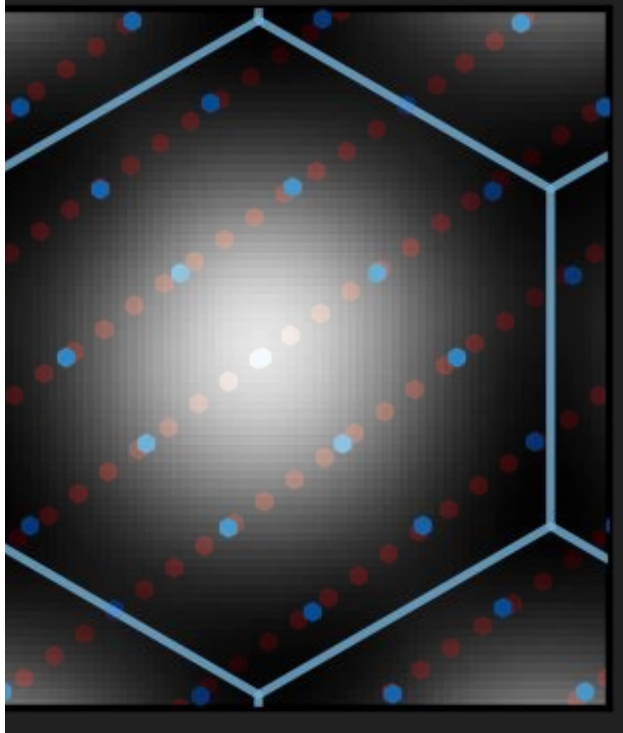
25 deg


Actual Twist Angle: 24.9752302897
Total Atoms: 111
W Atoms (Top Layer): 18
Mo Atoms (Bottom Layer): 19
Actual Twist Angle: 24.9866894456
Total Atoms: 426
W Atoms (Top Layer): 68
Mo Atoms (Bottom Layer): 74

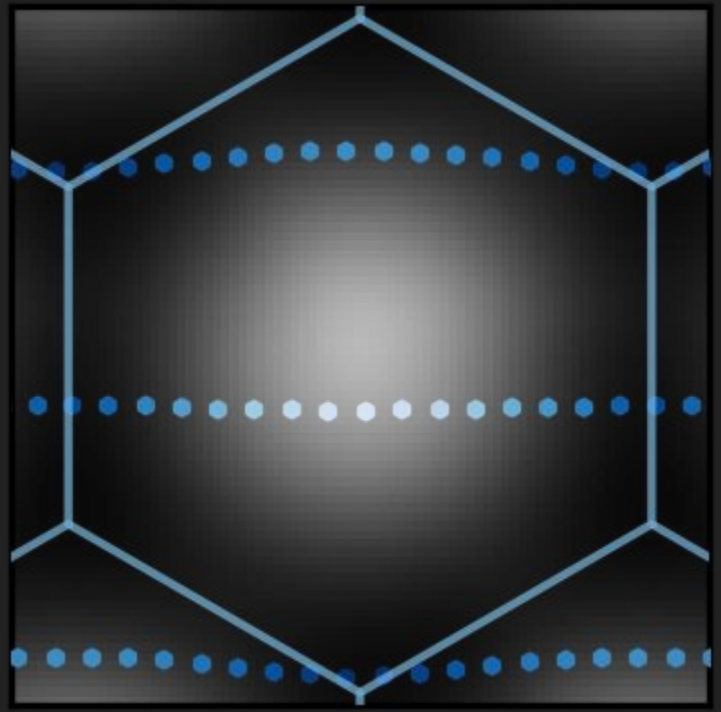

MoS2 WSe2 1D Disregistry (25 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

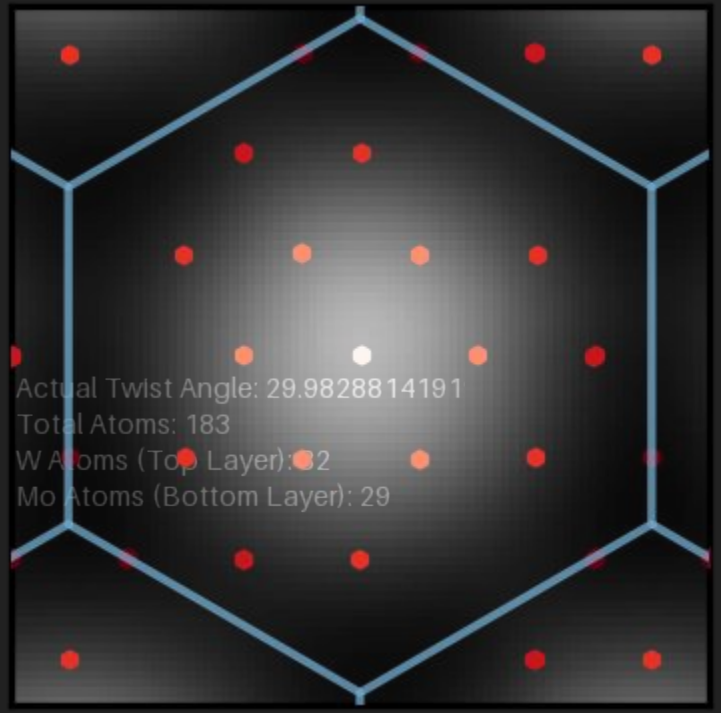

MoS2 WSe2 2D Disregist
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5


MoS2 WSe2 1D/2D Disregistry (25 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

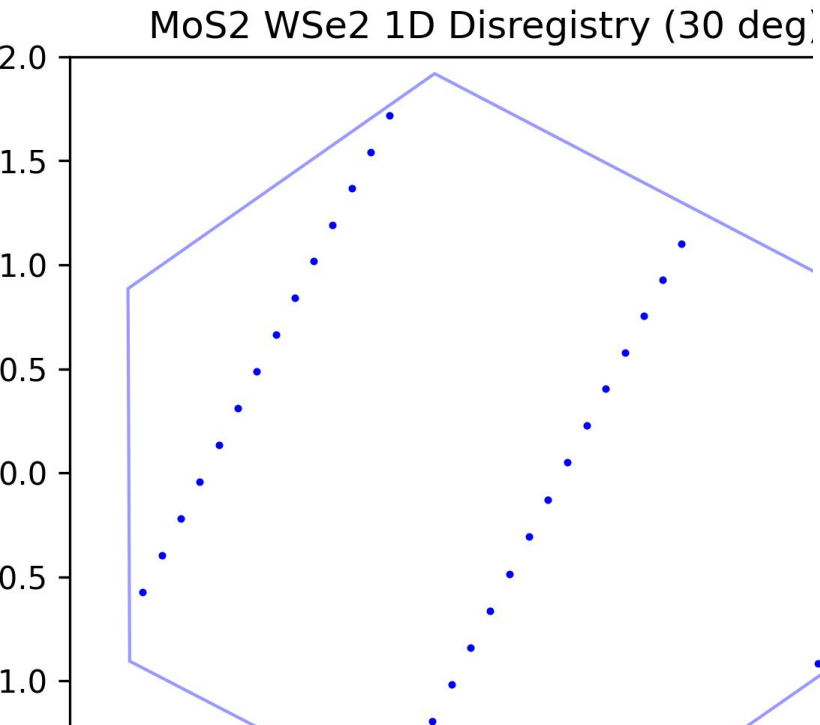


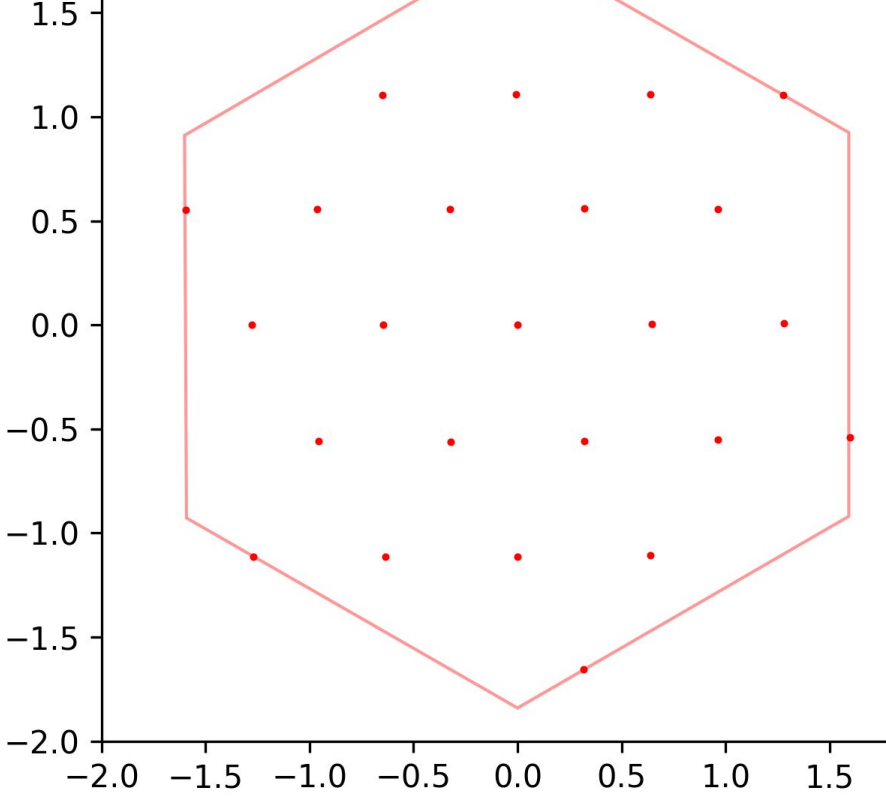
30 deg

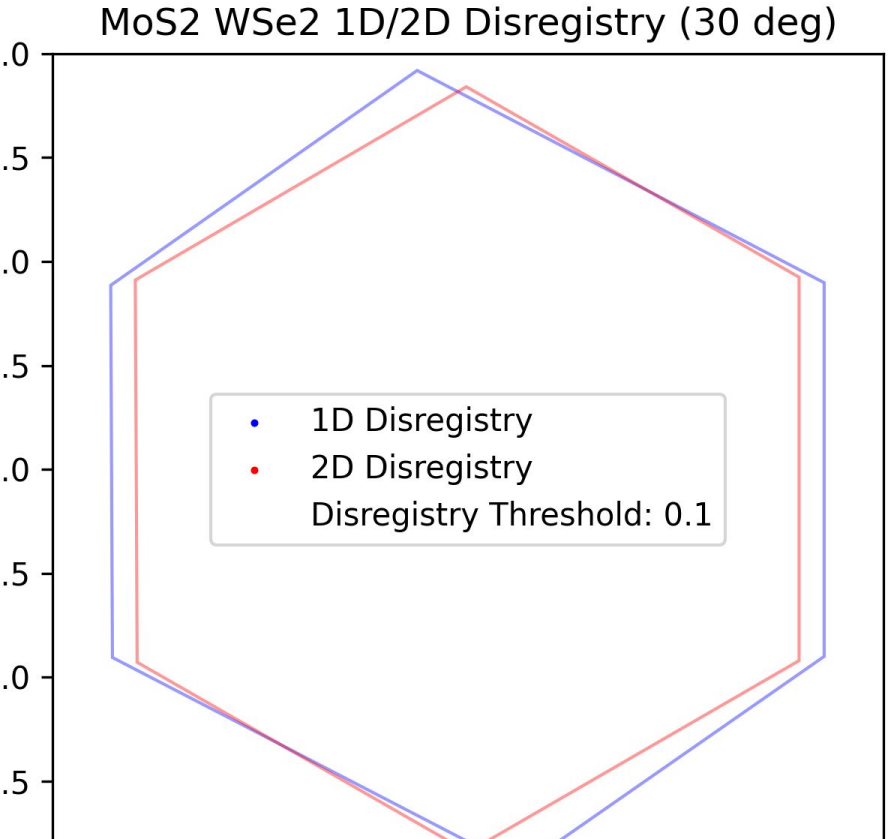


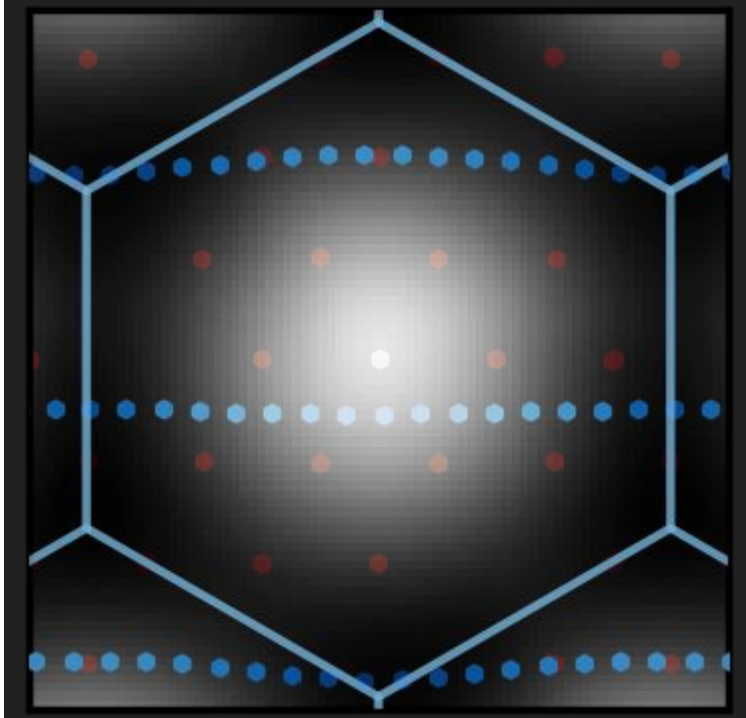


Actual Twist Angle: 30.0172588869
Total Atoms: 156
W Atoms (Top Layer): 25
Mo Atoms (Bottom Layer): 27

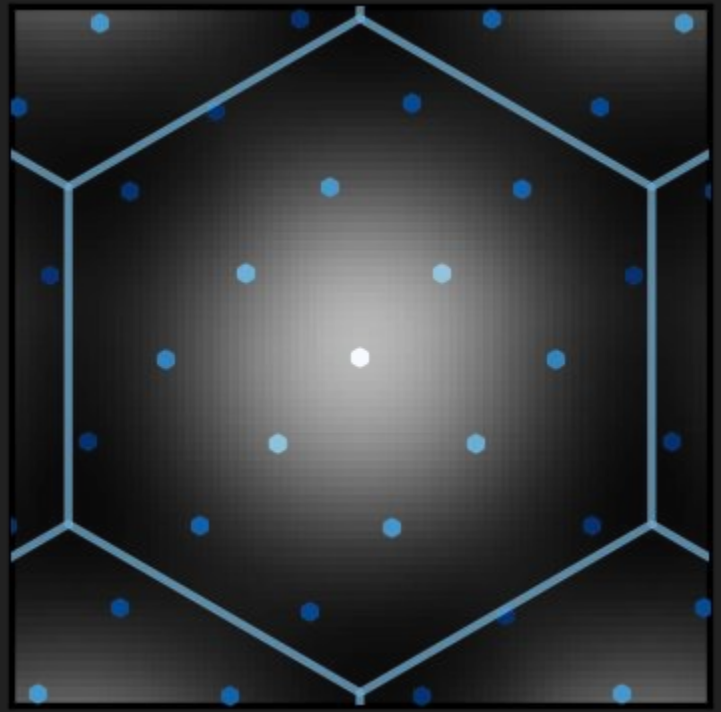

MoS2 WSe2 1D Disregistry (30 deg)
2.0
1.5
1.0
0.5
0.0
0.5
1.0


1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

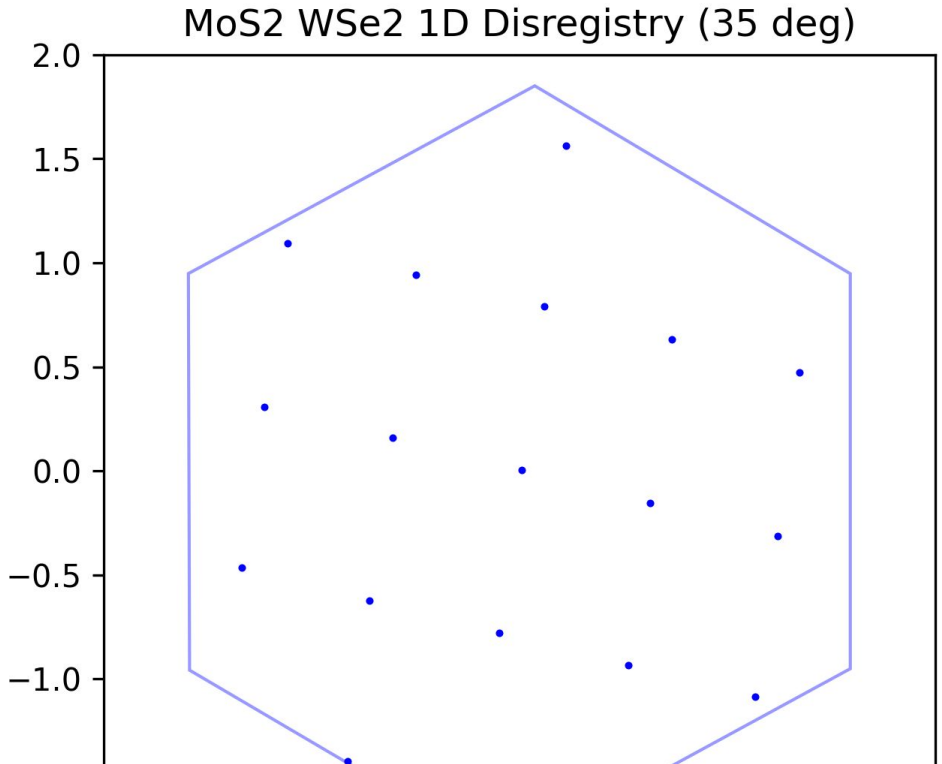

MoS2 WSe2 1D/2D Disregistry (30 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

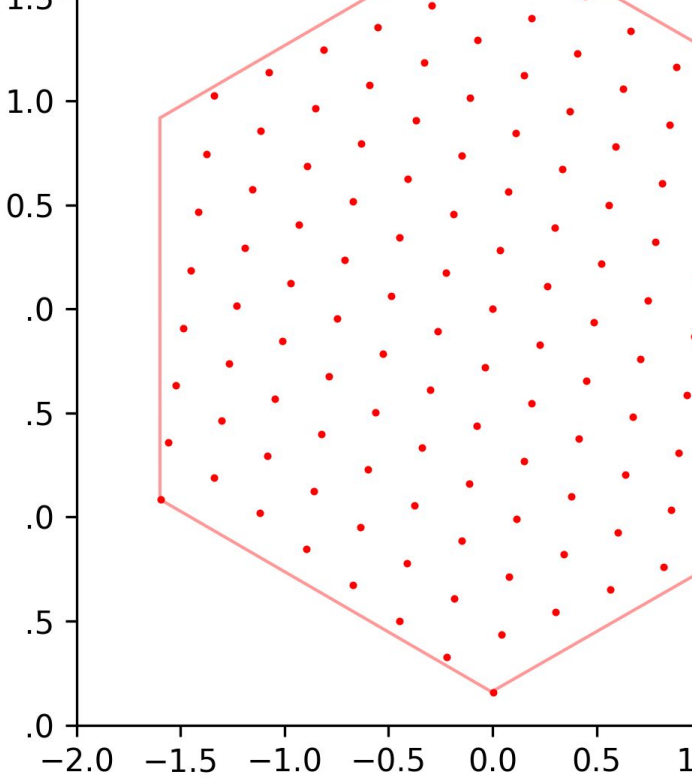


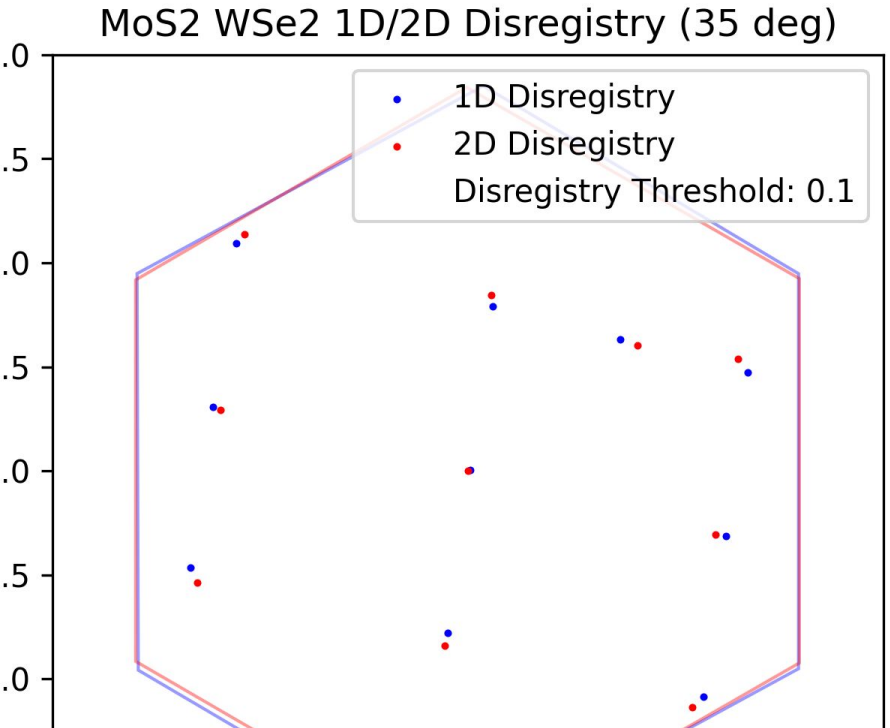
35 deg

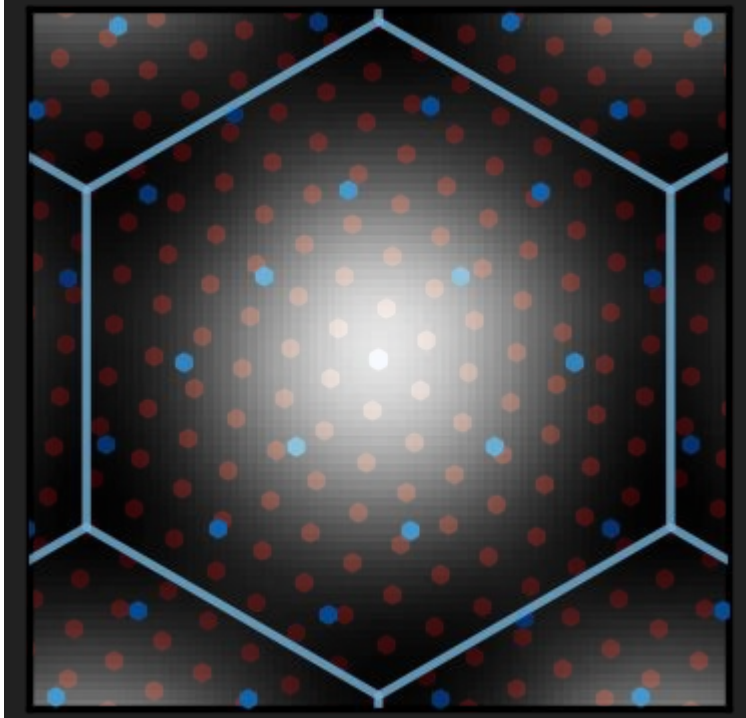


Actual Twist Angle: 34.9790733927
Total Atoms: 804
W Atoms (Top Layer): 129
Mo Atoms (Bottom Layer): 139

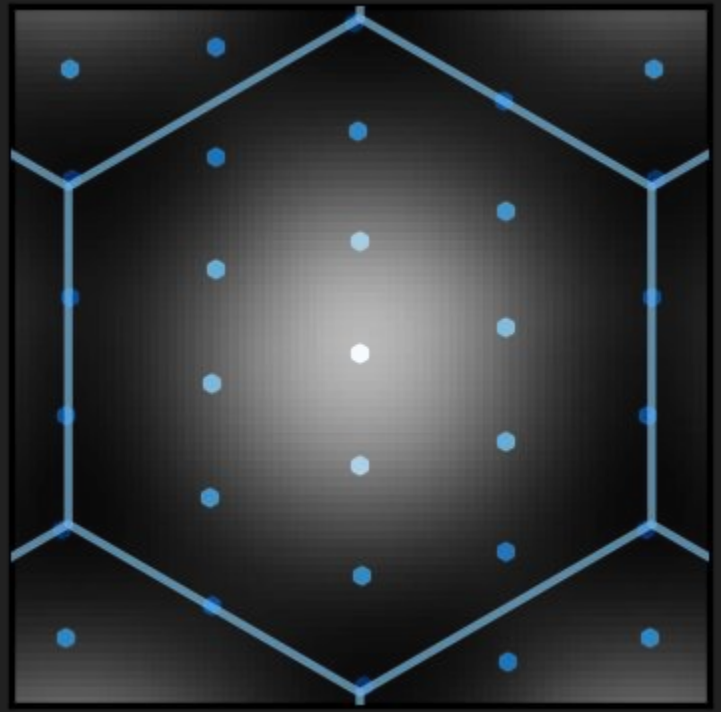

MoS2 WSe2 1D Disregistry (35 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

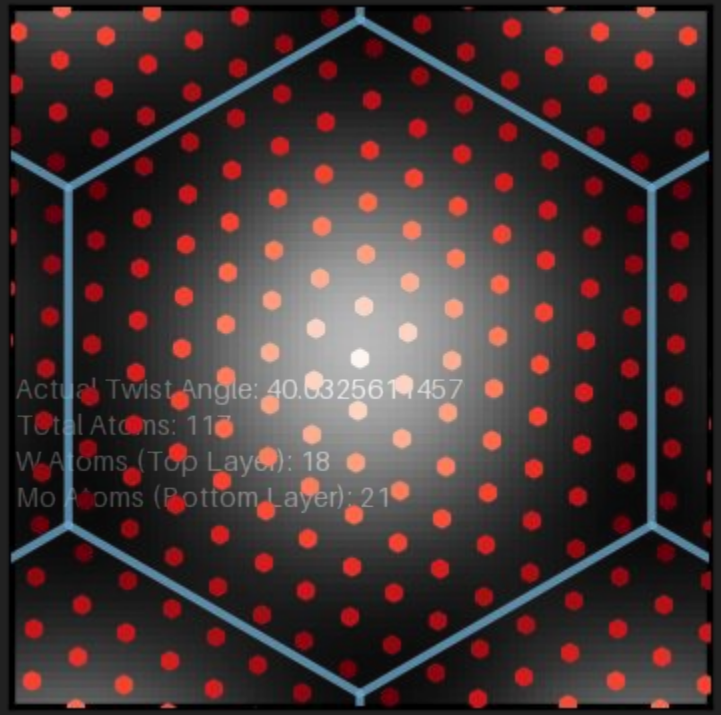

1.0
0.5
.0
.5
.0
.5
.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5


MoS2 WSe2 1D/2D Disregistry (35 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1



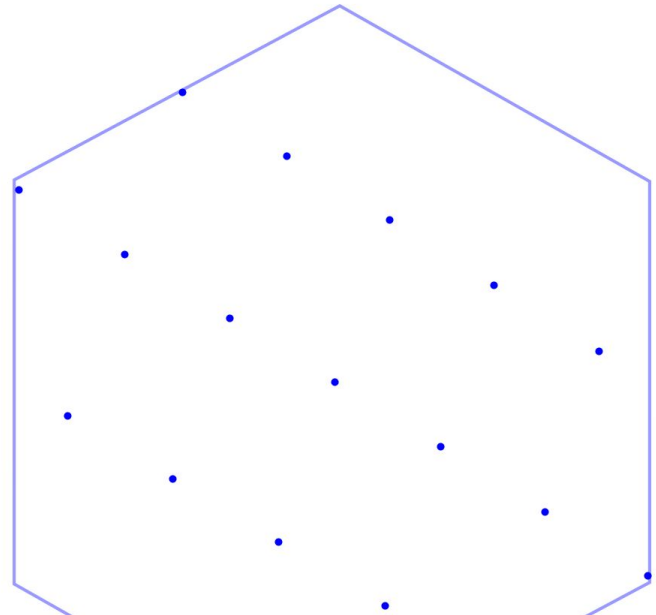
40 deg

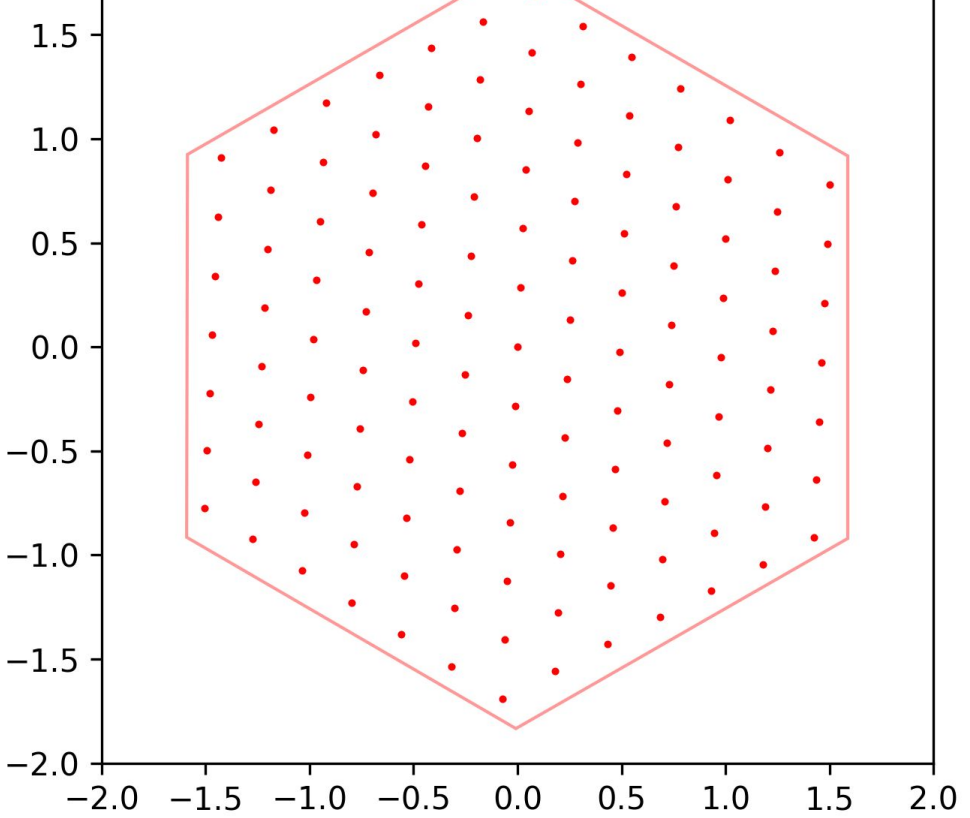


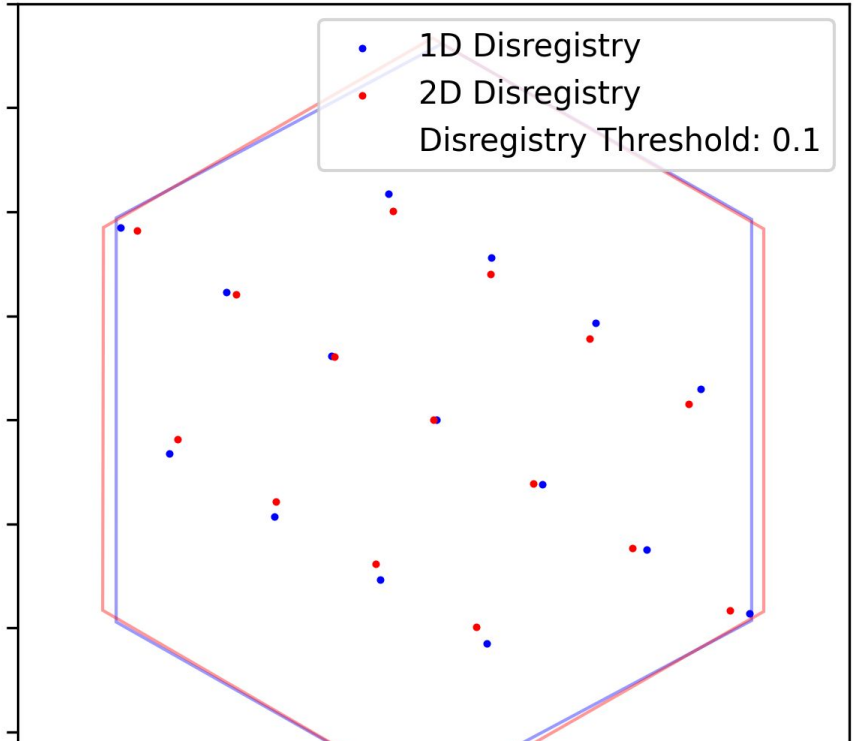


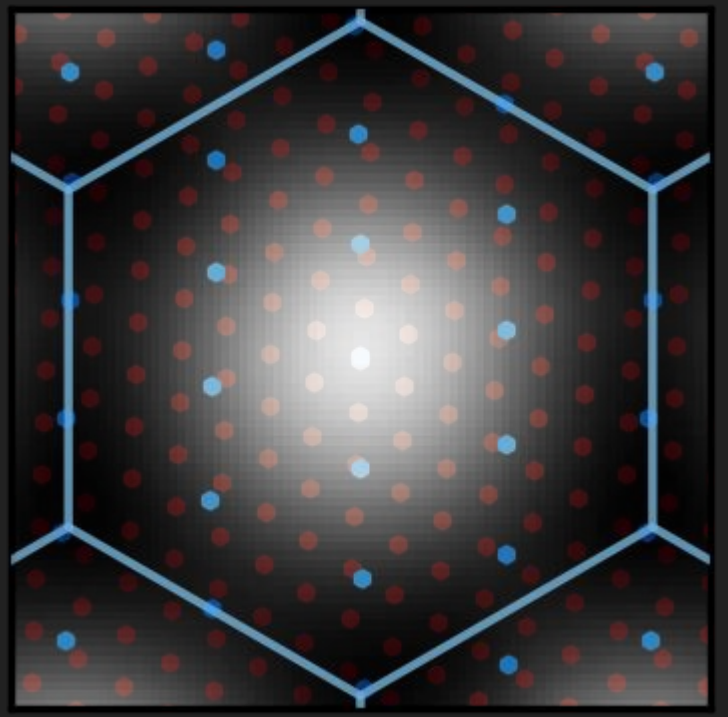
Actual Twist Angle: 40.0153724119
Total Atoms: 798
W Atoms (Top Layer): 127
Mo Atoms (Bottom Layer): 139

MoS2 WSe2 1D Disregistry (40 deg

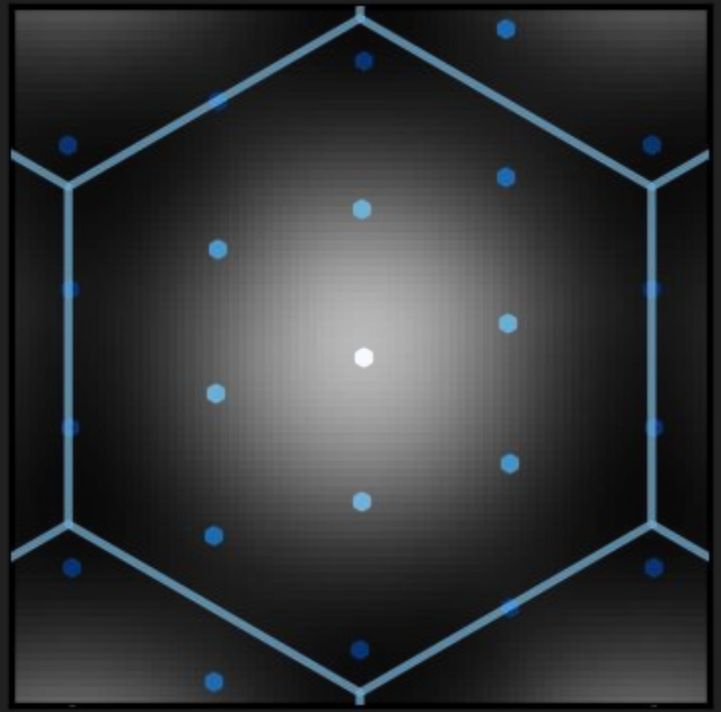


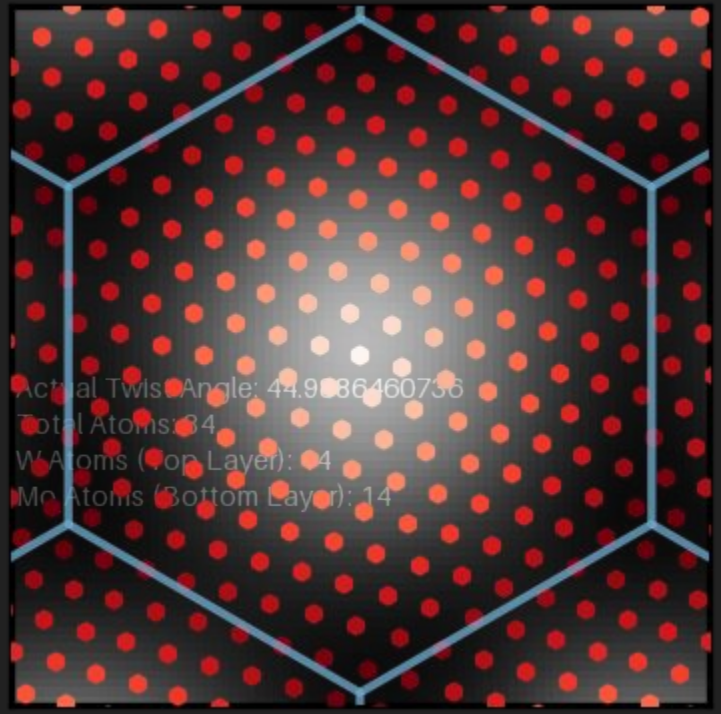


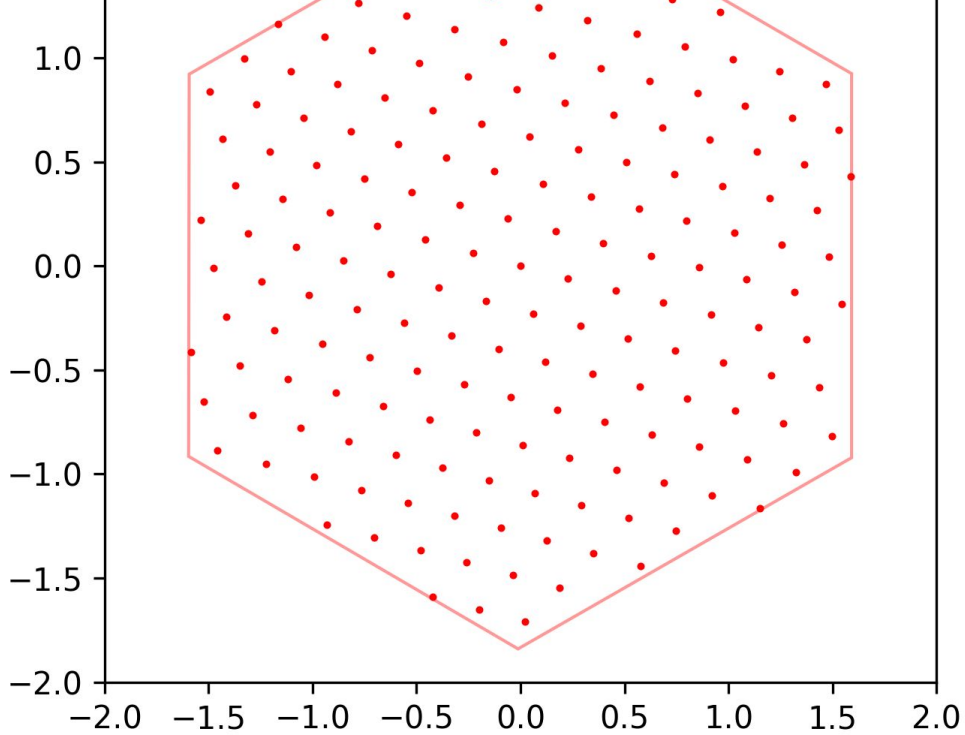

MoS2 WSe2 1D/2D Disregistry (40 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

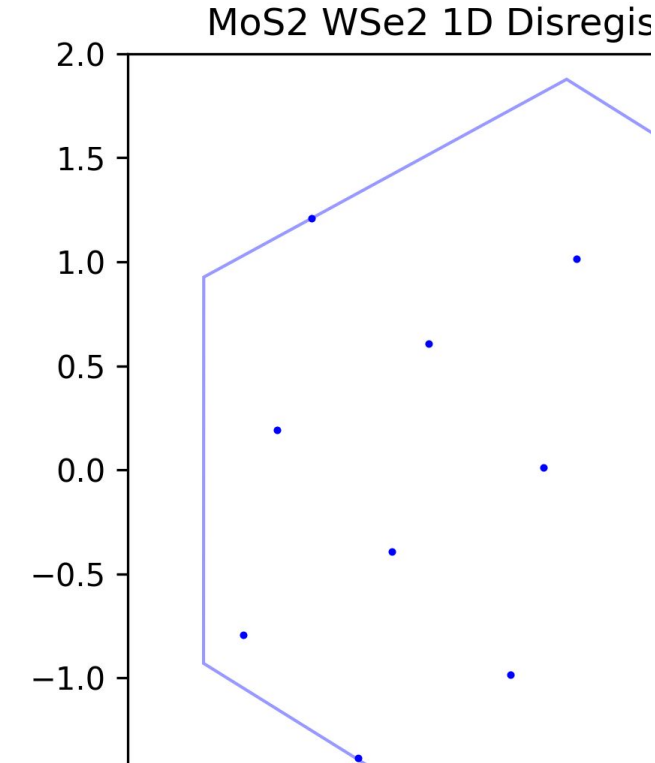


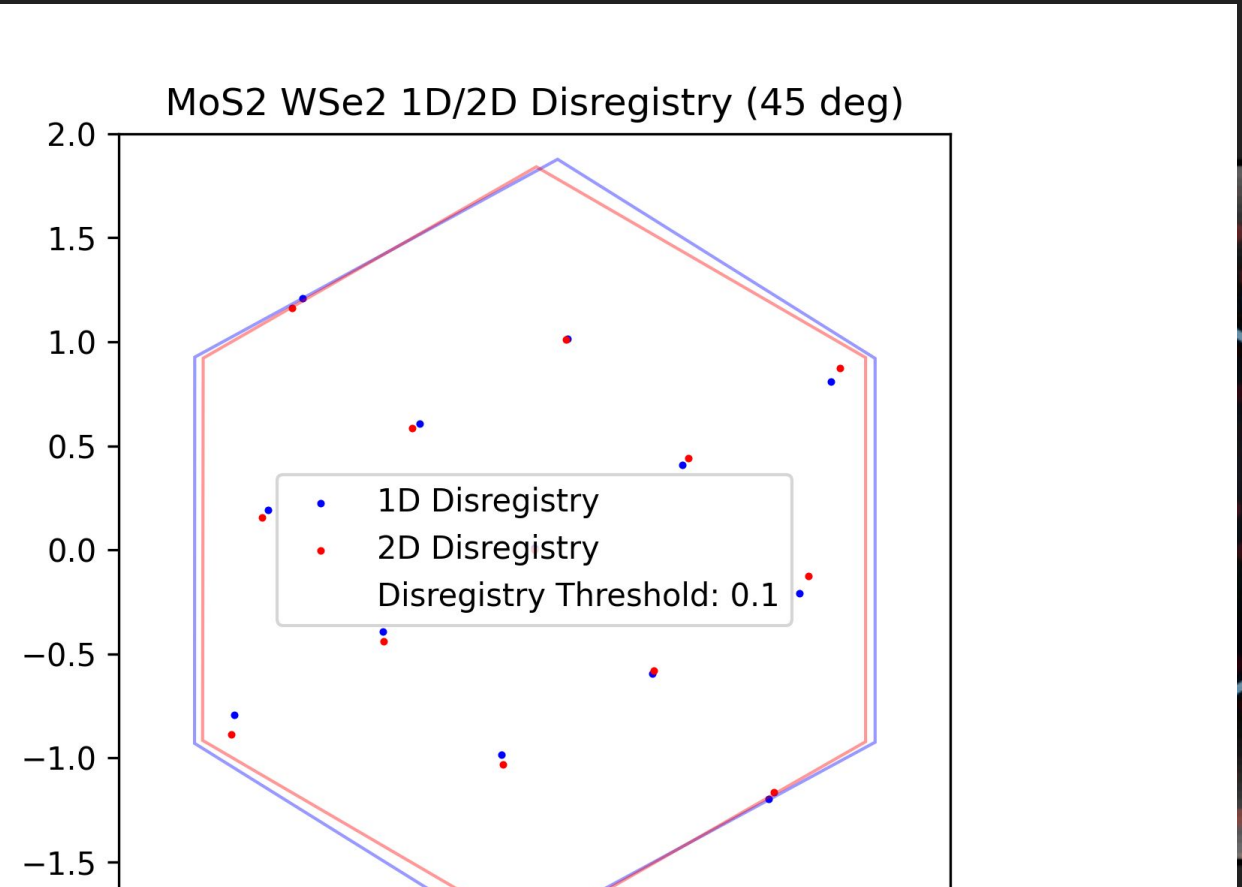
45 deg

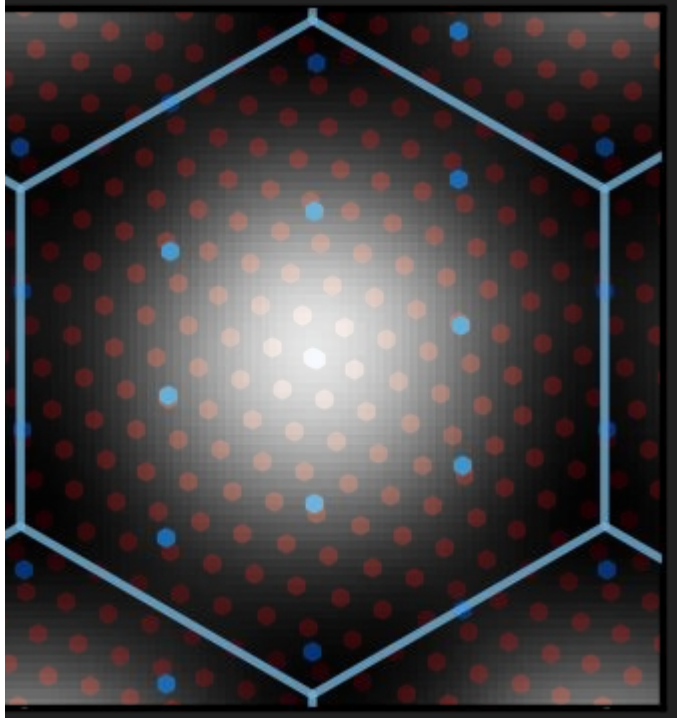



Actual Twist Angle: 44.9829164957
Total Atoms: 1131
W Atoms (Top Layer): 181
Mo Atoms (Bottom Layer): 196

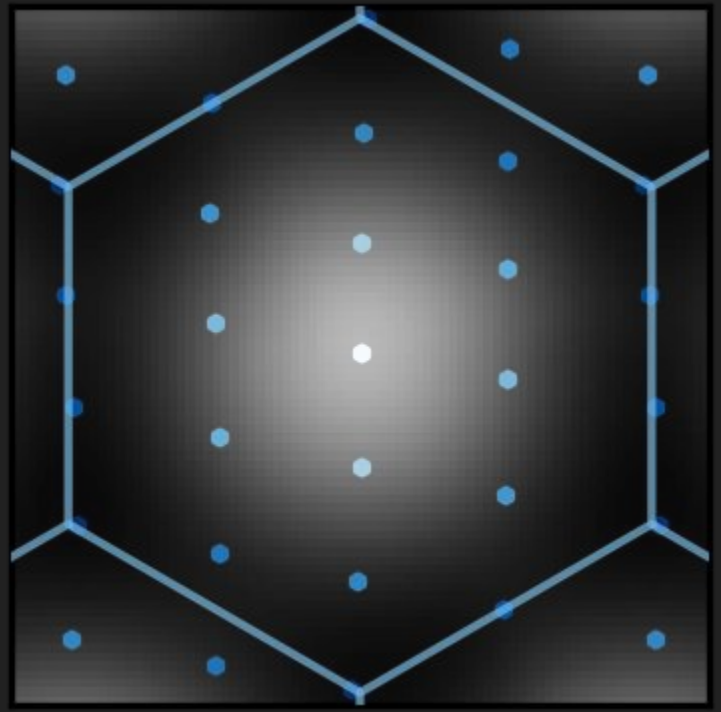

1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

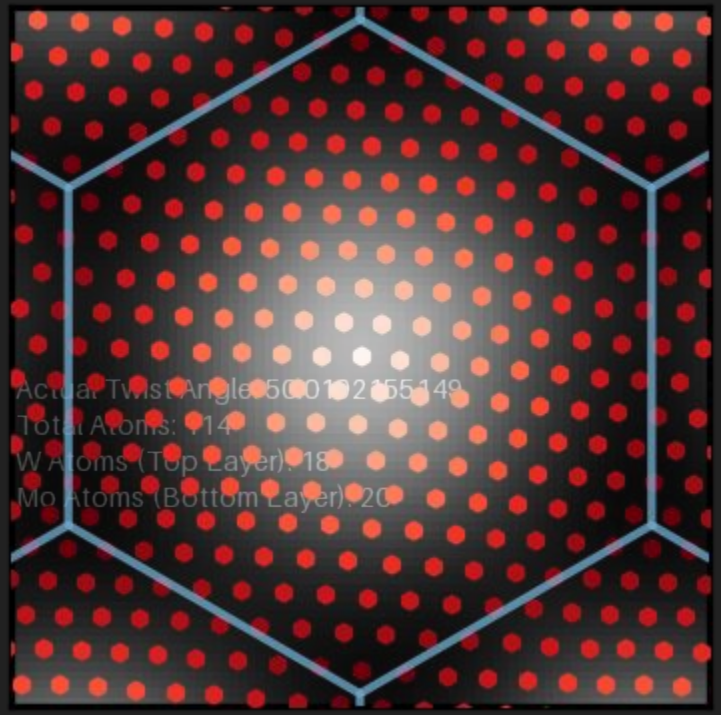

MoS2 WSe2 1D Disregis
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


MoS2 WSe2 1D/2D Disregistry (45 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

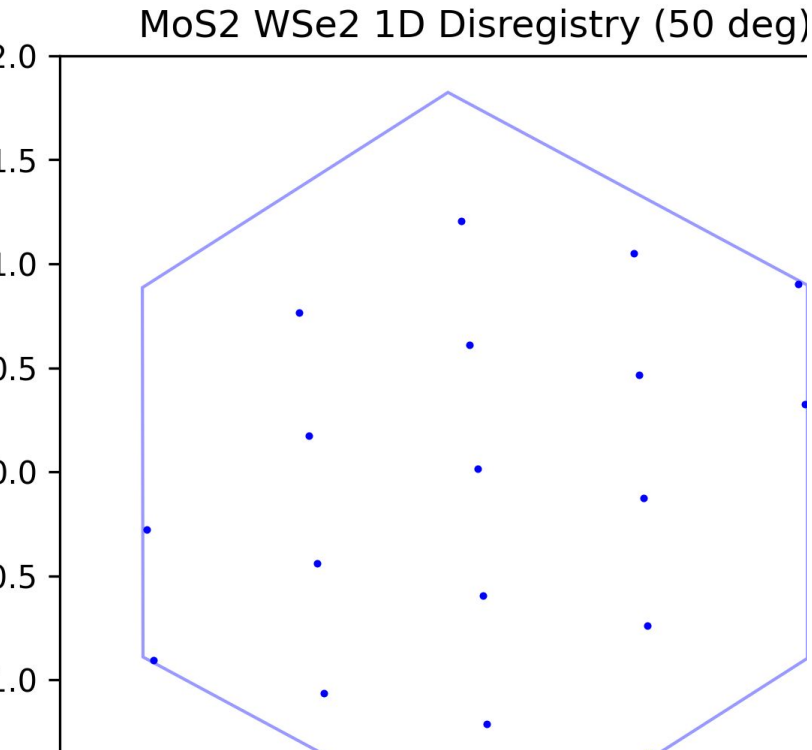


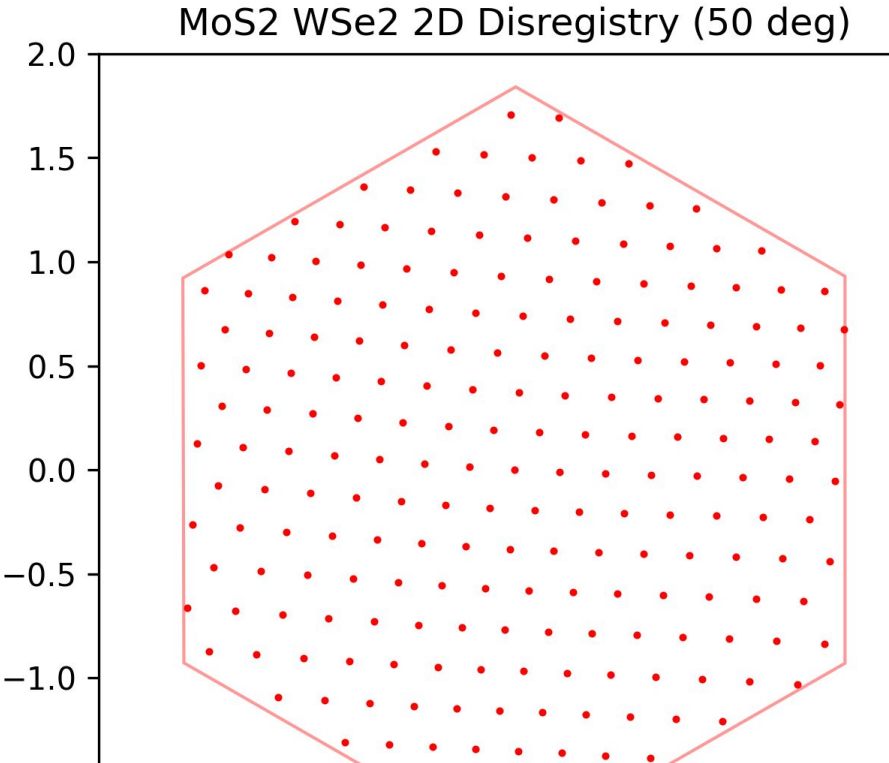
50 deg

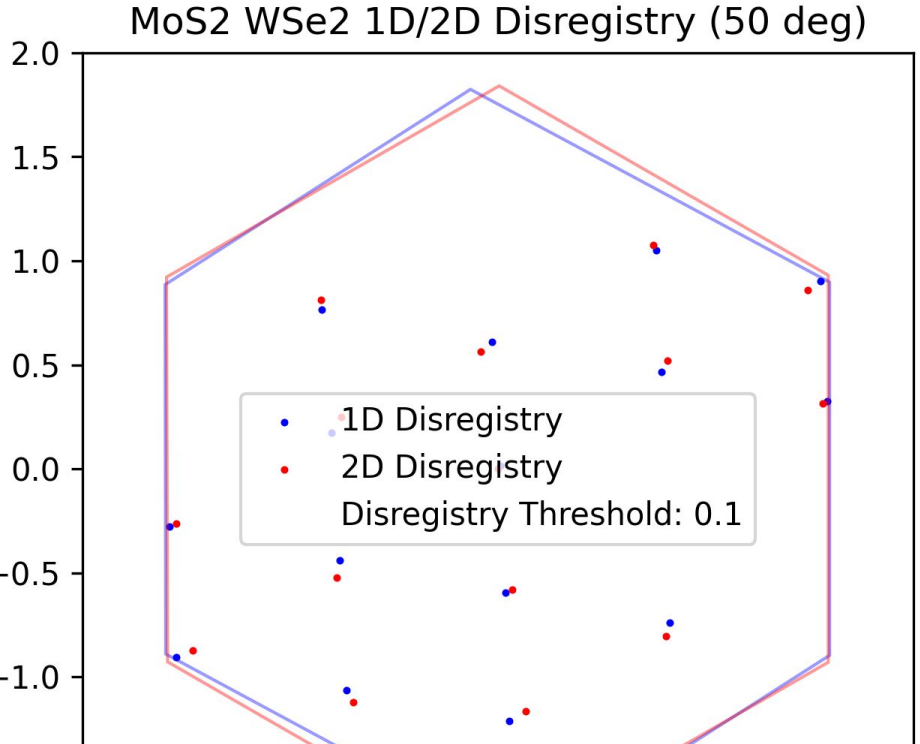


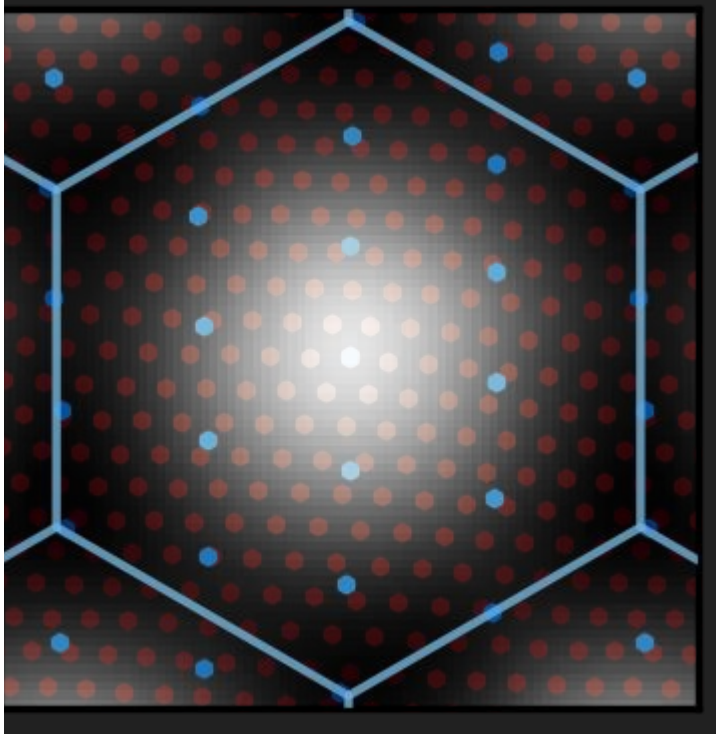


Actual Twist Angle: 50.0192155149
Total Atoms: 1317
W Atoms (Top Layer): 211
Mo Atoms (Bottom Layer): 228

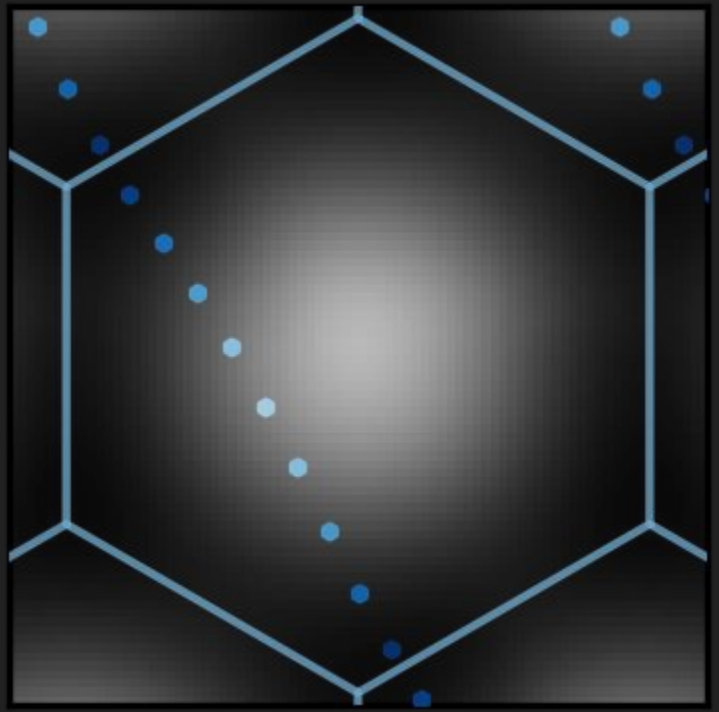

MoS2 WSe2 1D Disregistry (50 deg)
2.0
1.5
1.0
0.5
0.0
0.5
1.0

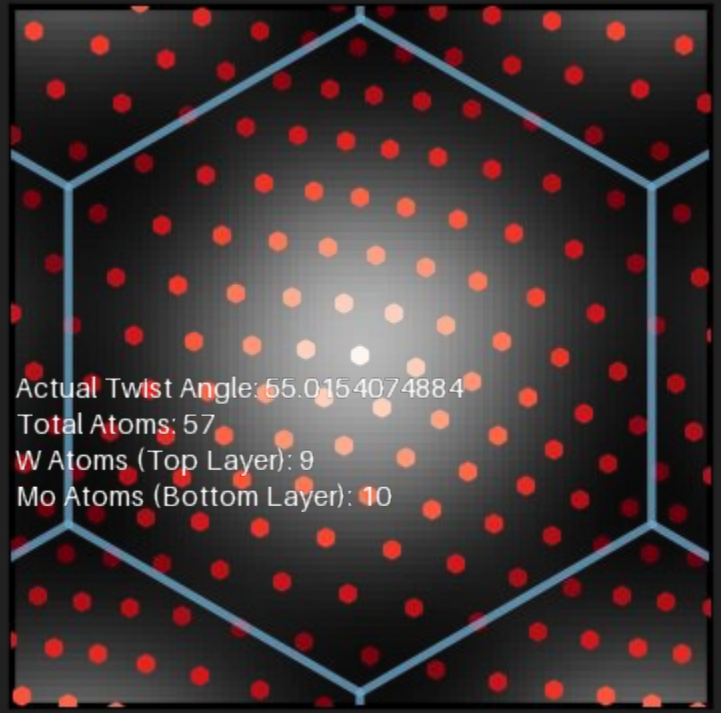

MoS2 WSe2 2D Disregistry (50 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


MoS2 WSe2 1D/2D Disregistry (50 deg)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1



55 deg

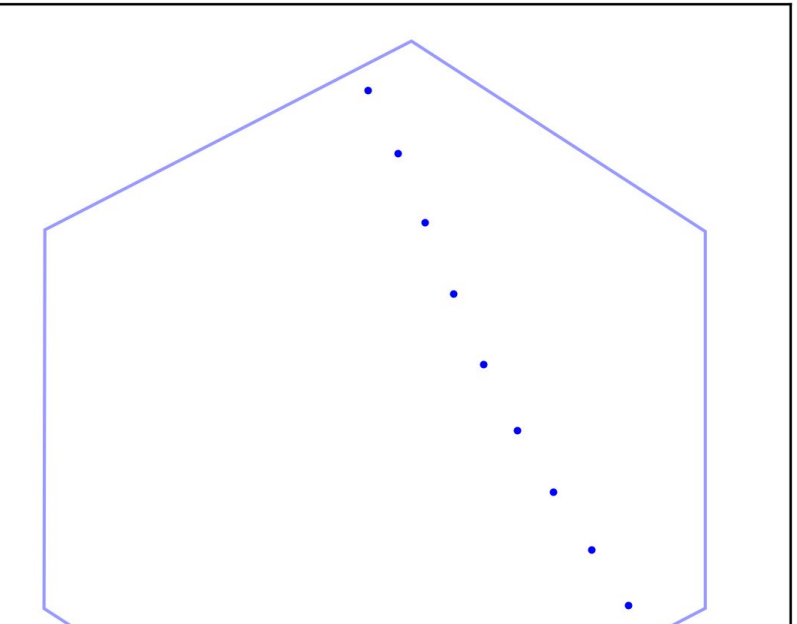


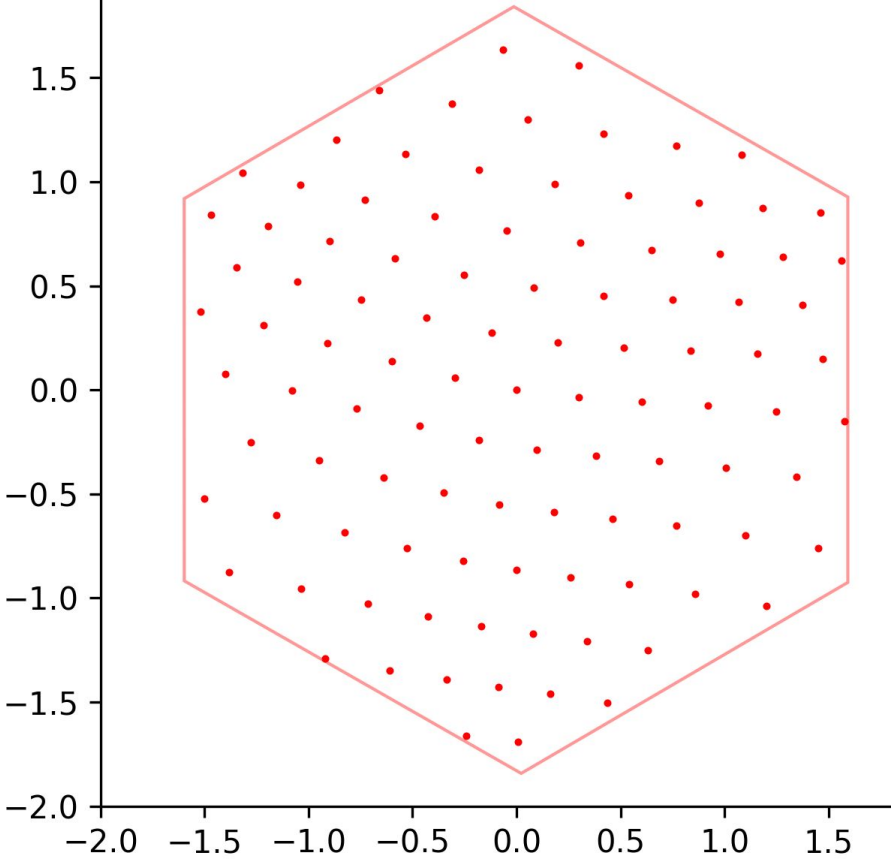


Actual Twist Angle: 55.0154074884
Total Atoms: 642
W Atoms (Top Layer): 103
Mo Atoms (Bottom Layer): 111

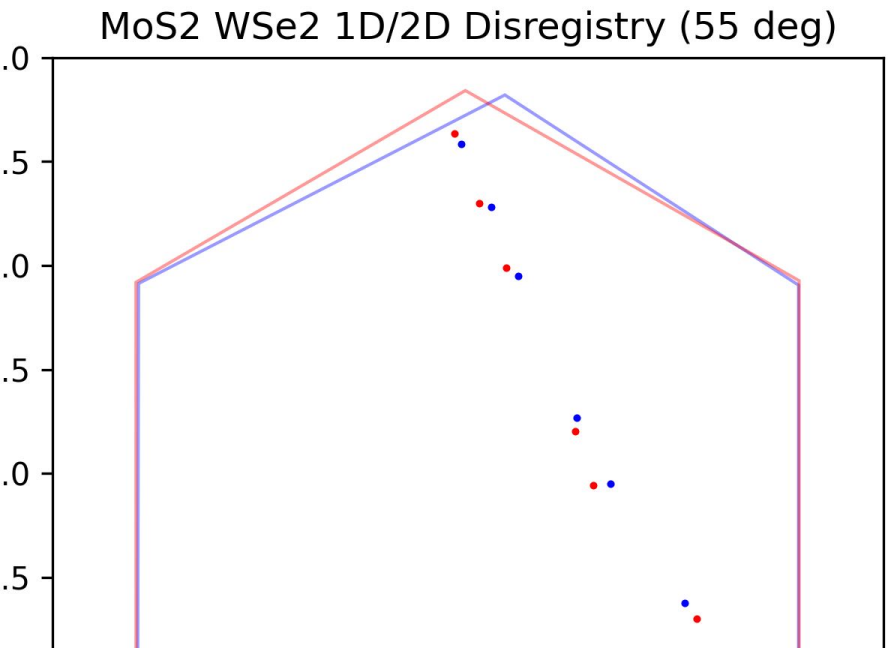
[redacted]

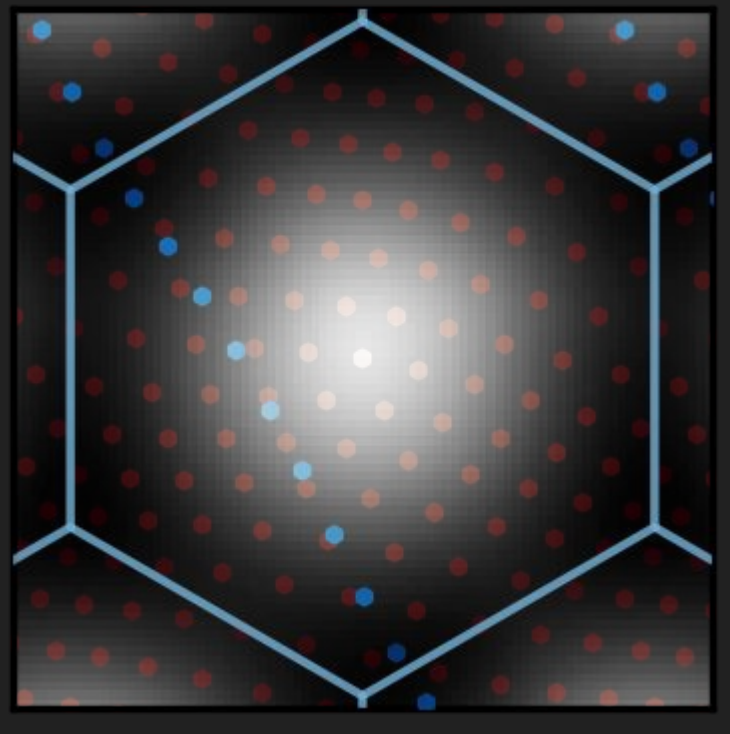
MoS2 WSe2 1D Disregistry (55 deg)



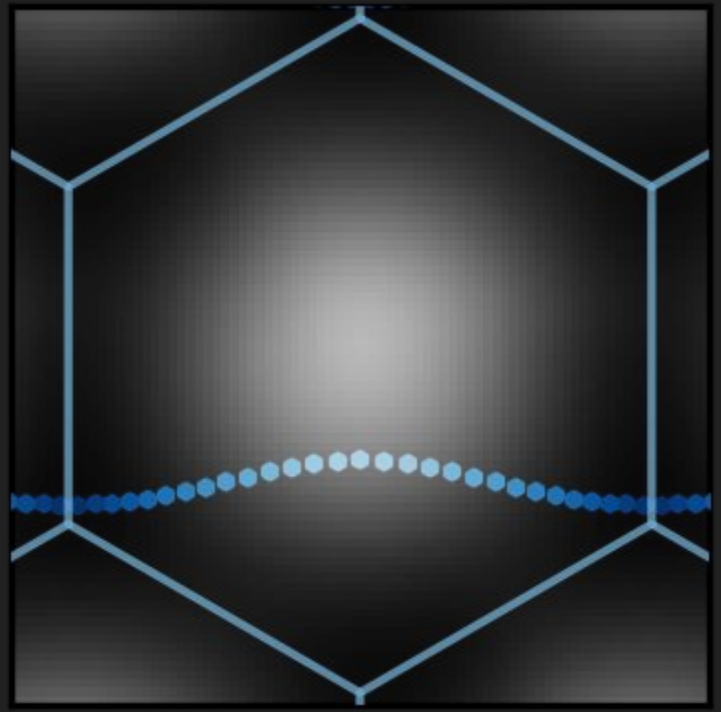


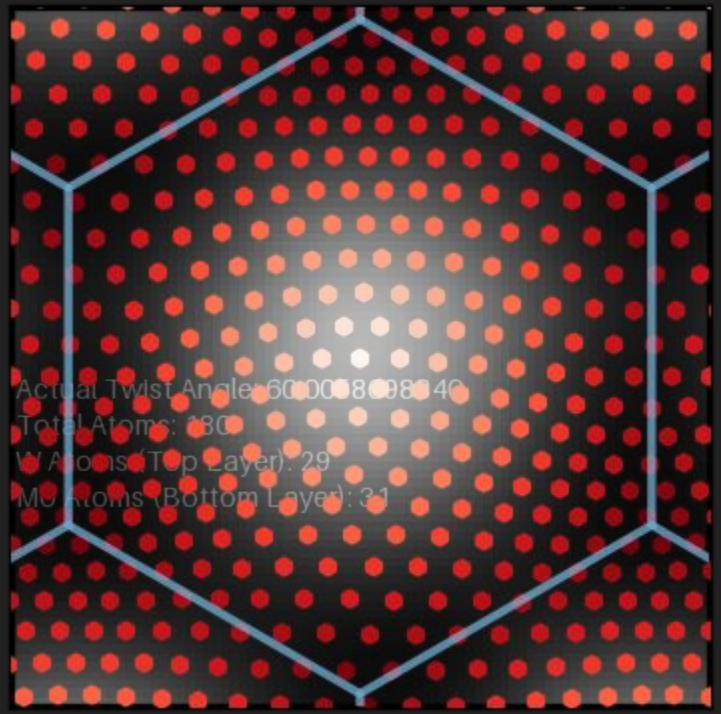
[redacted]


MoS2 WSe2 1D/2D Disregistry (55 deg)
.0
.5
.0
.5
.0
.5

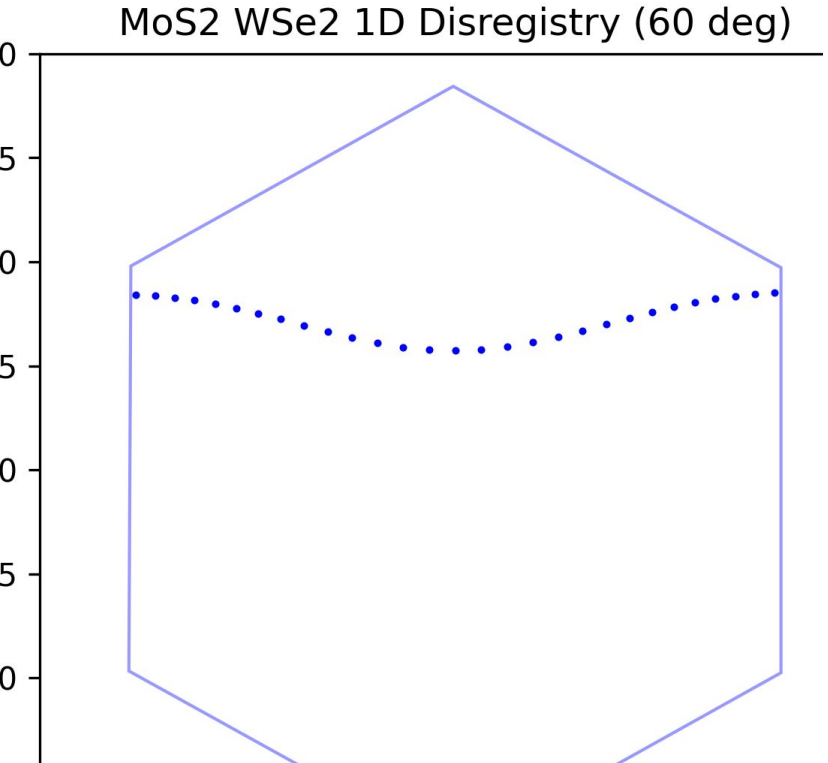


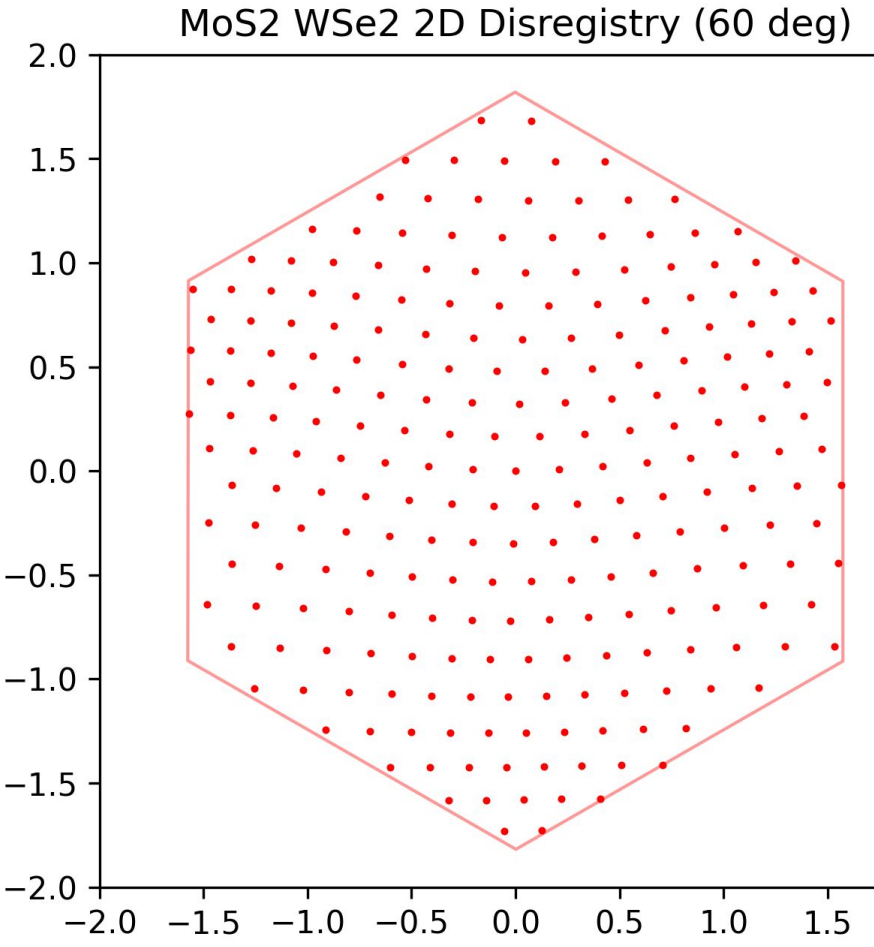
60 deg

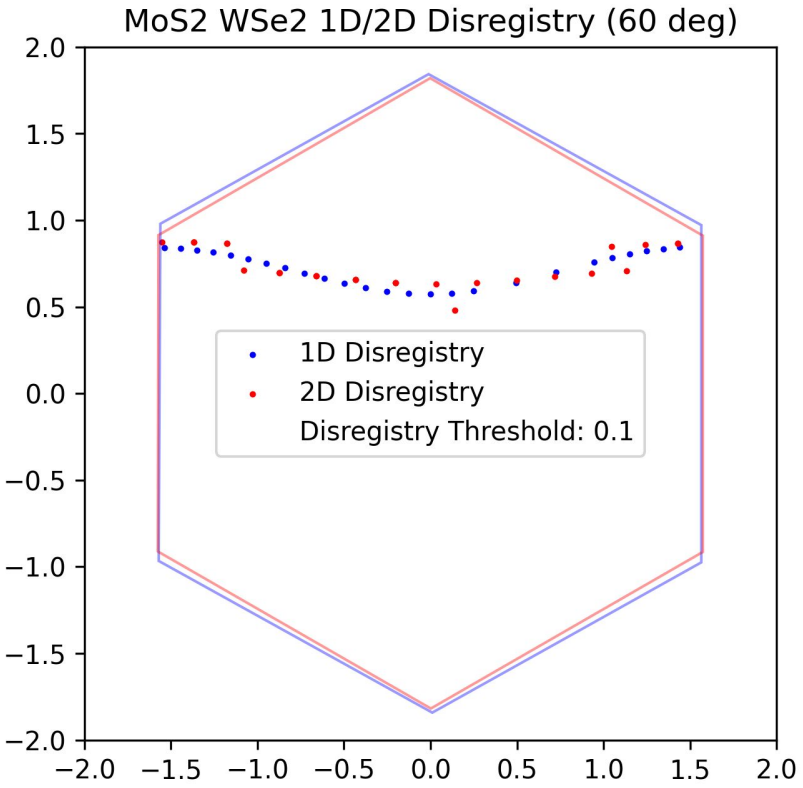


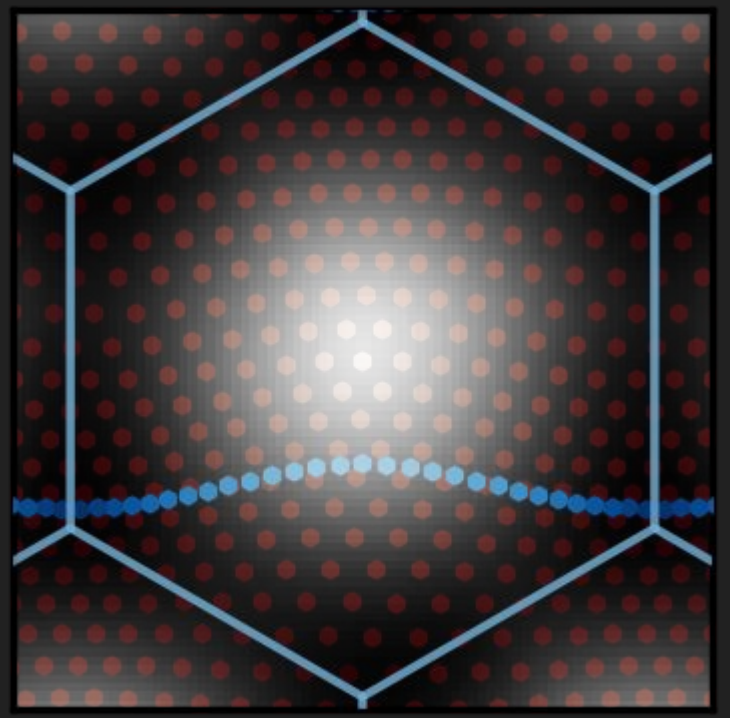


Actual Twist Angle: 59.97722199420
Total Atoms: 1536
W Atoms (Top Layer): 240
Mo Atoms (Bottom Layer): 272


MoS2 WSe2 1D Disregistry (60 deg)


MoS2 WSe2 2D Disregistry (60 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5


MoS2 WSe2 1D/2D Disregistry (60 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1



- [ ] 1 piece of conclusion is a summary of what i was looking at, what i did, along with code and files I worked on put that together
- [ ] Then work on a 10 min powerpoint presentation, 15 min presentation at group meeting
- [ ] Instead of writing new reports, just write something in the style of a paper in the style of a report, make it comprehensive, less on results and more on methods I used and what I learned
- [ ] I've generated structures, relaxed them, visualized in ovito and disregistry, compared structures
- [ ] Take next 3-4 days for this friday come up with a presentation outline ⇒ deliver presntation
- [ ] Motivate the subproject, the understanding of how these 1D structures sample disregistry space ⇒ can we actually deconstruct/properly sample 2d strucs with 1d ⇒ comparing positions/similarities
- [ ] use presentation to construct high-level points
- [ ] parallel paper, this is what we set outto do, methods used, qualitative/quantitative measures, make a conclusion, that q1d samples this (or something) well
- [ ] q1d structs are valid in this regime
- [ ] what is the argument
- [ ] could also conclude there is no pattern
- [ ] showing 1 of the voronoi cell
- [ ] show multiple plots, throw leftovers all in a backup slides

Tools I used

Pymoire

ASE (Python)

Scipy

Numpy

matplotlib

What did I do?

Learned how to use the tools, lots of trial and error for figuring out how they work

Constructed q1d and 2d structures at varying twist angles with pymoire

Used scipy spatial to measure disregistries, construct voronoi cells, fold them together to construct disregistry plots.

Used that data to make comparisons between q1d and 2d structures using scipy spatial to measure similarities via mean disregistry error (from q1d to closest 2d disregistries)

Constructed plots showcasing those at different angles

Relaxed the structures with mace-interlayer (Jornada group flavor)

Performed a similar analysis there

Graphics I want to show

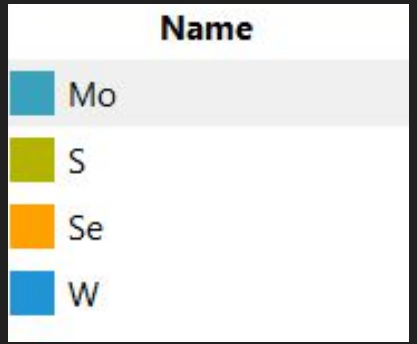
Angle vs mean disregistry error (before/after relaxation)

Johnathan's code plots => overlay between q1d and 2d

My simple plots of nearby real-space disregistries

Ovito constructions of relaxed/unrelaxed structures

- Highlight q1d structures, compare to 2d
- Show 1d and 2d compared to relaxed counterparts
- Show spiralling pattern for certain ones
-



Learning about motivation behind this direction for research

Reading through Johnathan/Akash’s paper

Learned how to use Ovito to visualize,

Learned how to use ASE libraries to construct, deconstruct, evaluate atom positions

Relaxations using LAMMPS python/ase module

Pymoire to construct structures at varying twist angles

Learned about voronoi analysis

Developed Code to connect process between construction to analysis

Ran relaxations then analyzed those structures