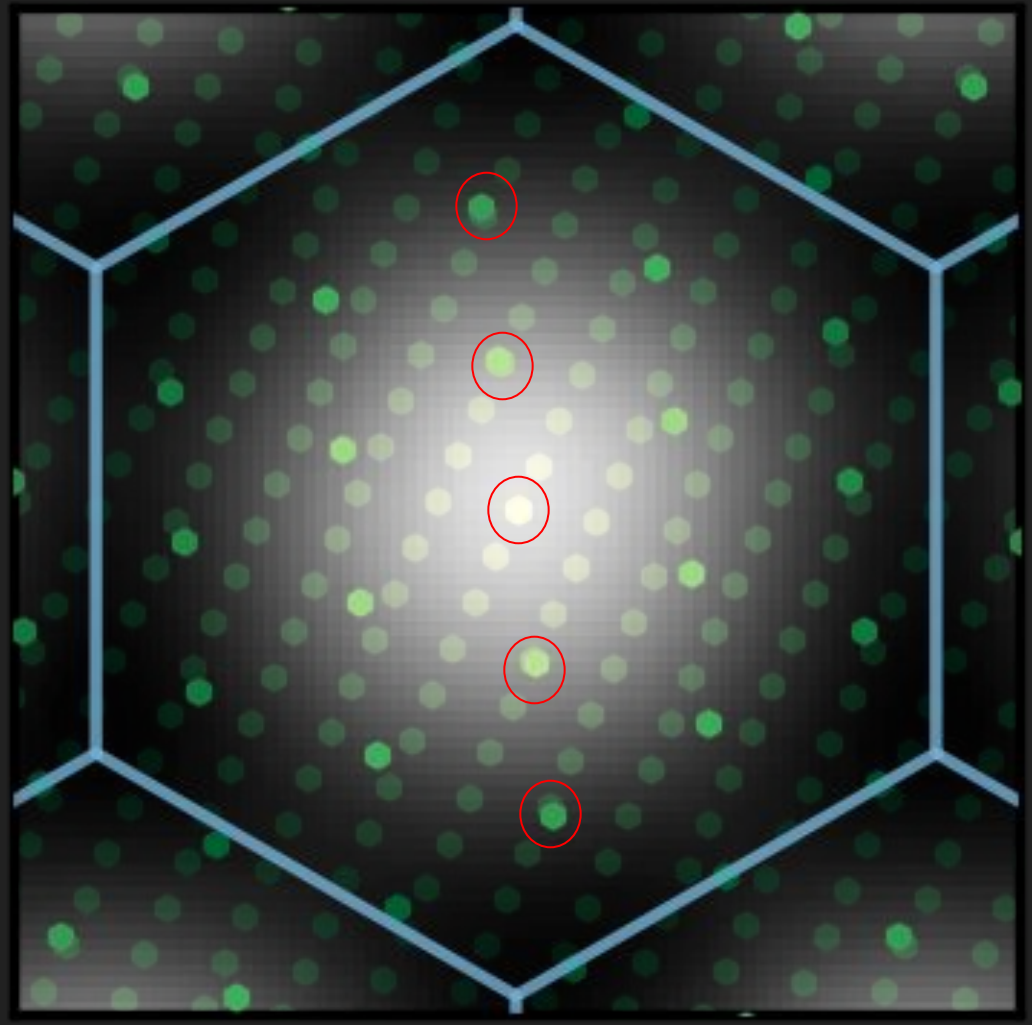
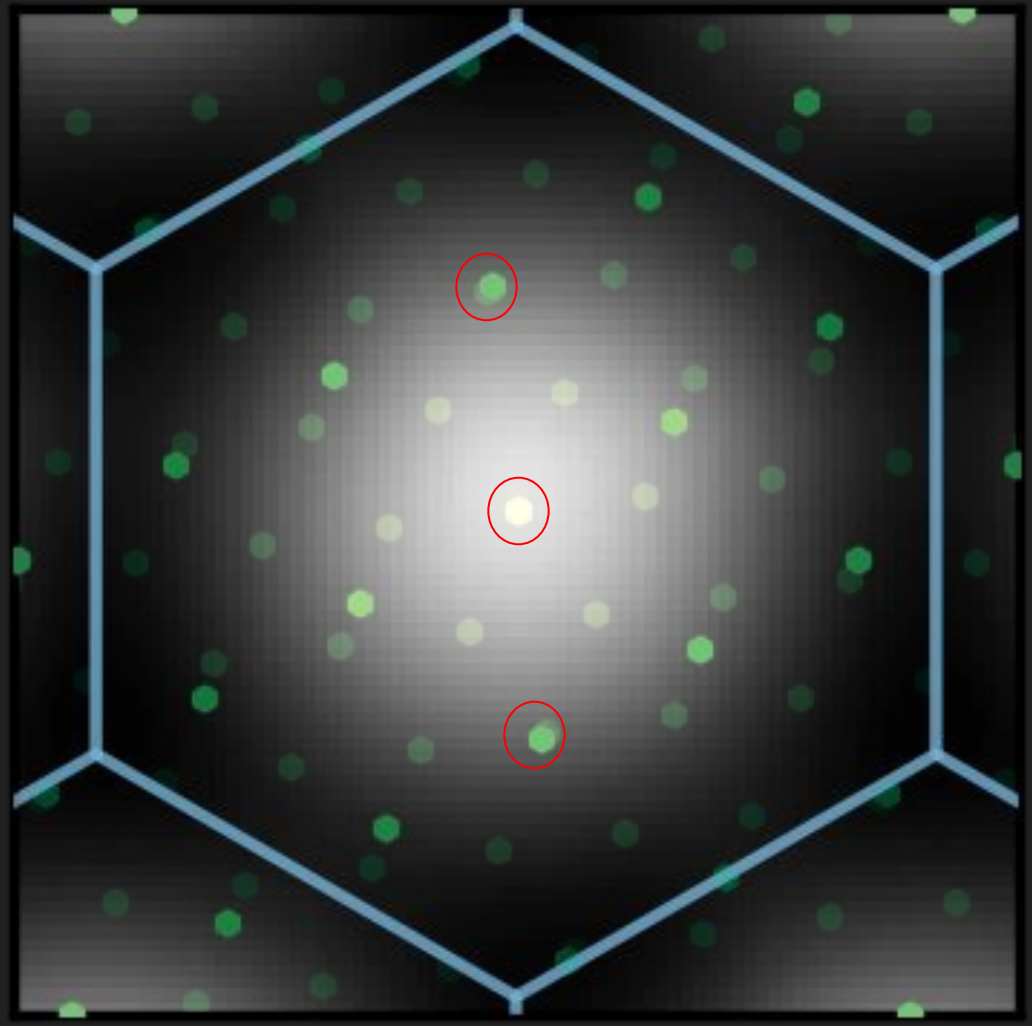
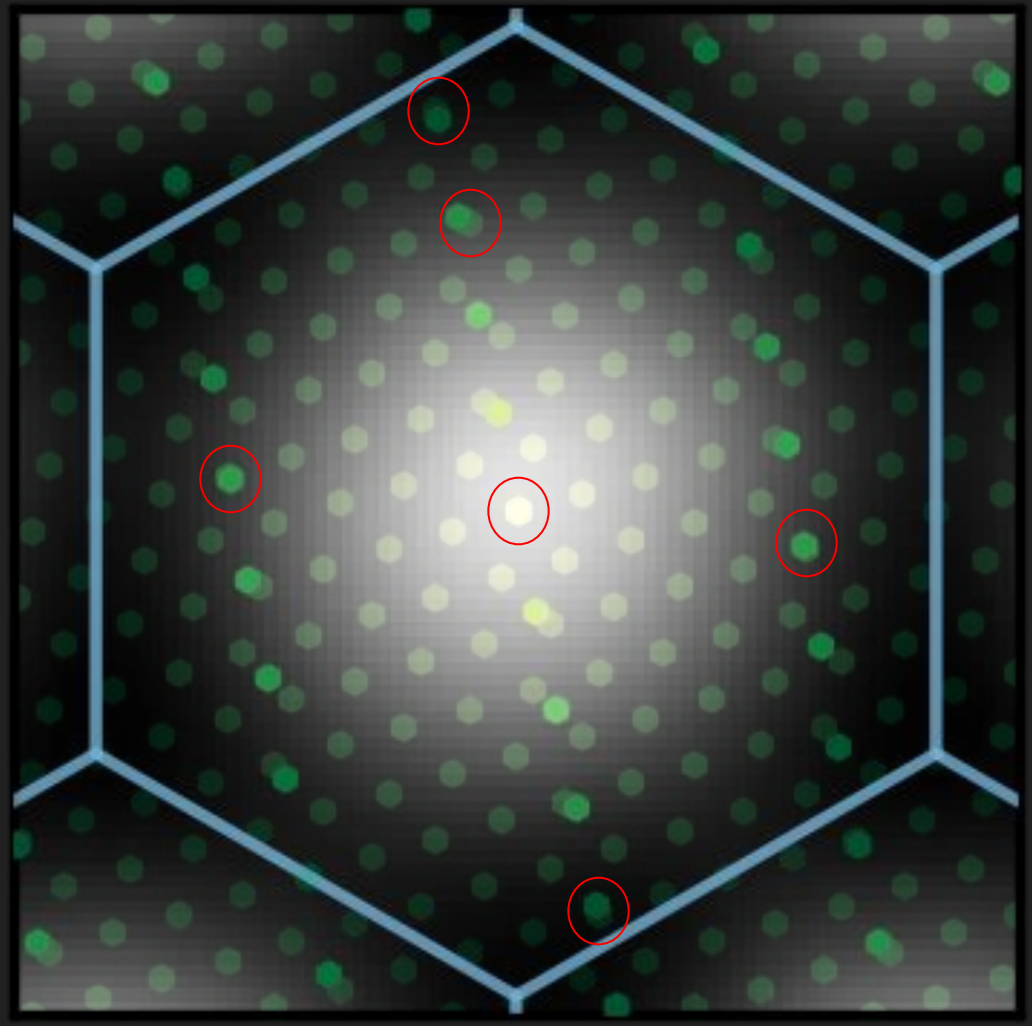
MoS2 - MoS2 Q1D/2D Overlay



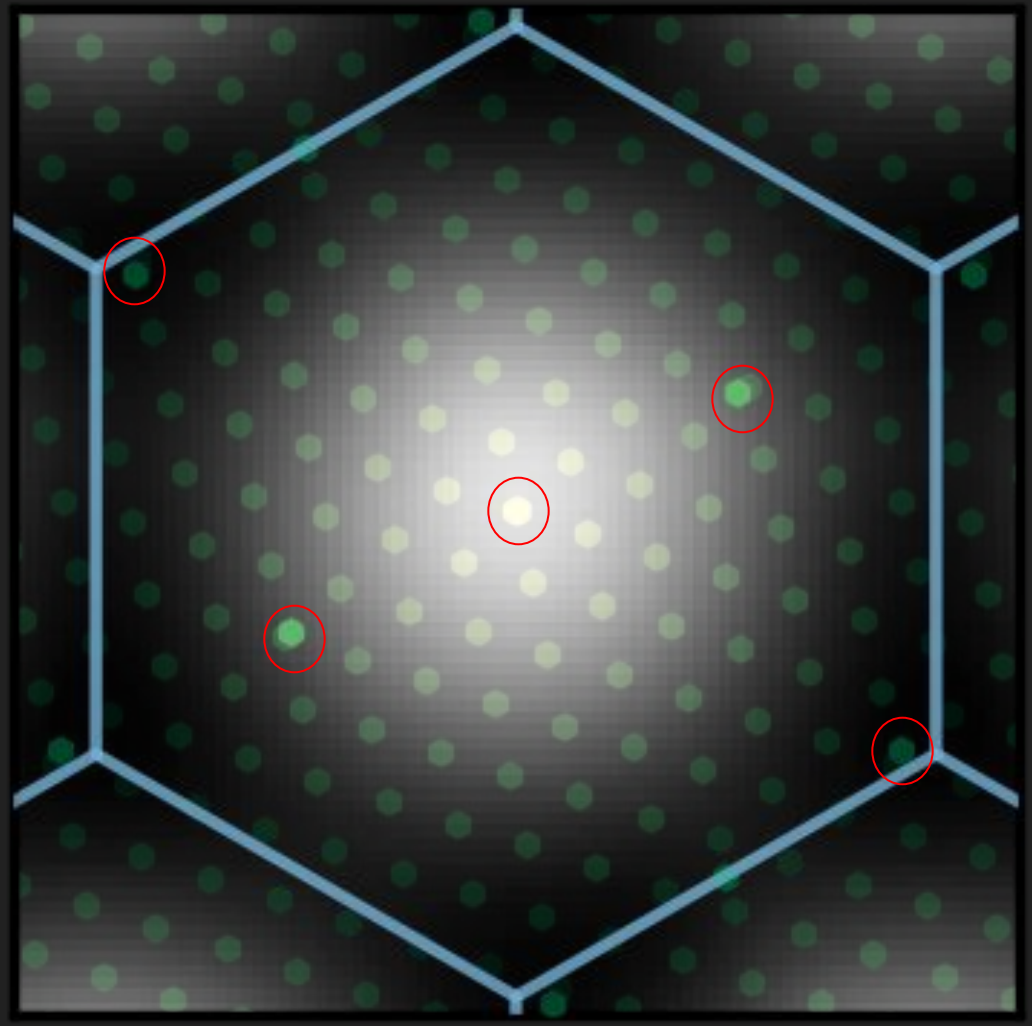
twist_min_search: 9.98
twist_max_search: 10.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 148
Mo Atoms (Top Layer): 74
Mo Atoms (Bottom Layer): 74



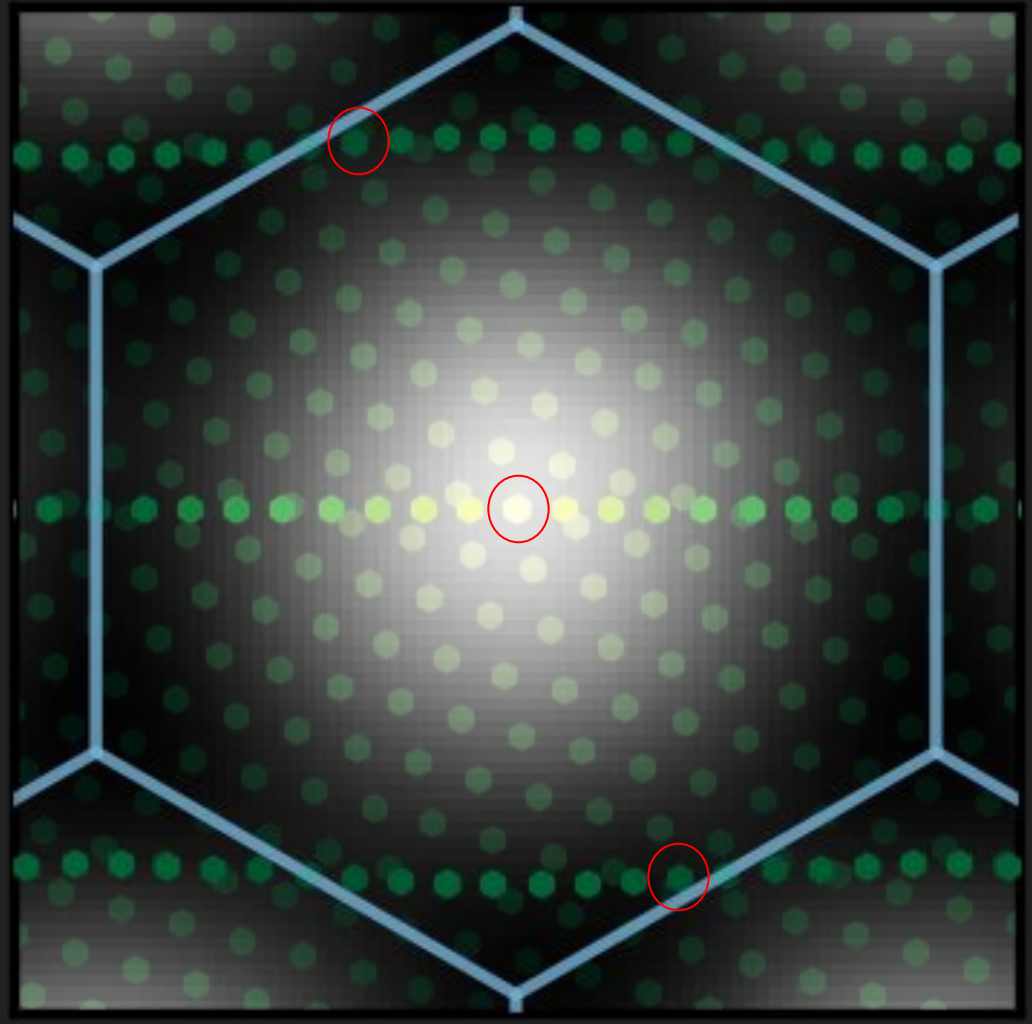
twist_min_search: 14.98
twist_max_search: 15.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 258
Mo Atoms (Top Layer): 43
Mo Atoms (Bottom Layer): 43



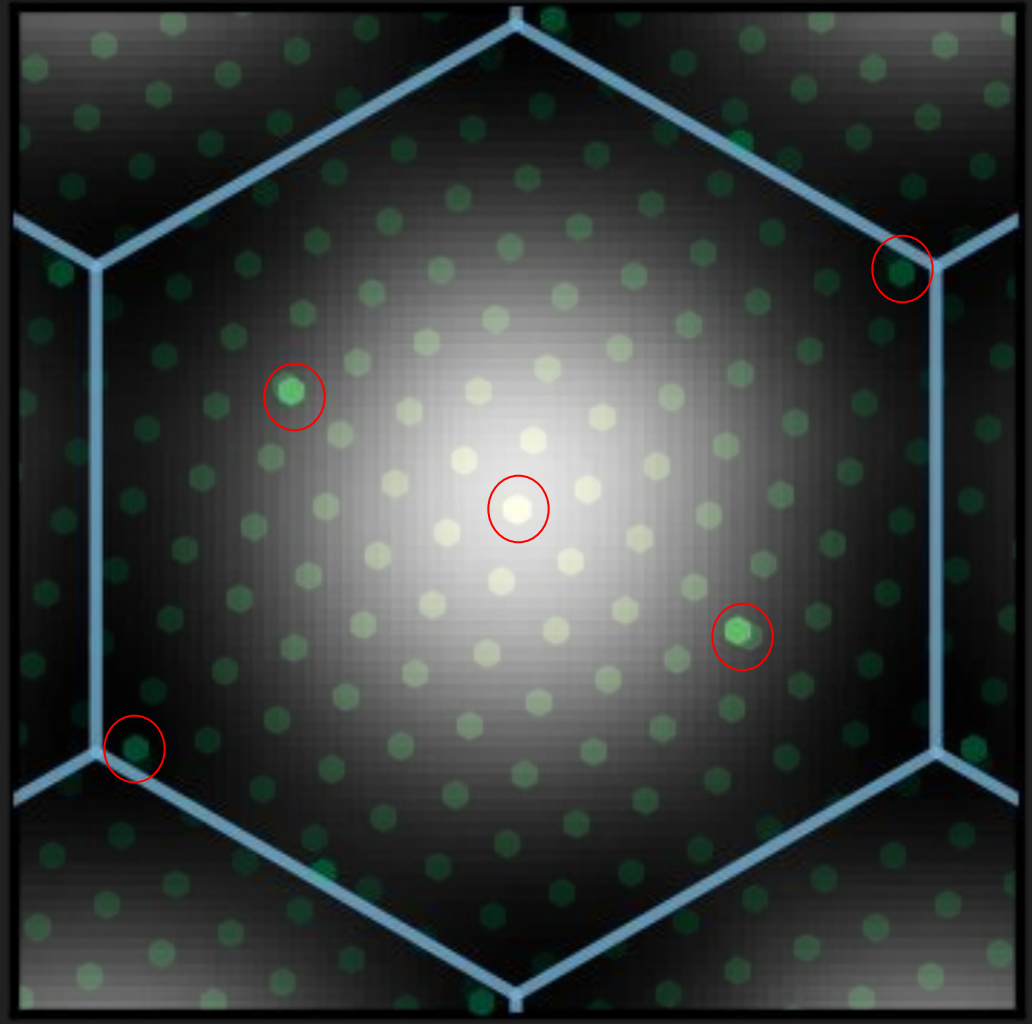
twist_min_search: 19.98
twist_max_search: 20.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 935
Mo Atoms (Top Layer): 256
Mo Atoms (Bottom Layer): 257



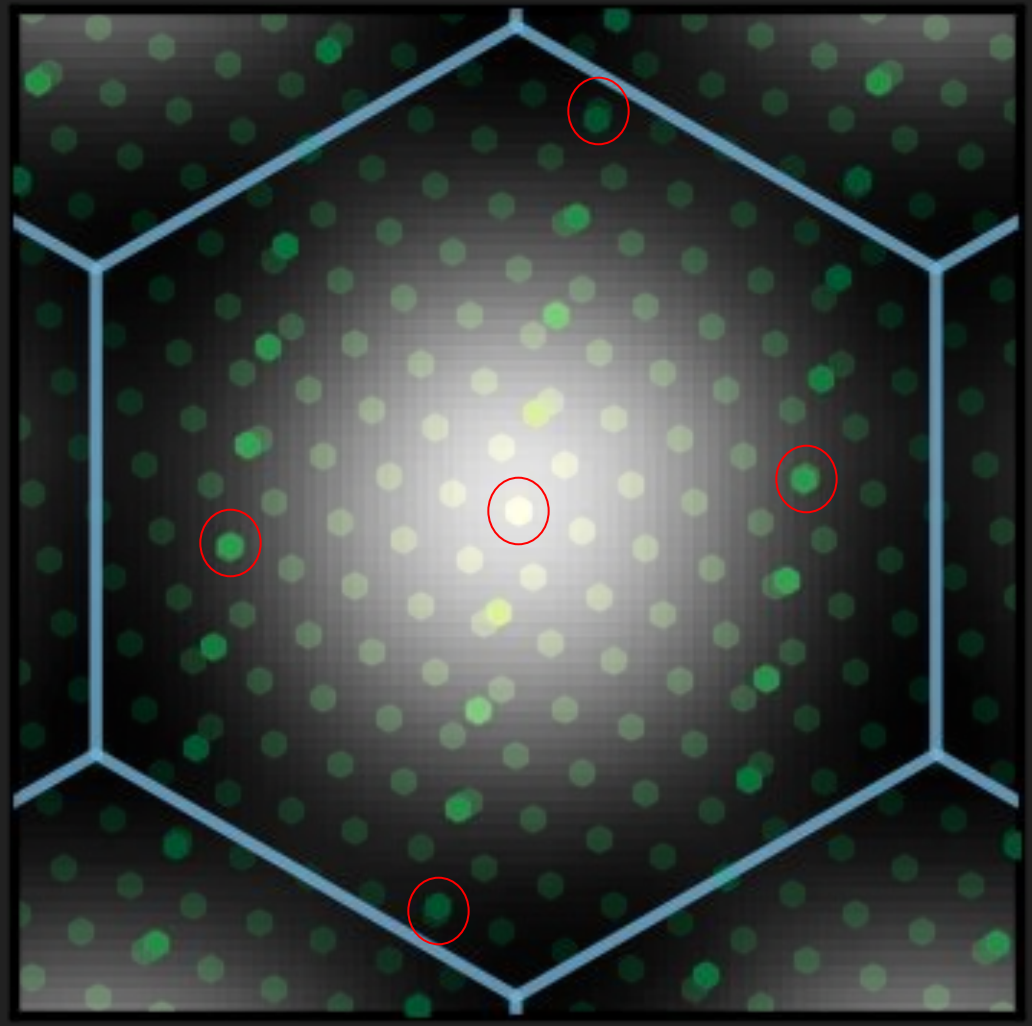
twist_min_search: 24.98
twist_max_search: 25.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 368
Mo Atoms (Top Layer): 133
Mo Atoms (Bottom Layer): 133



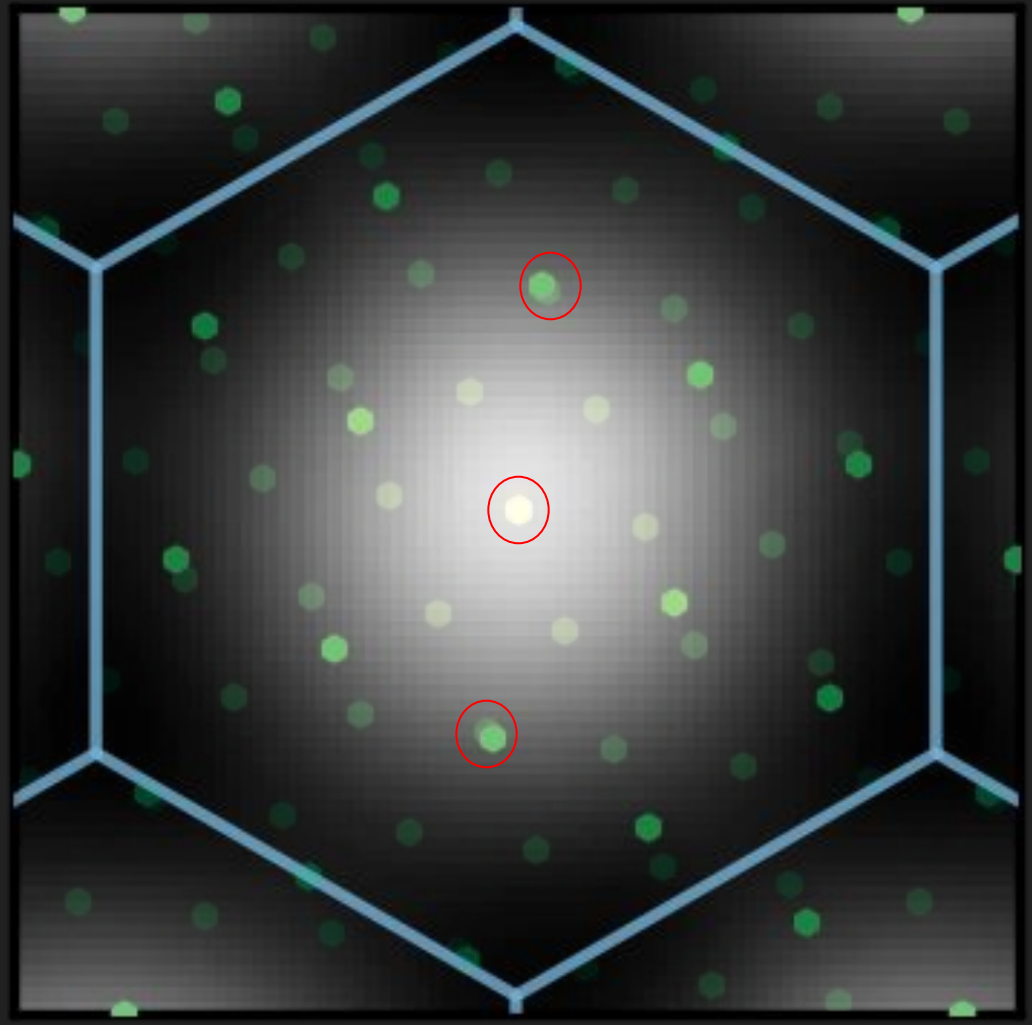
twist_min_search: 29.98
twist_max_search: 30.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 2086
Mo Atoms (Top Layer): 381
Mo Atoms (Bottom Layer): 381



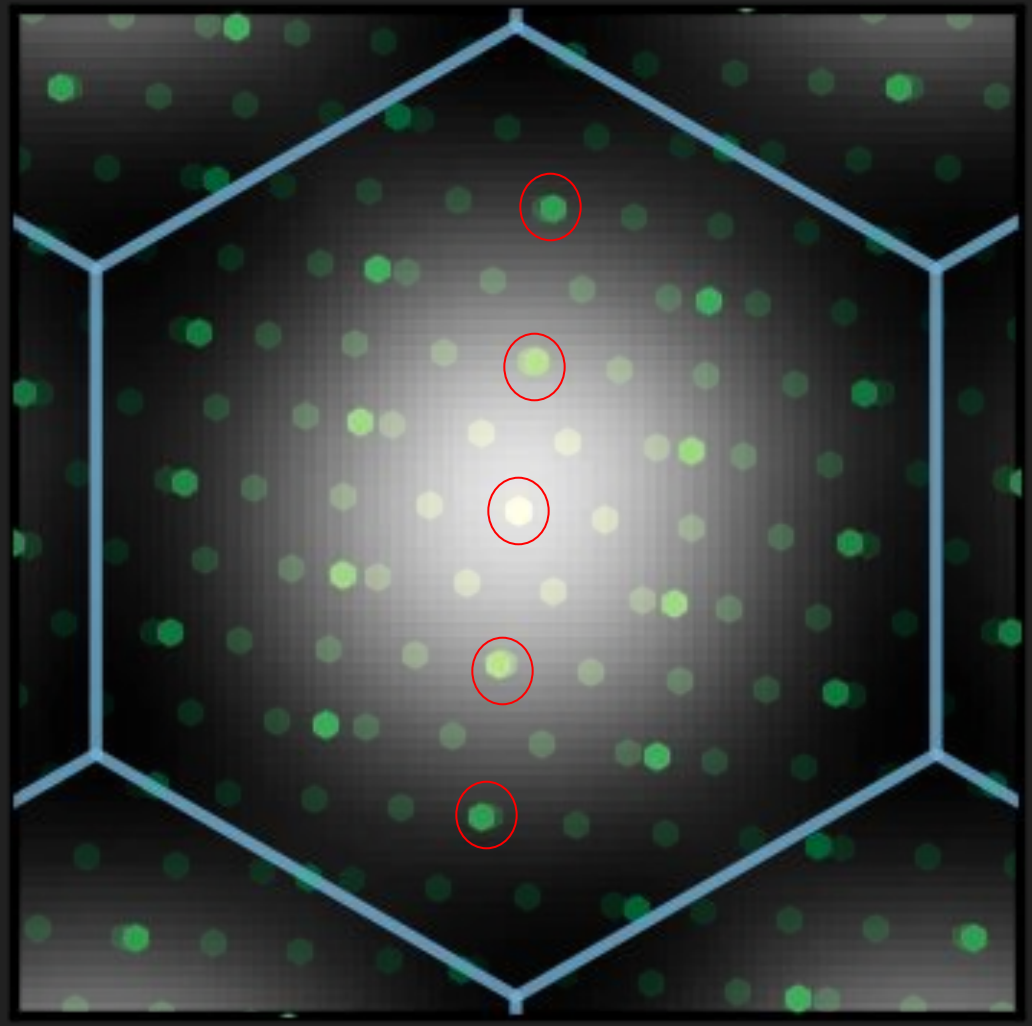
twist_min_search: 34.98
twist_max_search: 35.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 368
Mo Atoms (Top Layer): 133
Mo Atoms (Bottom Layer): 133



twist_min_search: 39.98
twist_max_search: 40.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 939
Mo Atoms (Top Layer): 256
Mo Atoms (Bottom Layer): 257



twist_min_search: 44.98
twist_max_search: 45.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 258
Mo Atoms (Top Layer): 43
Mo Atoms (Bottom Layer): 43



twist_min_search: 49.98
twist_max_search: 50.02
max_strain: 0.02
is_1D_dir_1: False
is_1D_dir_2: False
Rmax_max_search: 16
max_iter_twist_search: 5
Total Atoms: 546
Mo Atoms (Top Layer): 294
Mo Atoms (Bottom Layer): 294

MoS_2 WSe_2 Q1D Structures

0 degree

twist_min_search = 0

twist_max_search = 0.1

max_strain = 0.2

is_1D_dir_1 = True

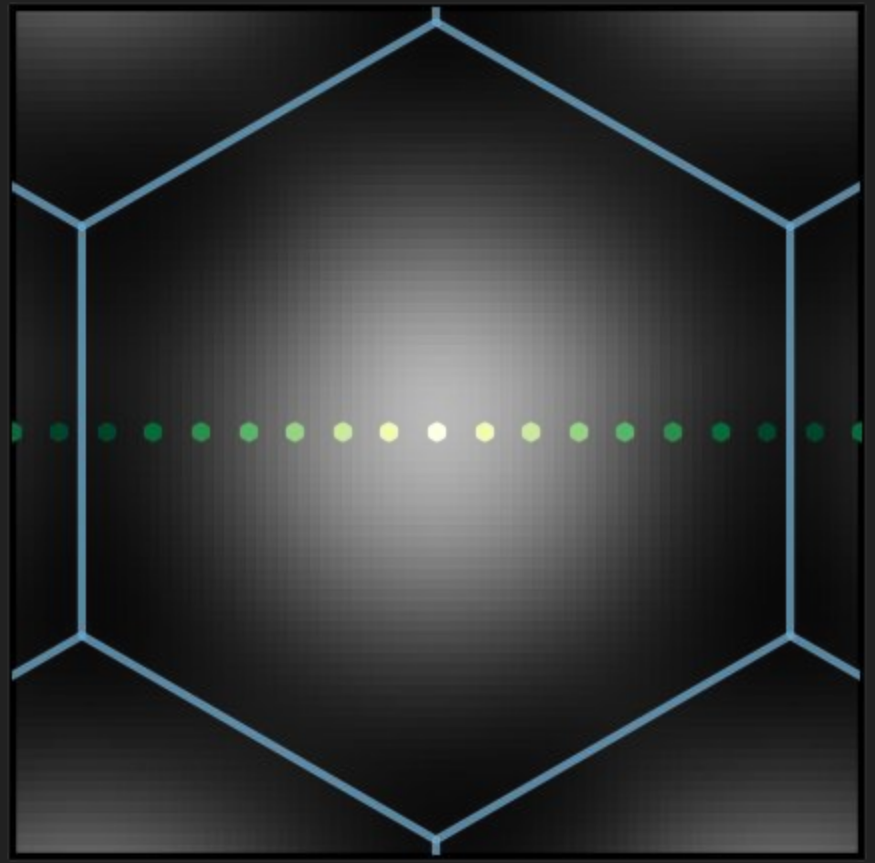
Rmax_max_search = 16

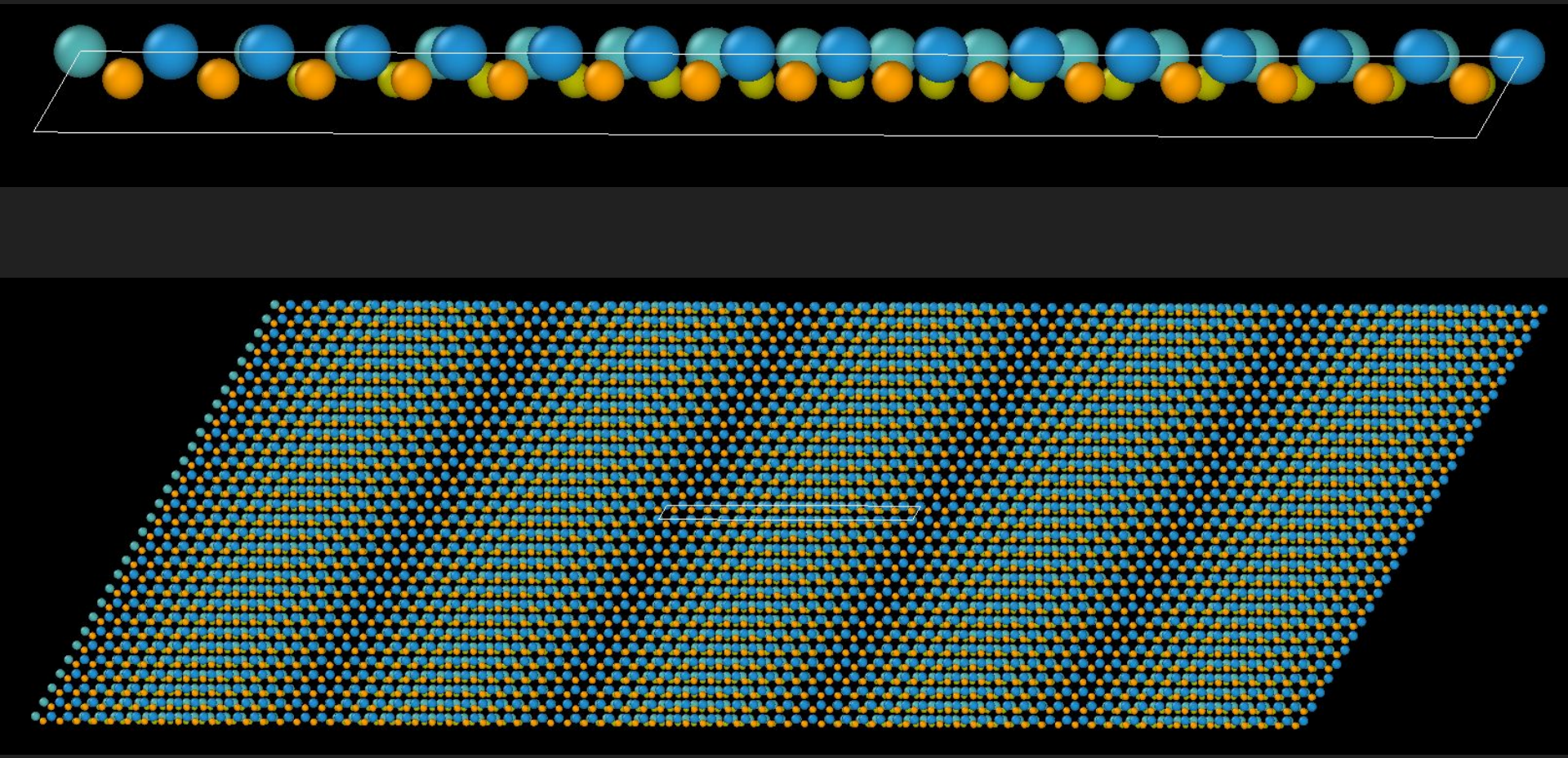
max_iter_twist_search = 5

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

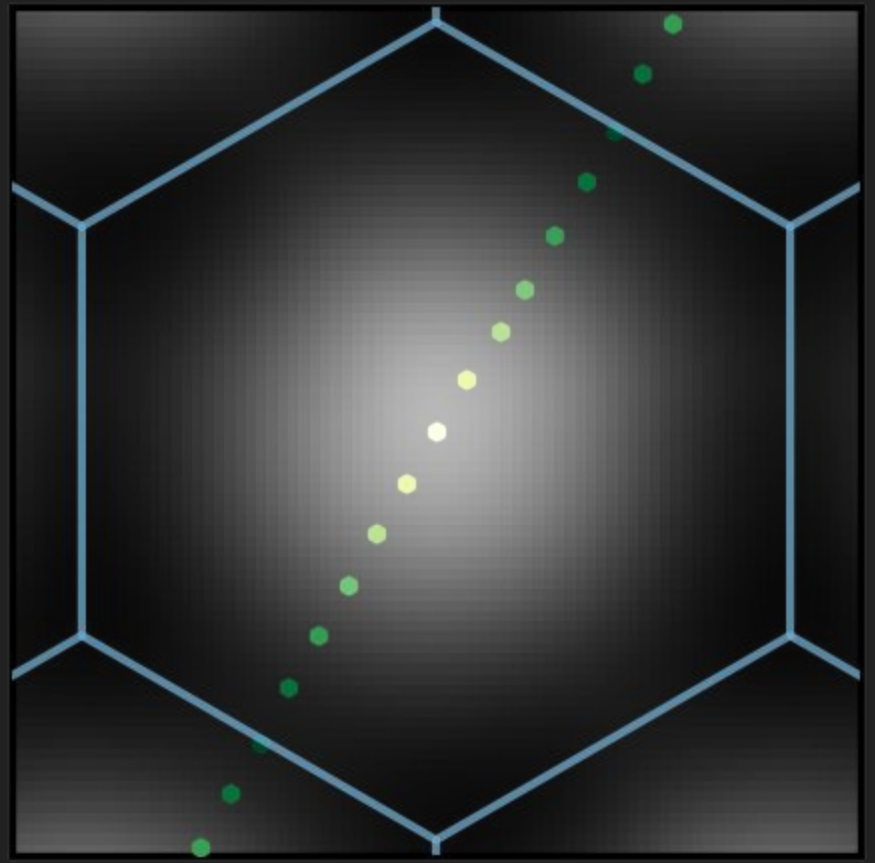
Rmax_max_search = 16

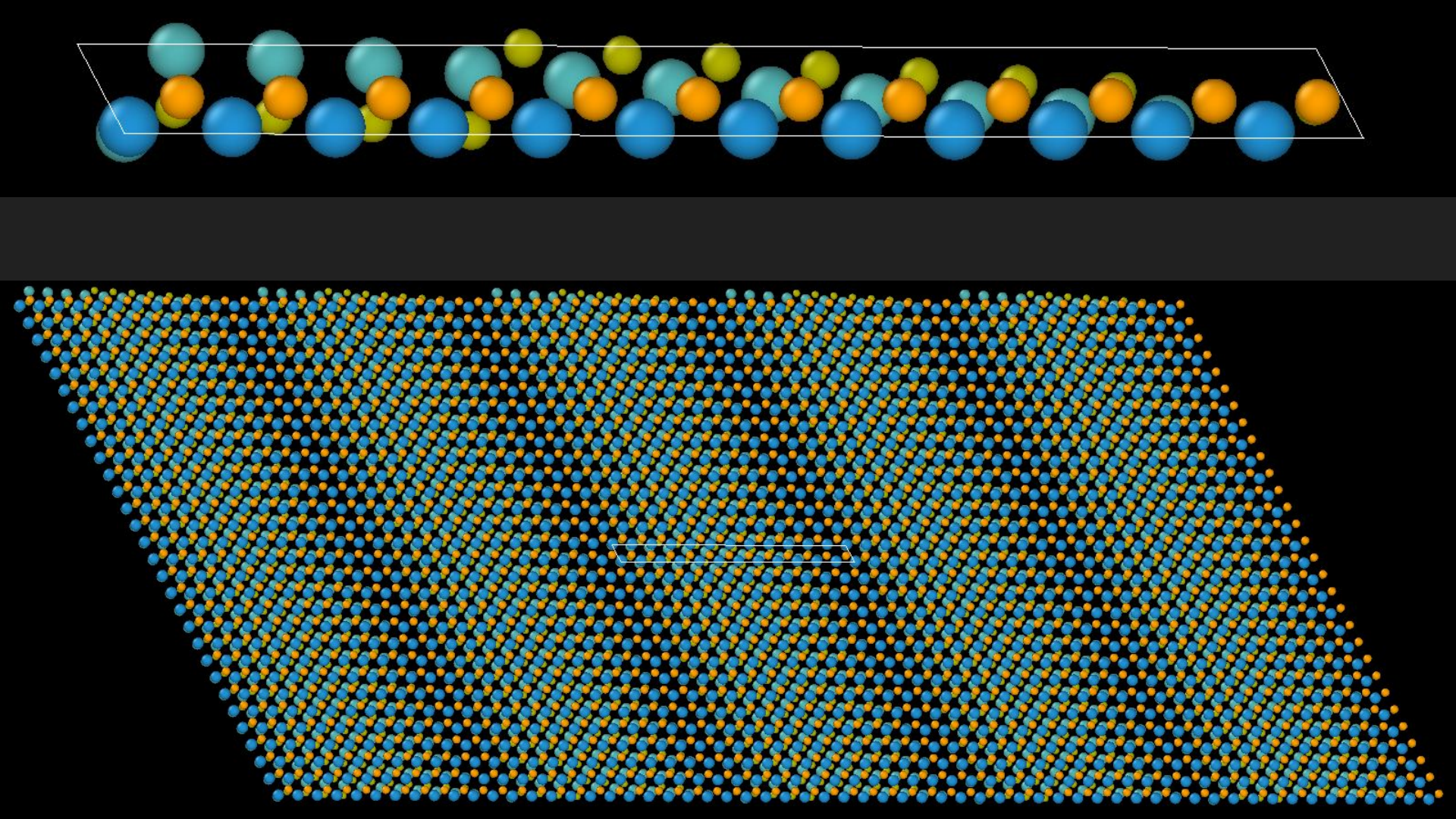
max_iter_twist_search = 5

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

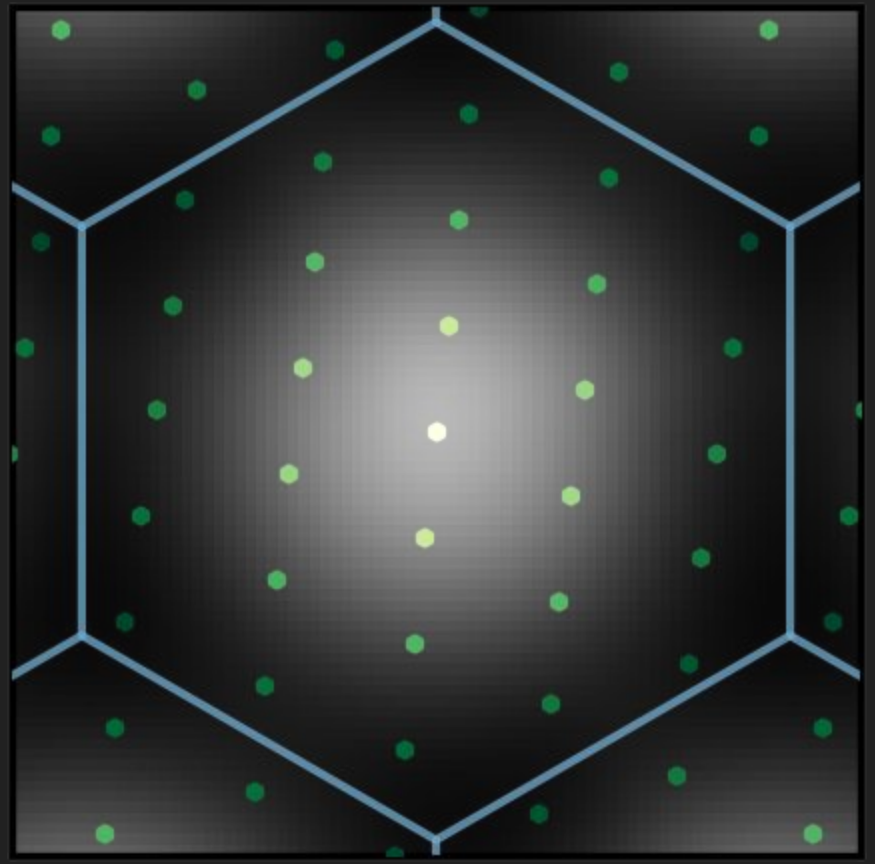
Rmax_max_search = 30

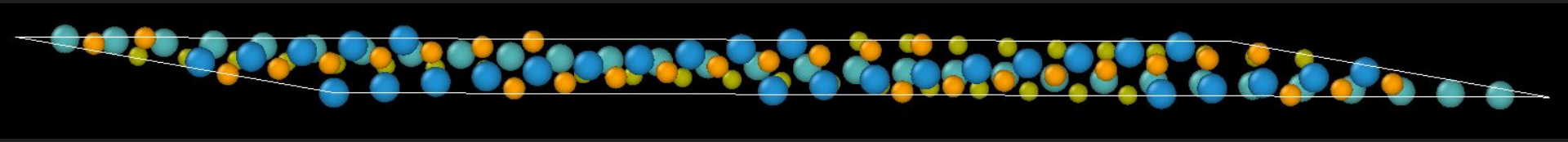
max_iter_twist_search = 5

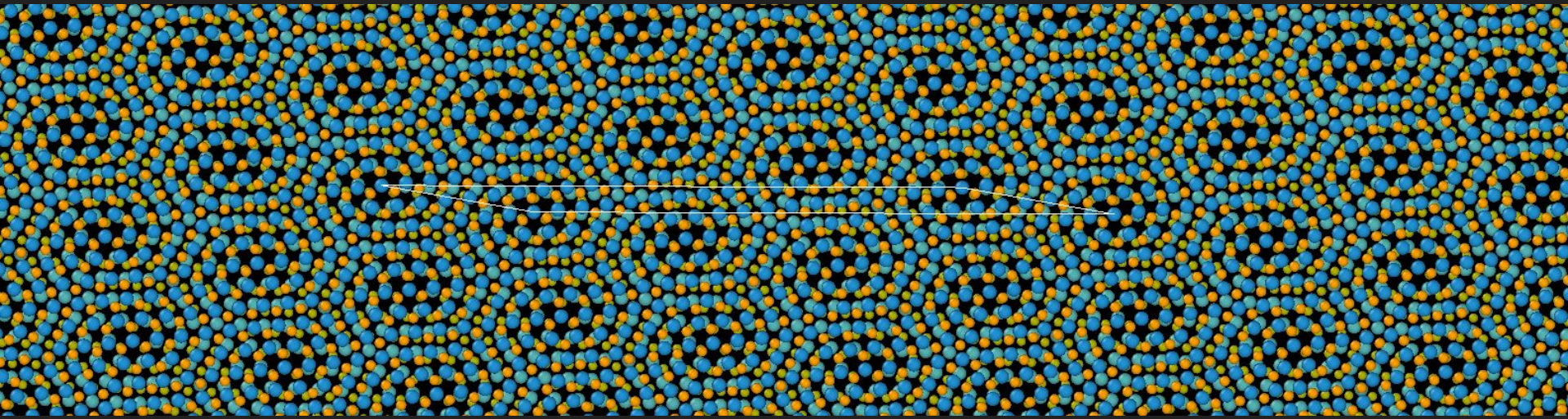
Total atoms: 180

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

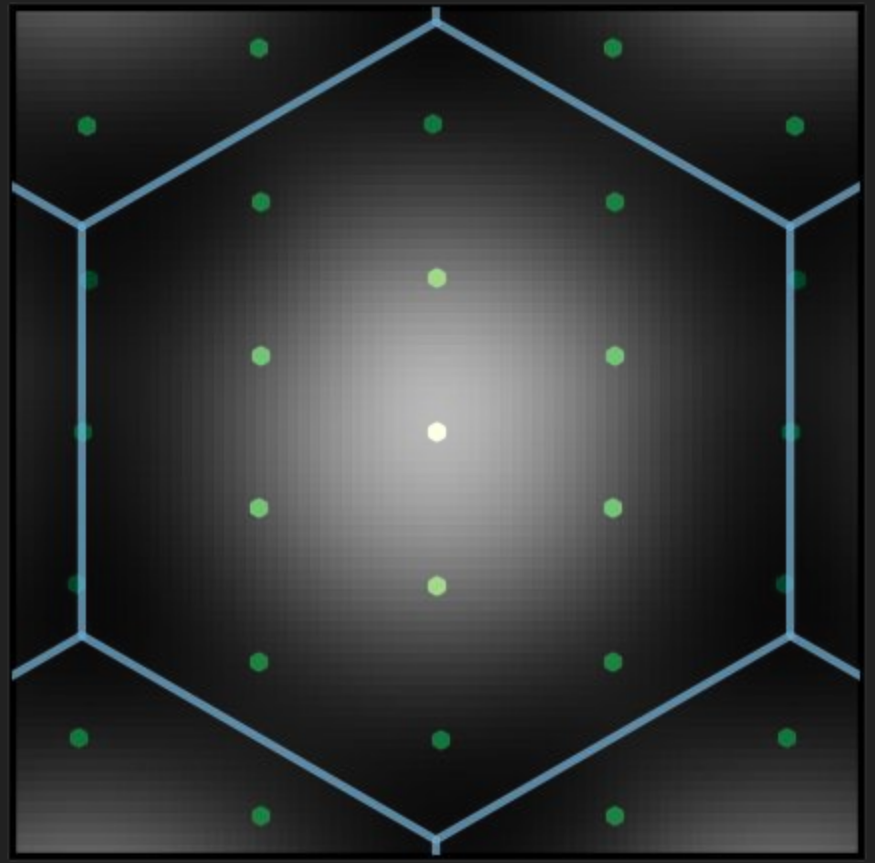
Rmax_max_search = 14

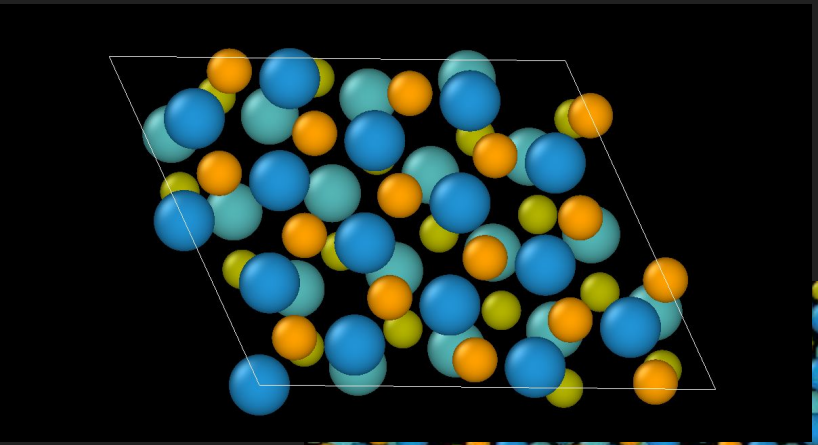
max_iter_twist_search = 5

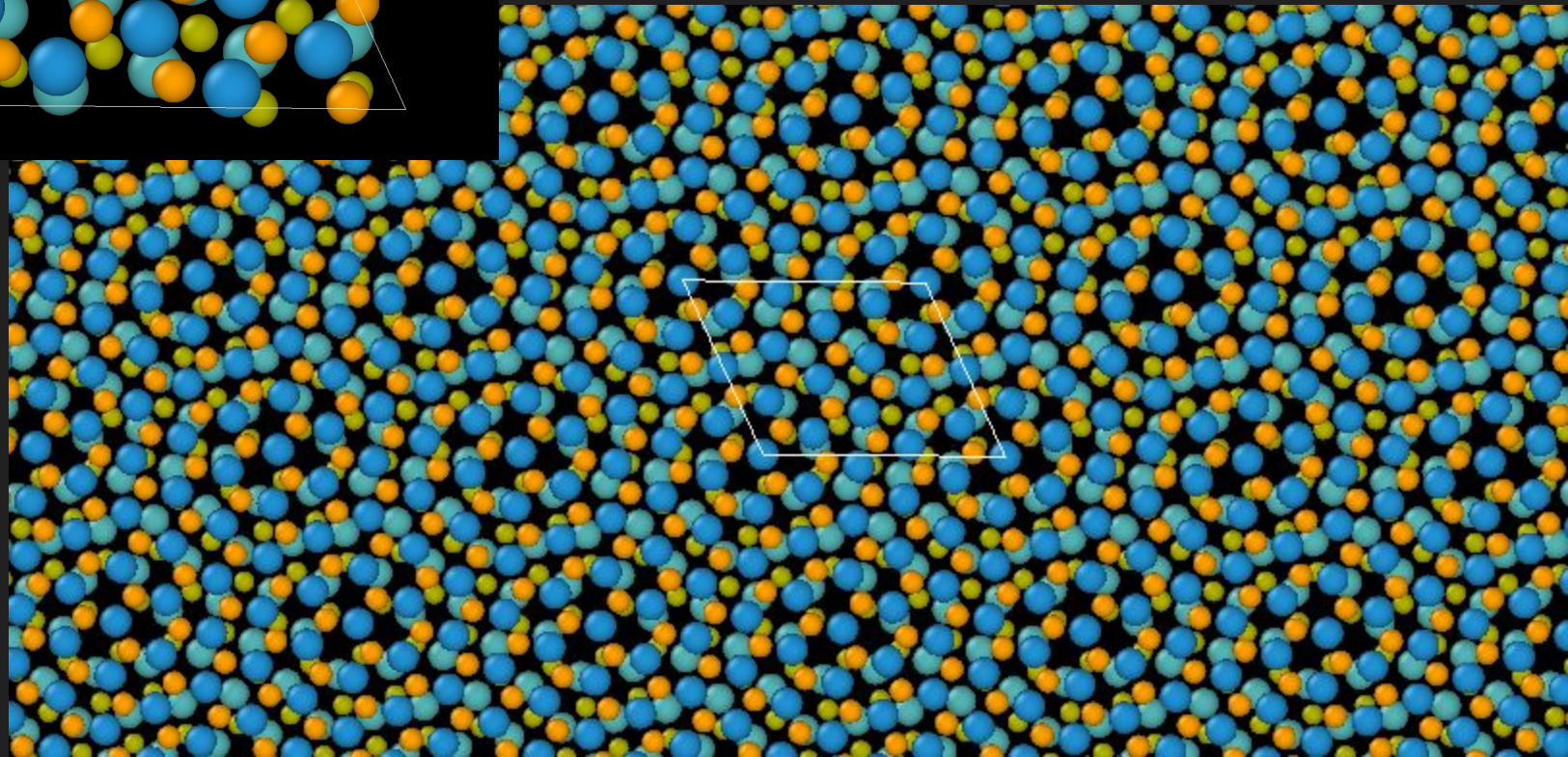
Total atoms: 99

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

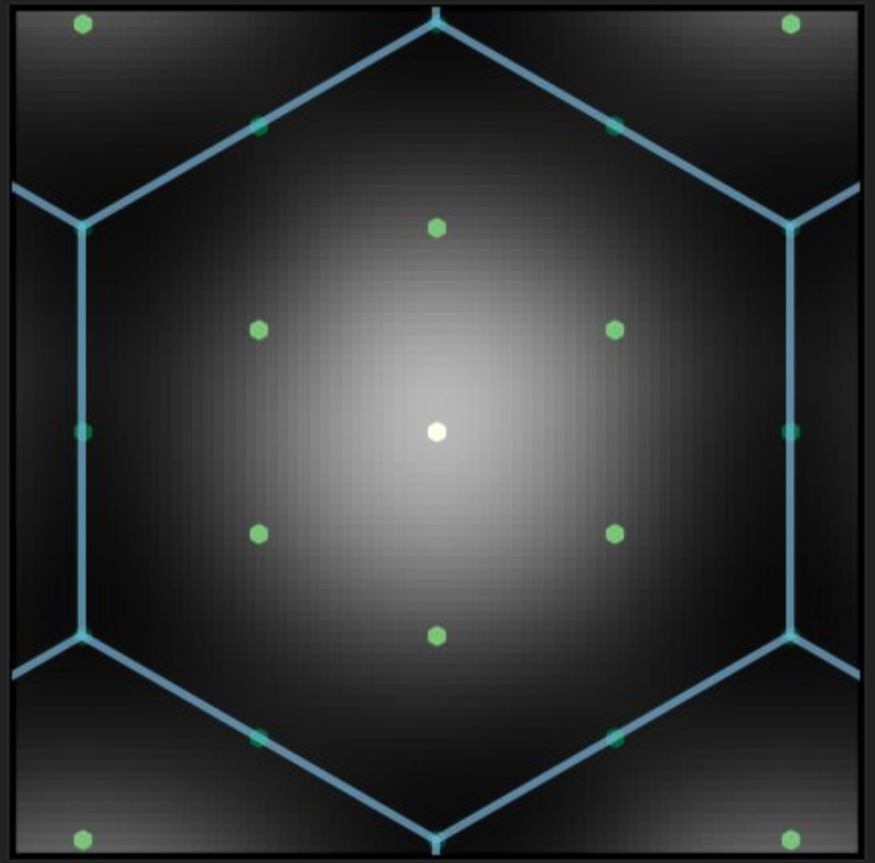
Rmax_max_search = 16

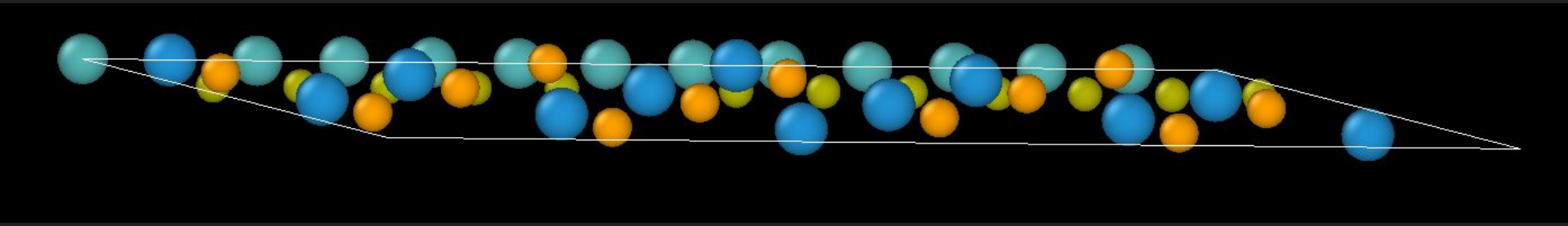
max_iter_twist_search = 5

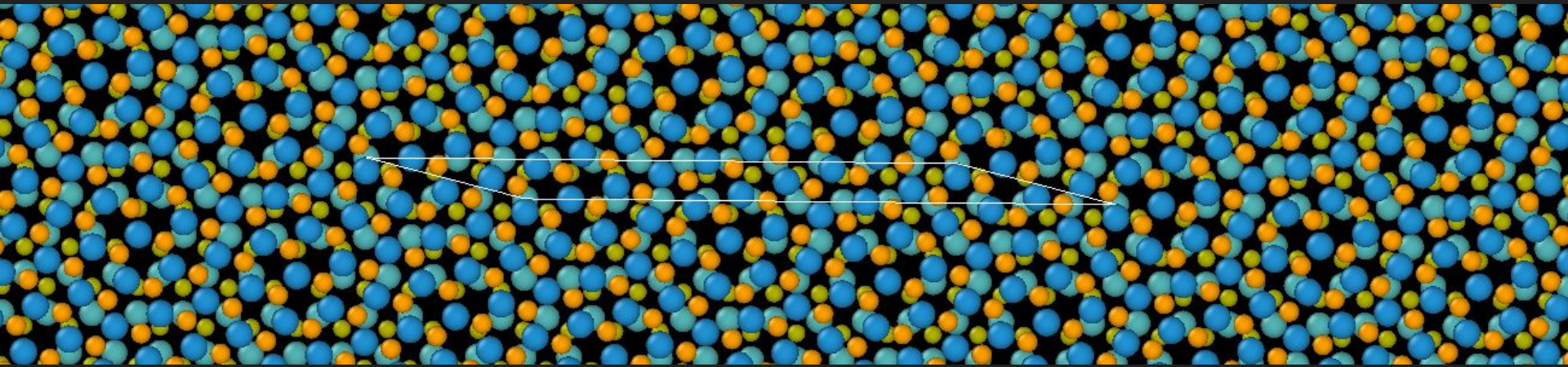
Total atoms: 75

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

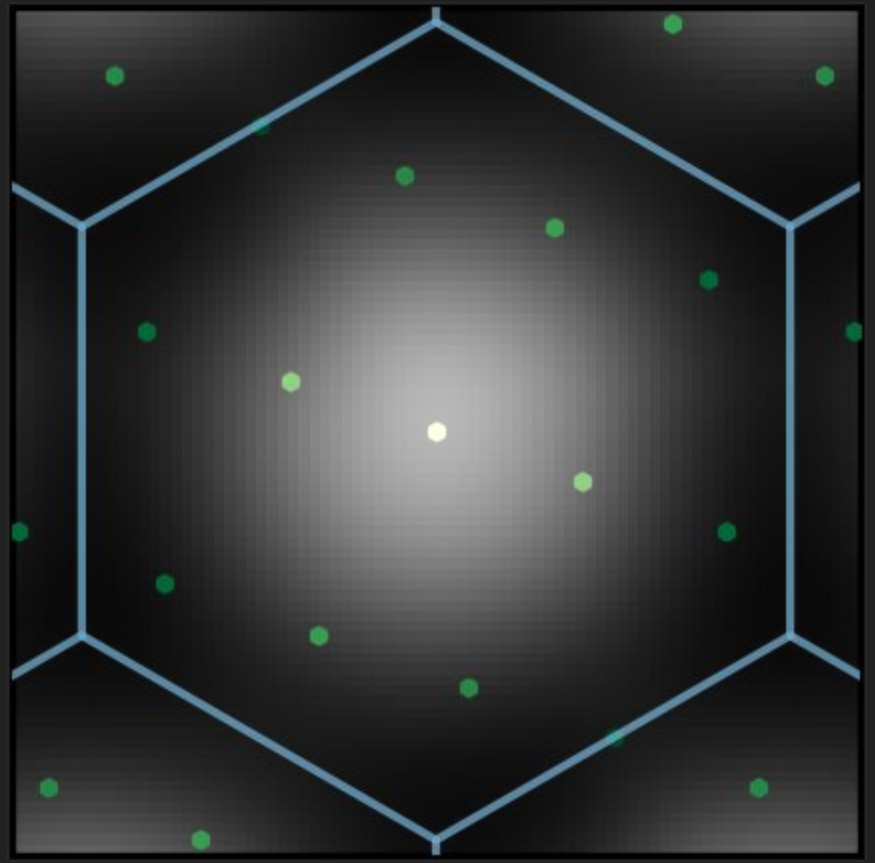
Rmax_max_search = 16

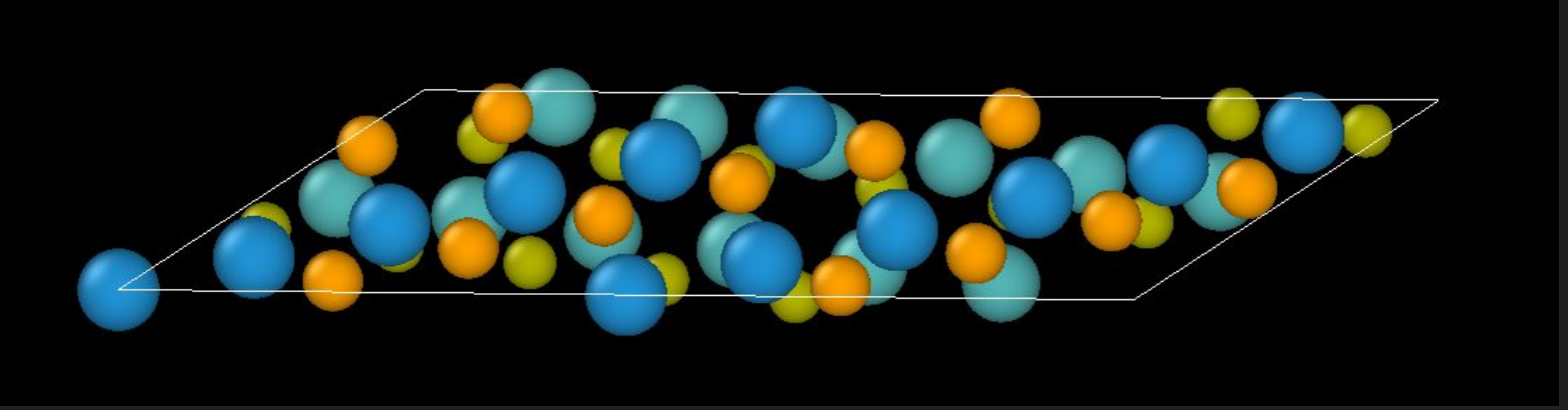
max_iter_twist_search = 5

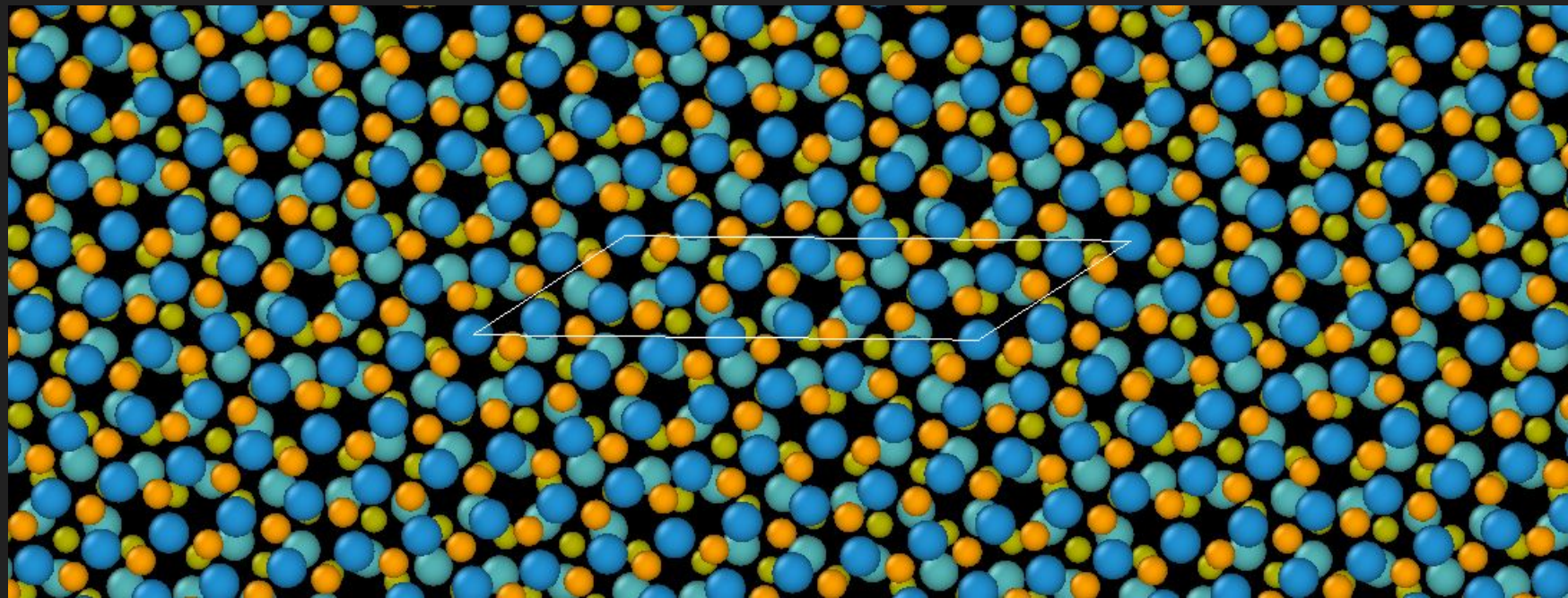
Total atoms: 75

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

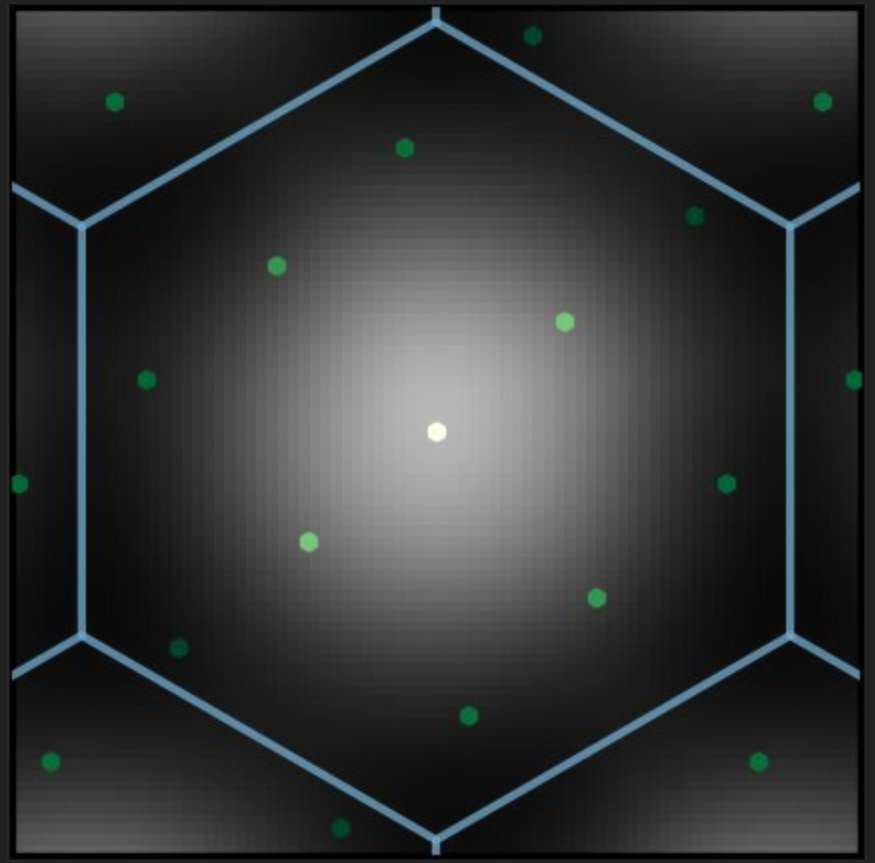
Rmax_max_search = 14

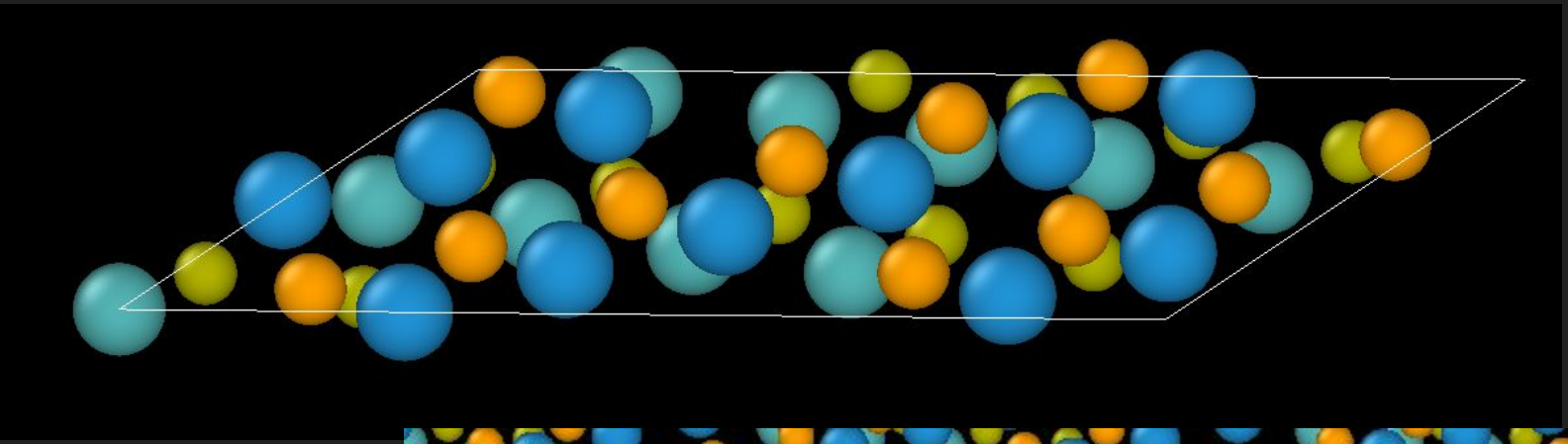
max_iter_twist_search = 5

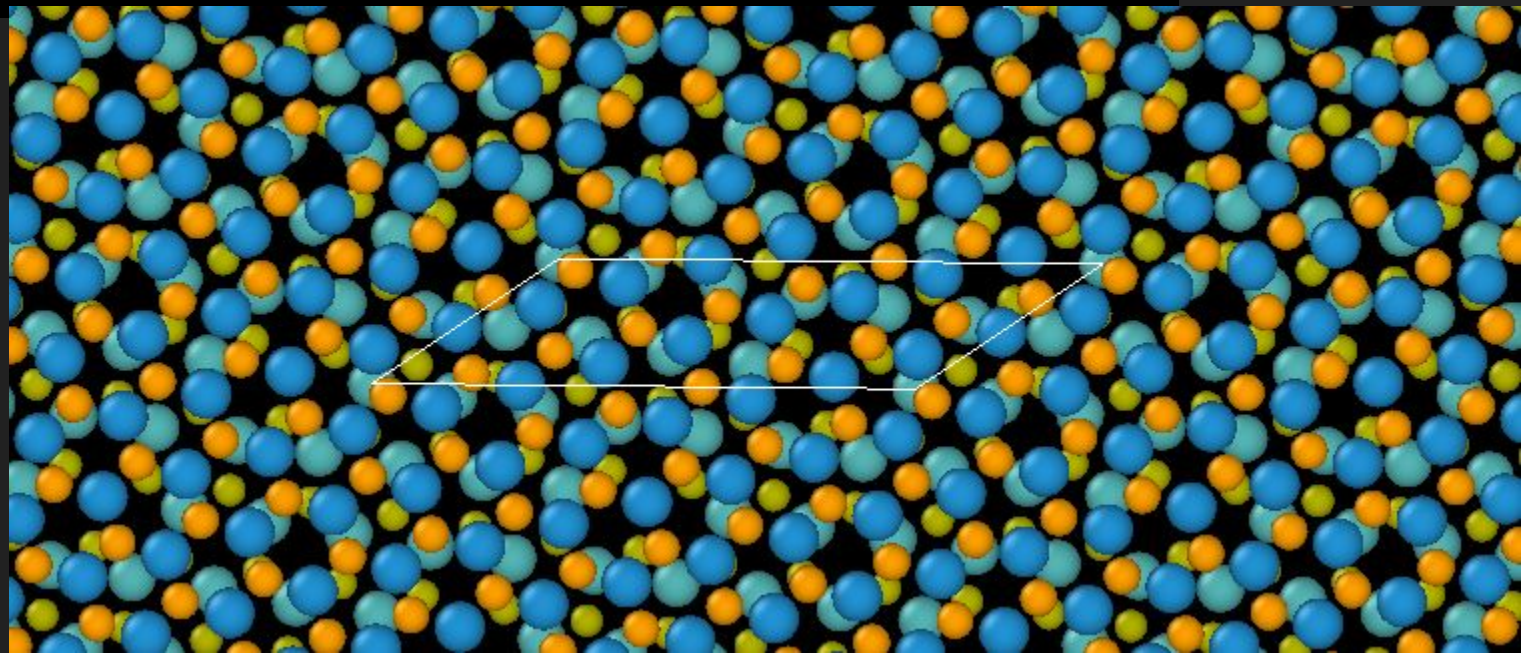
Total atoms: 66

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

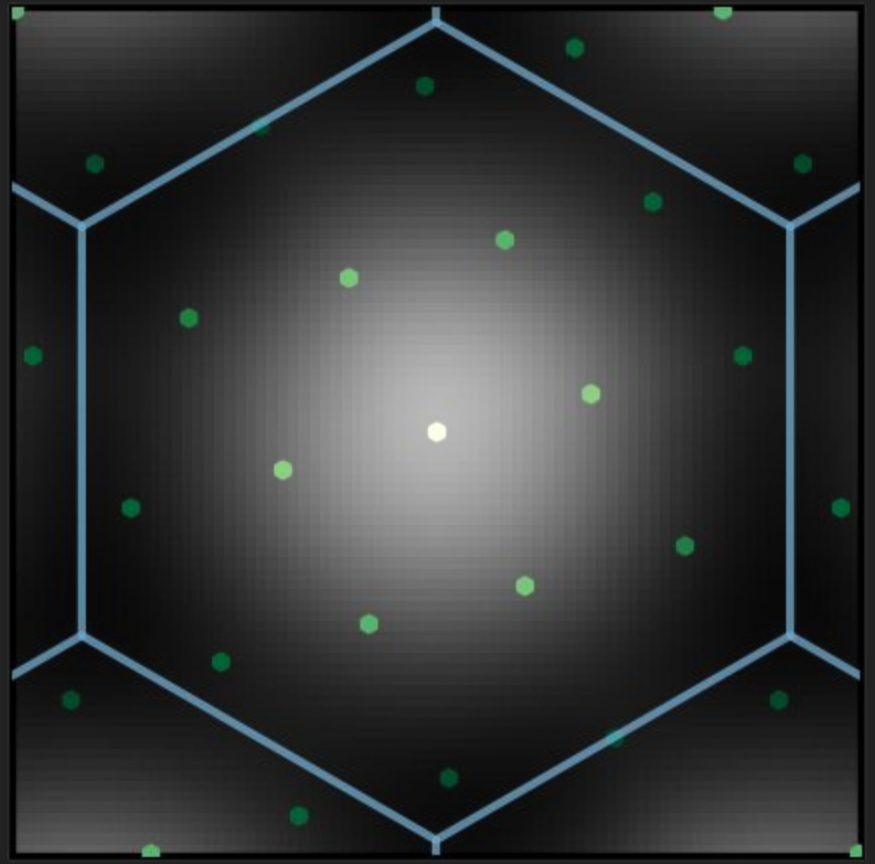
Rmax_max_search = 14

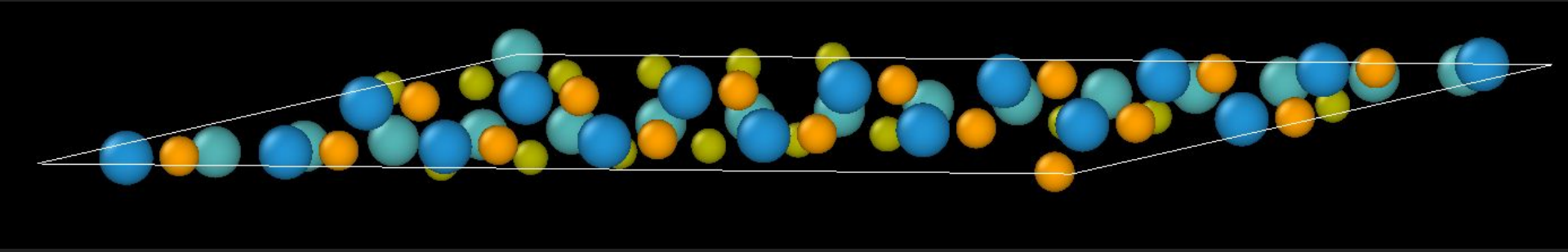
max_iter_twist_search = 5

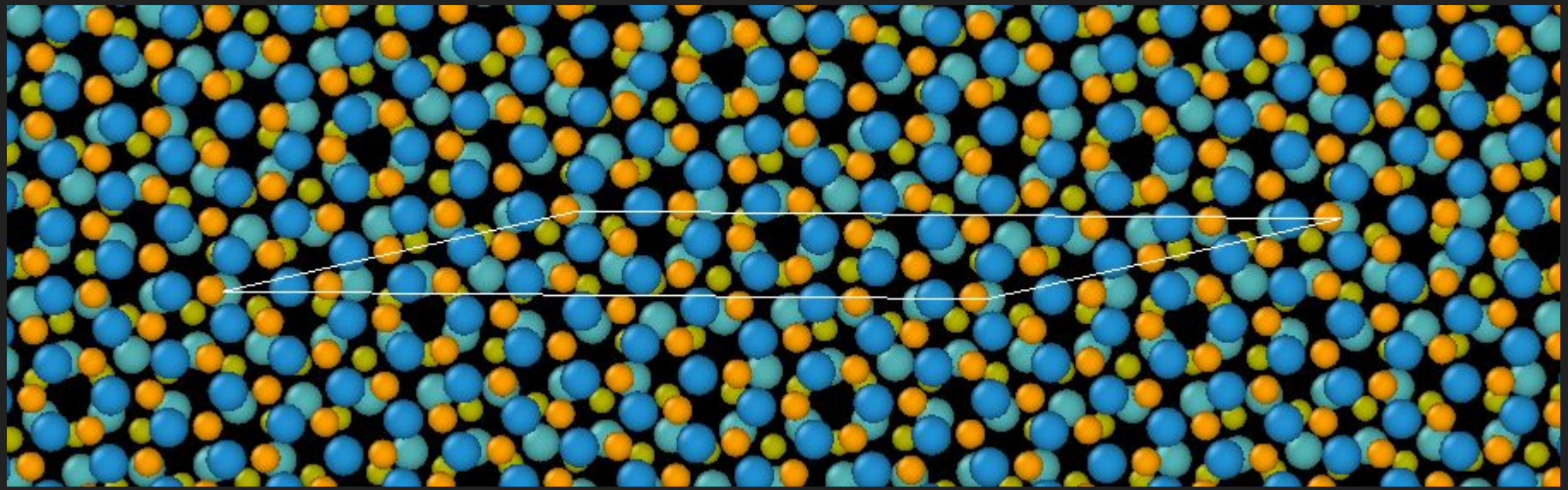
Total atoms: 99

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

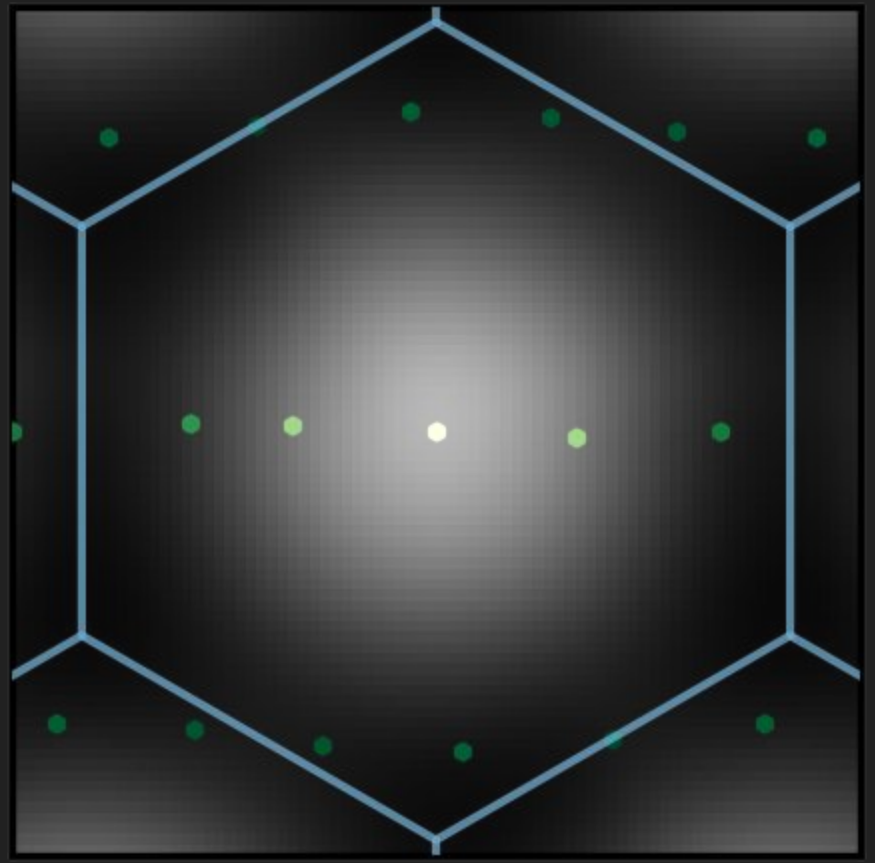
Rmax_max_search = 14

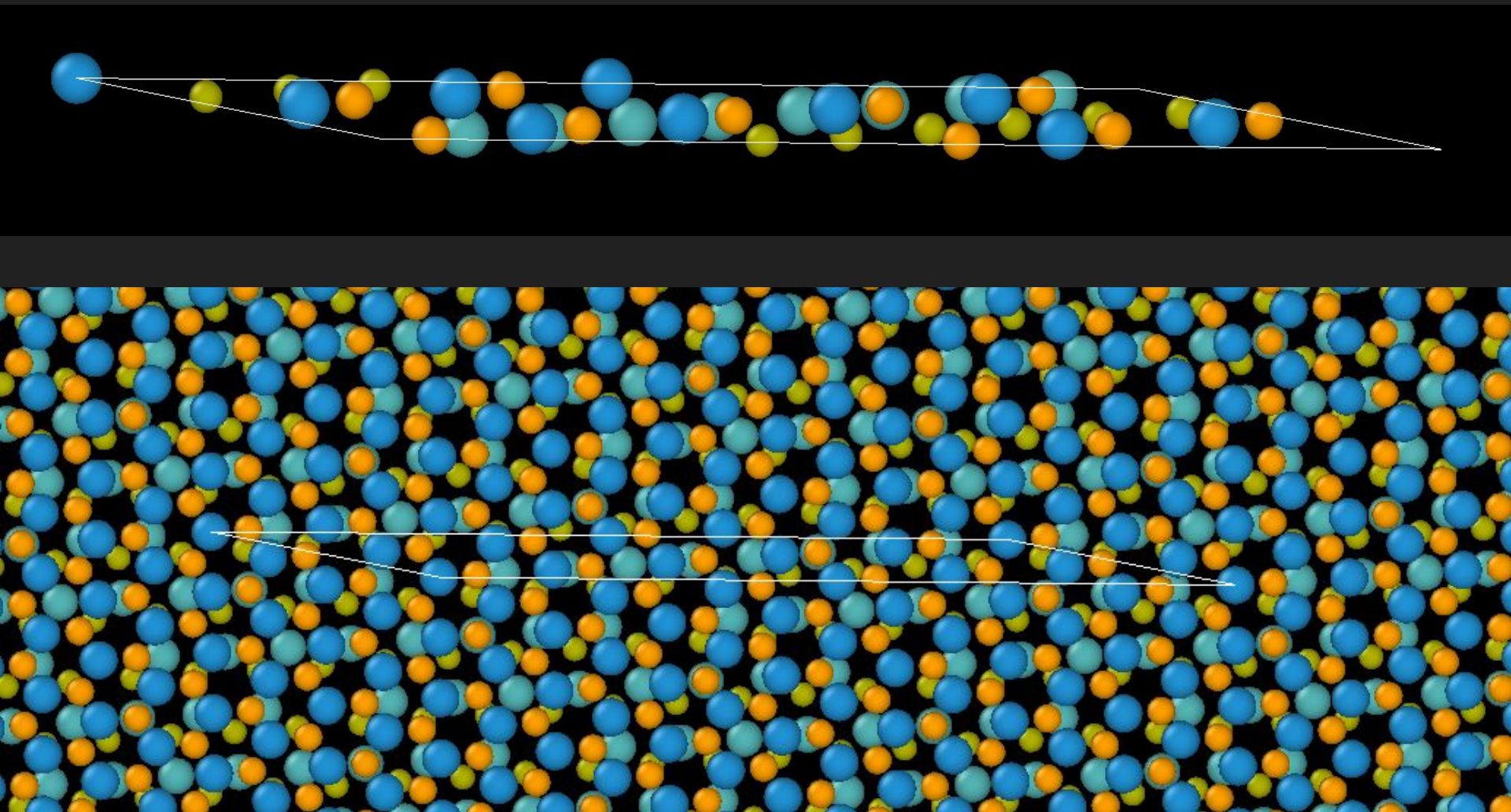
max_iter_twist_search = 5

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

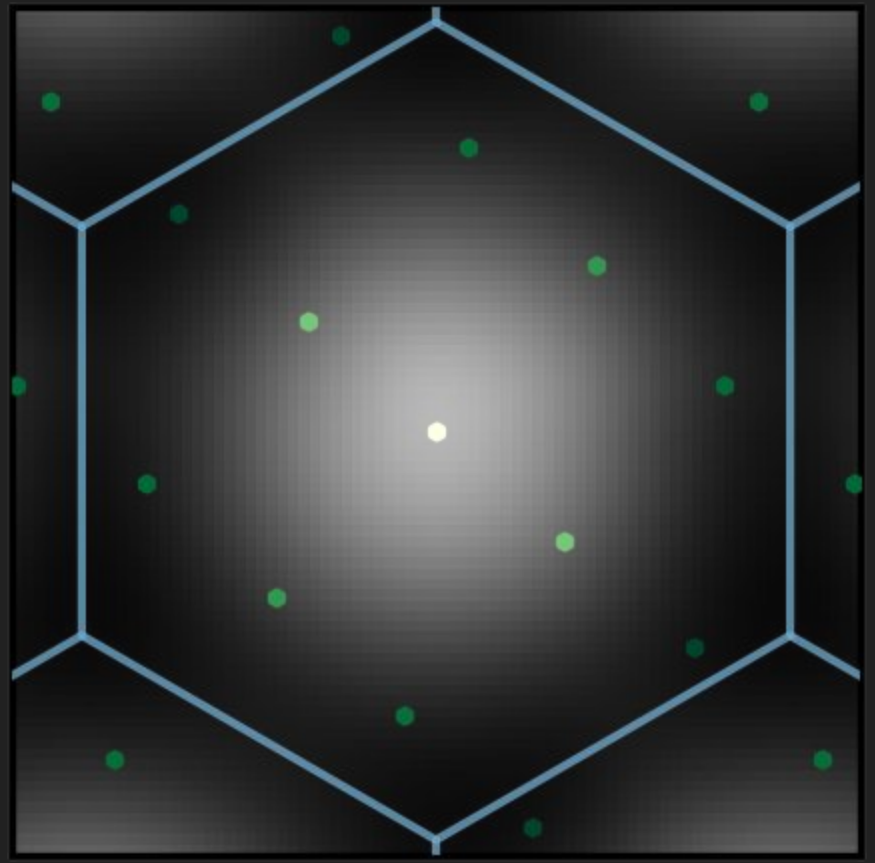
Rmax_max_search = 14

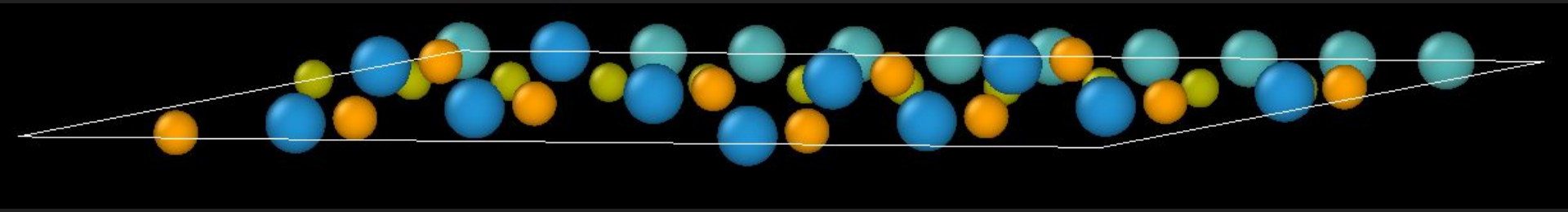
max_iter_twist_search = 5

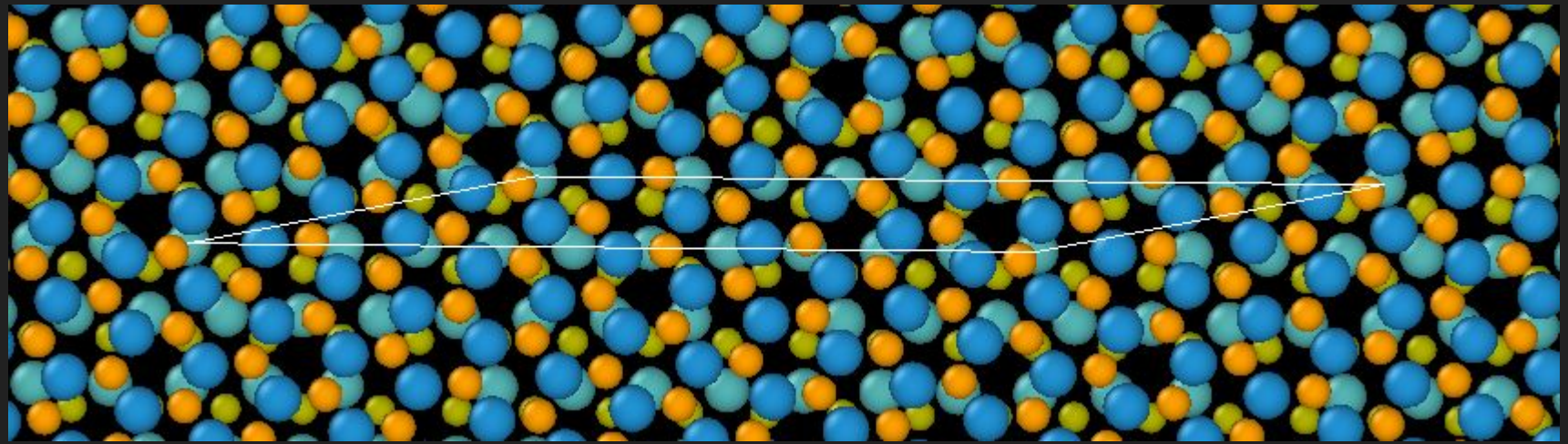
Total atoms: 66

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

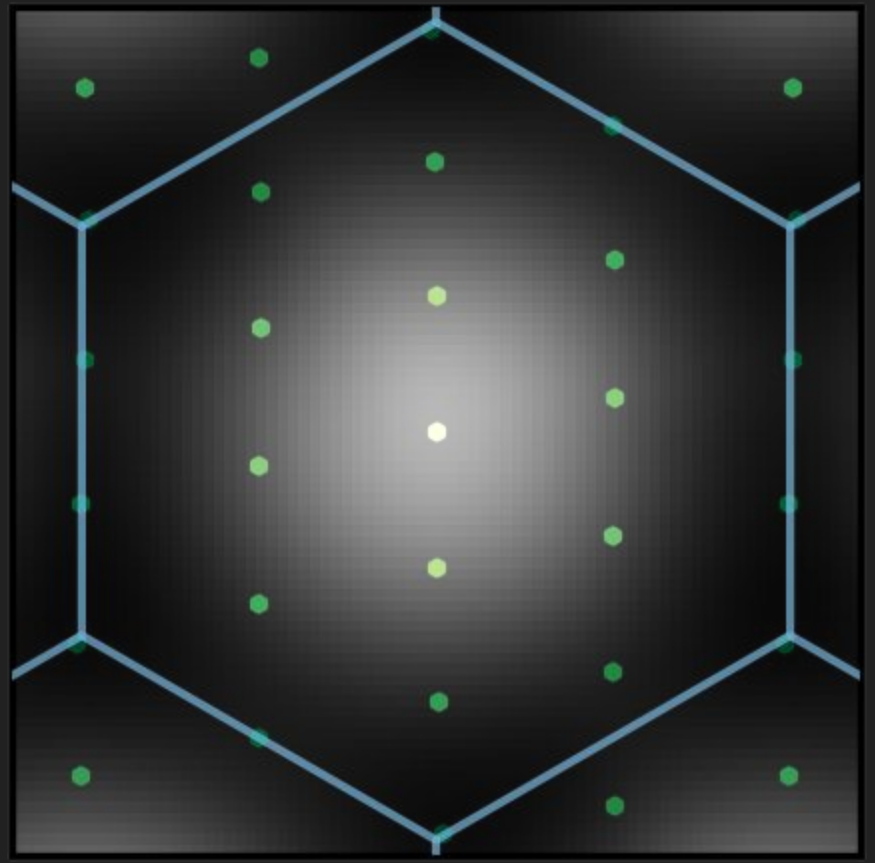
Rmax_max_search = 16

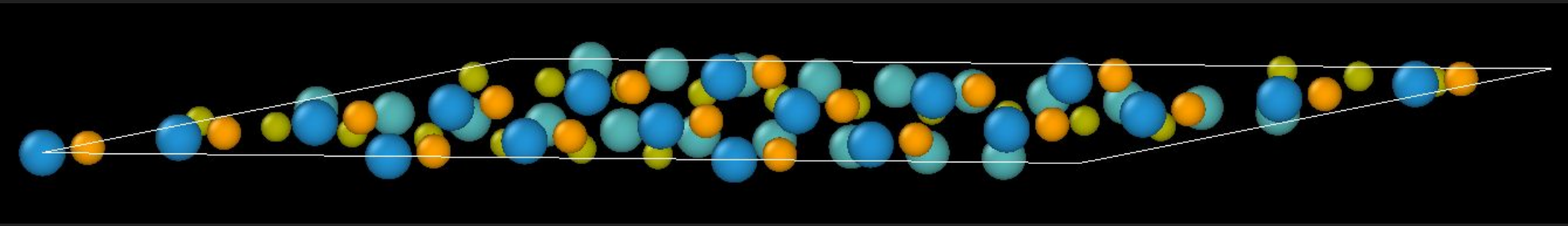
max_iter_twist_search = 5

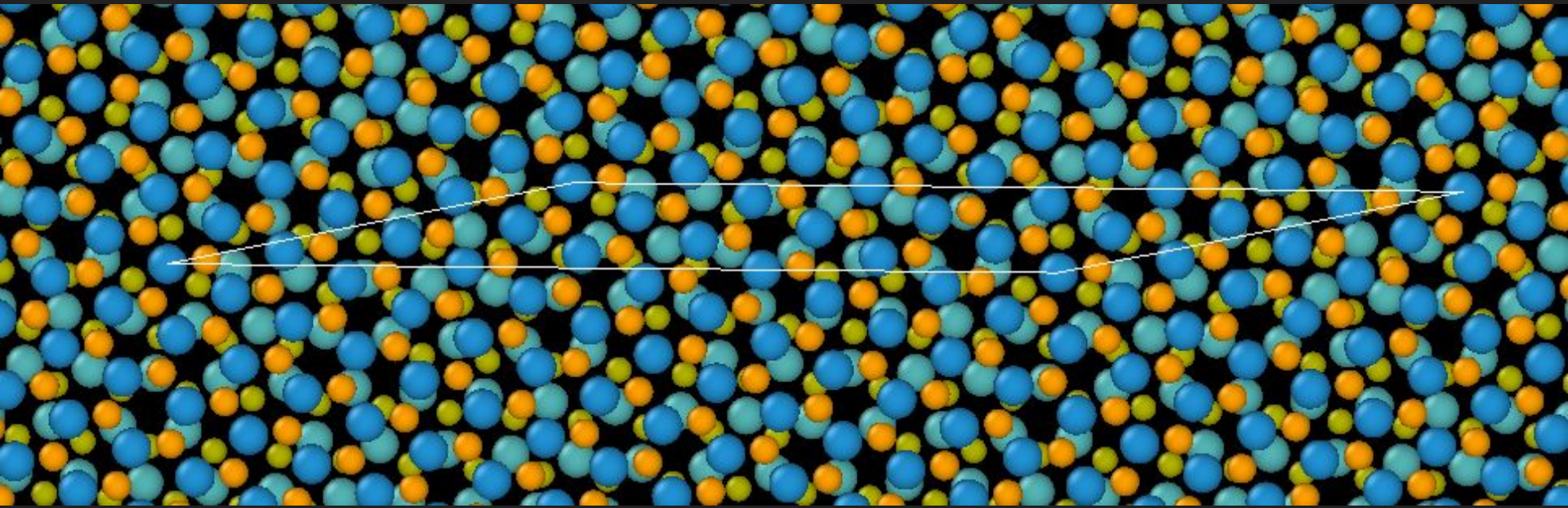
Total atoms: 117

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

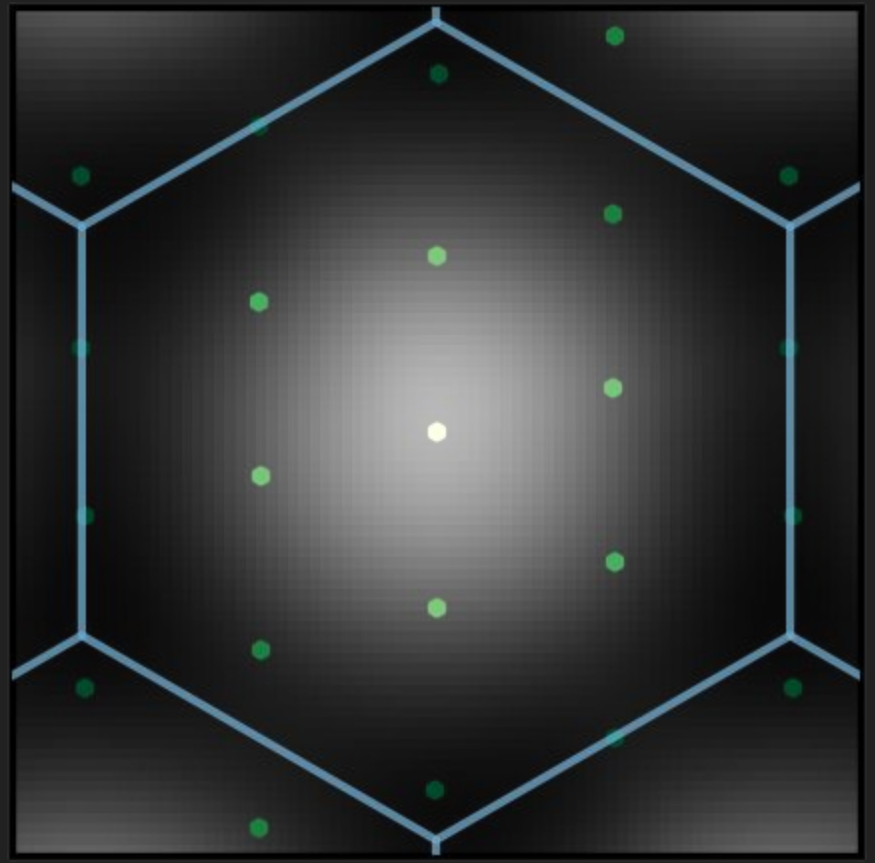
Rmax_max_search = 16

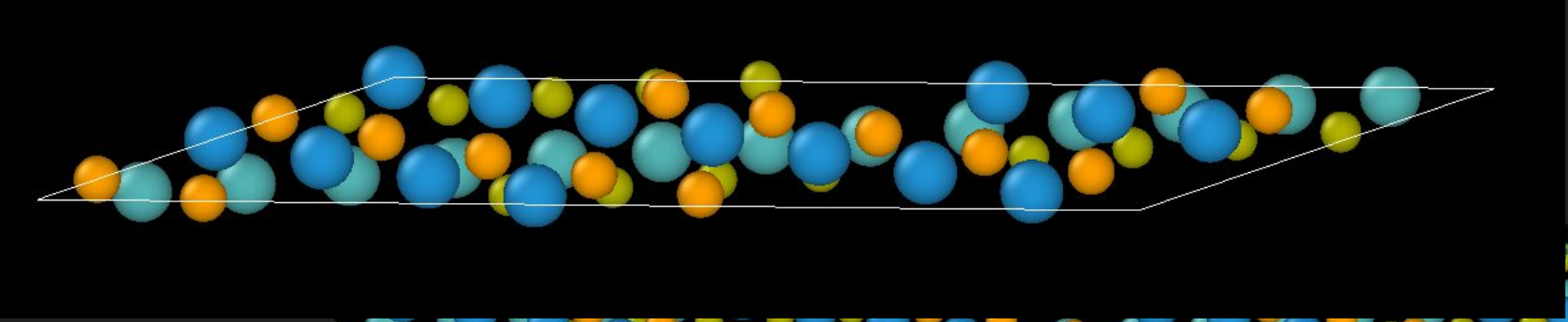
max_iter_twist_search = 5

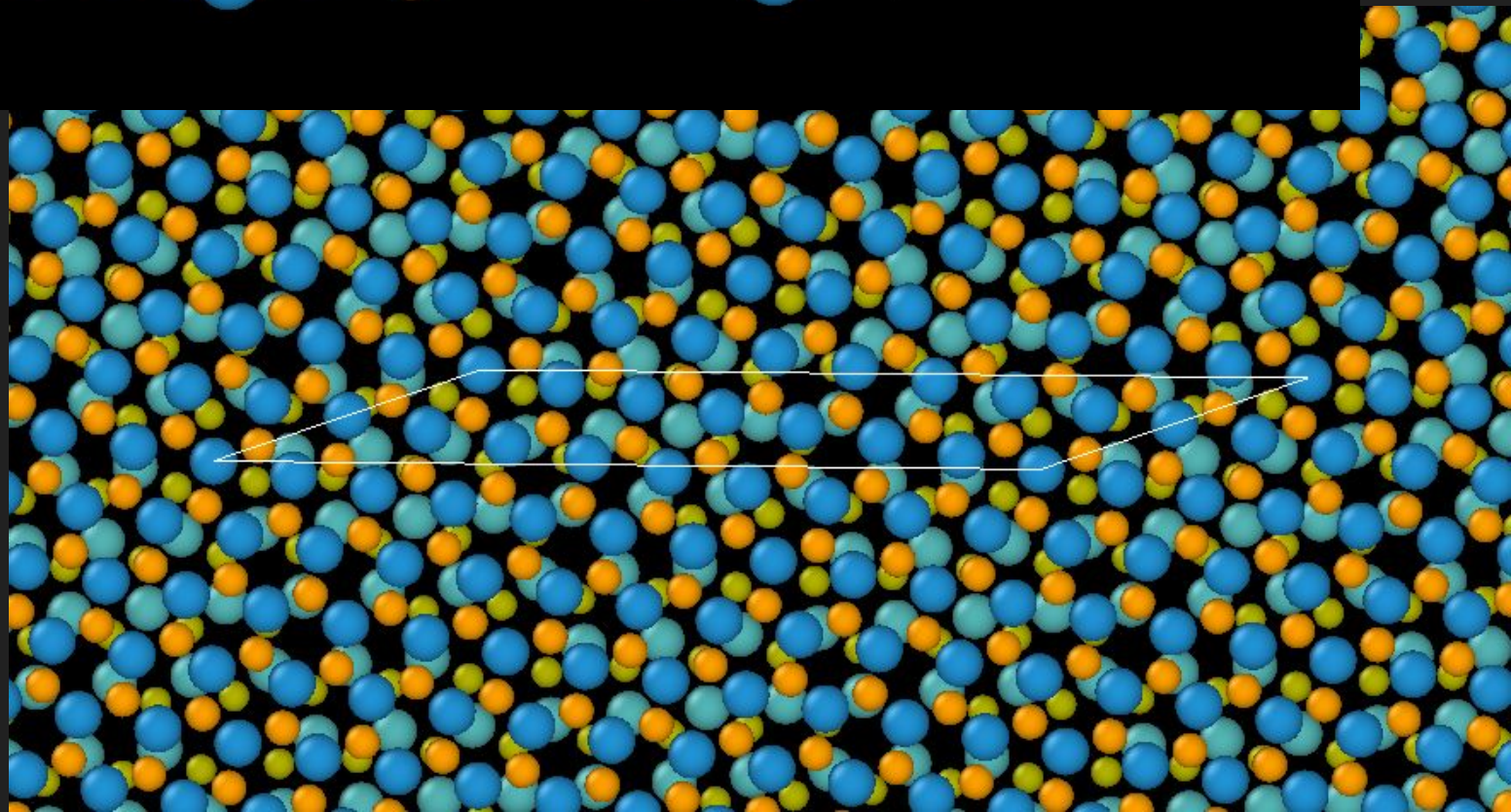
Total atoms: 84

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

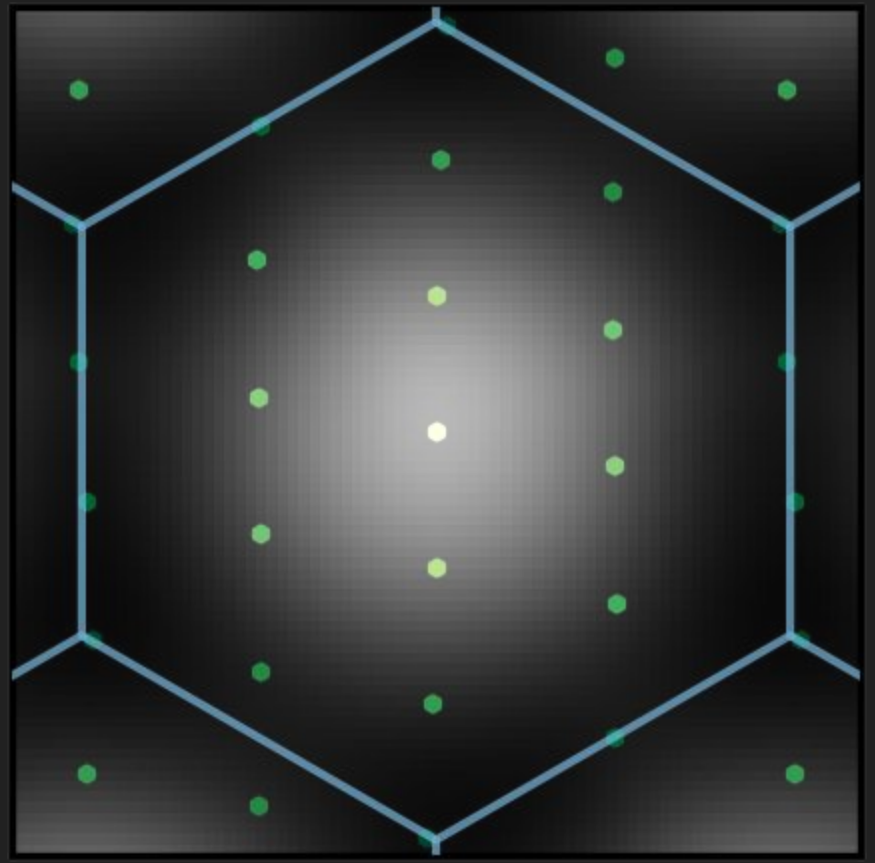
Rmax_max_search = 16

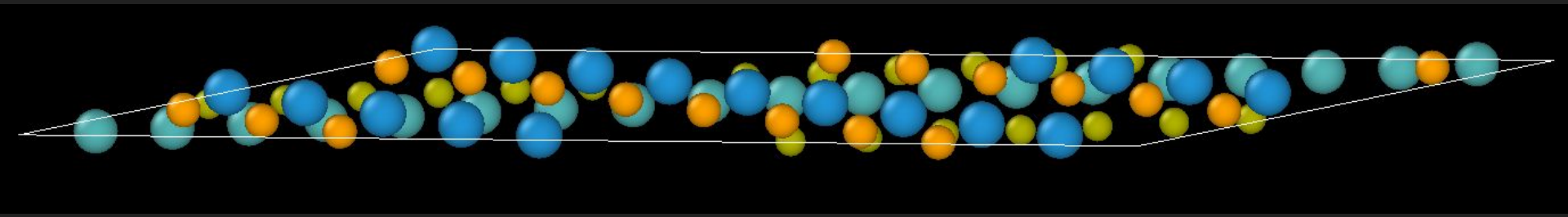
max_iter_twist_search = 5

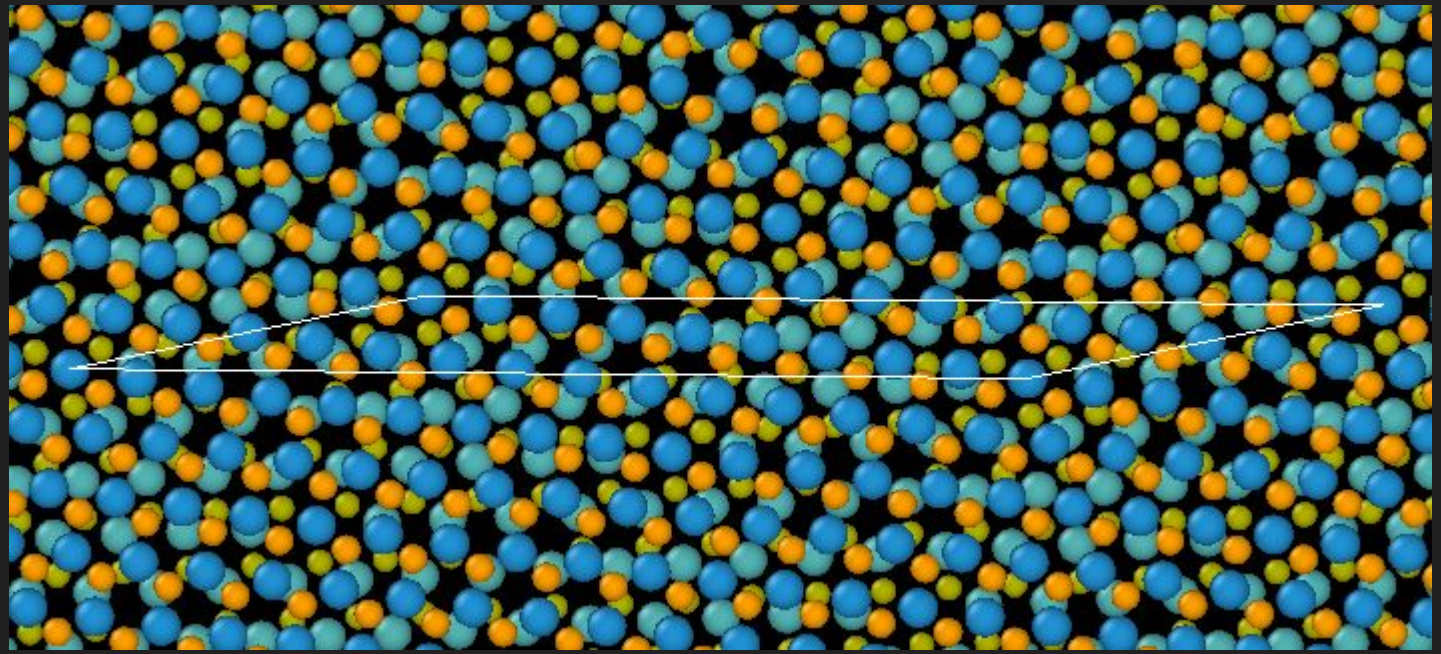
Total atoms: 114

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

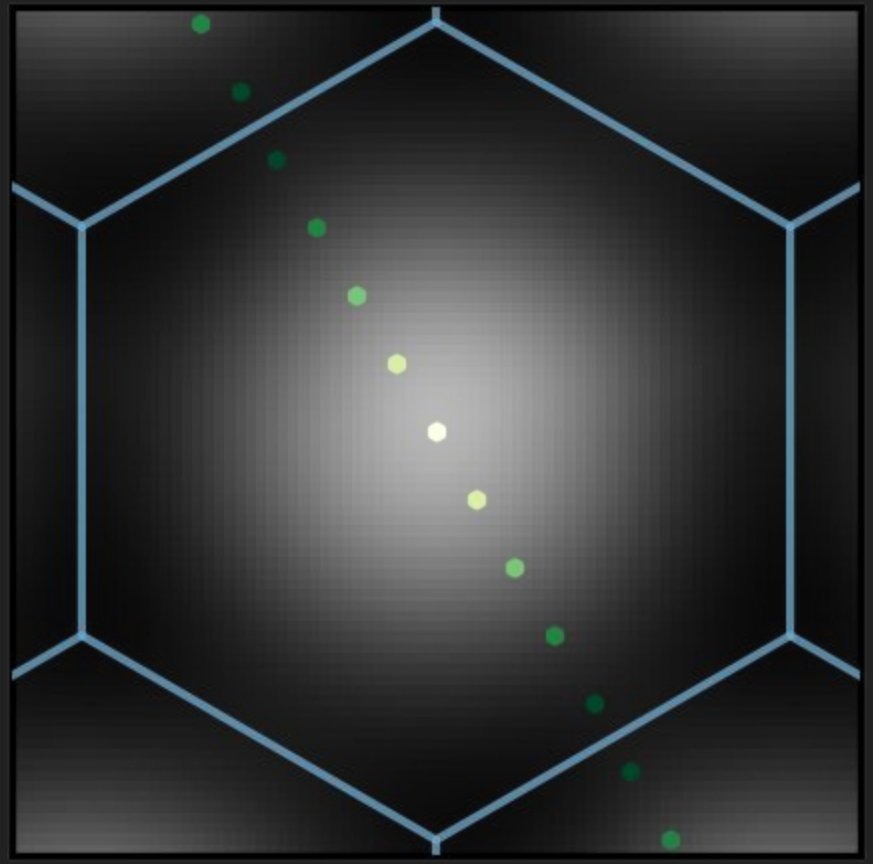
Rmax_max_search = 16

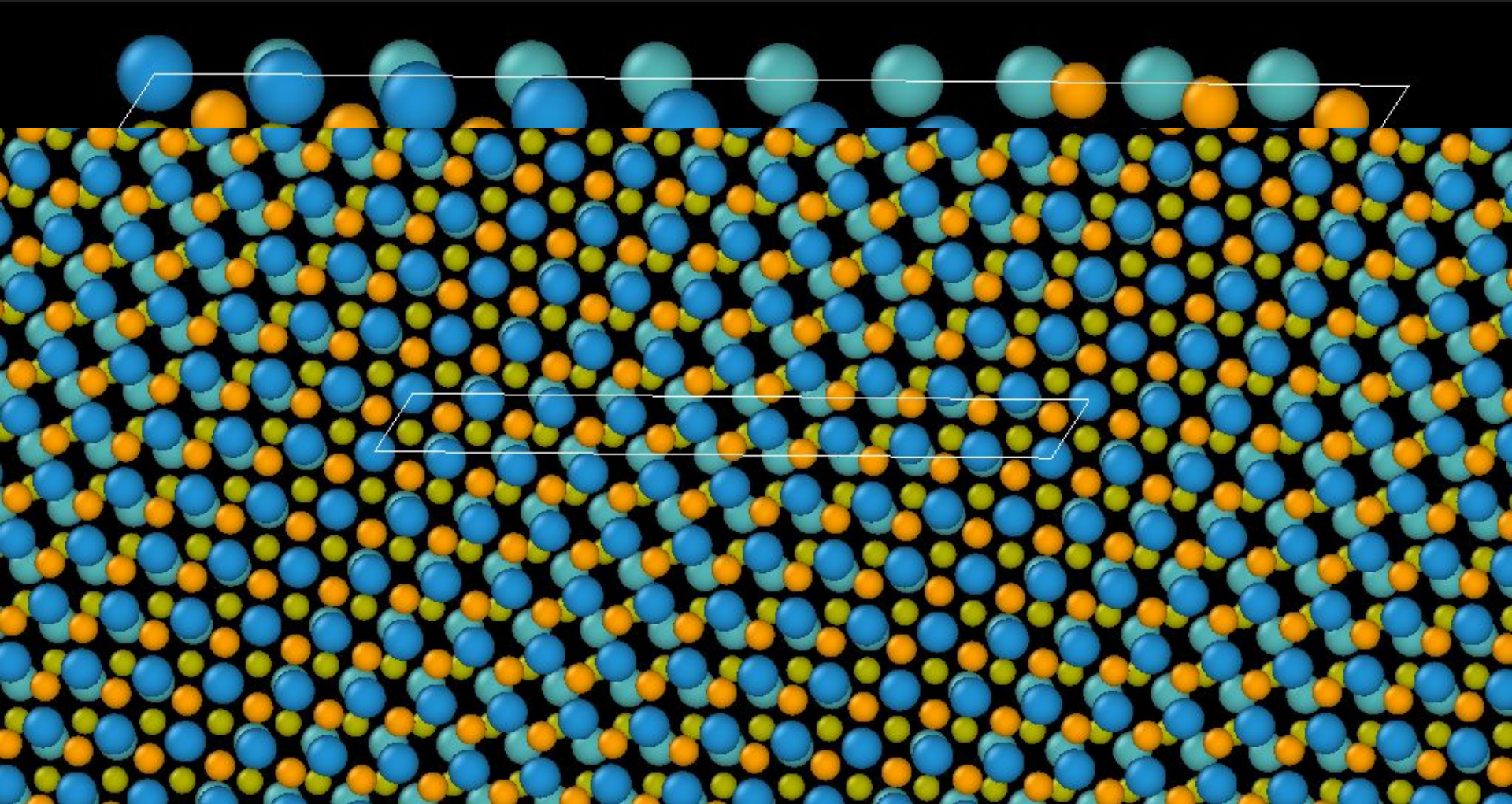
max_iter_twist_search = 5

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

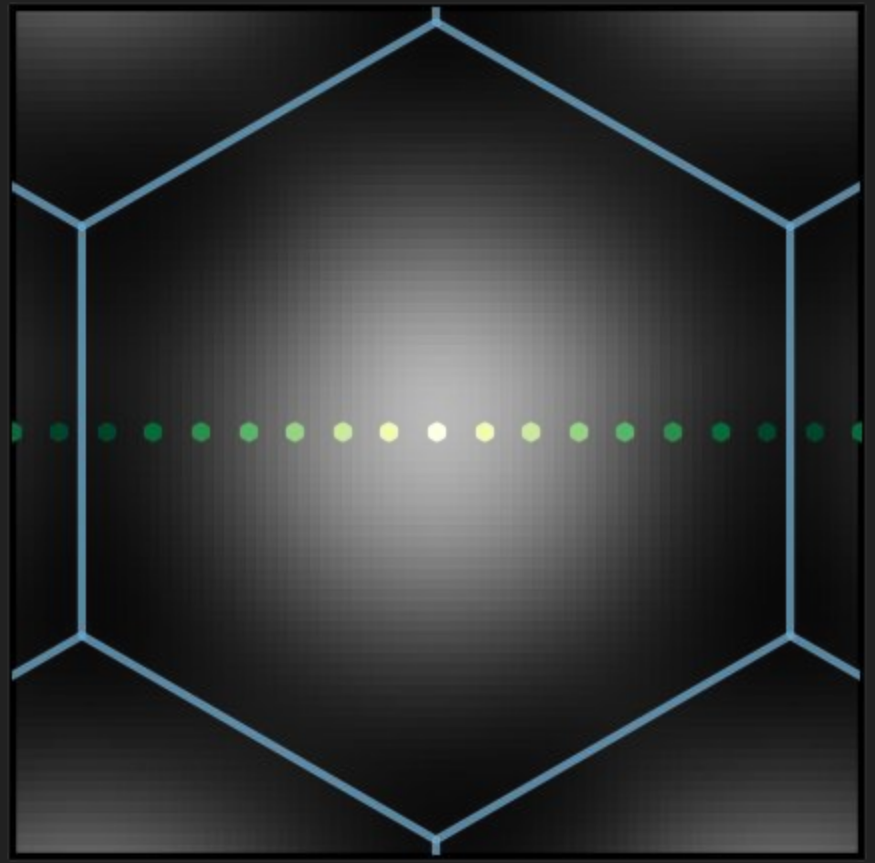
Rmax_max_search = 16

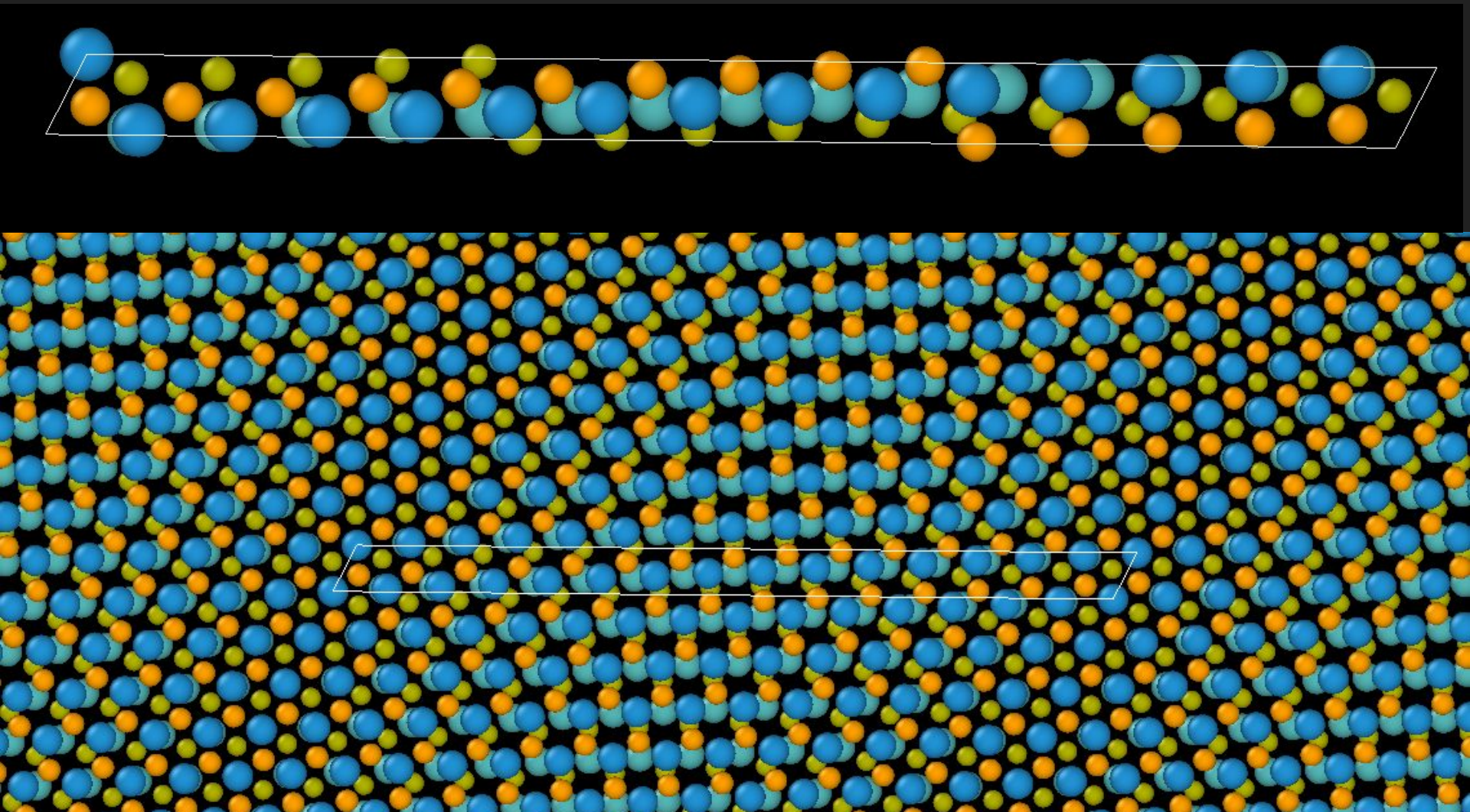
max_iter_twist_search = 5

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

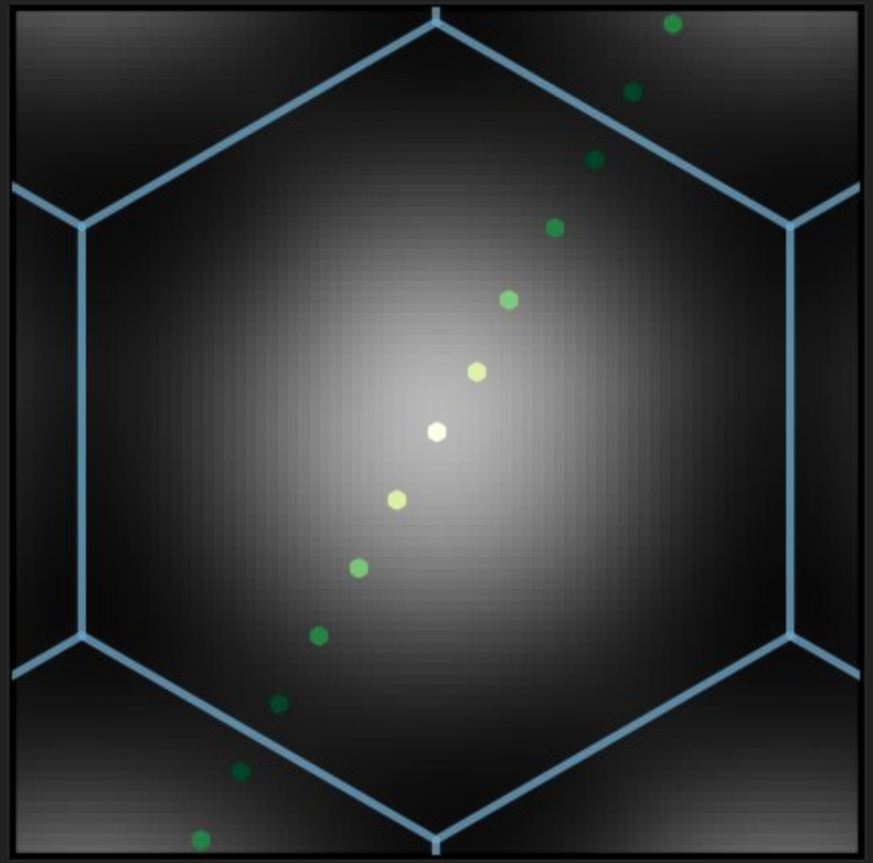
Rmax_max_search = 14

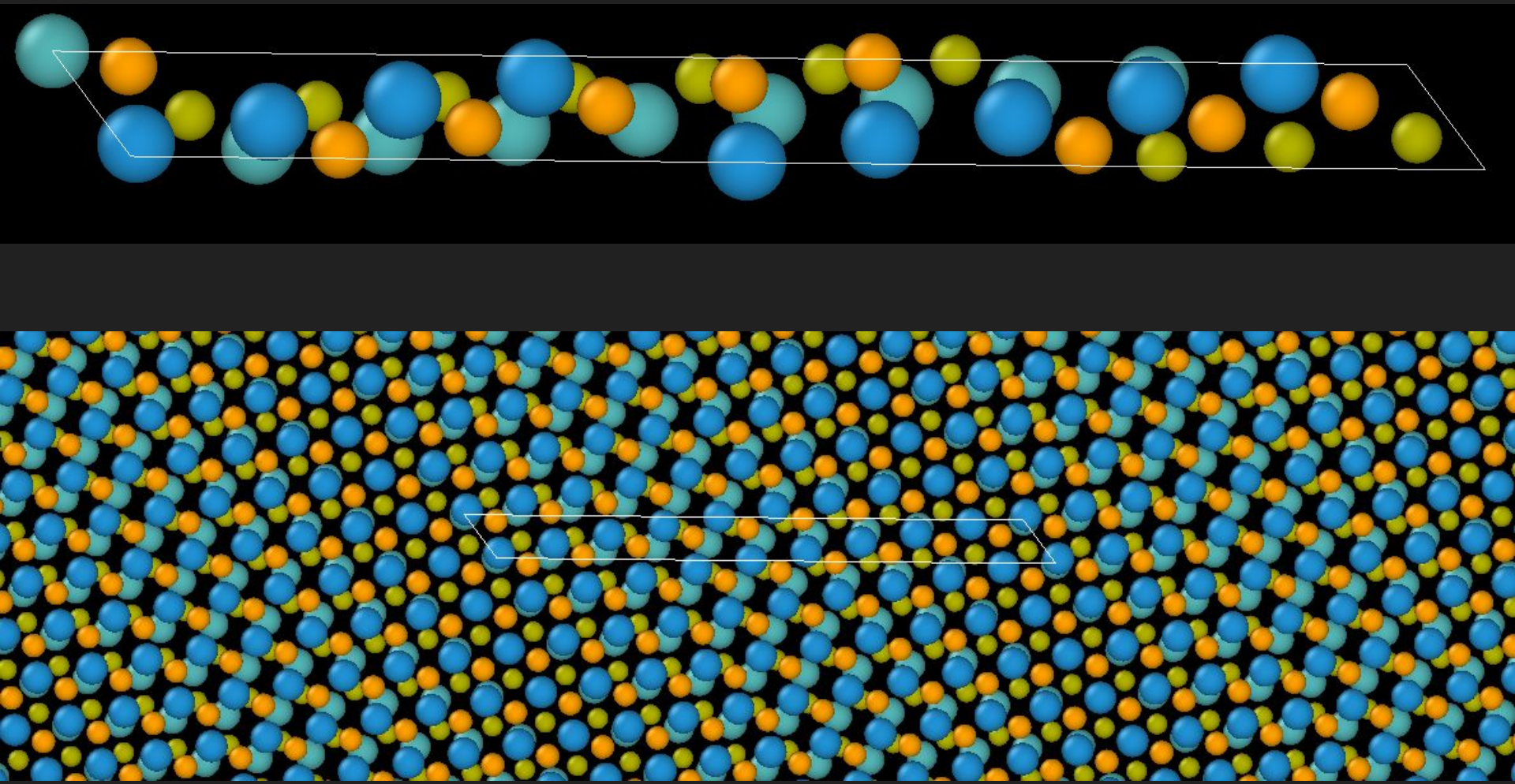
max_iter_twist_search = 5

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

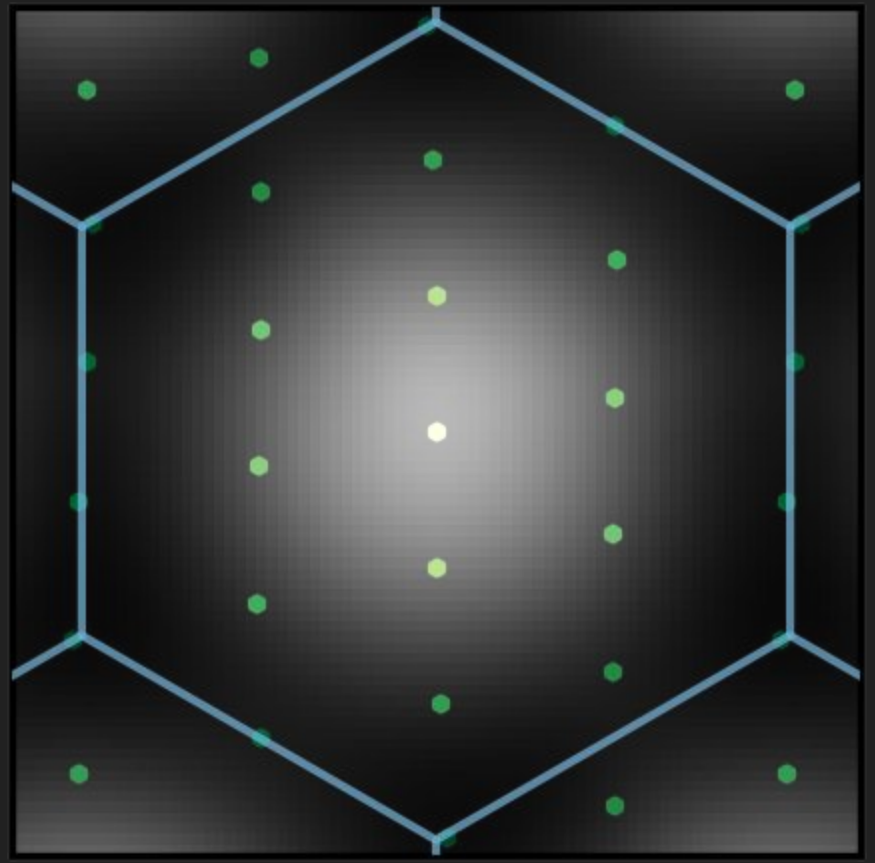
Rmax_max_search = 16

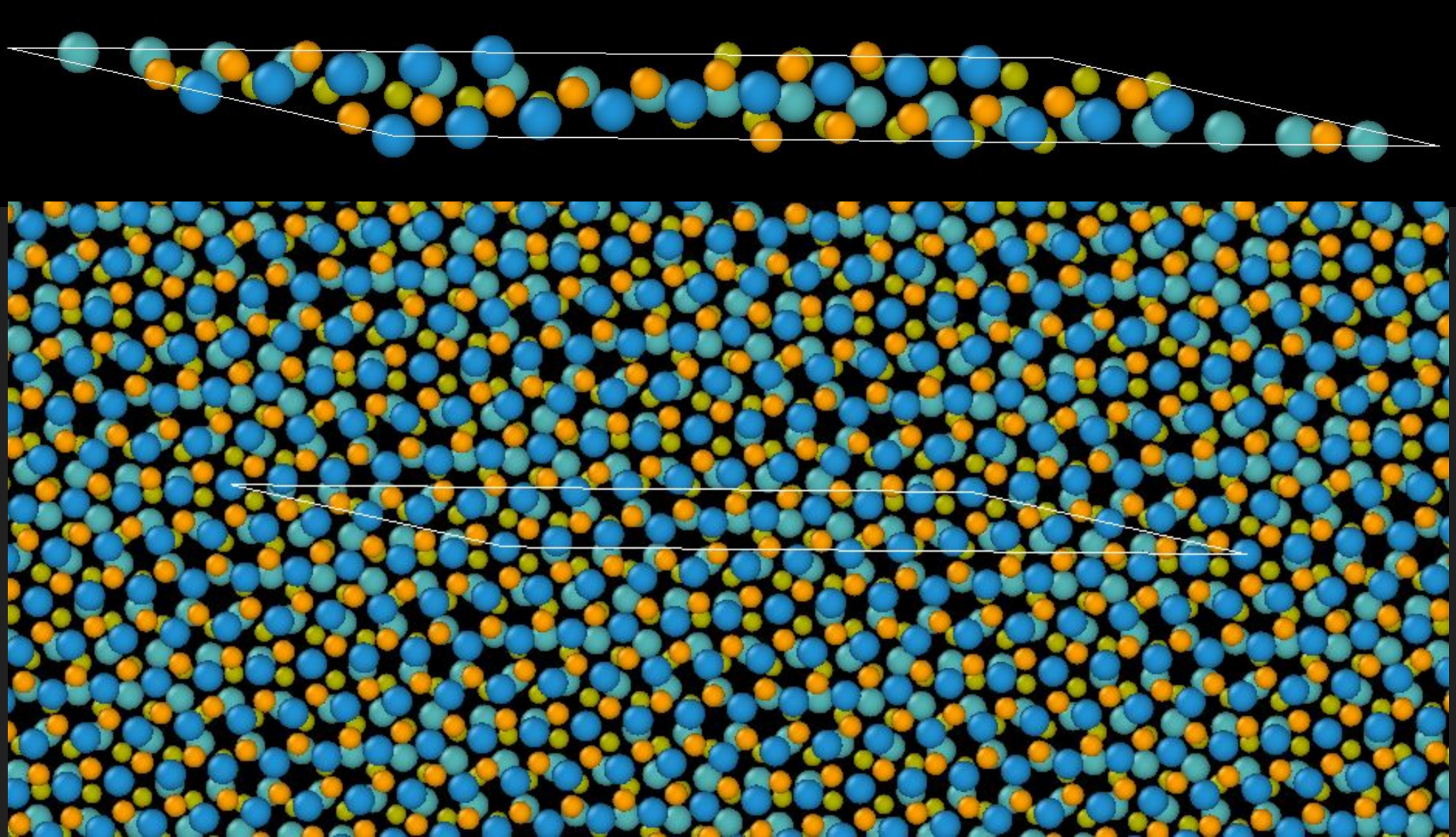
max_iter_twist_search = 5

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

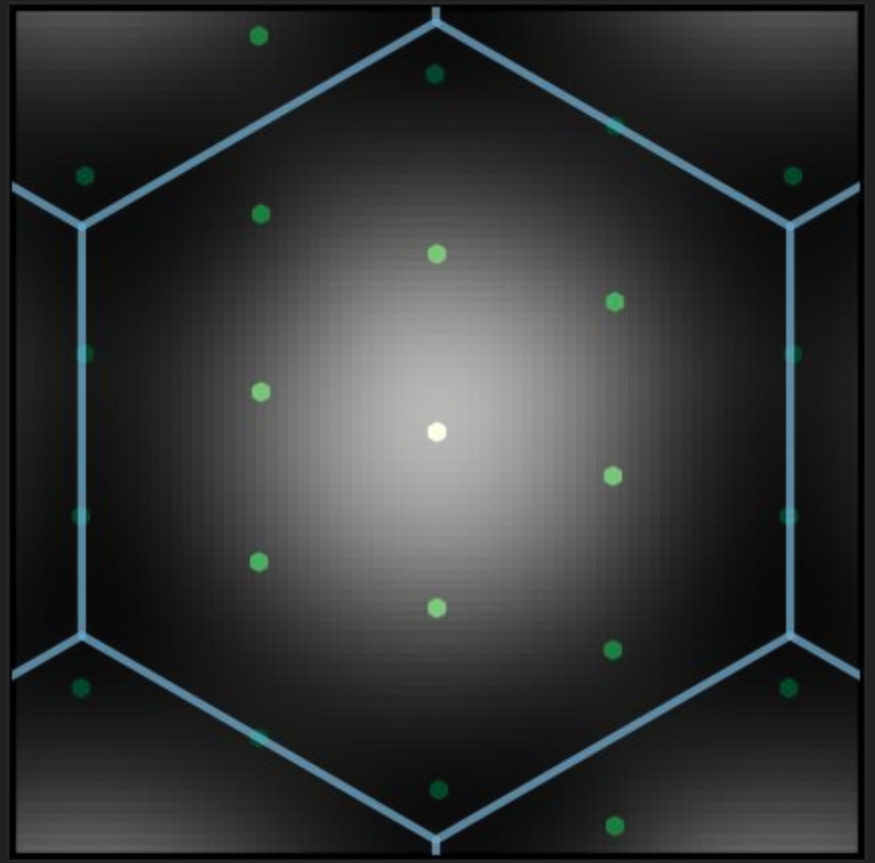
Rmax_max_search = 16

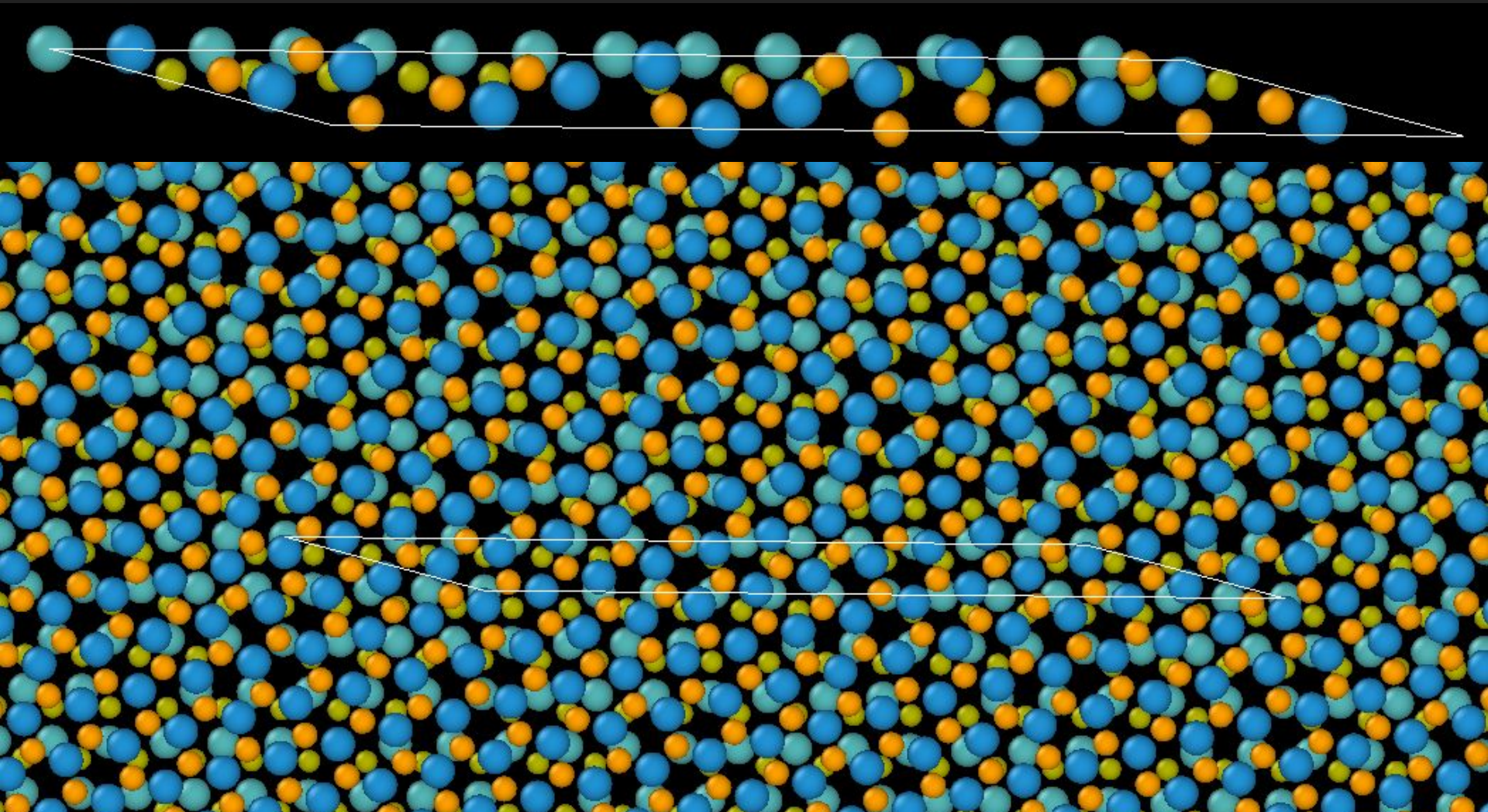
max_iter_twist_search = 5

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

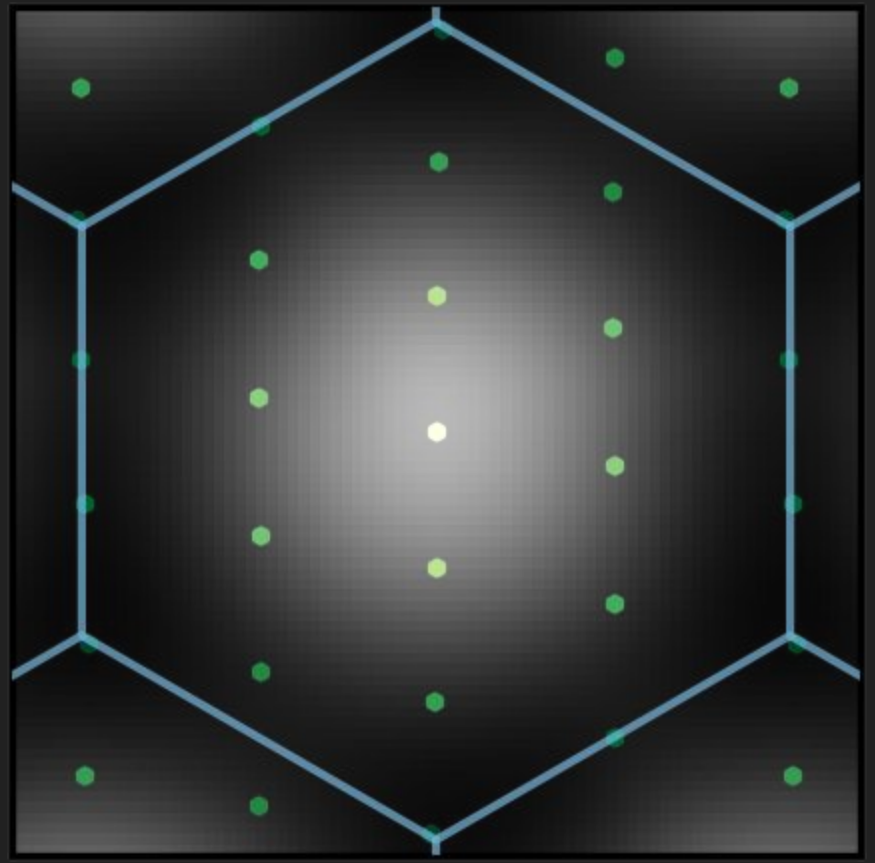
Rmax_max_search = 16

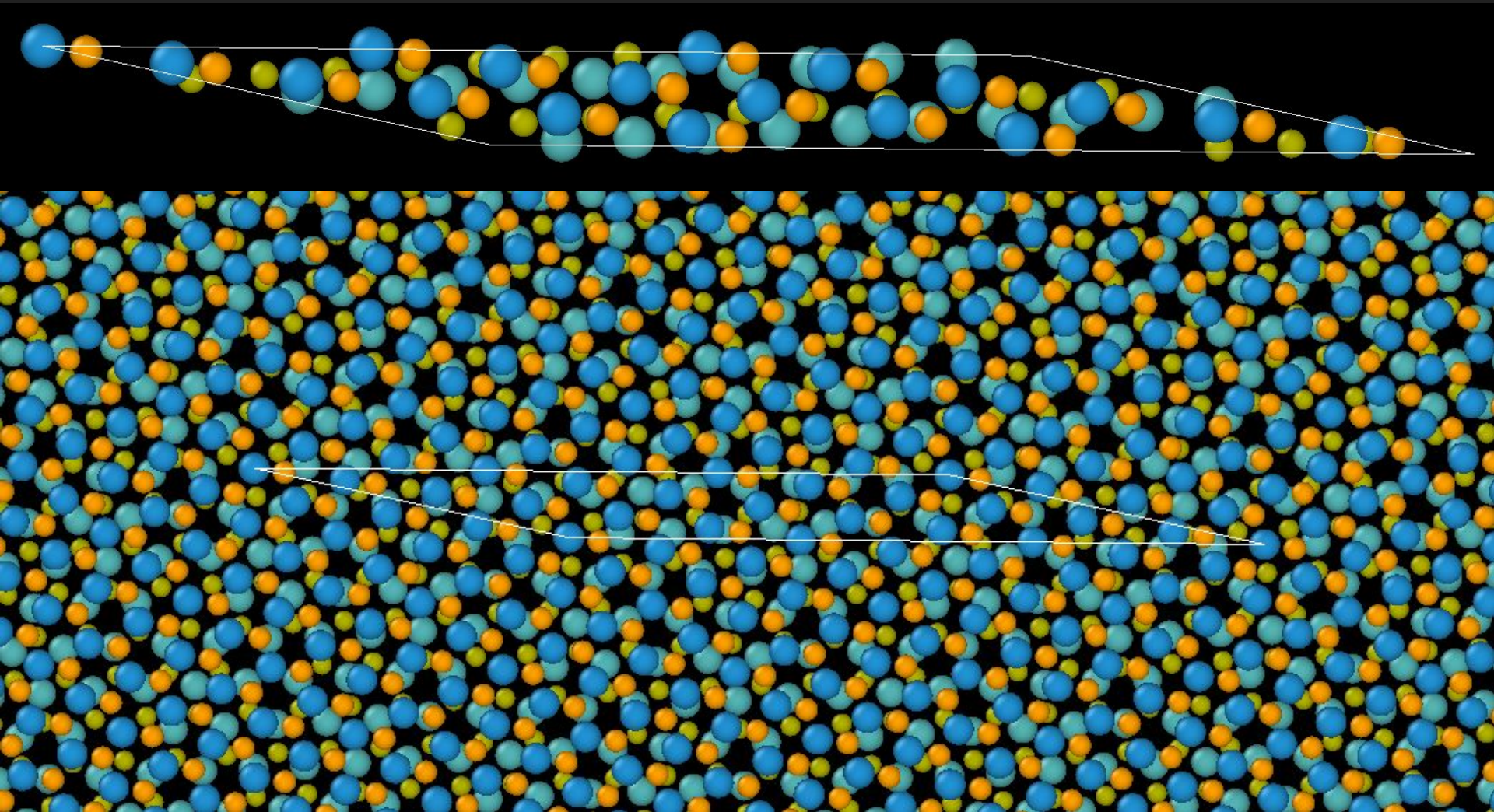
max_iter_twist_search = 5

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

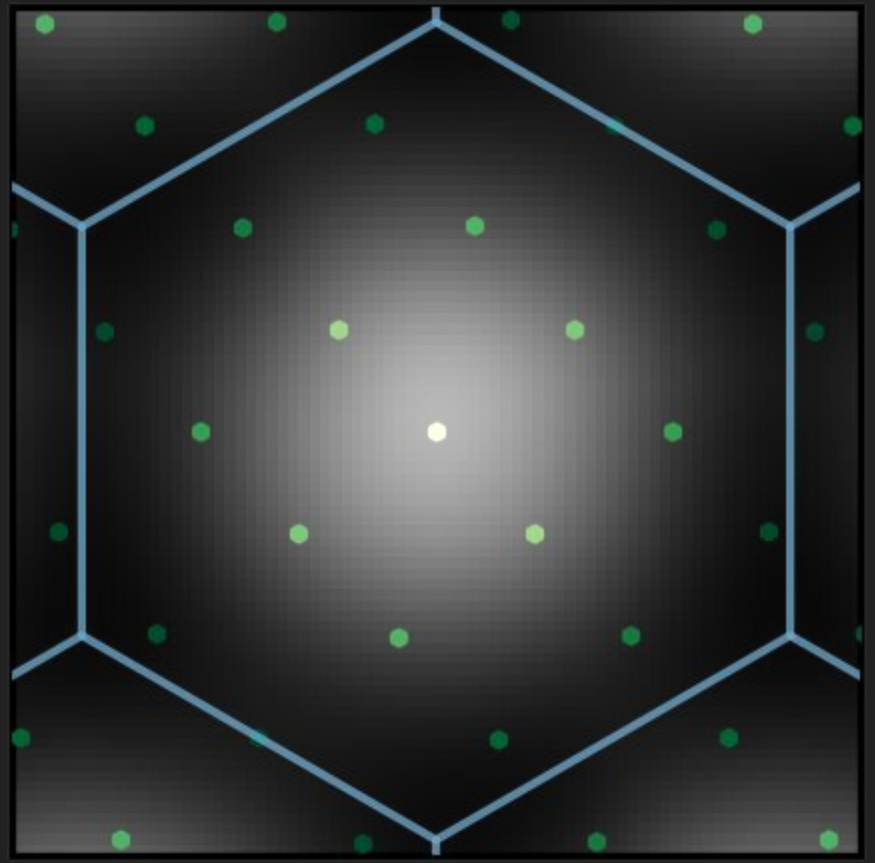
Rmax_max_search = 16

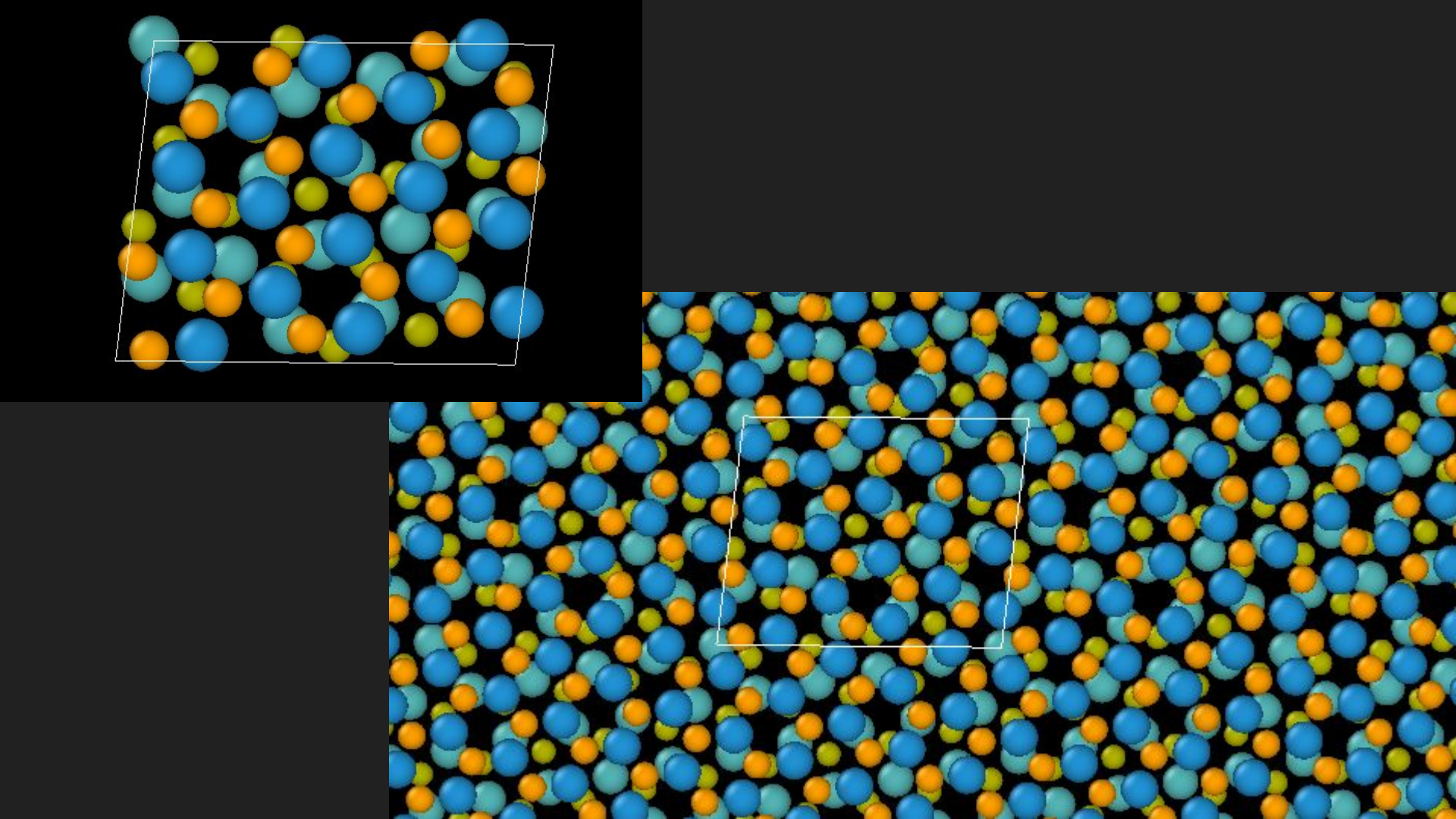
max_iter_twist_search = 5

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

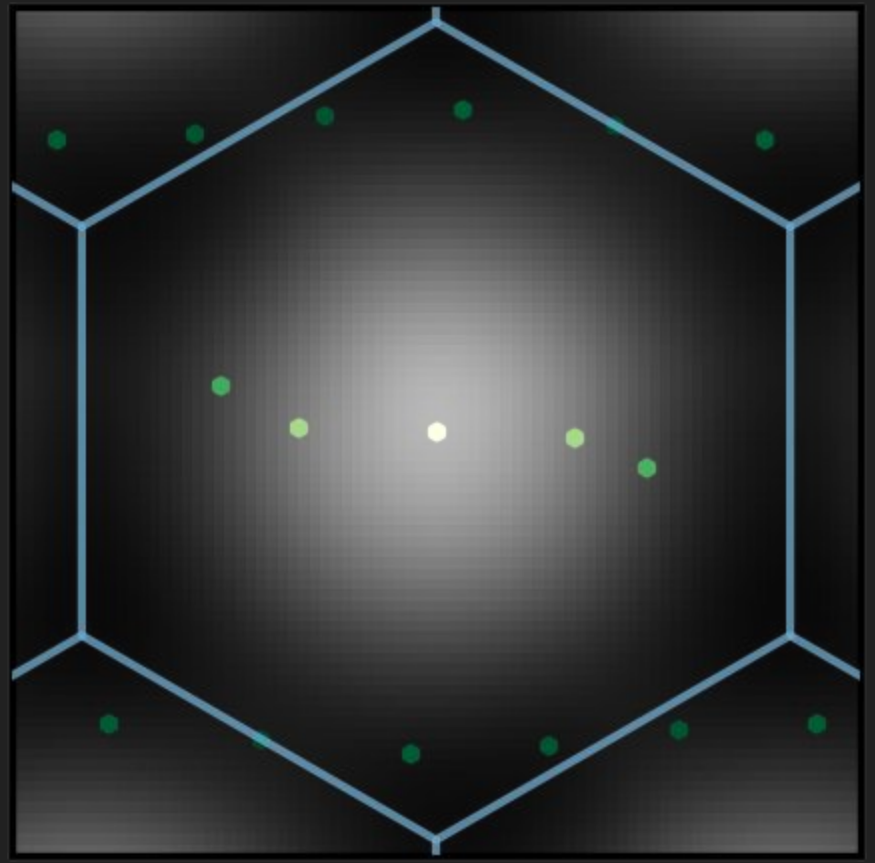
Rmax_max_search = 16

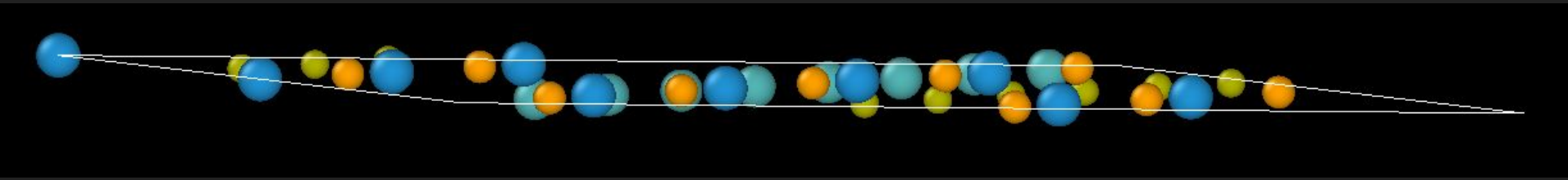
max_iter_twist_search = 5

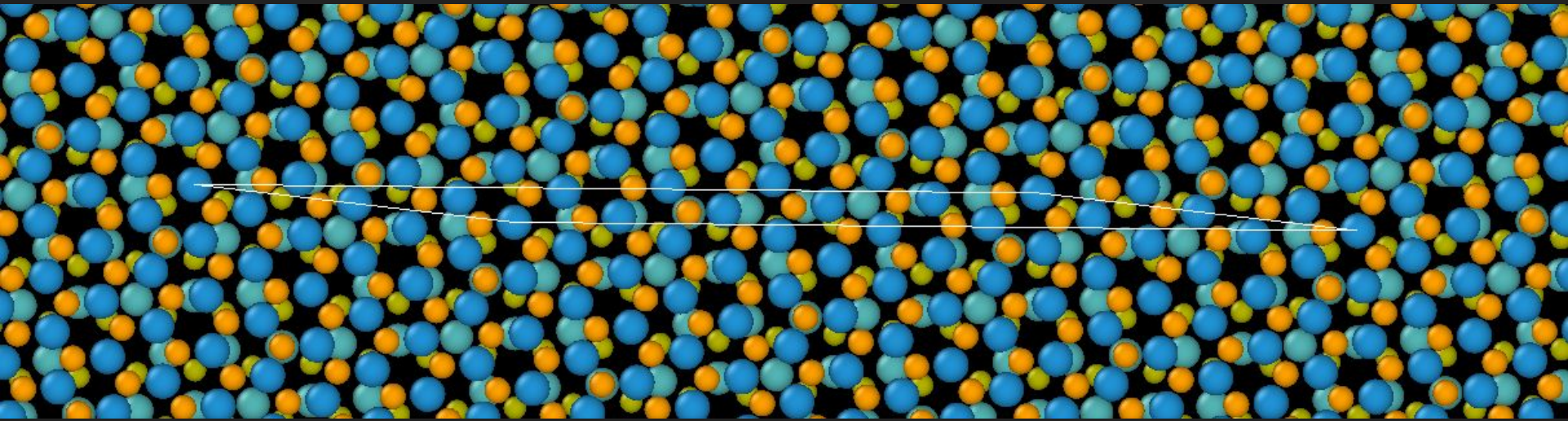
Total atoms: 57

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

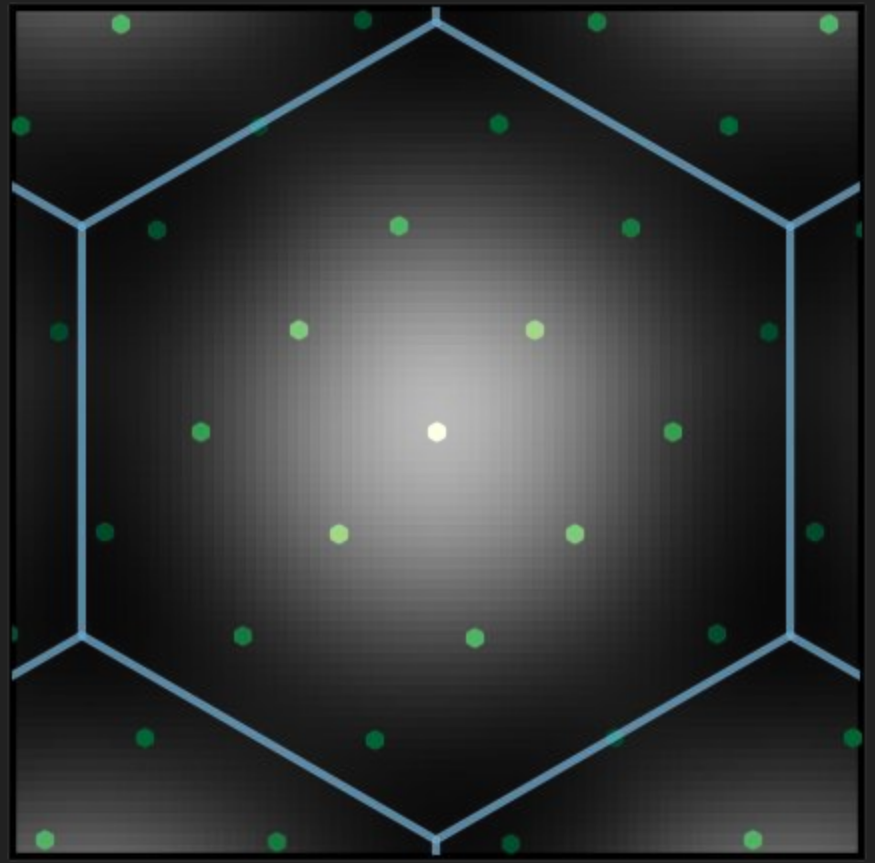
Rmax_max_search = 16

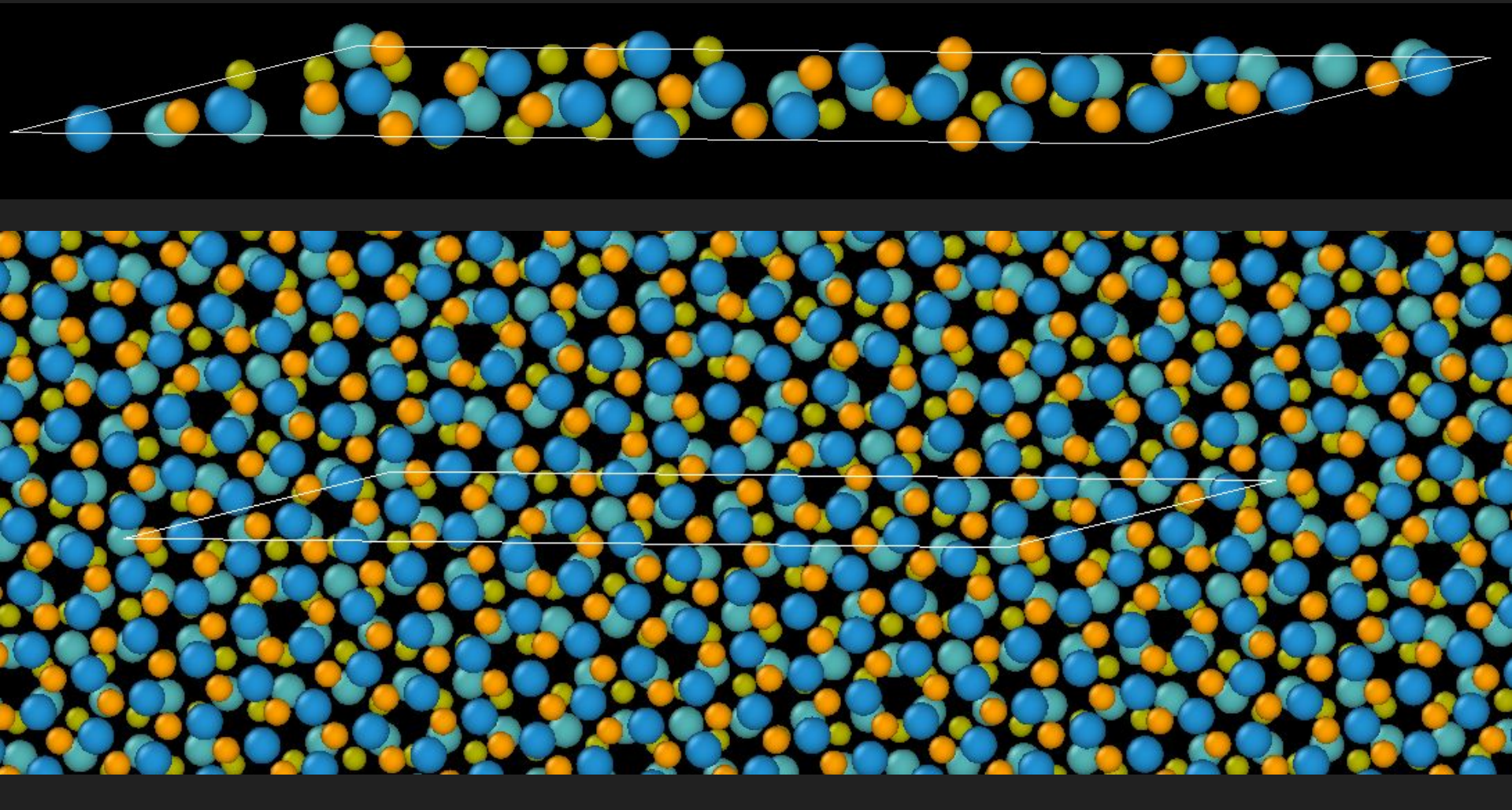
max_iter_twist_search = 5

Total atoms: 111

Mo count: 19

W count: 18





Pre-Relaxation

0 degree

twist_min_search = 0

twist_max_search = 0.1

max_strain = 0.2

is_1D_dir_1 = True

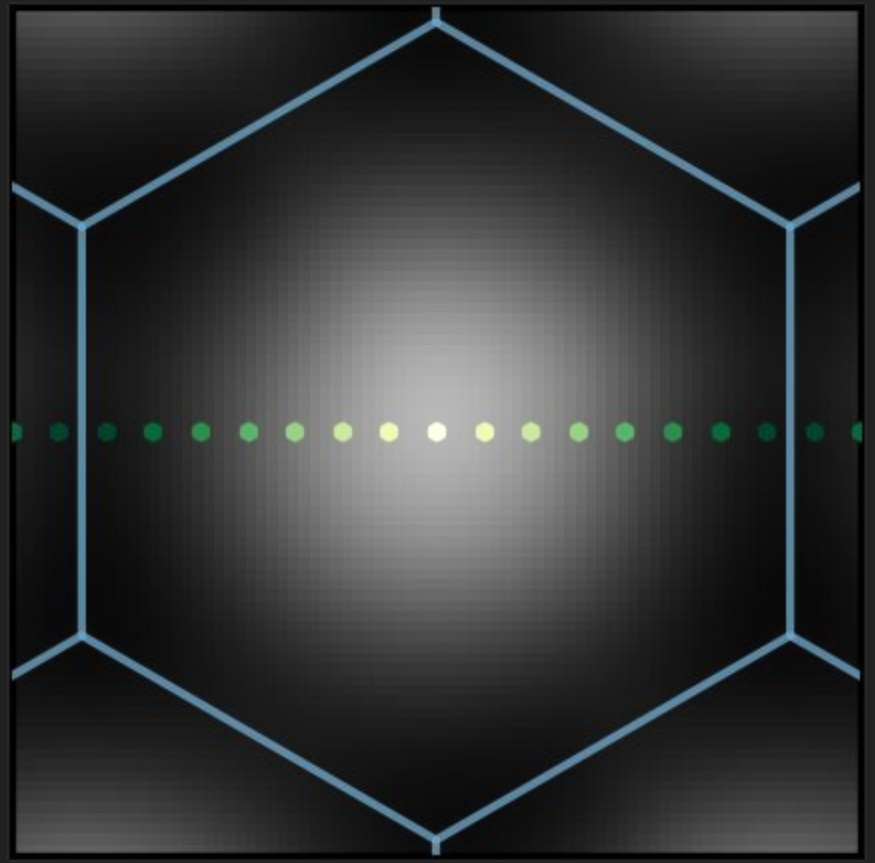
Rmax_max_search = 16

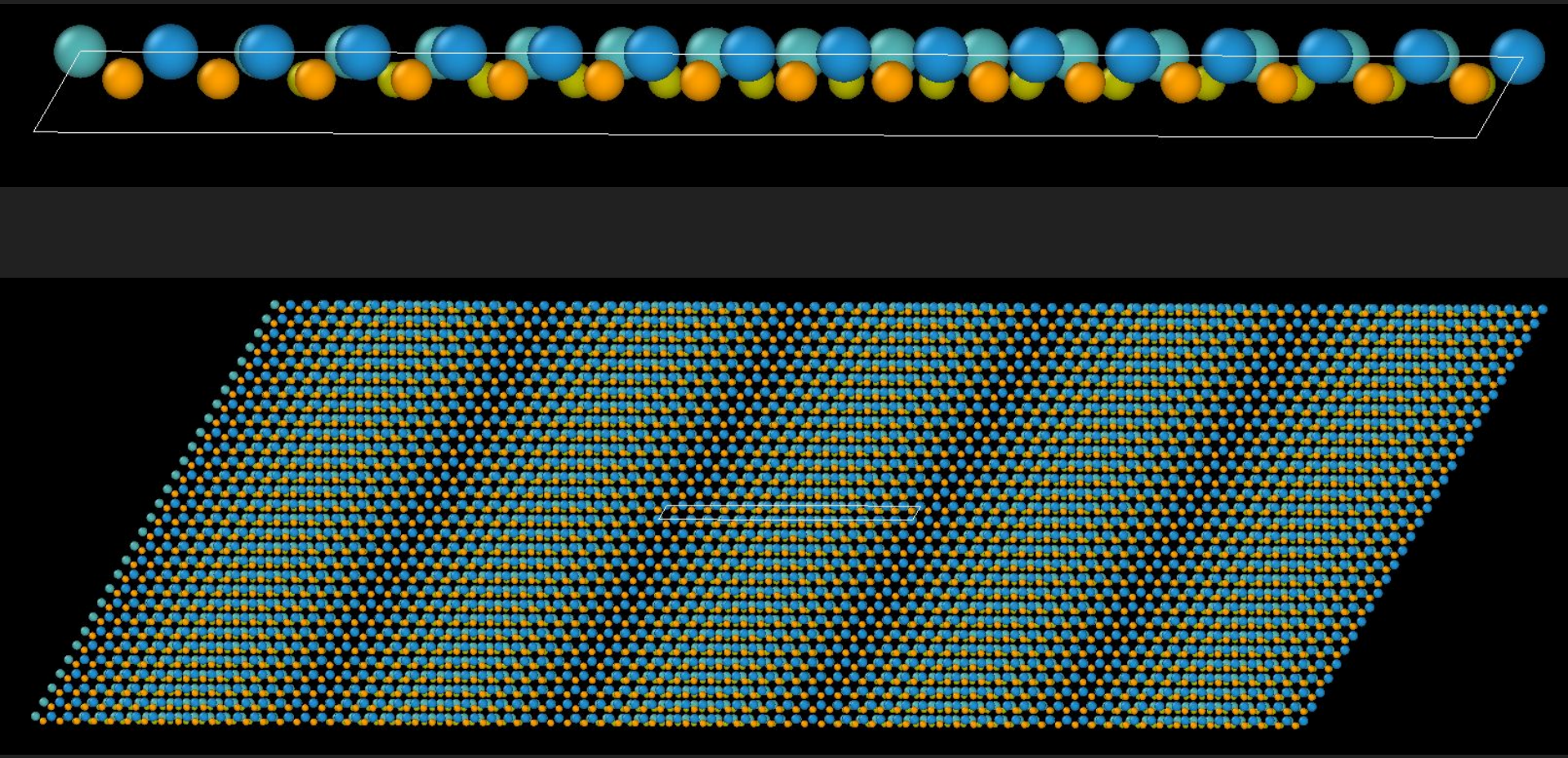
max_iter_twist_search = 5

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

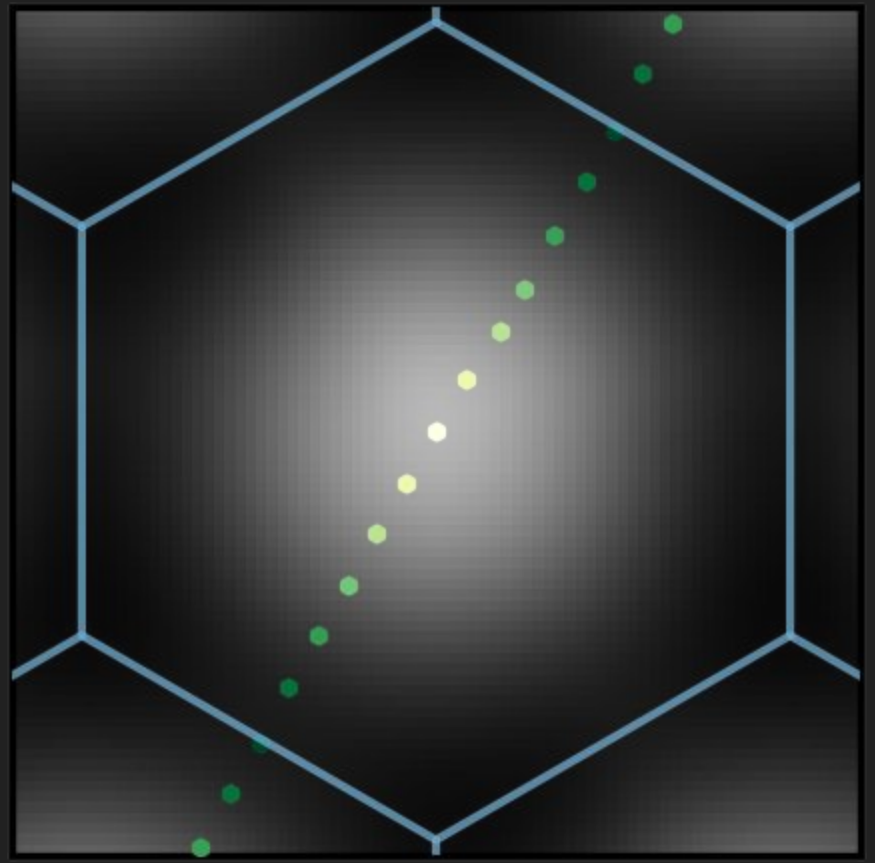
Rmax_max_search = 16

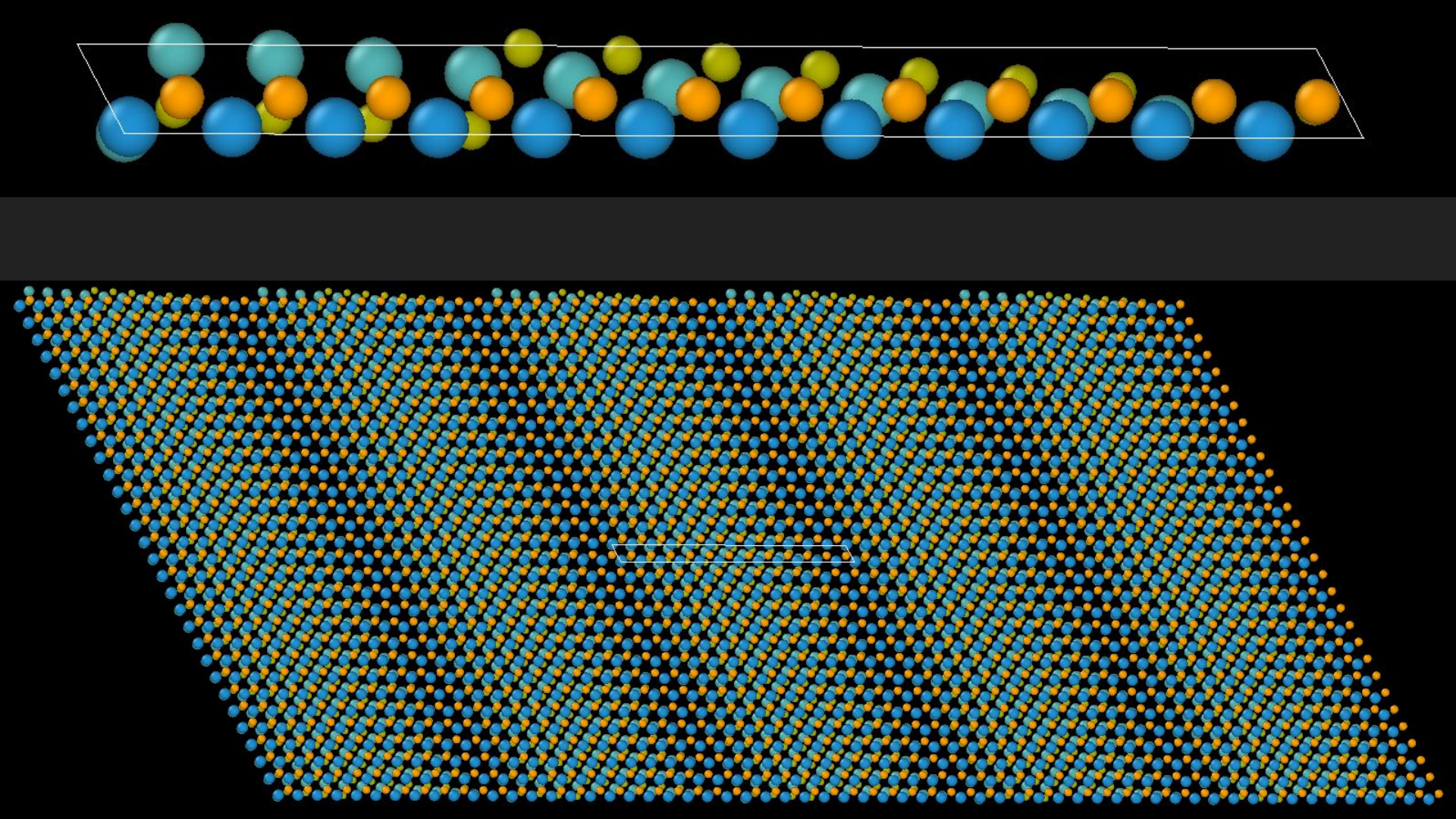
max_iter_twist_search = 5

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

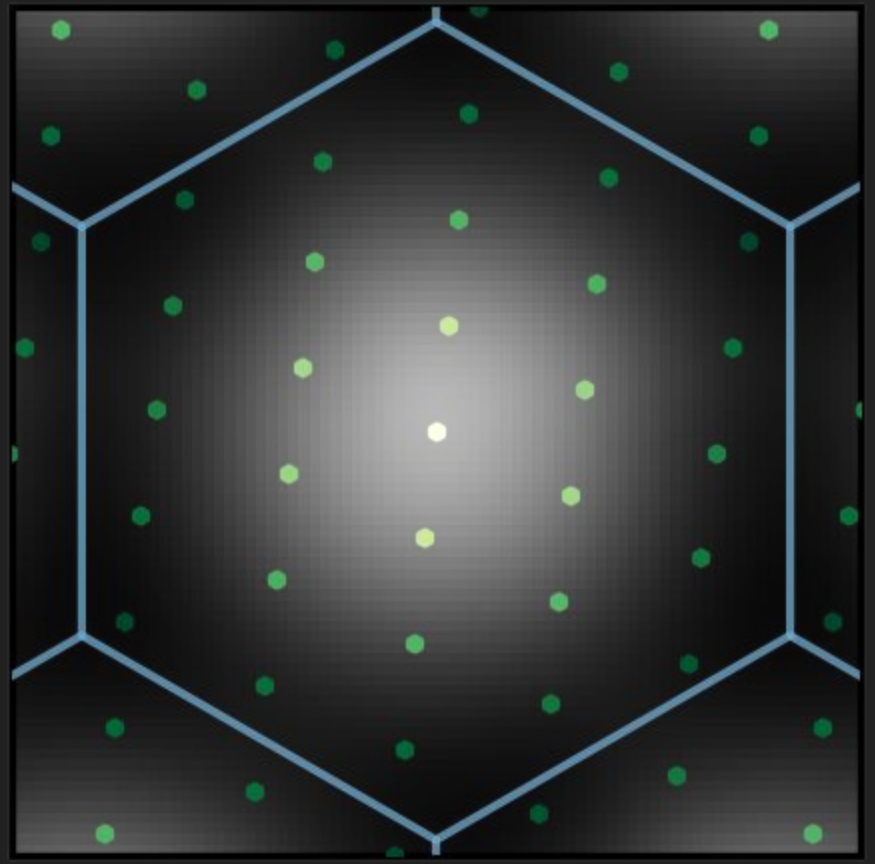
Rmax_max_search = 30

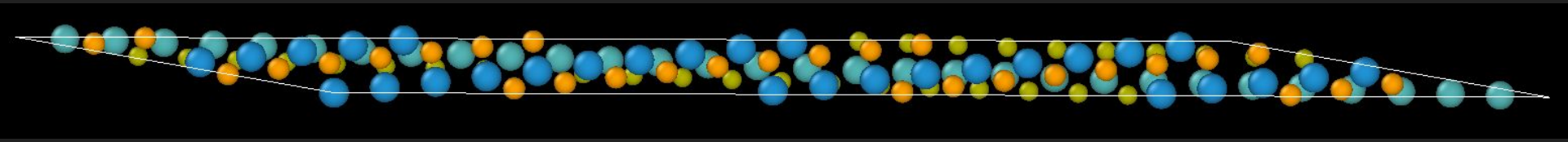
max_iter_twist_search = 5

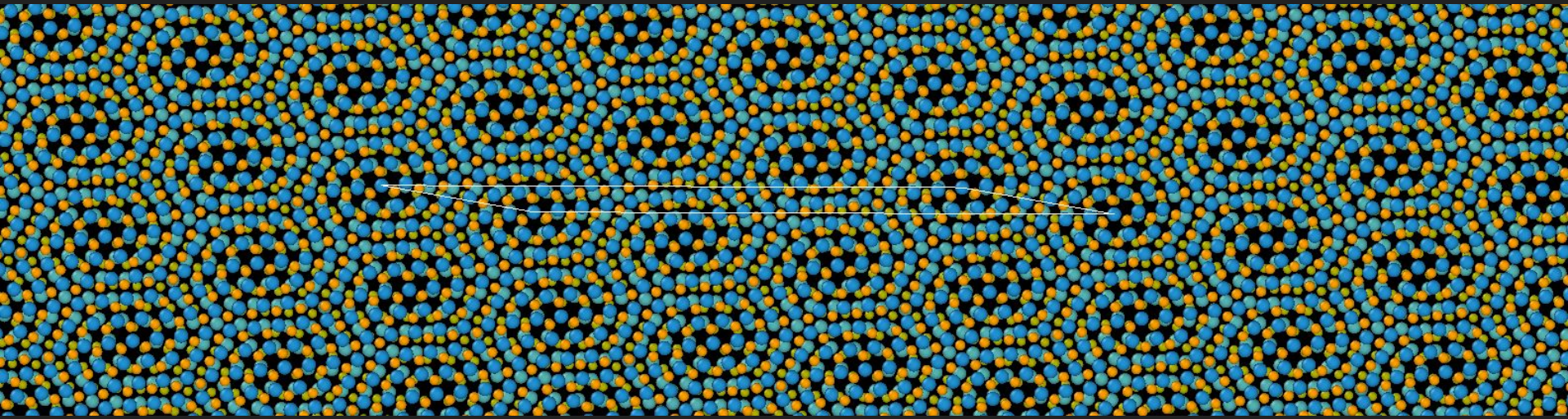
Total atoms: 180

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

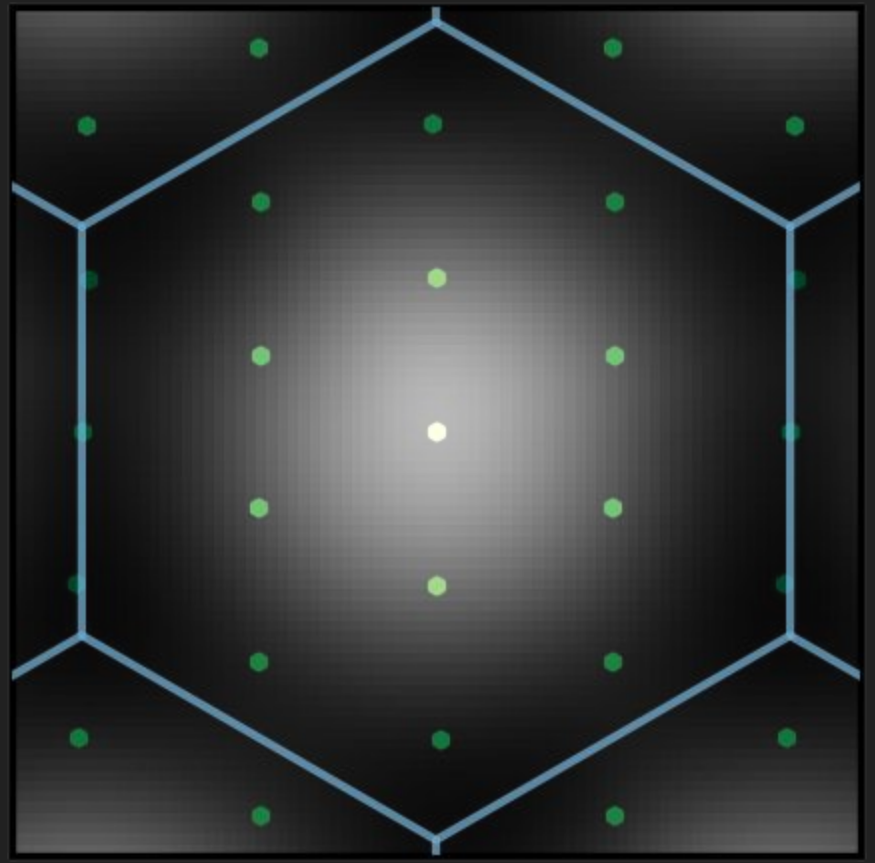
Rmax_max_search = 14

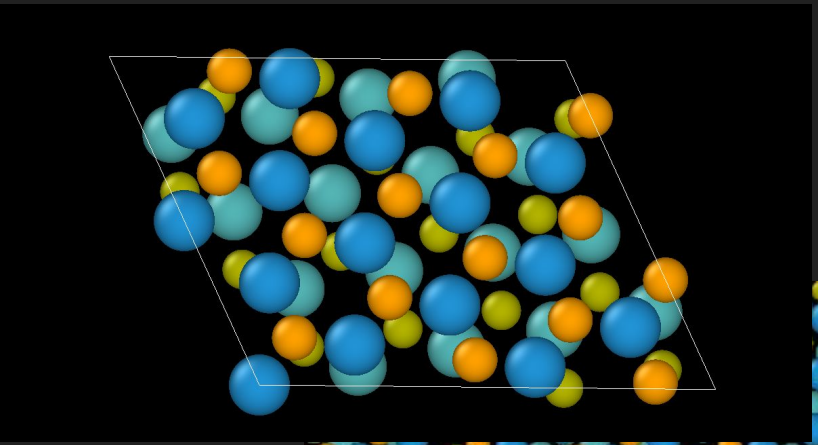
max_iter_twist_search = 5

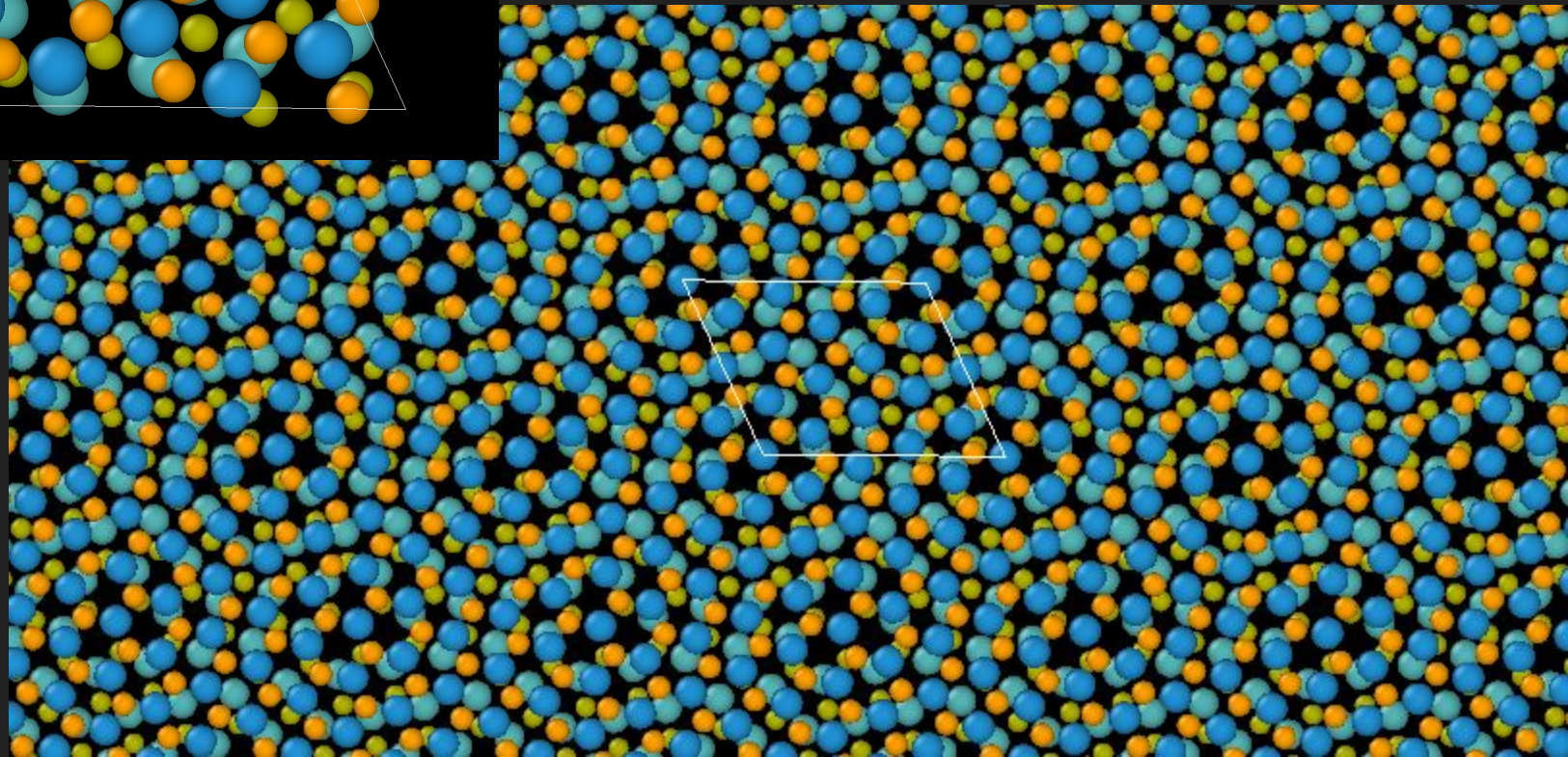
Total atoms: 99

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

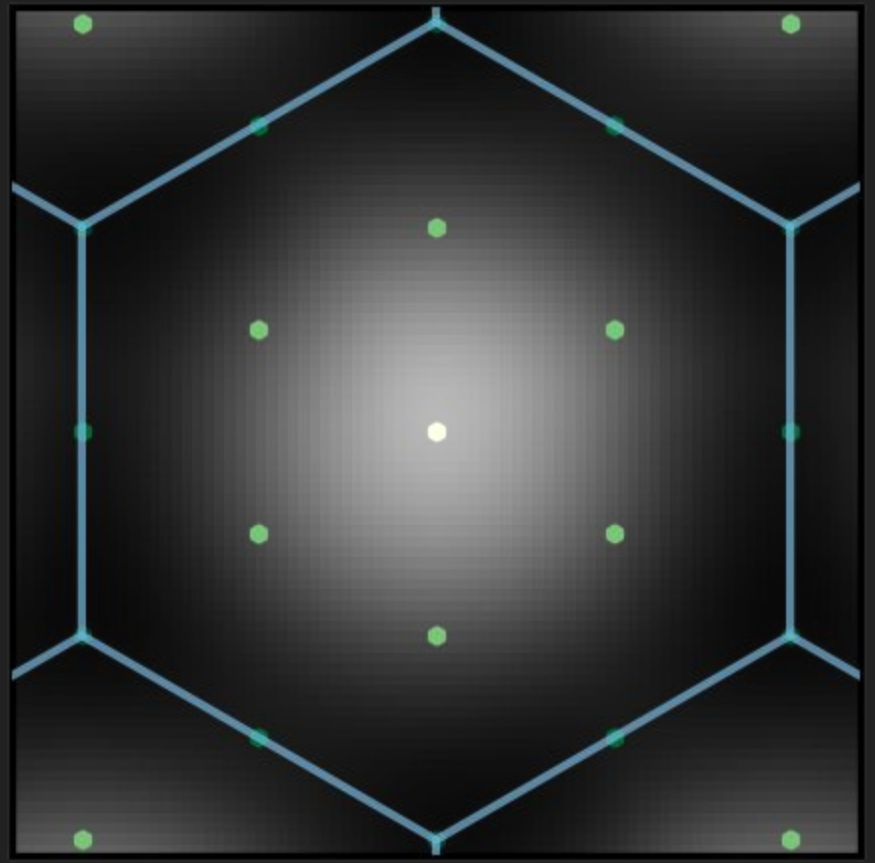
Rmax_max_search = 16

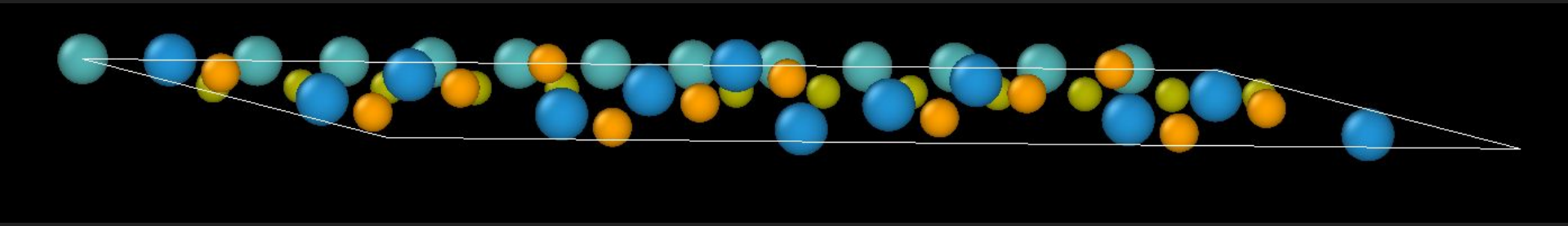
max_iter_twist_search = 5

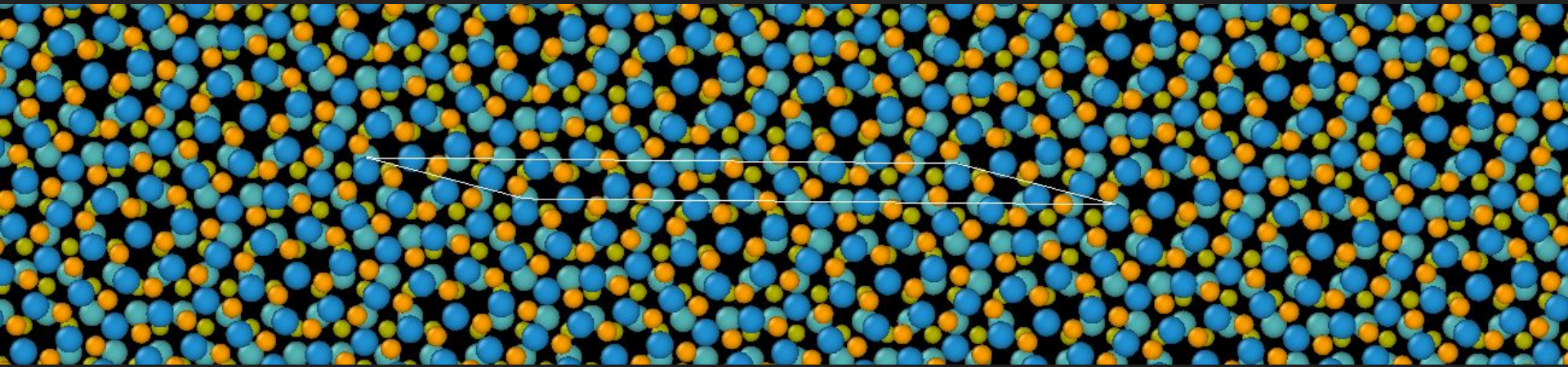
Total atoms: 75

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

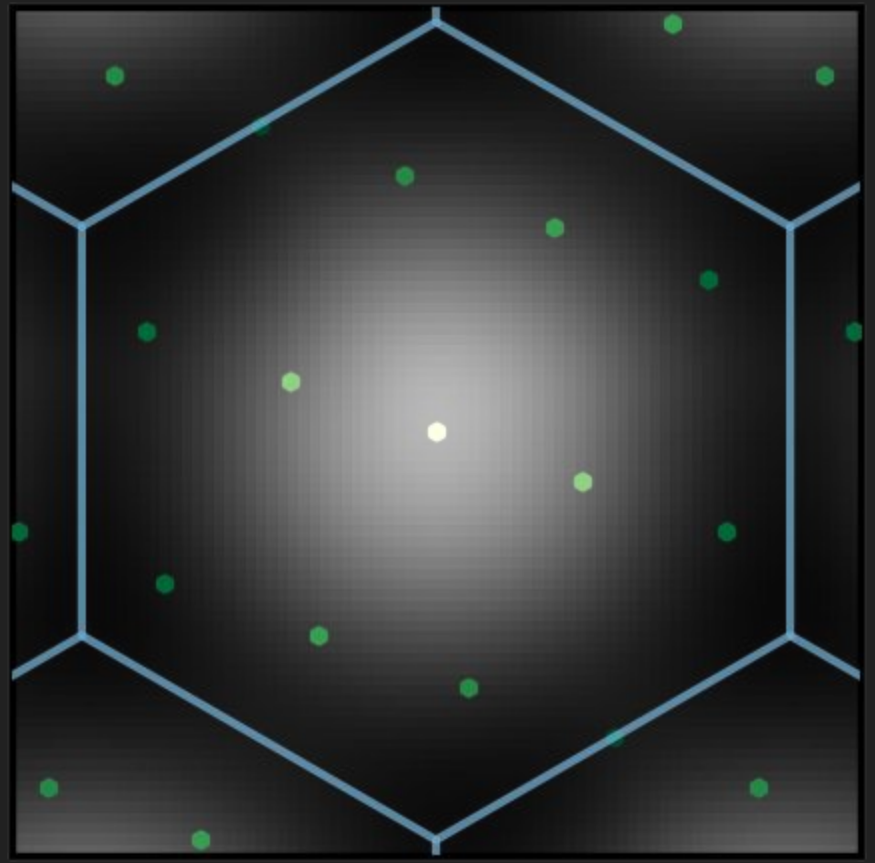
Rmax_max_search = 16

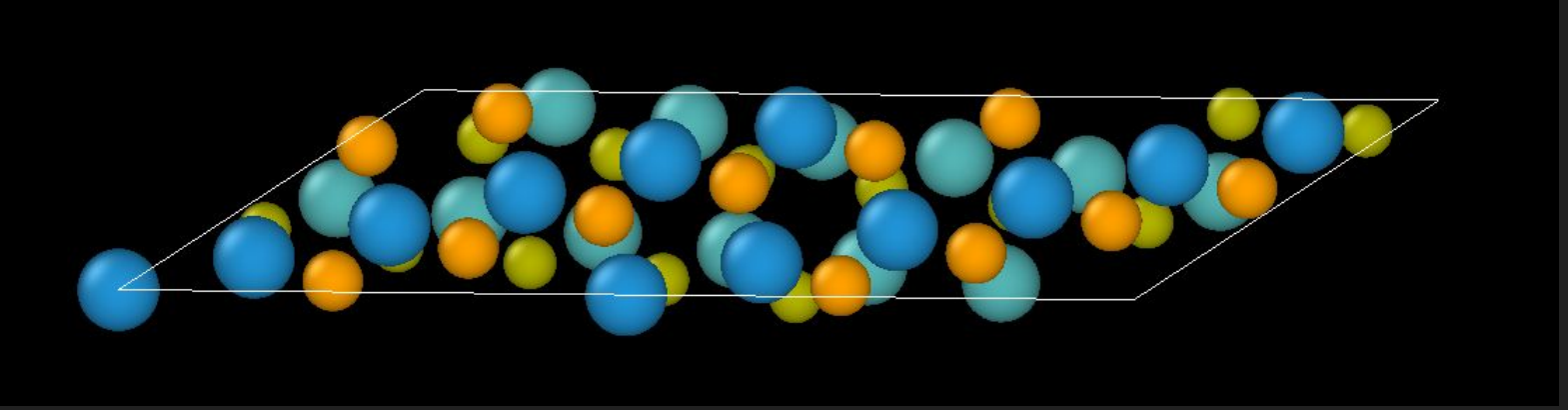
max_iter_twist_search = 5

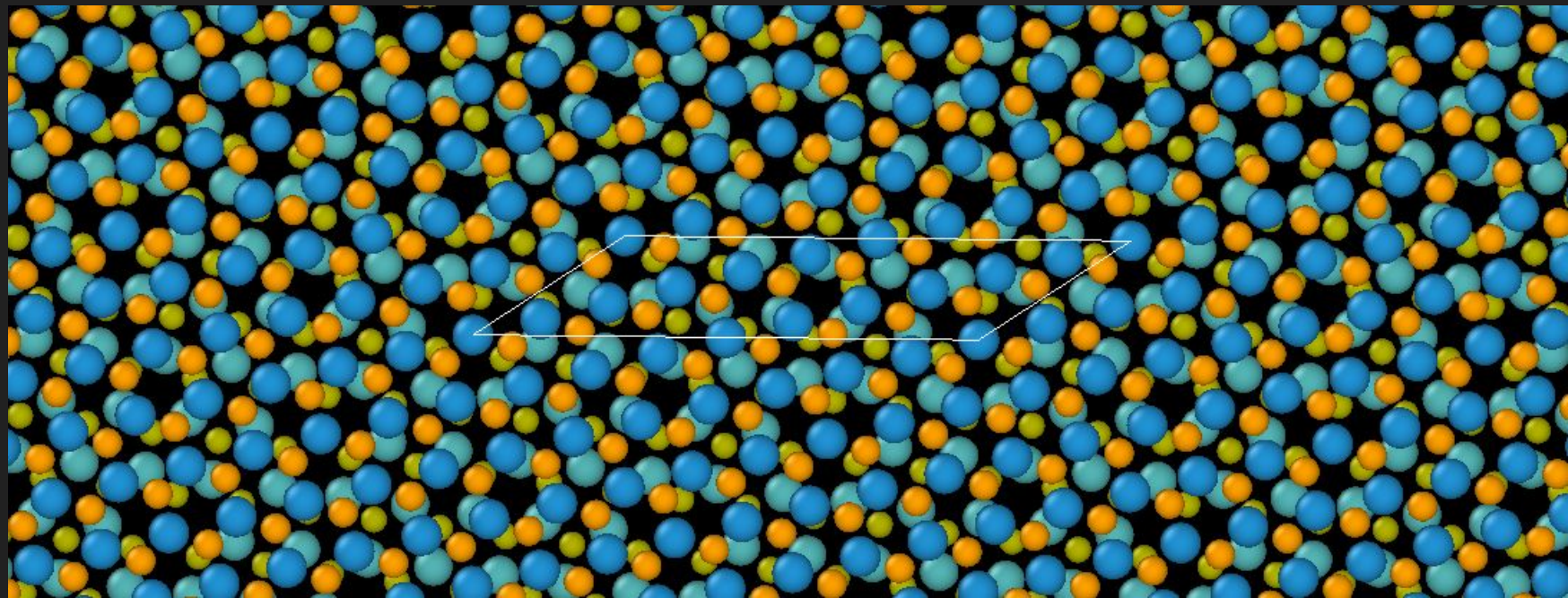
Total atoms: 75

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

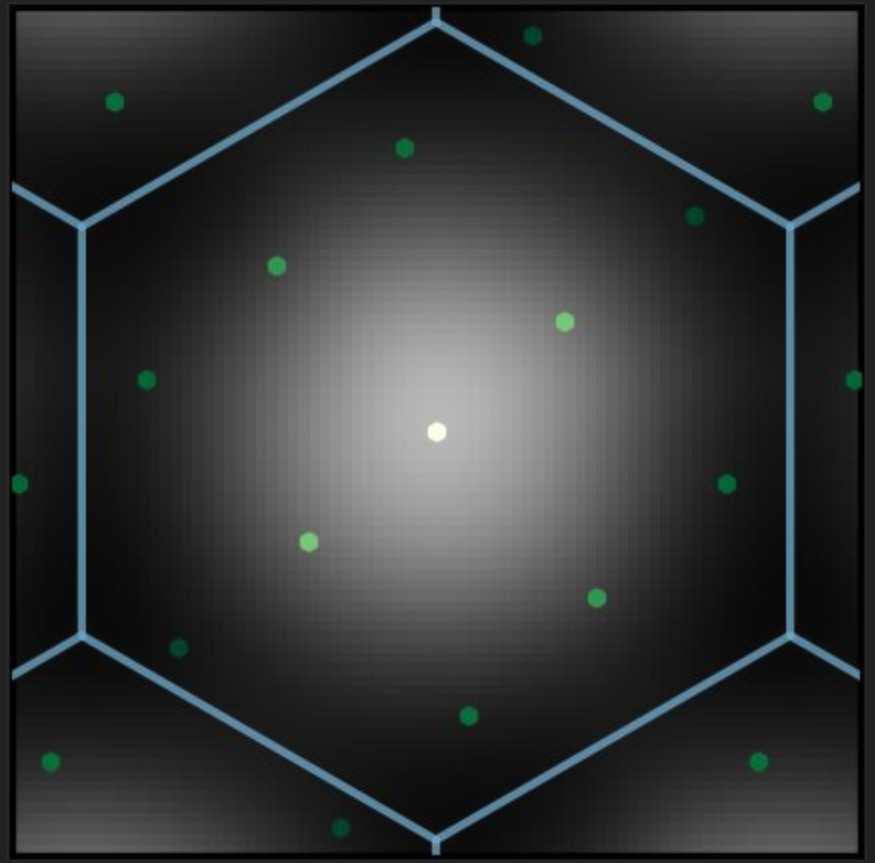
Rmax_max_search = 14

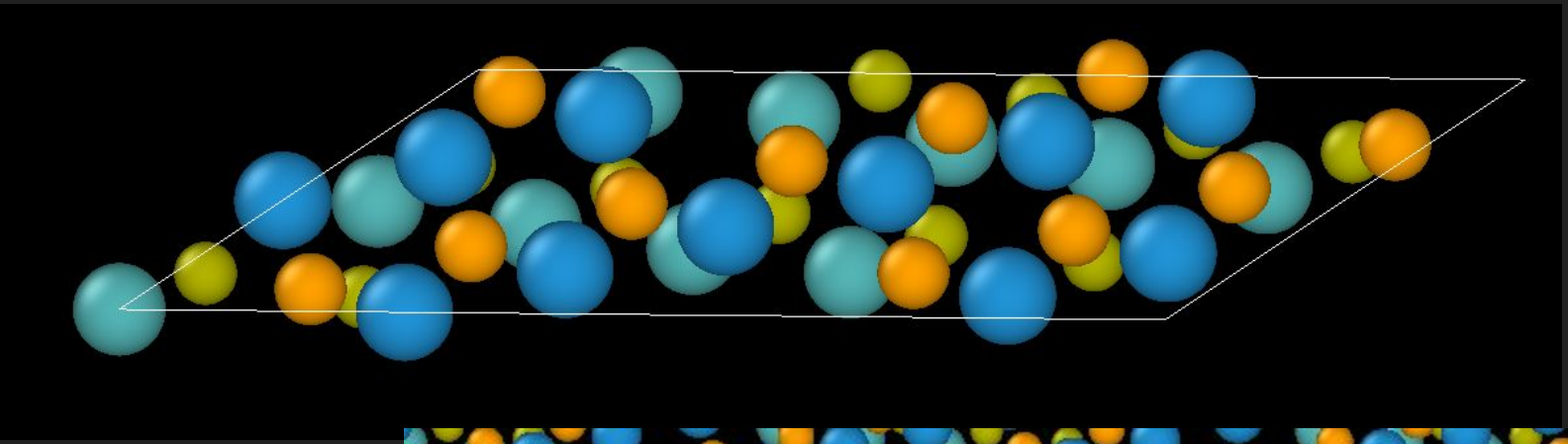
max_iter_twist_search = 5

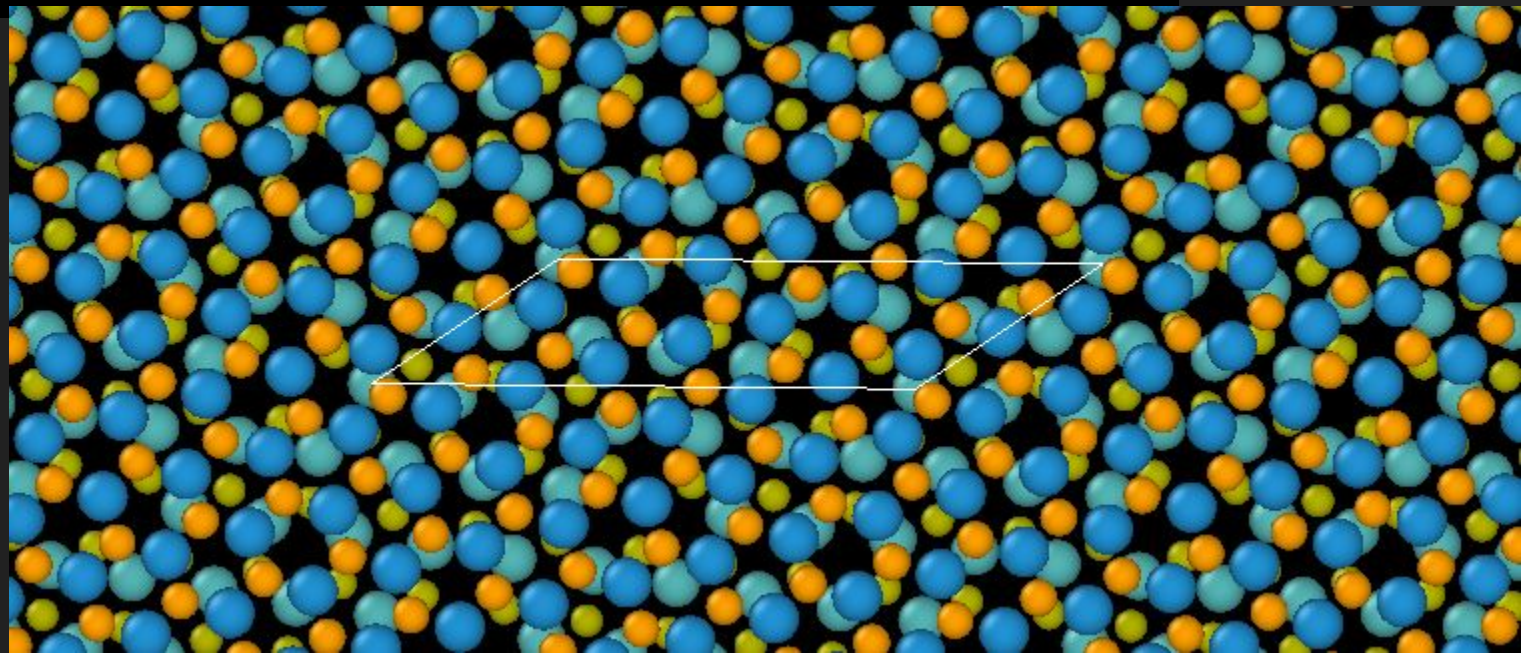
Total atoms: 66

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

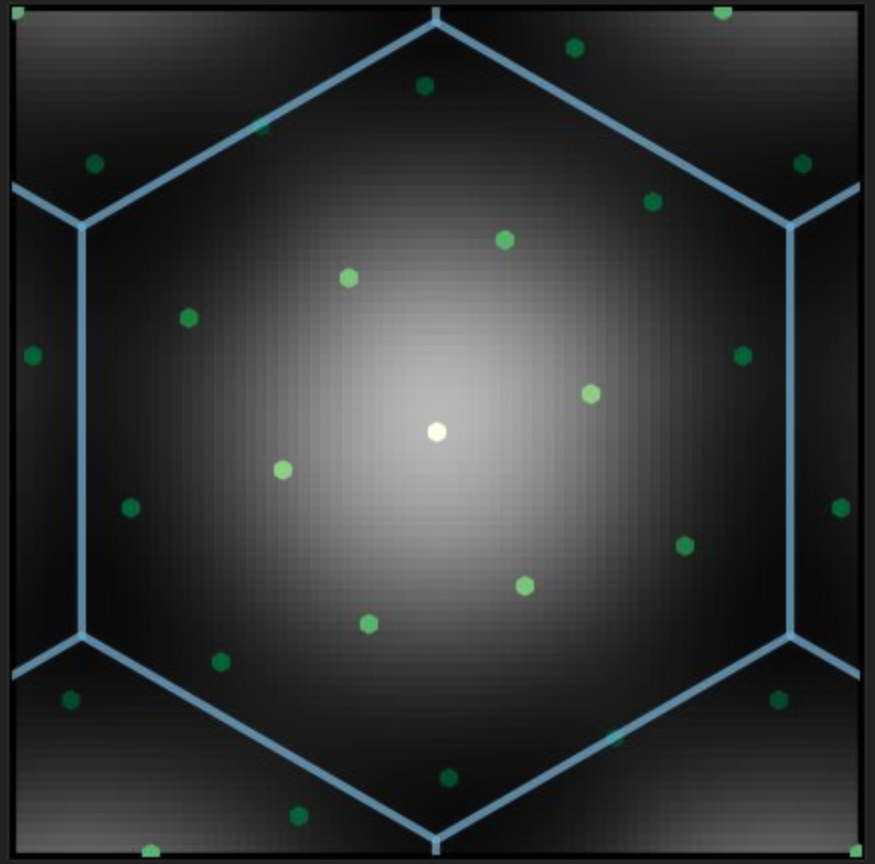
Rmax_max_search = 14

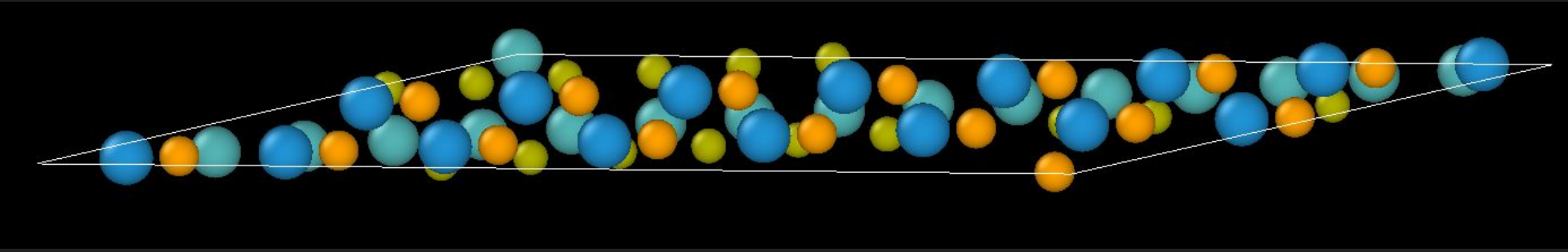
max_iter_twist_search = 5

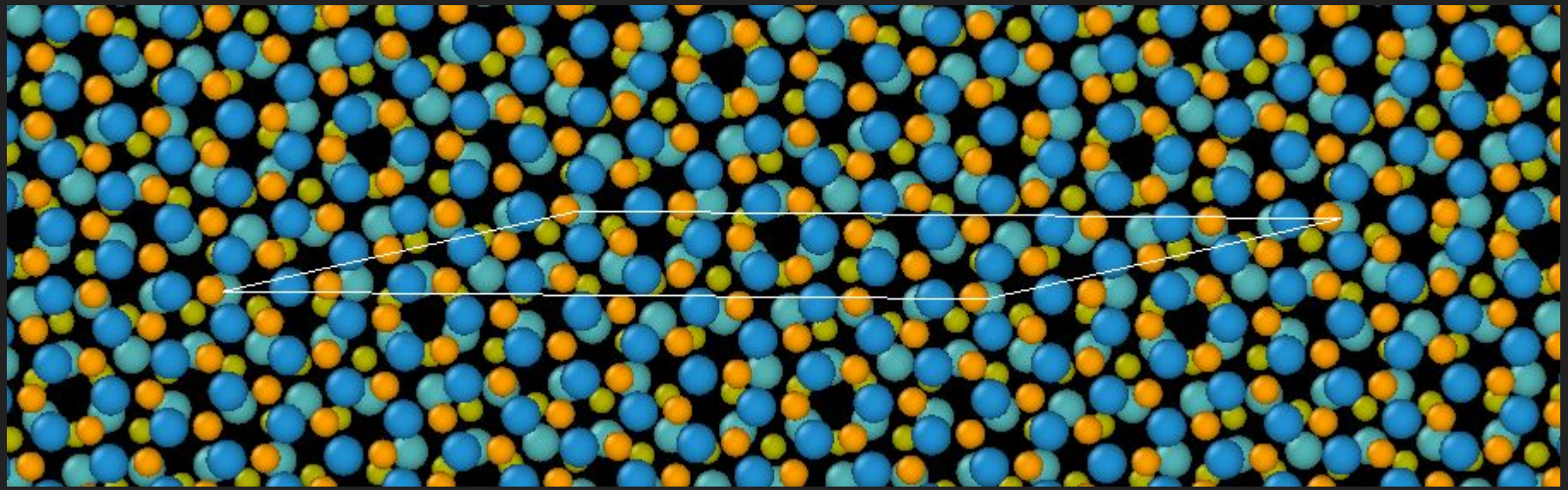
Total atoms: 99

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

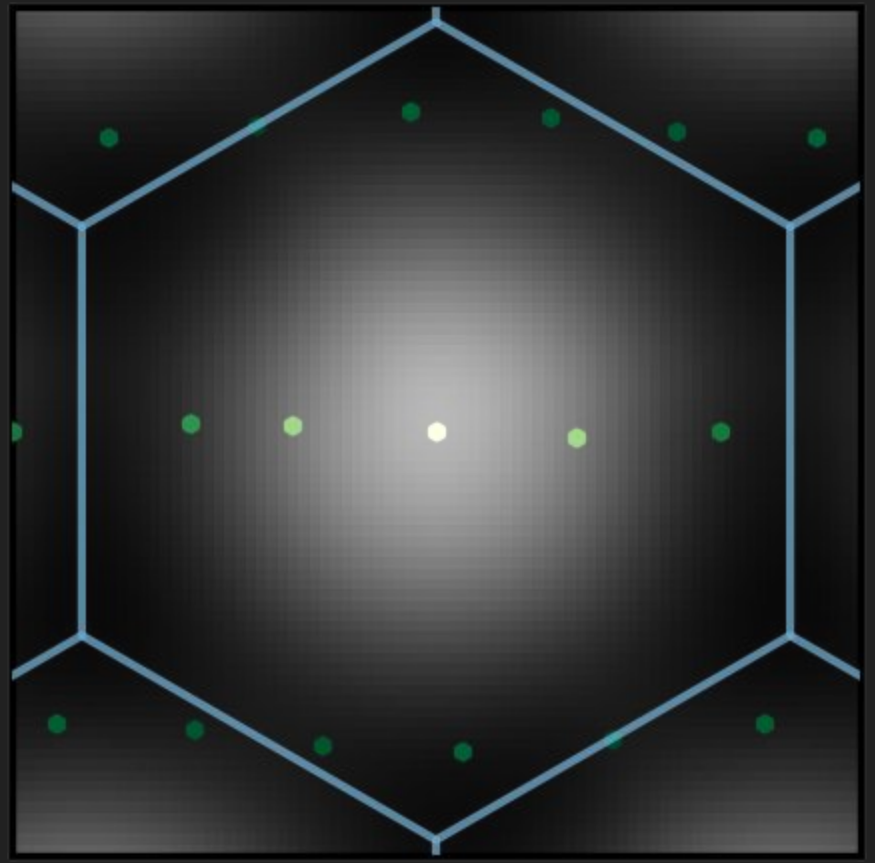
Rmax_max_search = 14

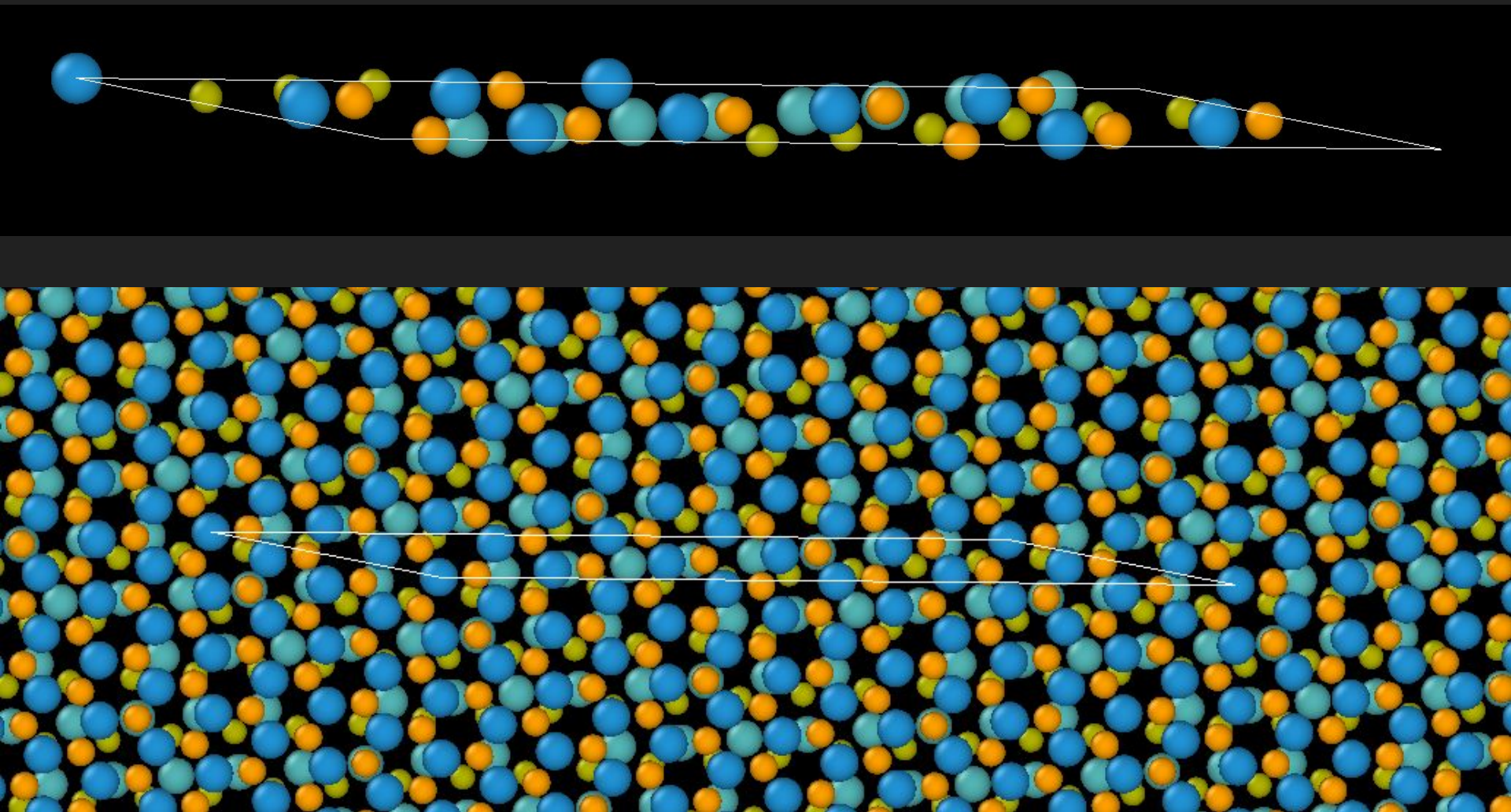
max_iter_twist_search = 5

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

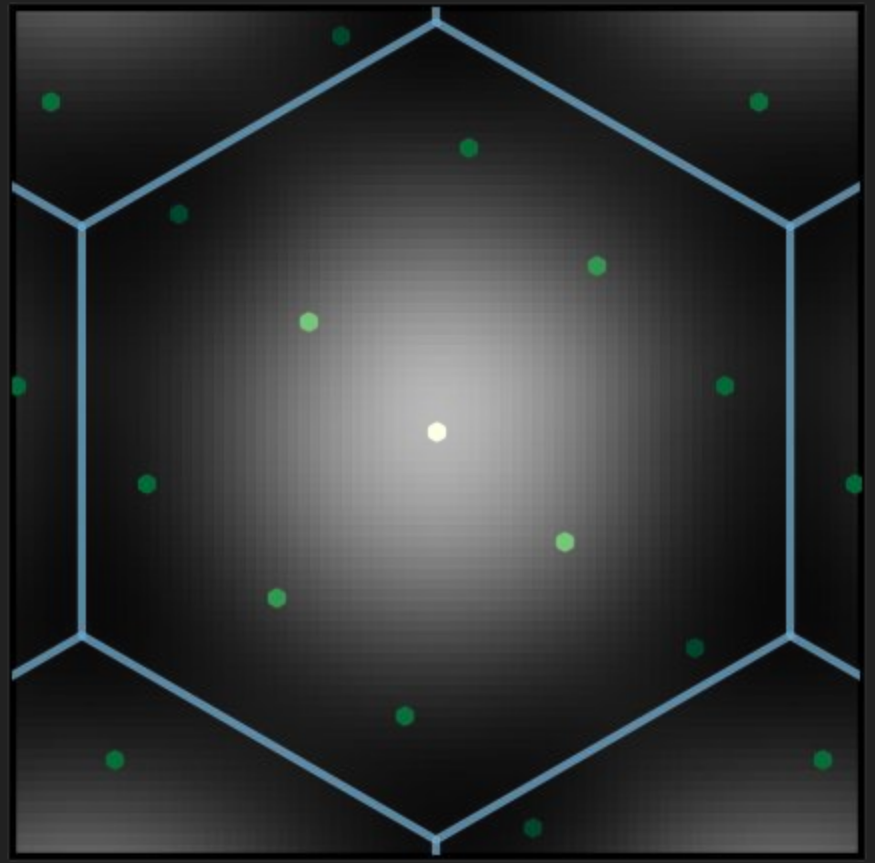
Rmax_max_search = 14

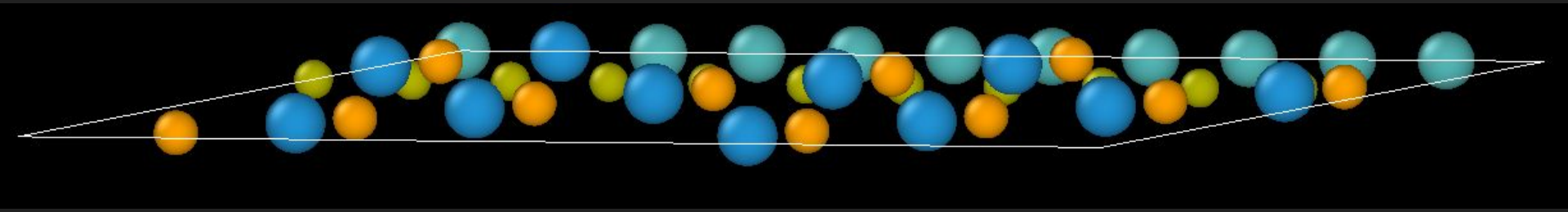
max_iter_twist_search = 5

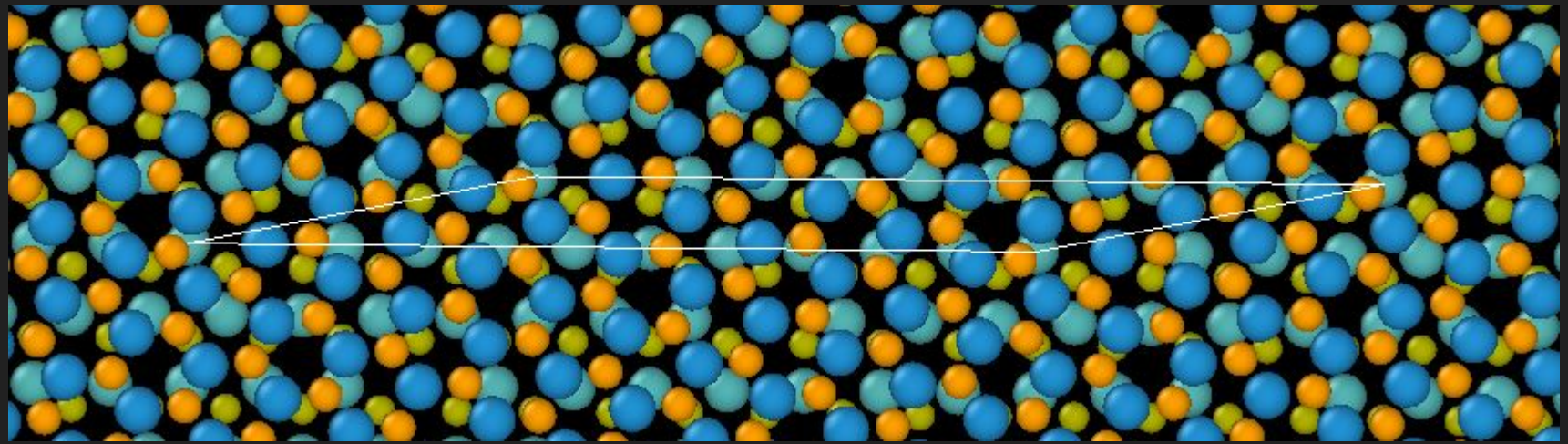
Total atoms: 66

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

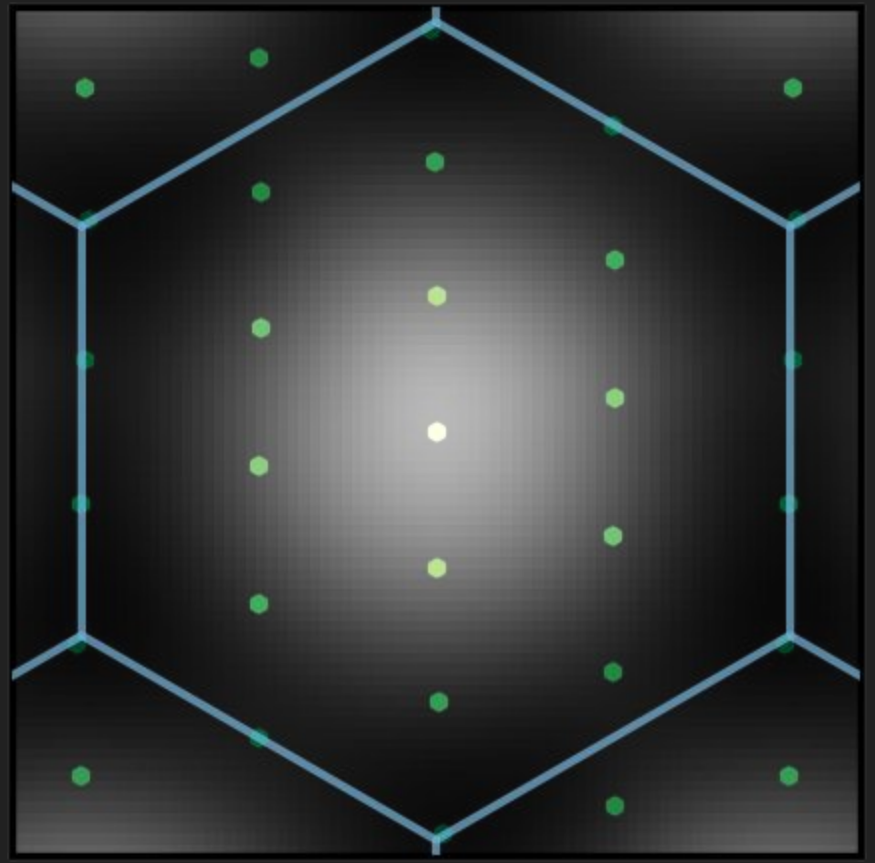
Rmax_max_search = 16

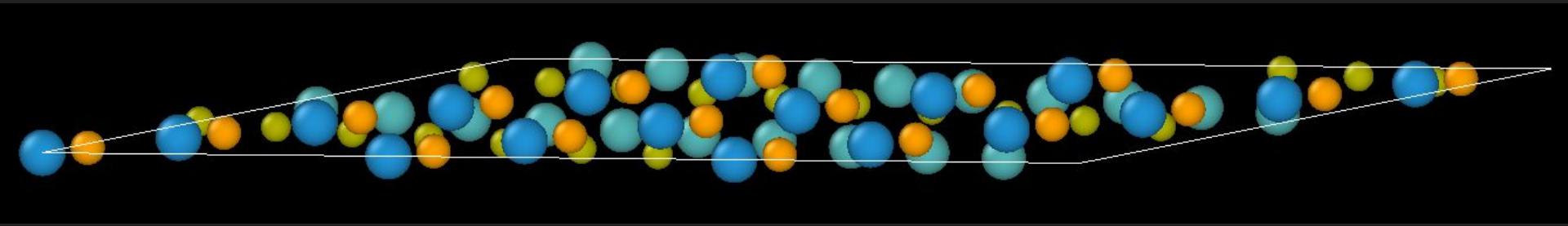
max_iter_twist_search = 5

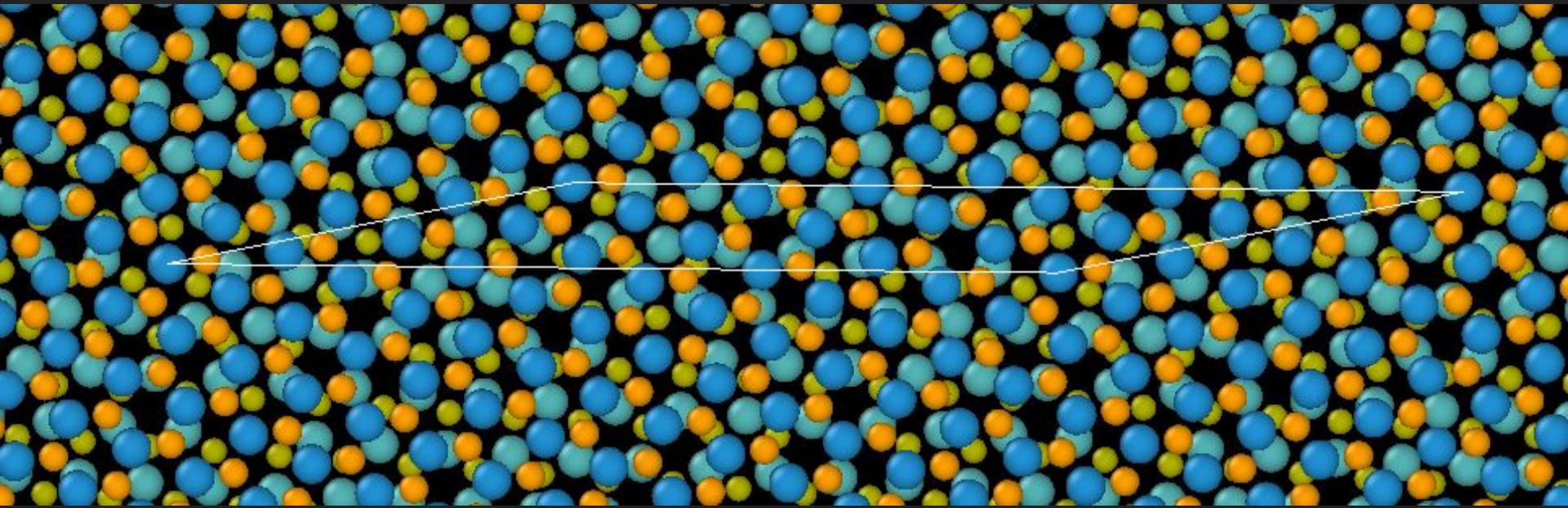
Total atoms: 117

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

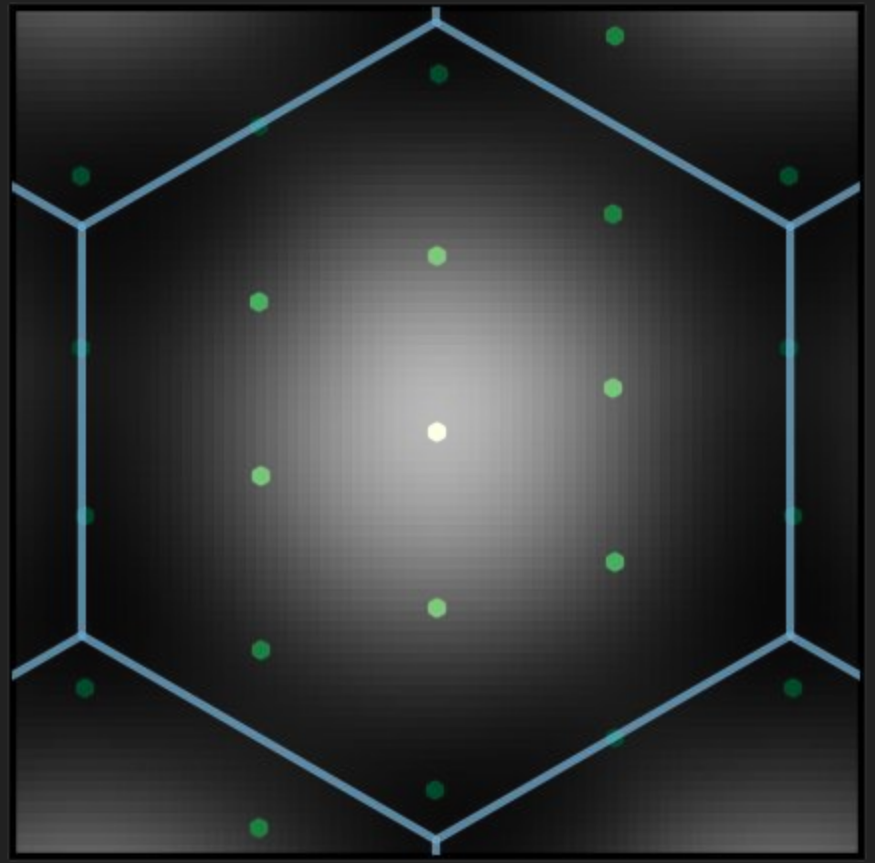
Rmax_max_search = 16

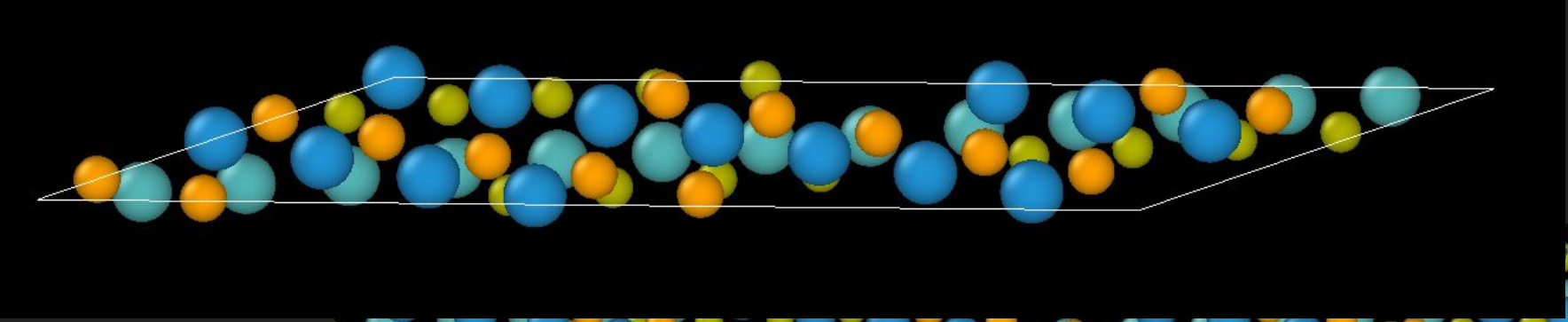
max_iter_twist_search = 5

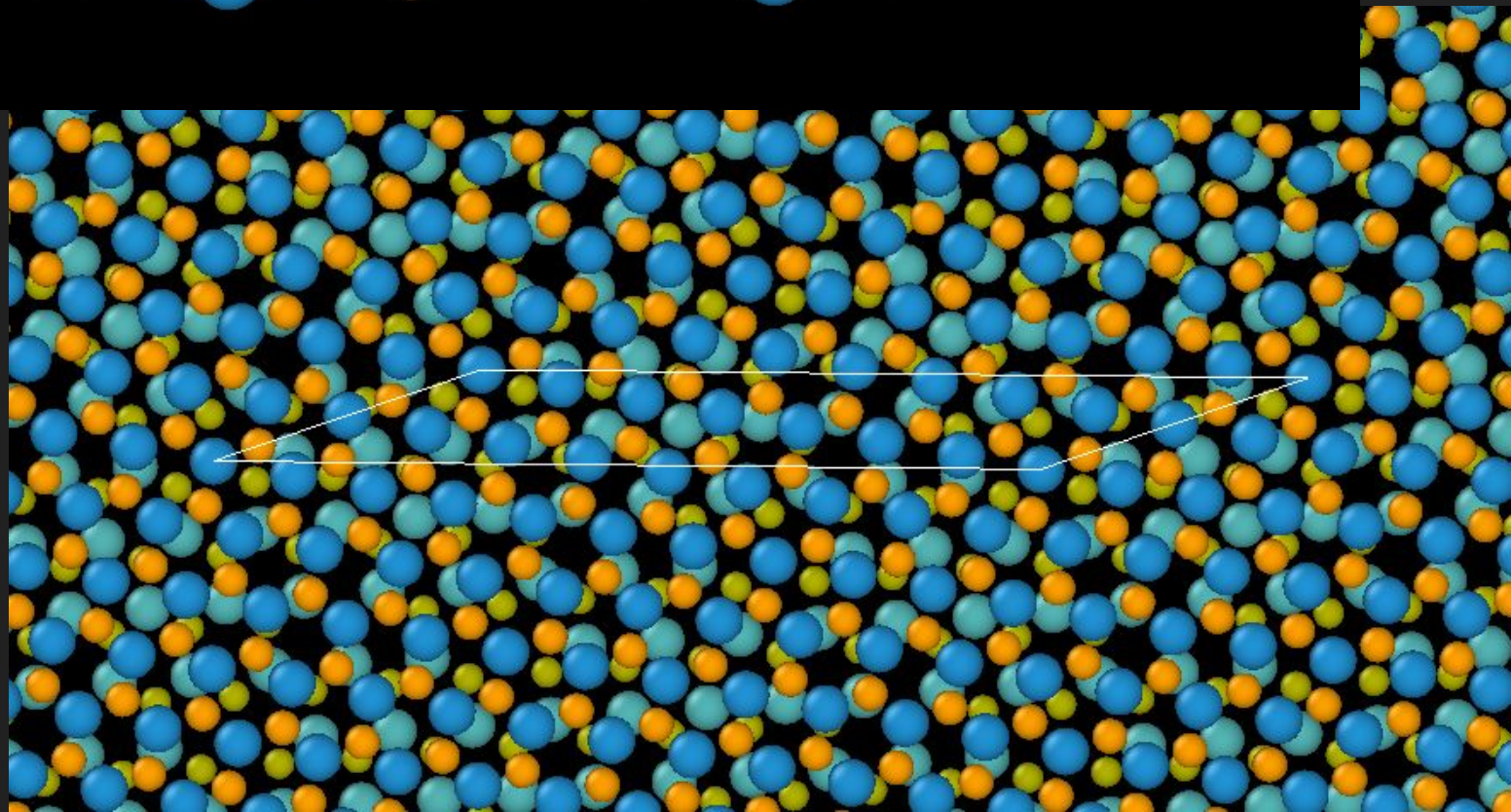
Total atoms: 84

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

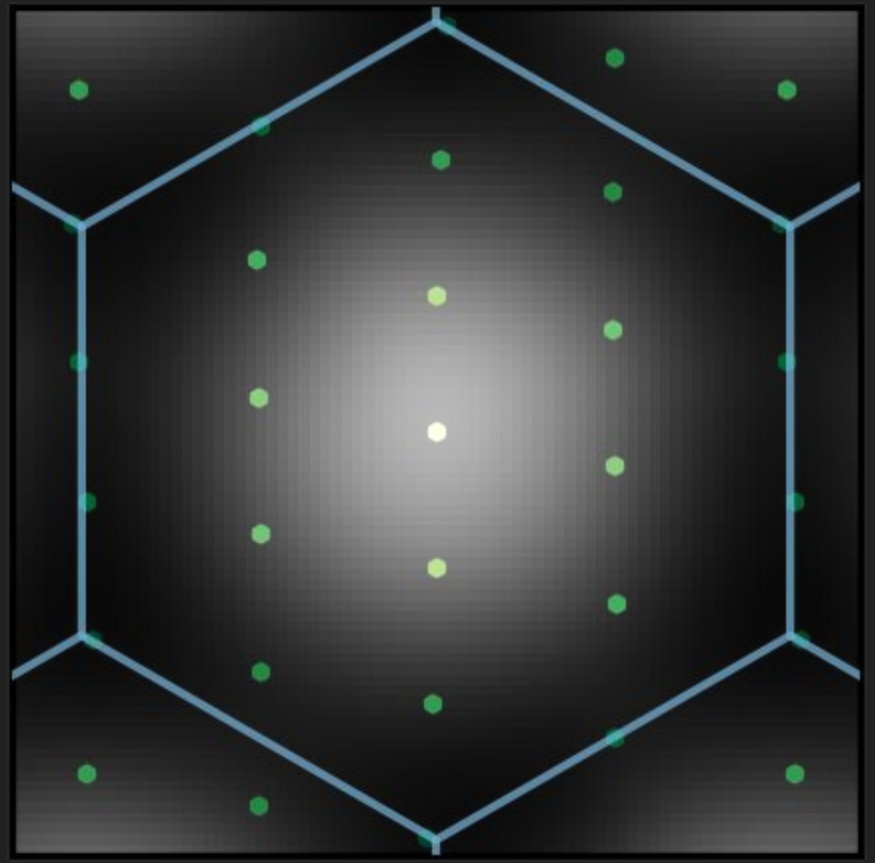
Rmax_max_search = 16

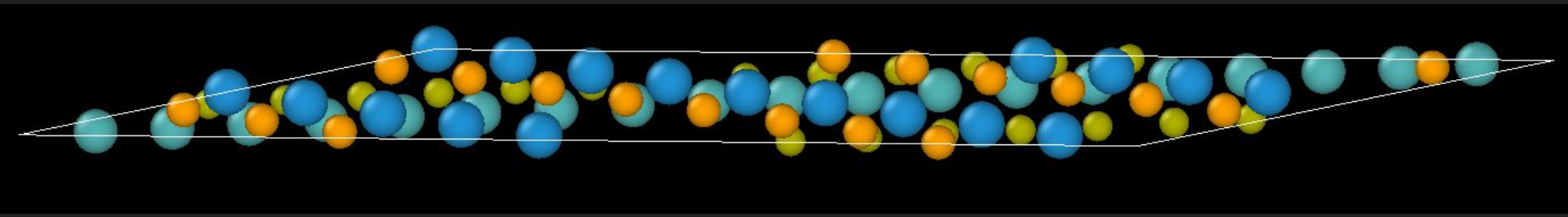
max_iter_twist_search = 5

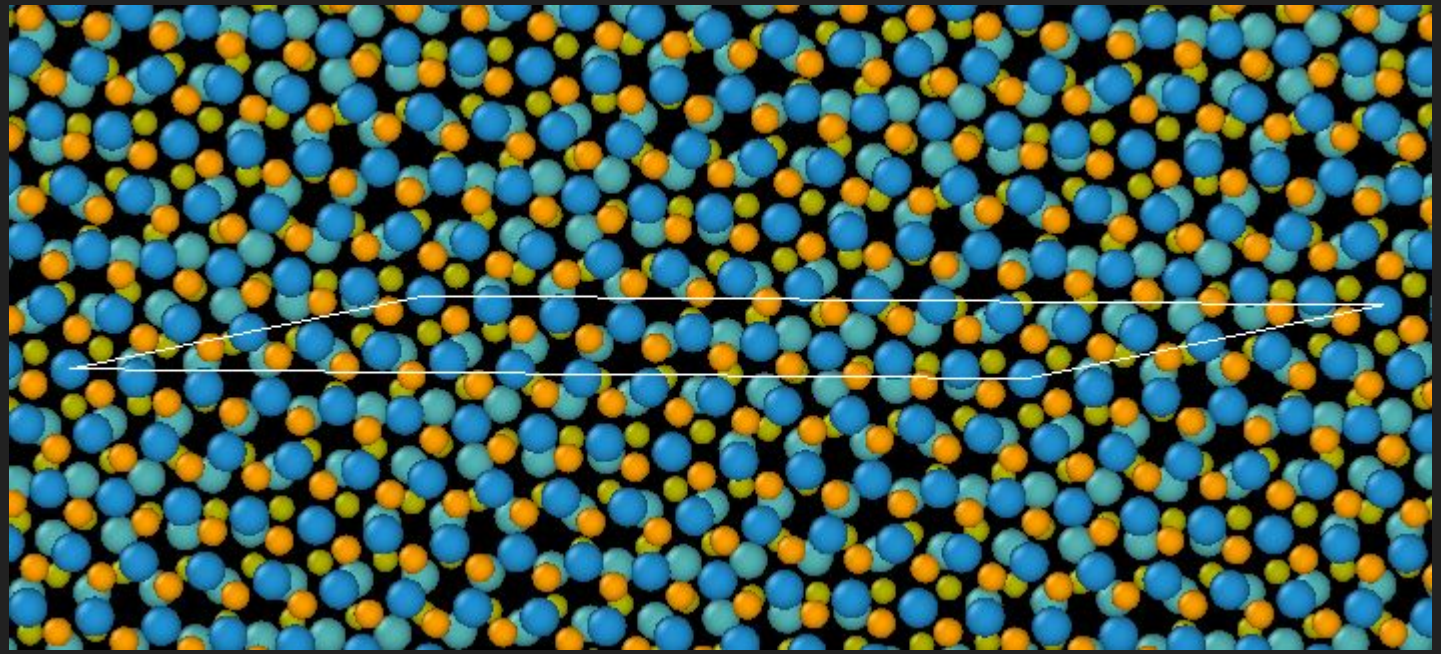
Total atoms: 114

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

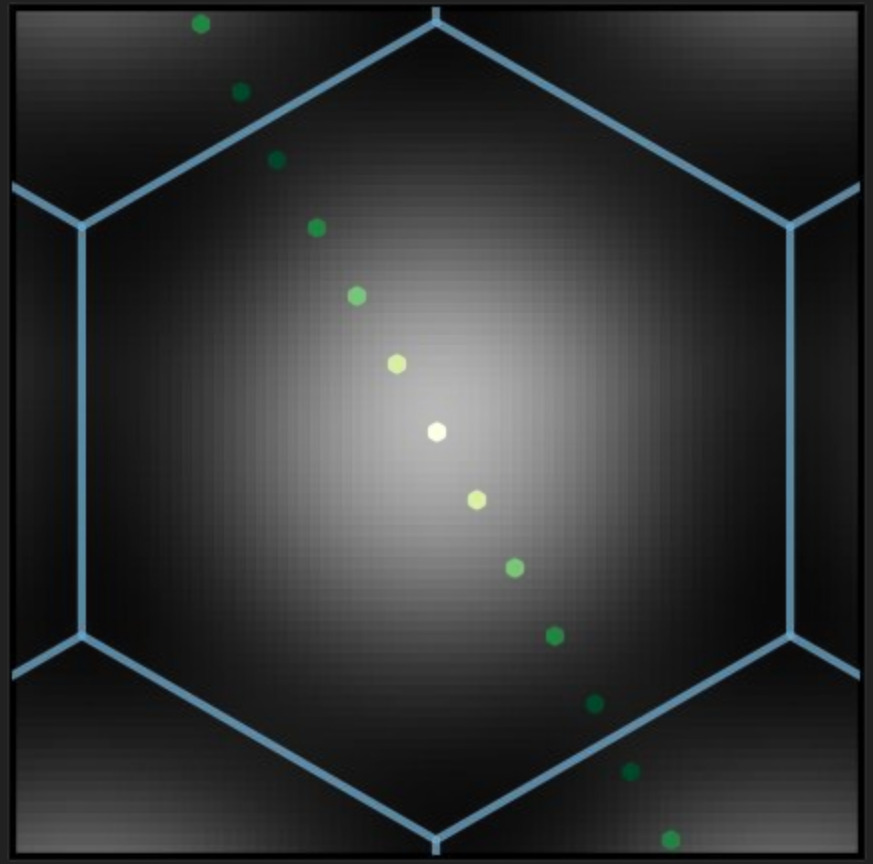
Rmax_max_search = 16

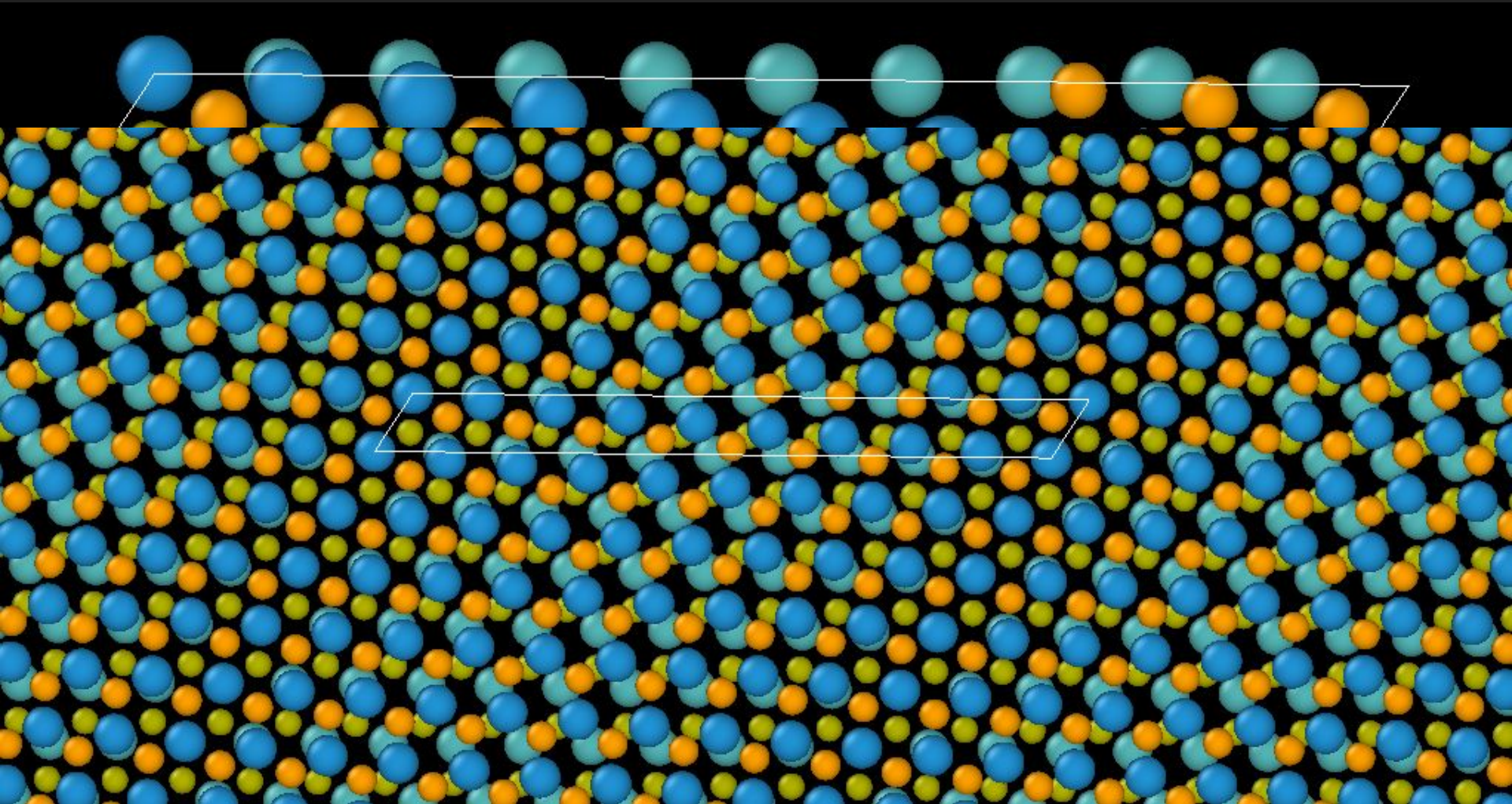
max_iter_twist_search = 5

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

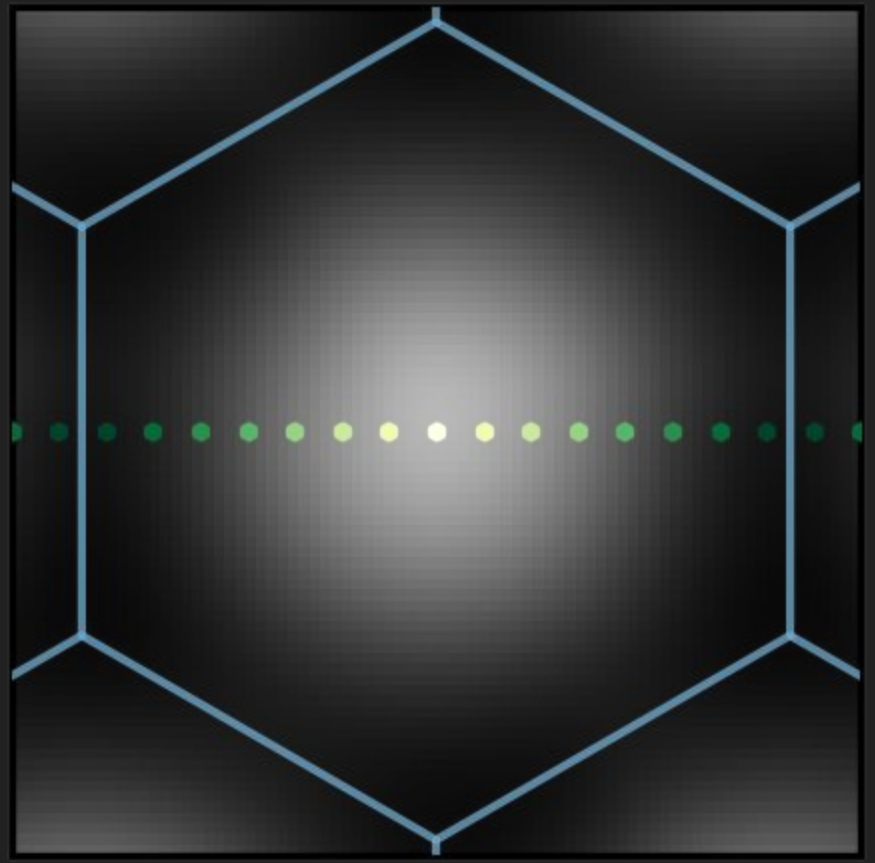
Rmax_max_search = 16

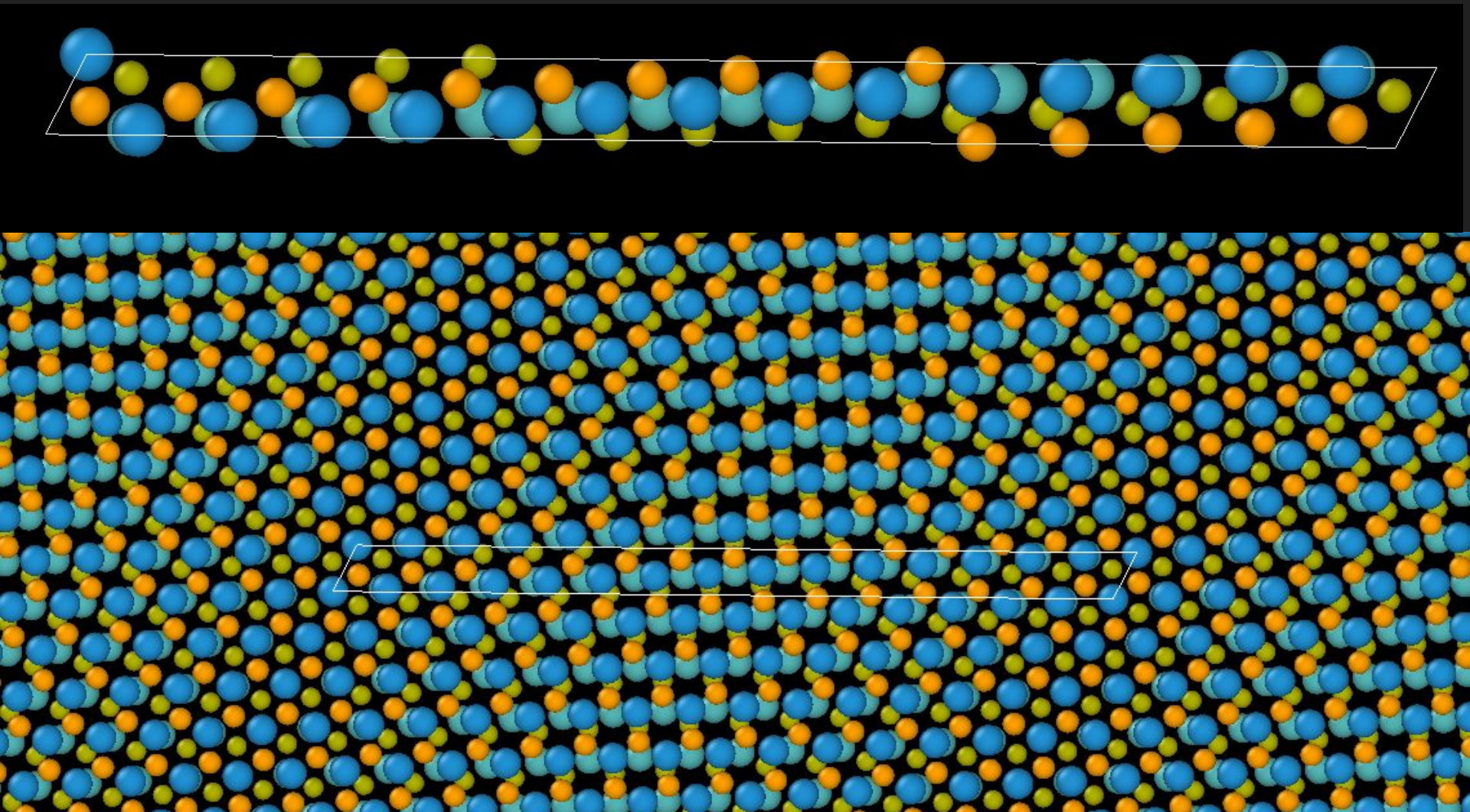
max_iter_twist_search = 5

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

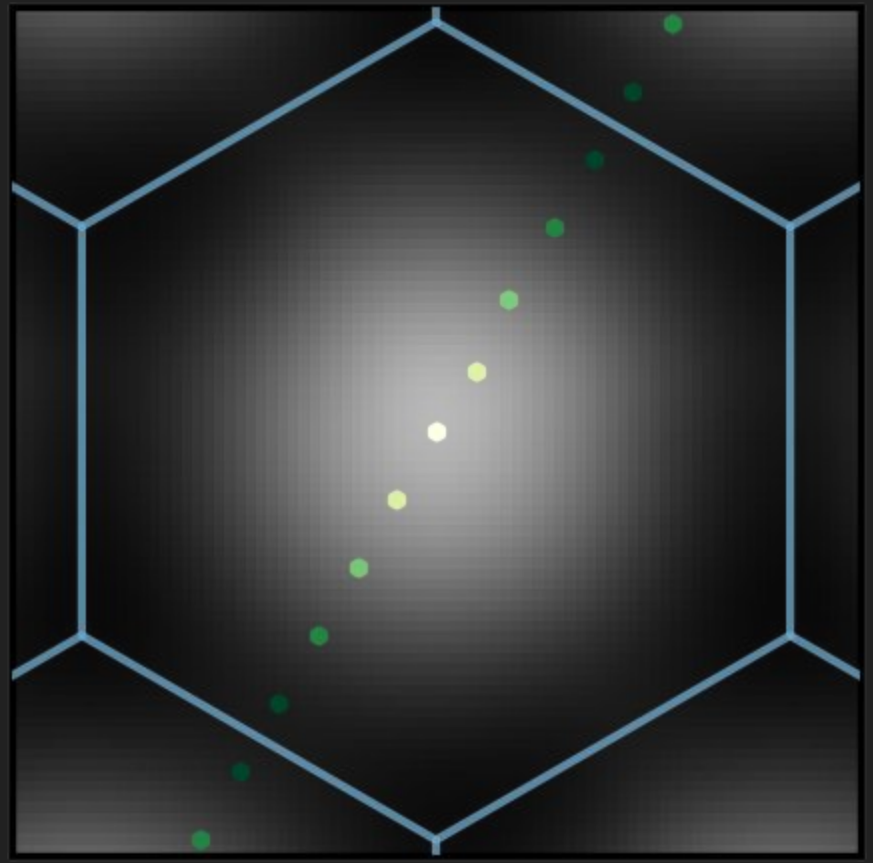
Rmax_max_search = 14

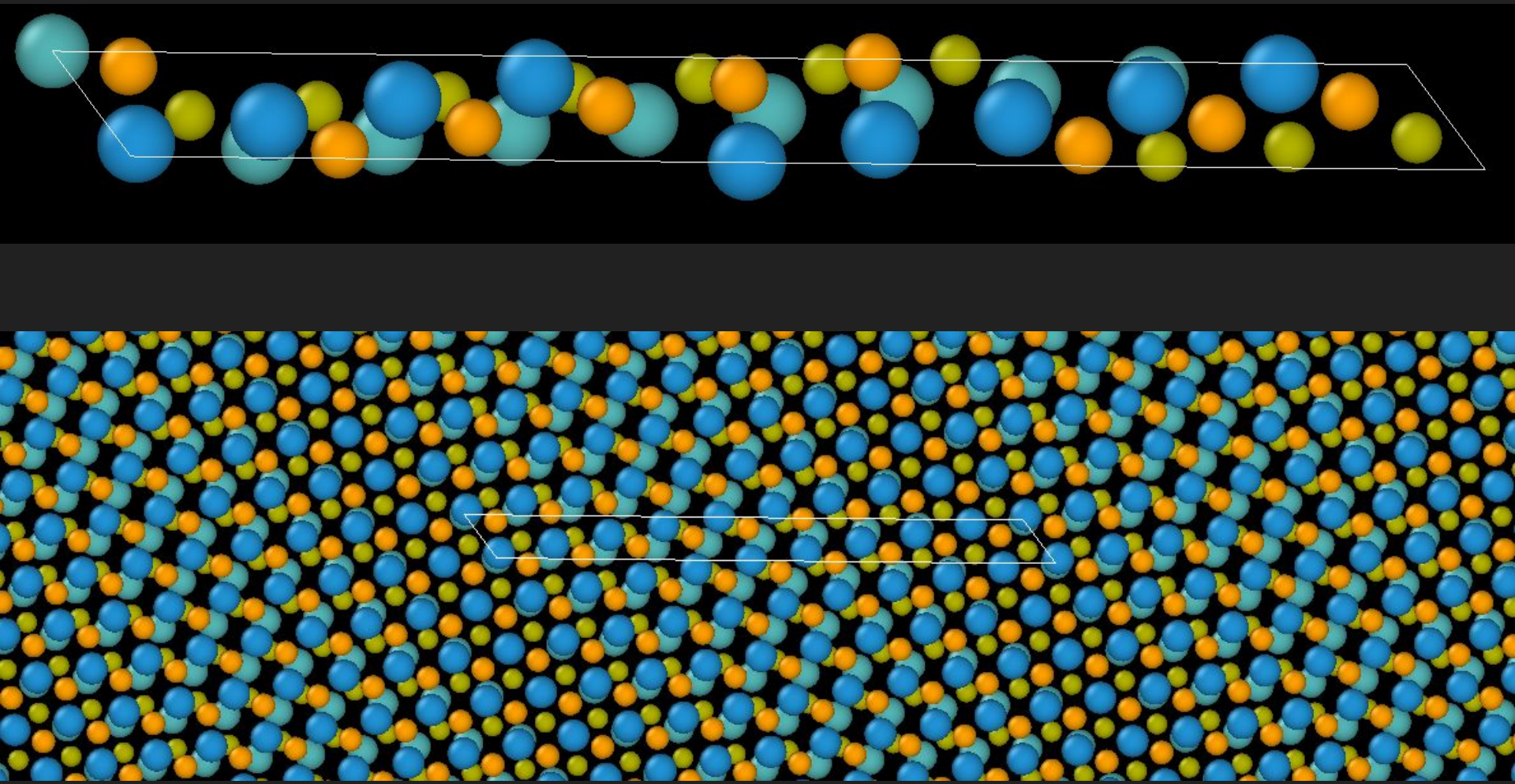
max_iter_twist_search = 5

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

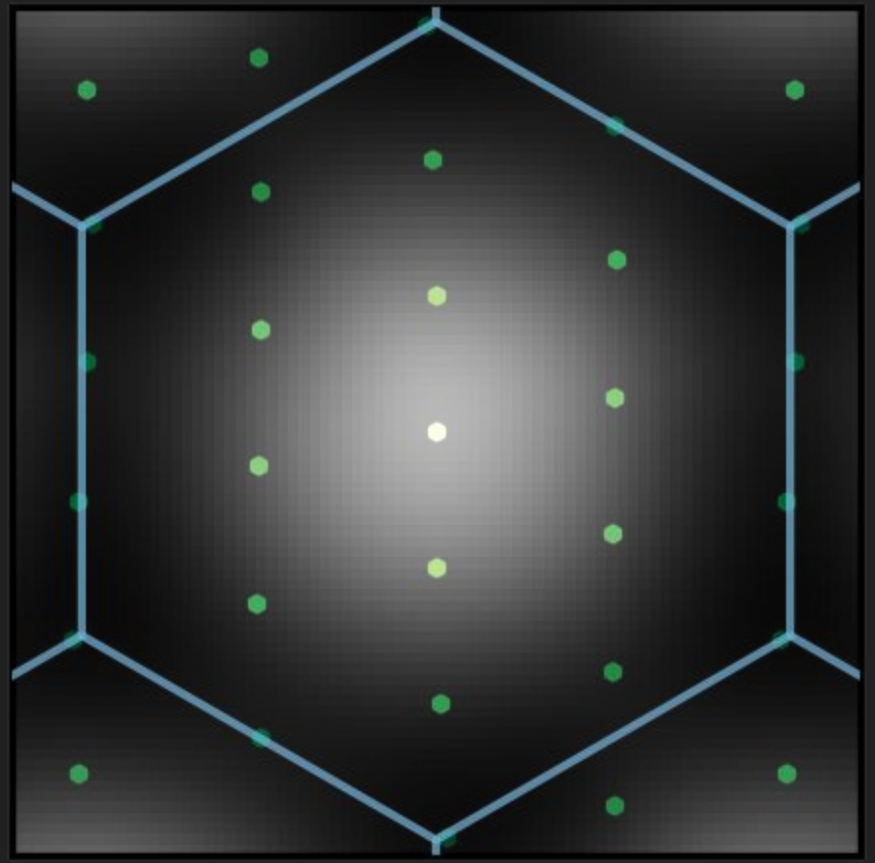
Rmax_max_search = 16

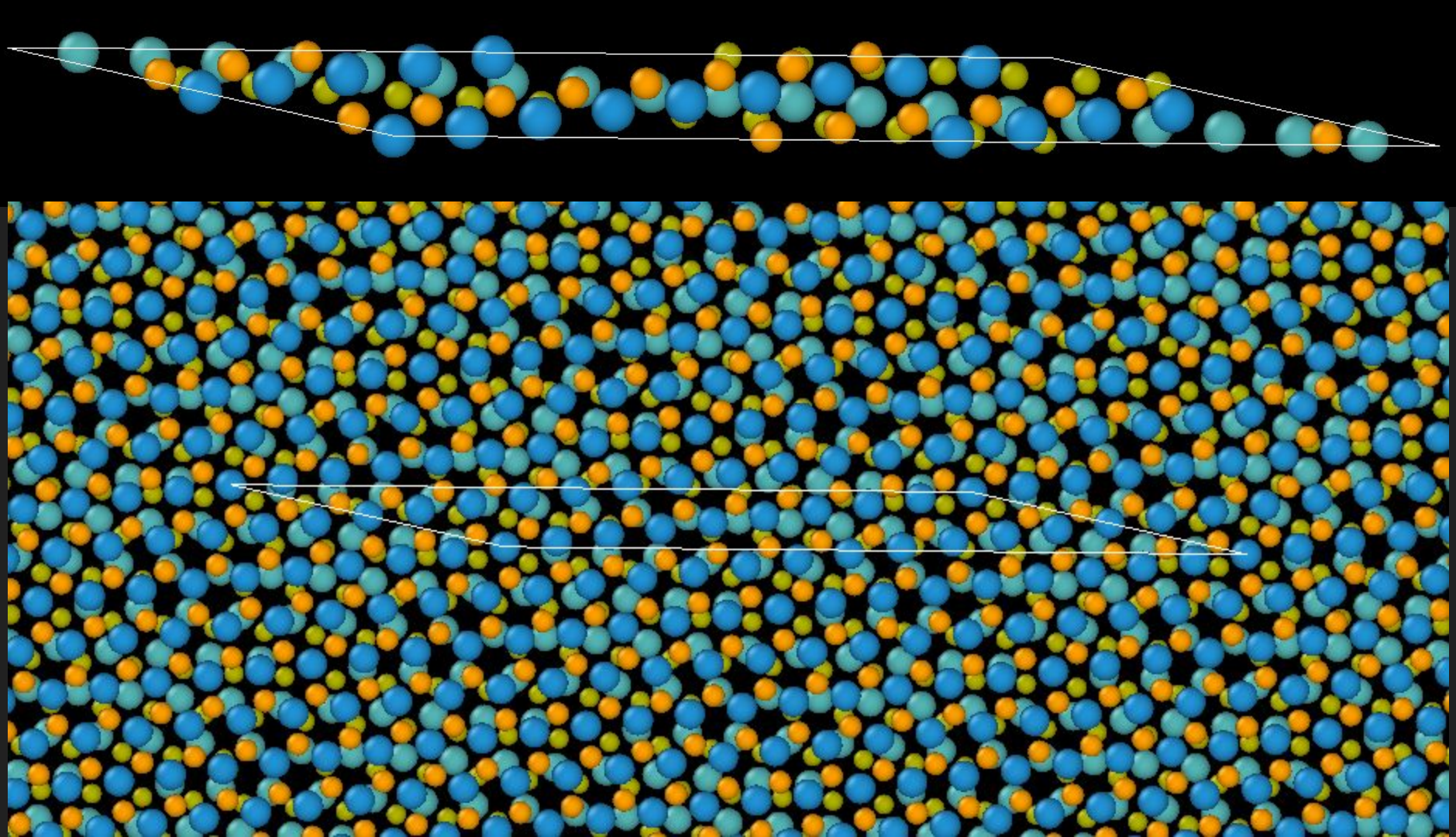
max_iter_twist_search = 5

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

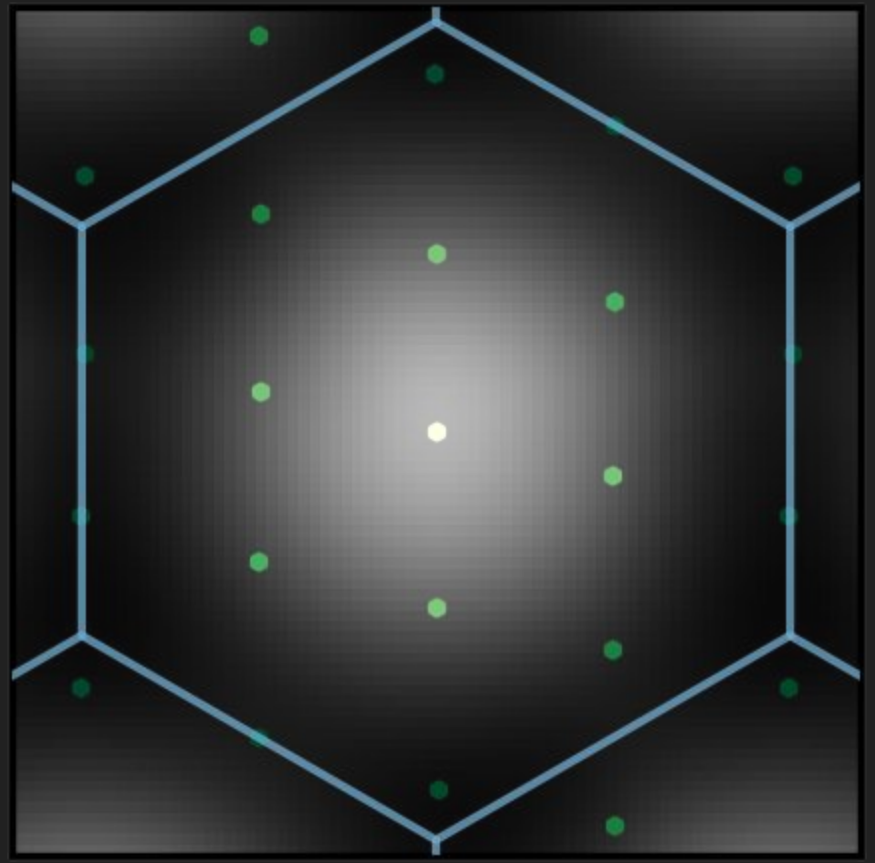
Rmax_max_search = 16

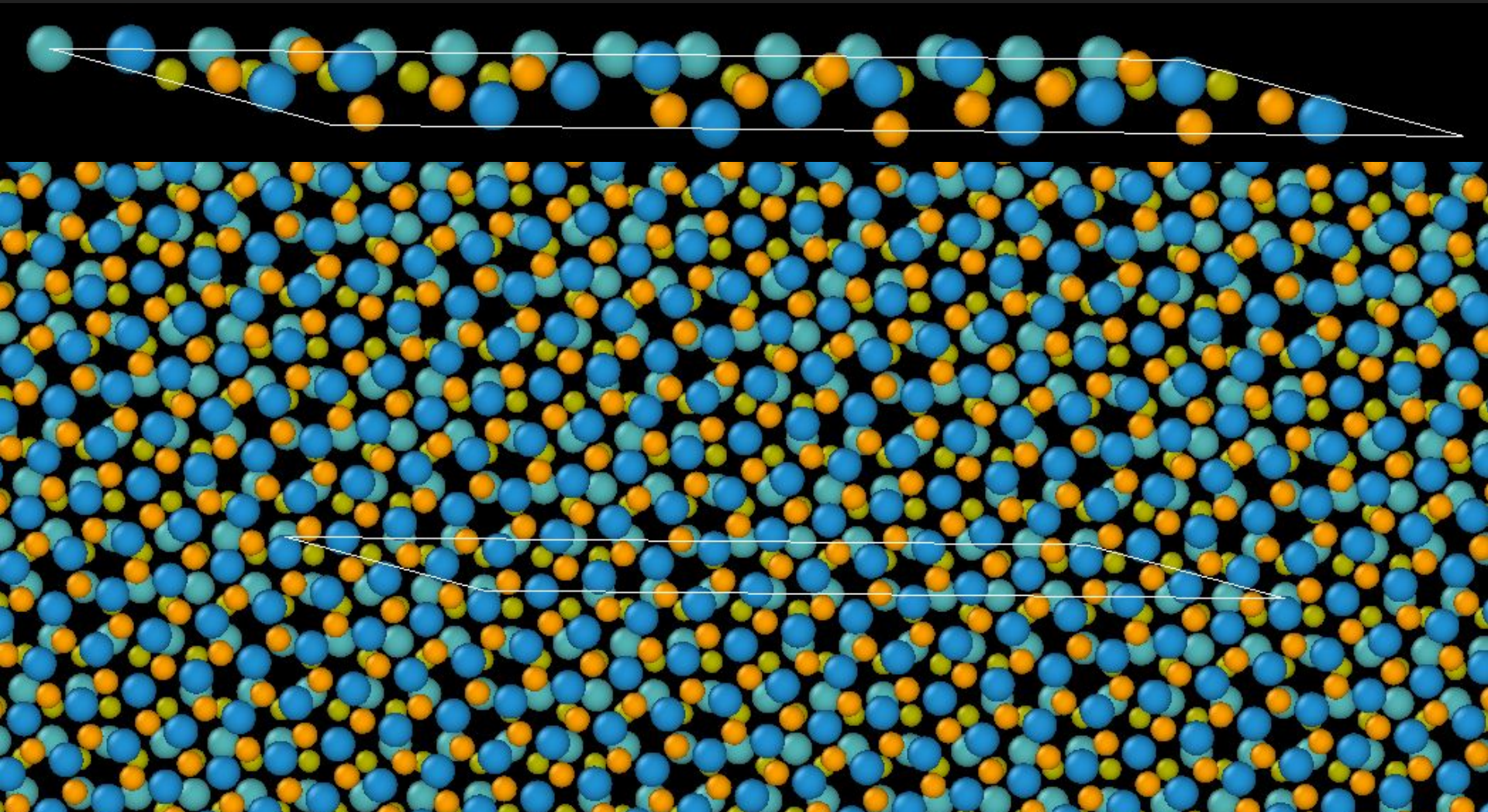
max_iter_twist_search = 5

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

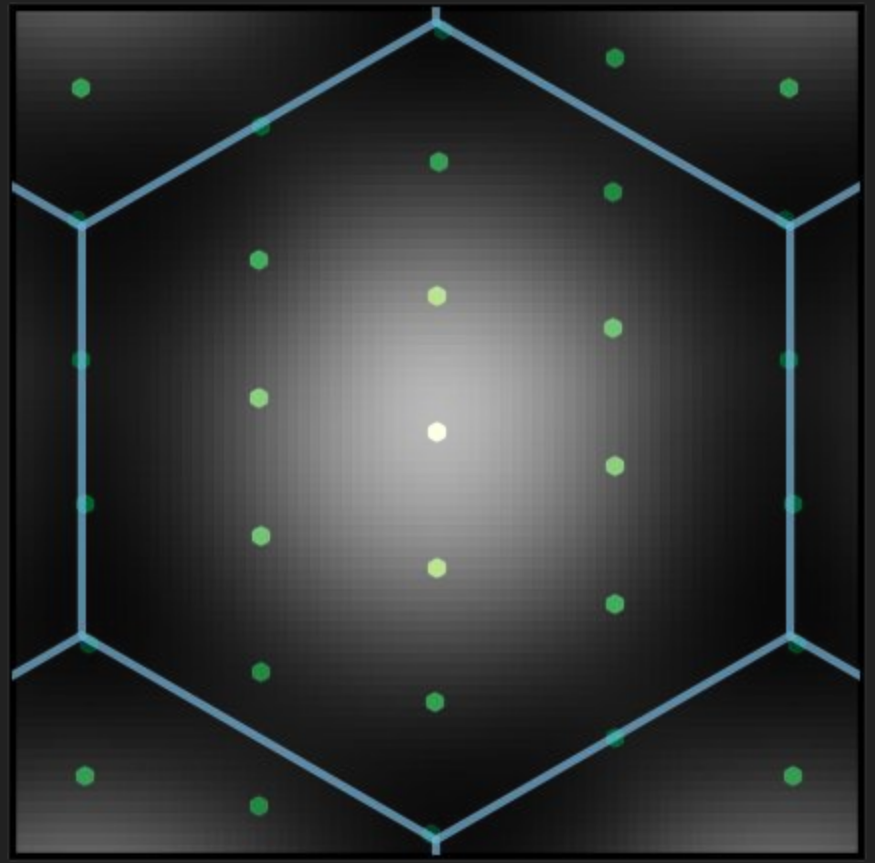
Rmax_max_search = 16

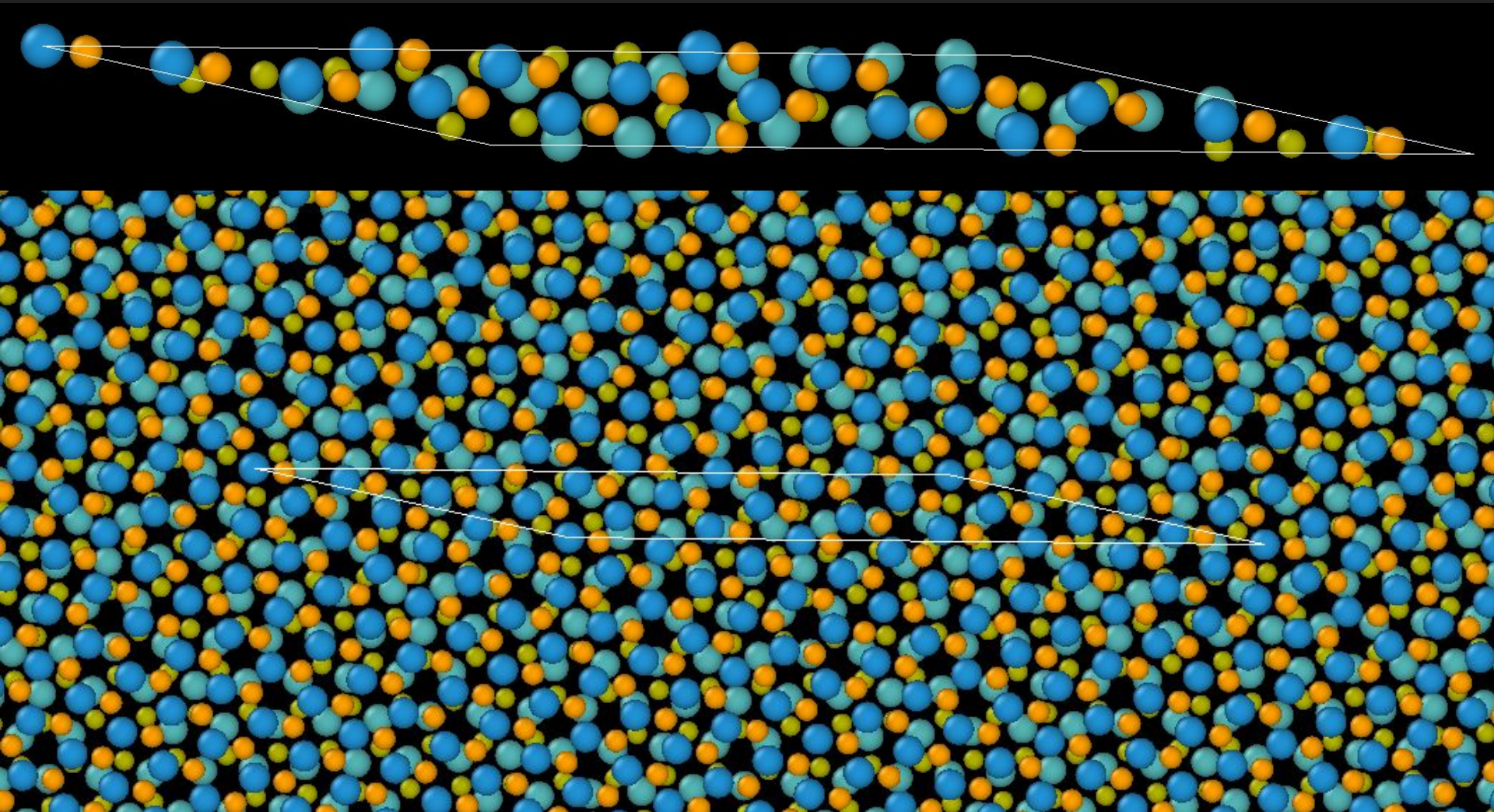
max_iter_twist_search = 5

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

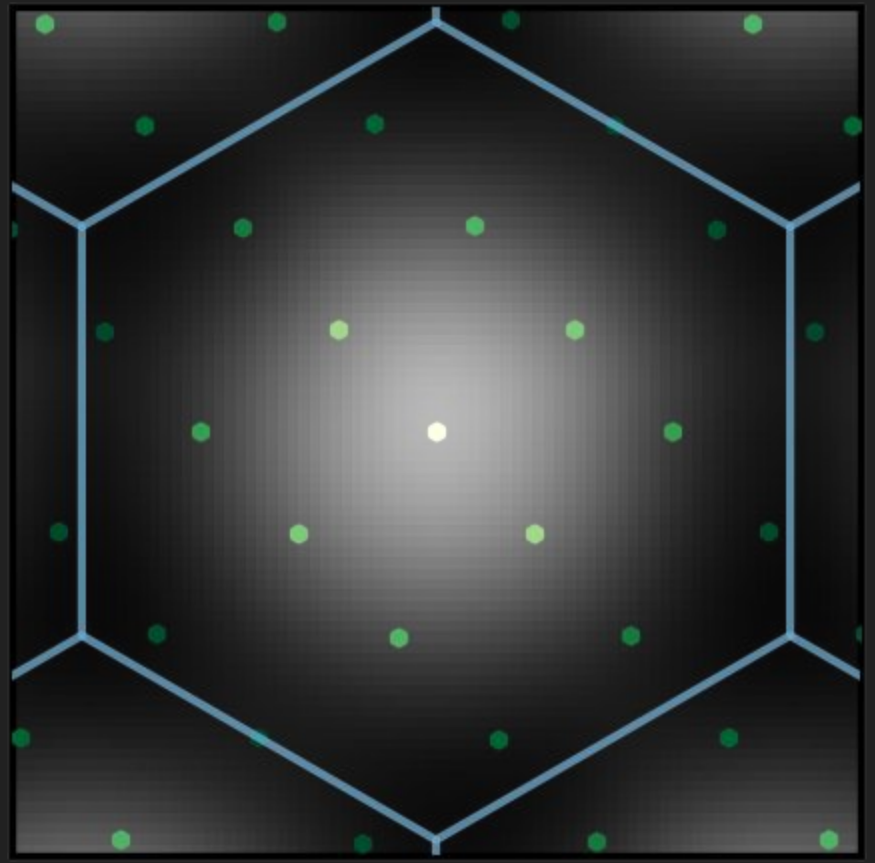
Rmax_max_search = 16

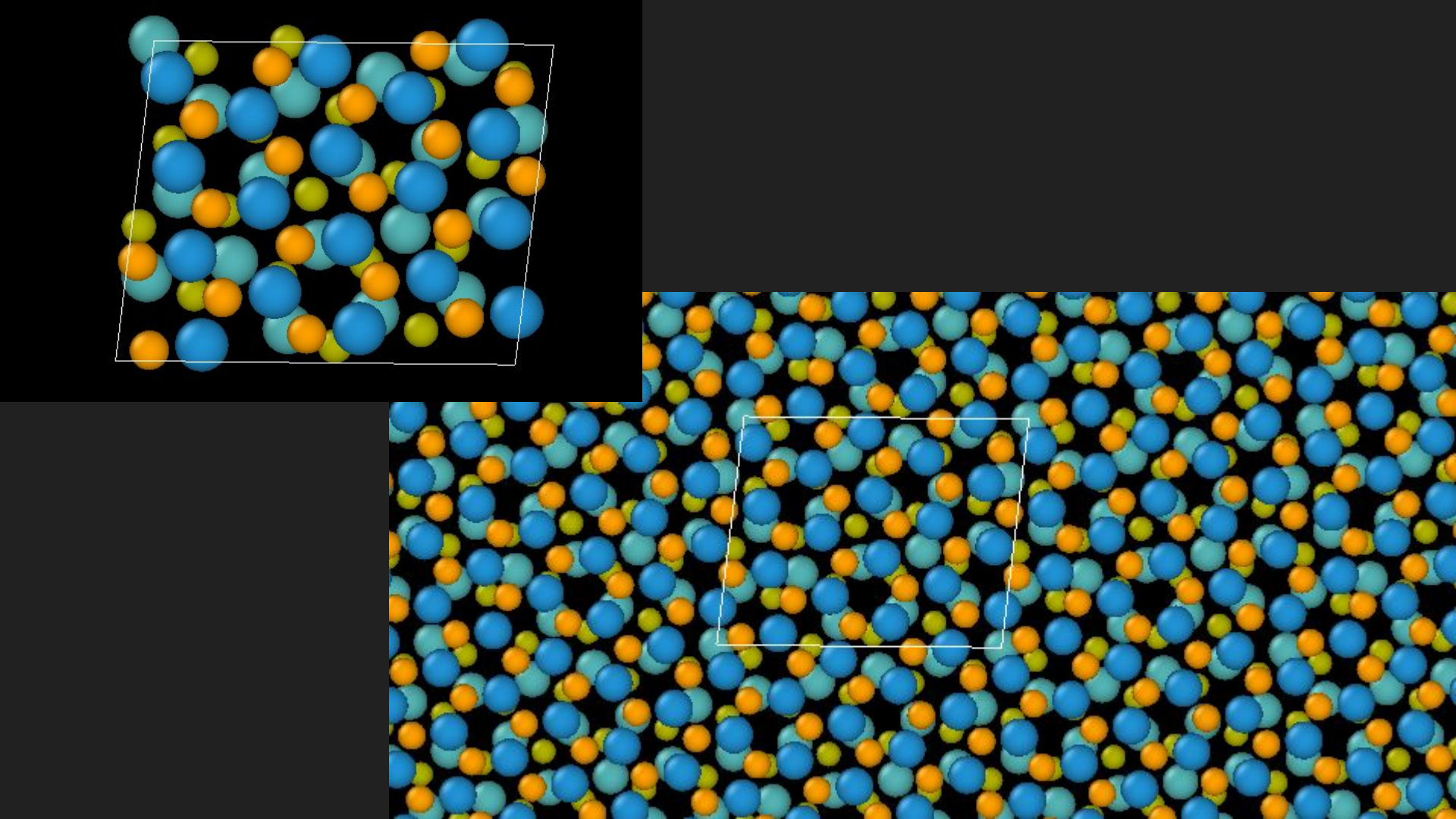
max_iter_twist_search = 5

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

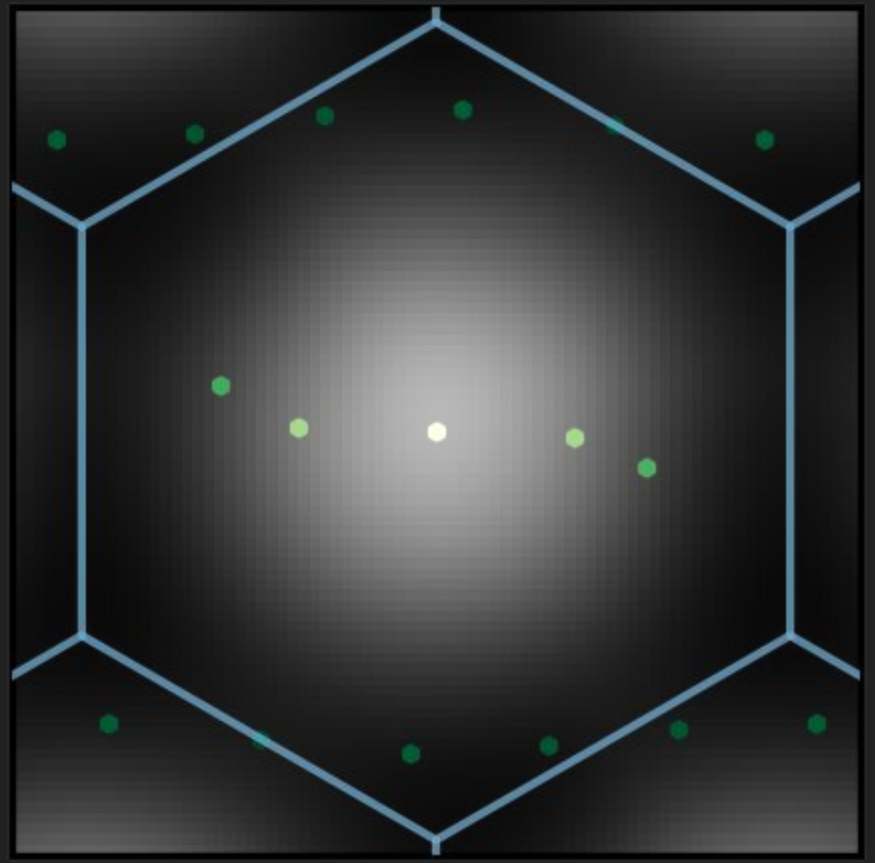
Rmax_max_search = 16

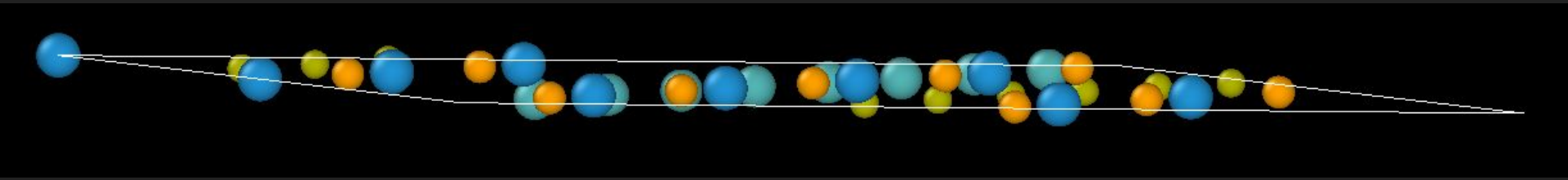
max_iter_twist_search = 5

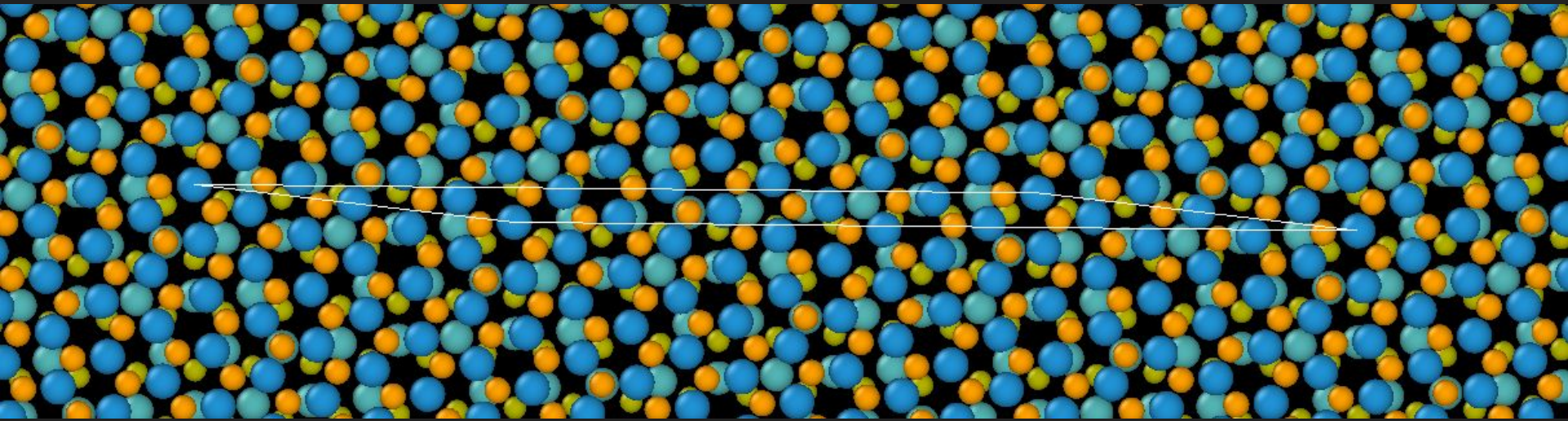
Total atoms: 57

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

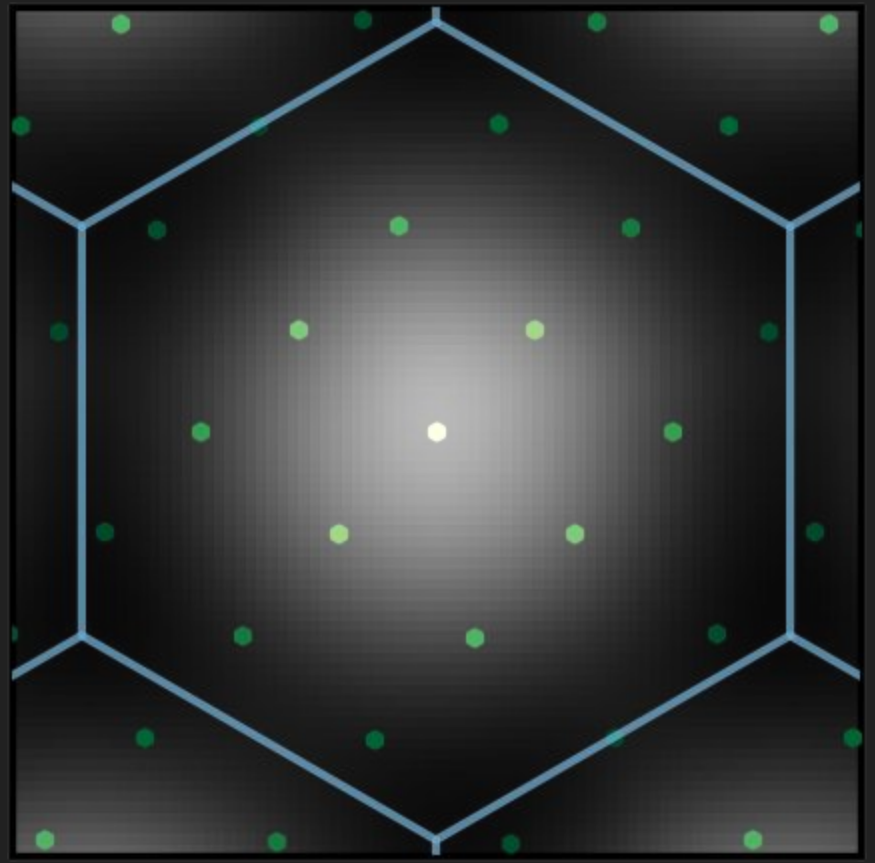
Rmax_max_search = 16

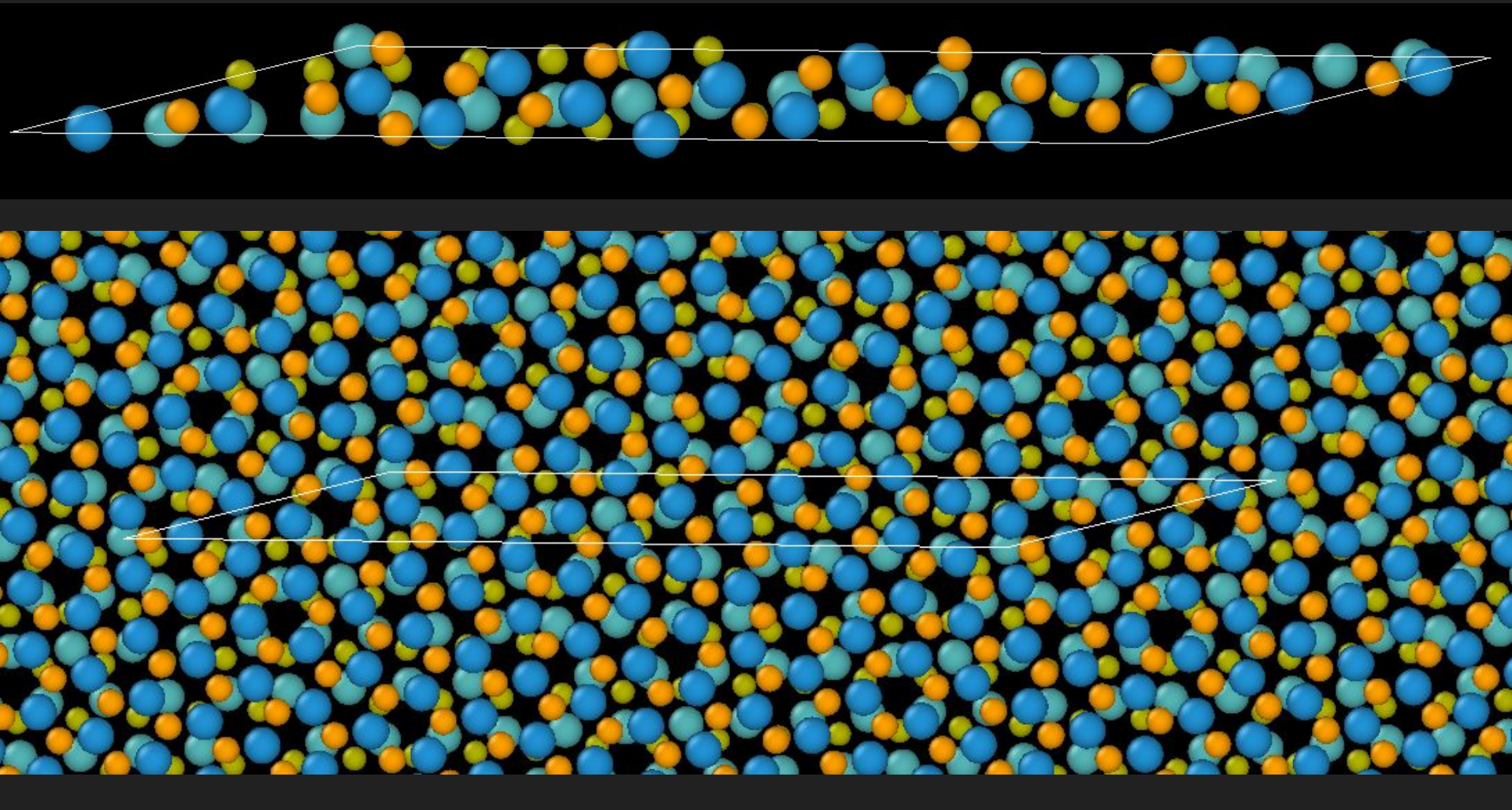
max_iter_twist_search = 5

Total atoms: 111

Mo count: 19

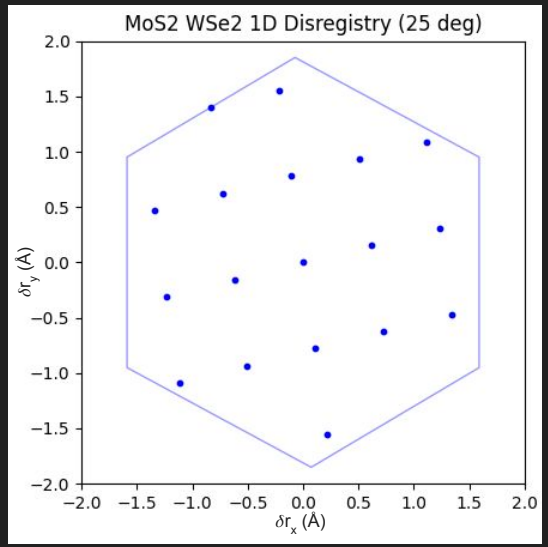
W count: 18

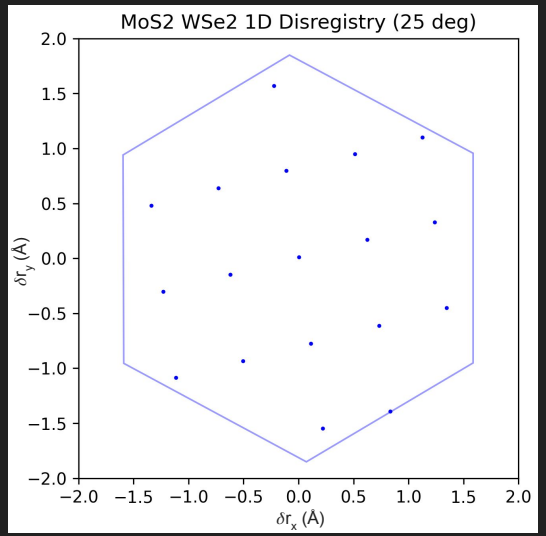




Pitfalls Cont.

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

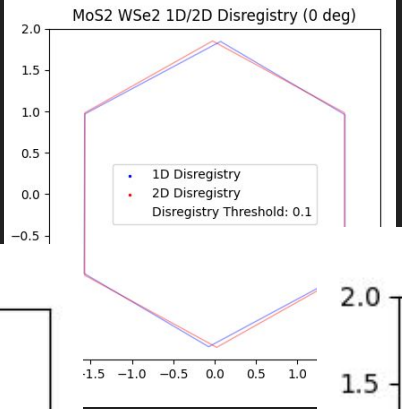


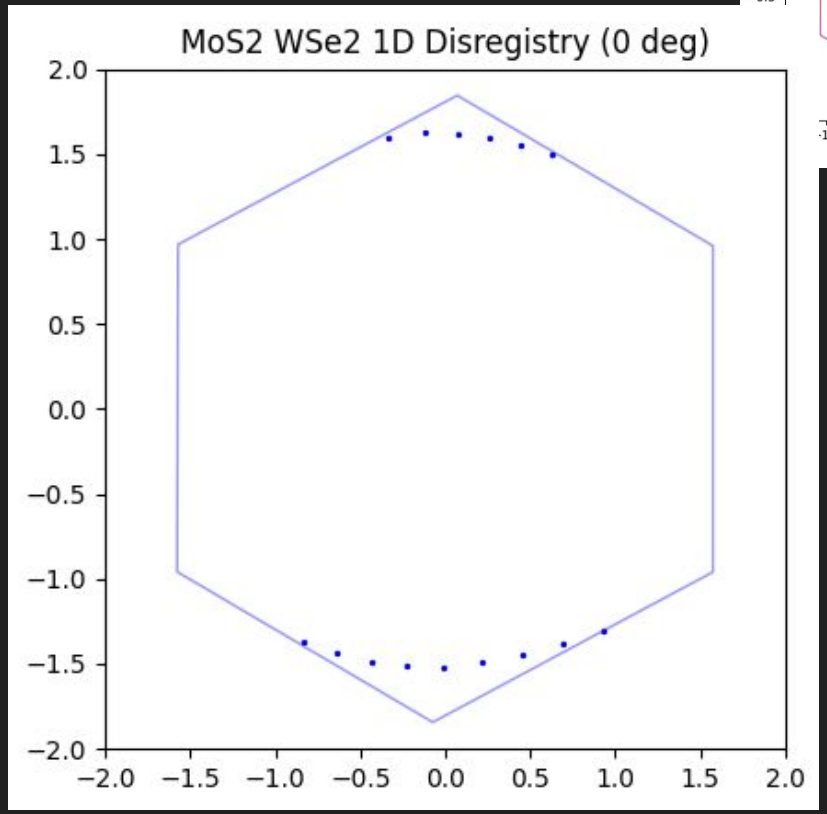


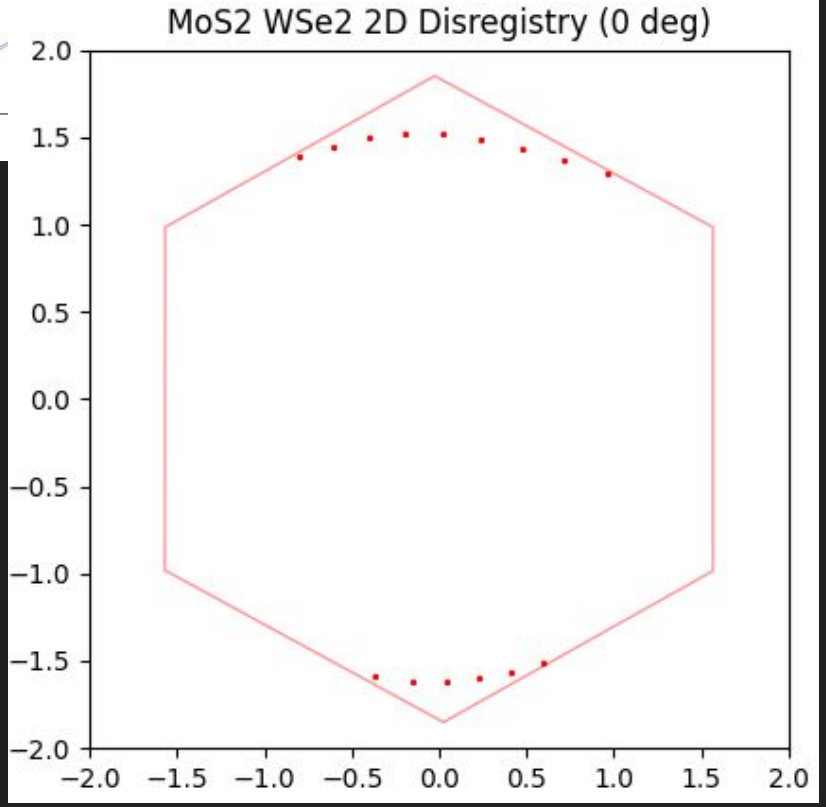
25 degree twist angle for Q1D Pre Relaxation vs. Post Relaxation

Post Relaxation

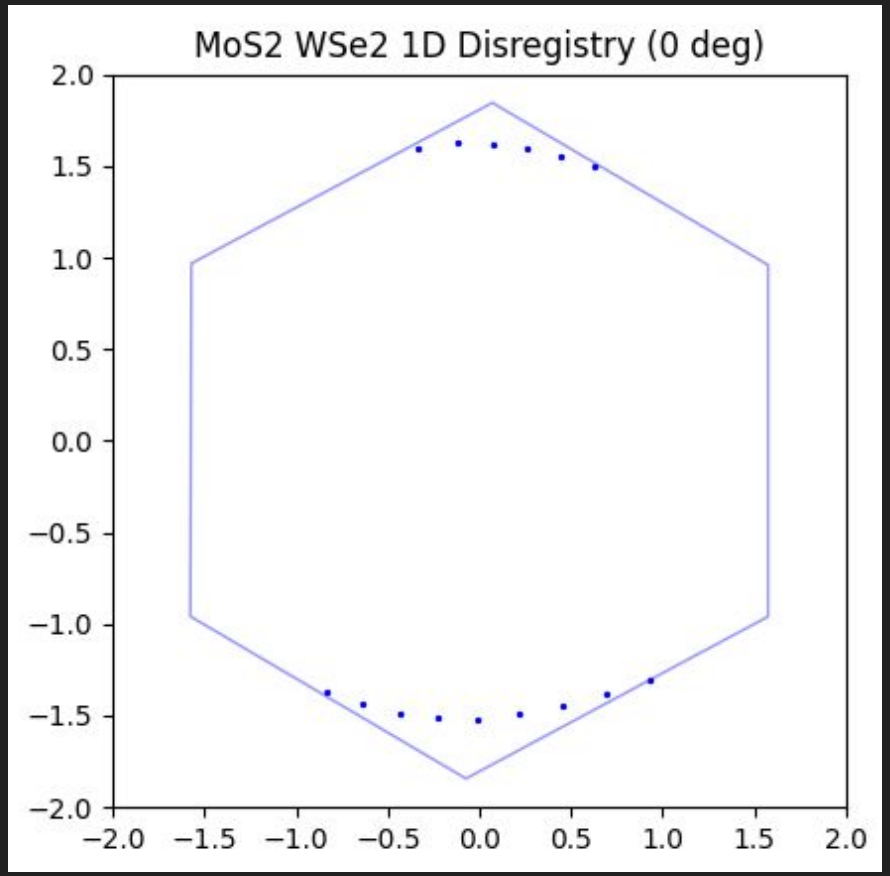
0 Degrees

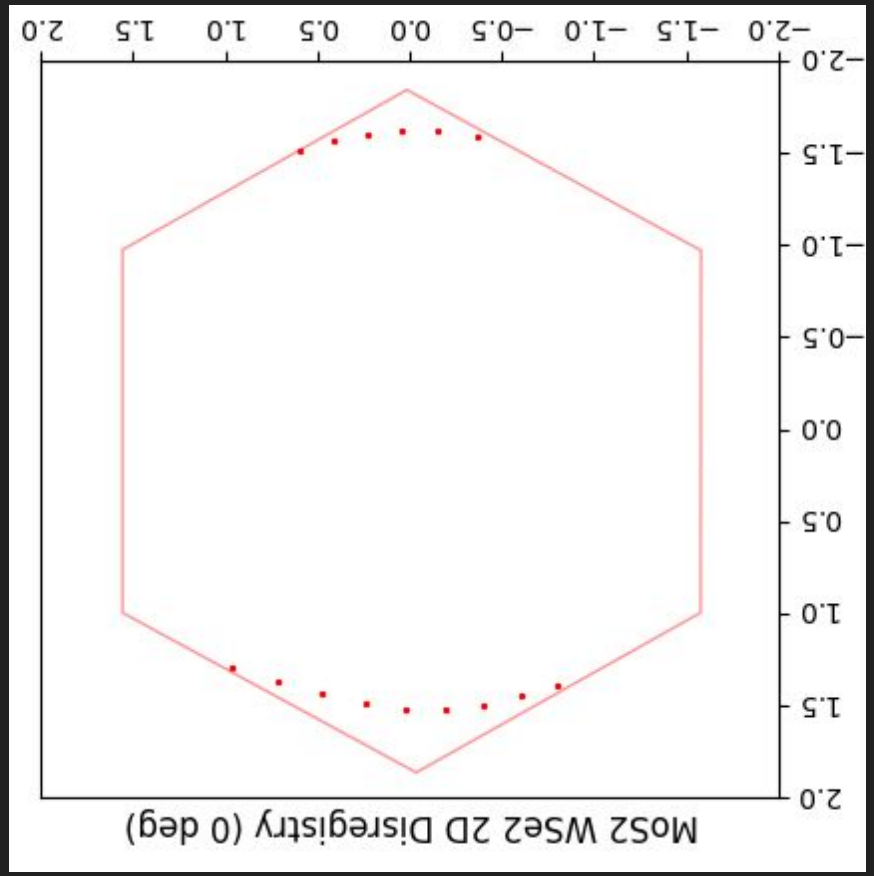

MoS2 WSe2 1D/2D Disregistry (0 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1


MoS2 WSe2 1D Disregistry (0 deg)

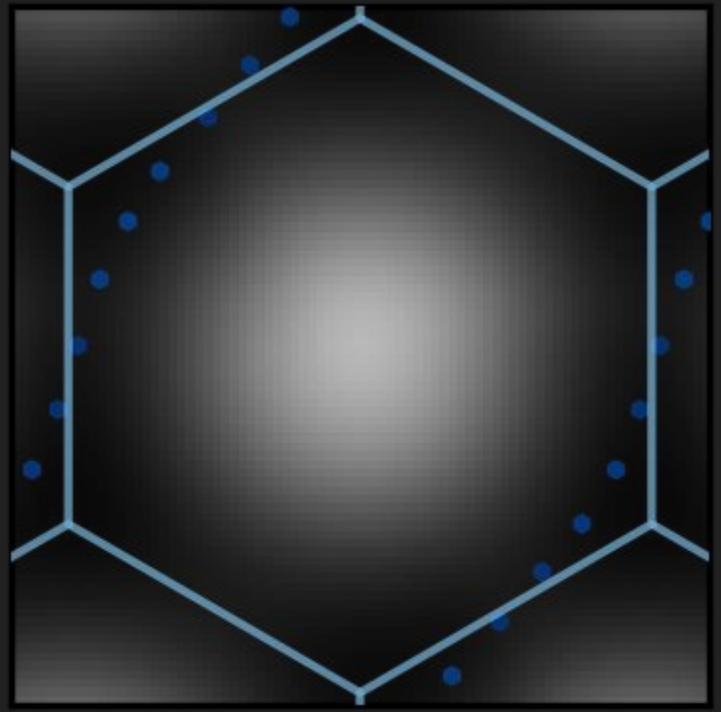

MoS2 WSe2 2D Disregistry (0 deg)

0 deg

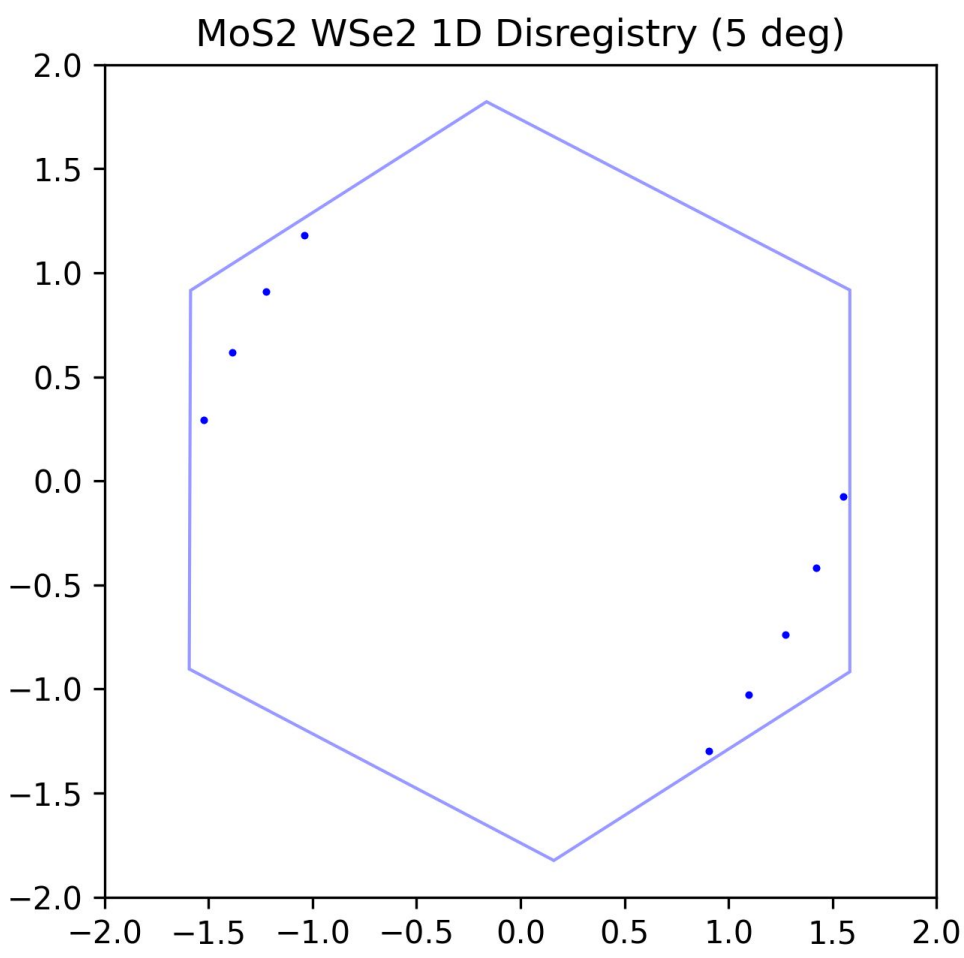

MoS2 WSe2 1D Disregistry (0 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

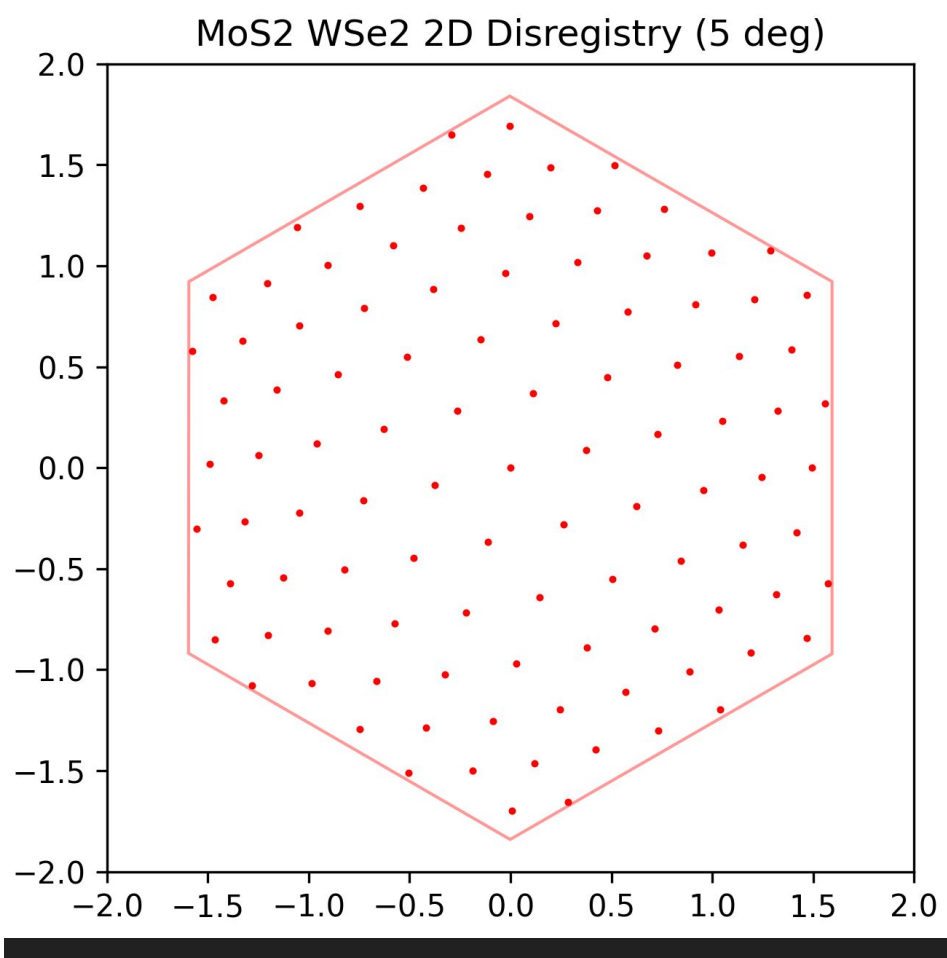

MoS2 WSe2 2D Disregistry (0 deg)

5 Degrees

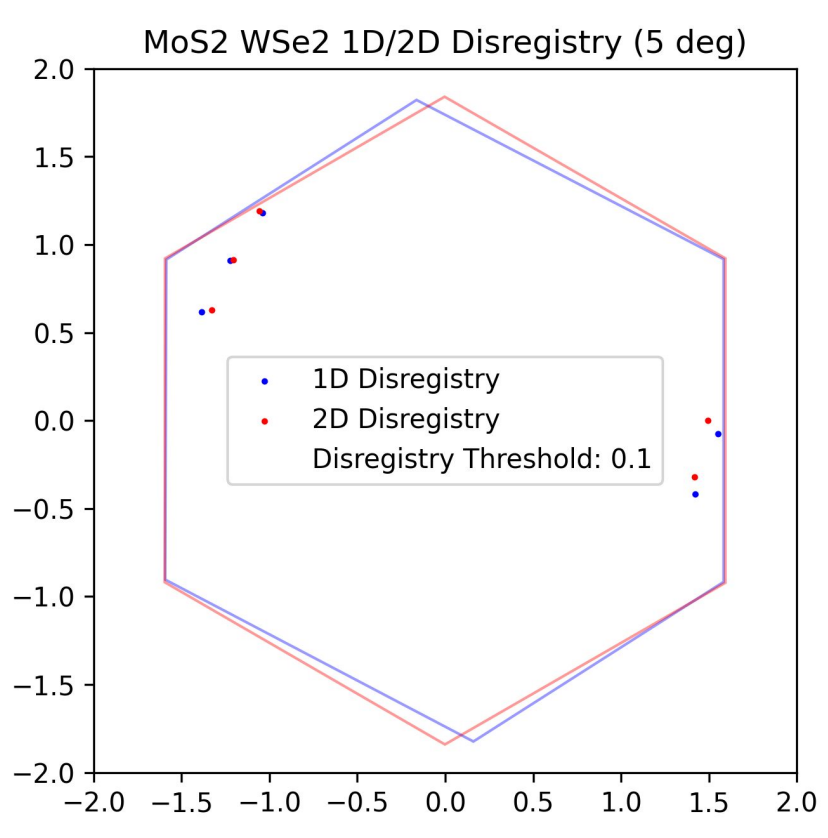


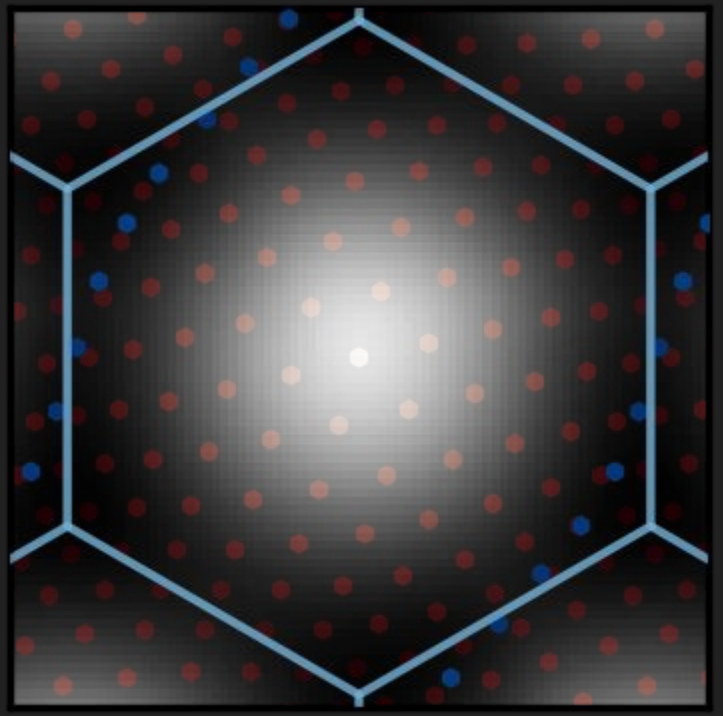
Actual Twist Angle: 4.97900323968
Total Atoms: 642
W Atoms (Top Layer): 103
Mo Atoms (Bottom Layer): 111


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

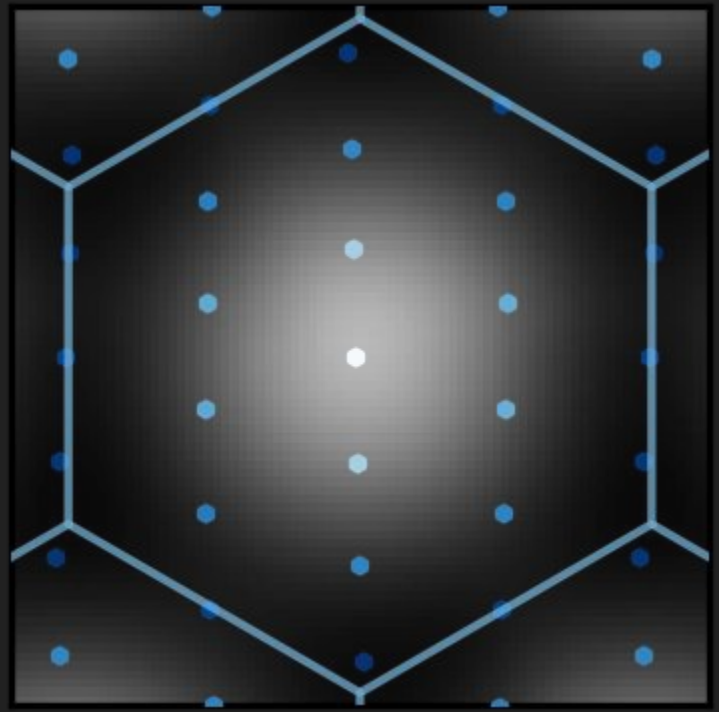

MoS2 WSe2 2D Disregistry (5 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0

5 deg

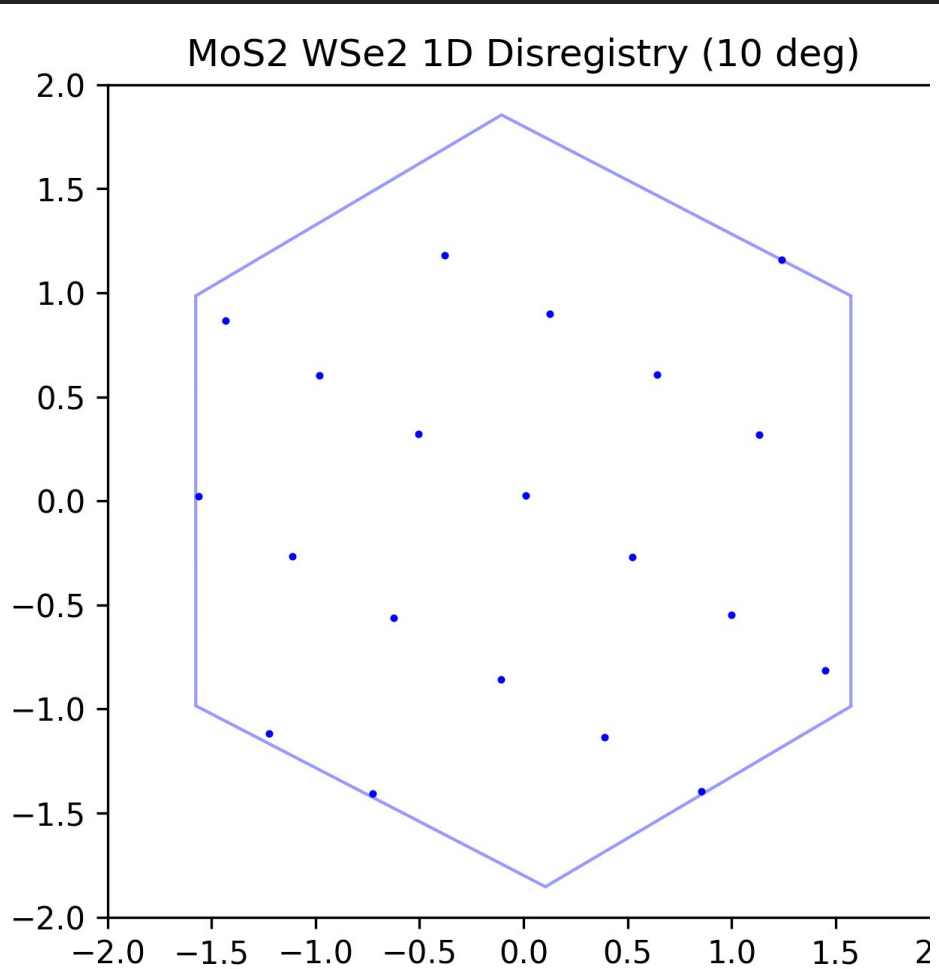

MoS2 WSe2 1D/2D Disregistry (5 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

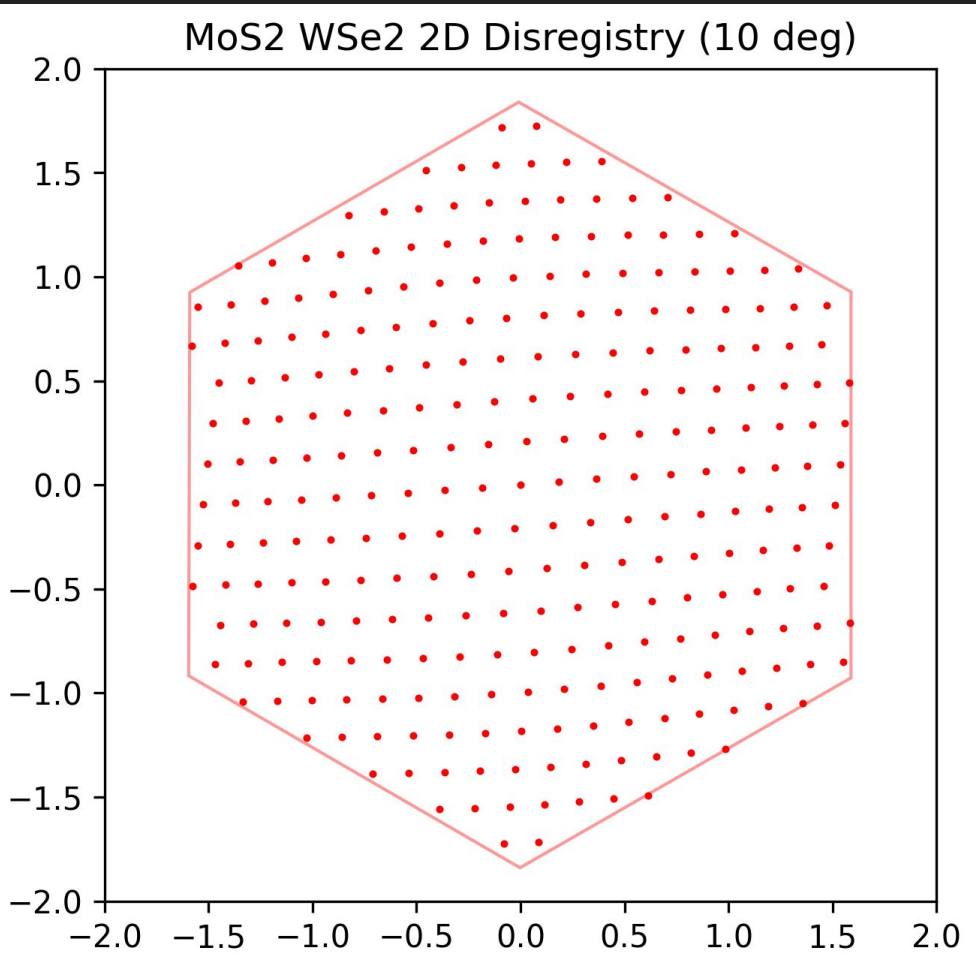


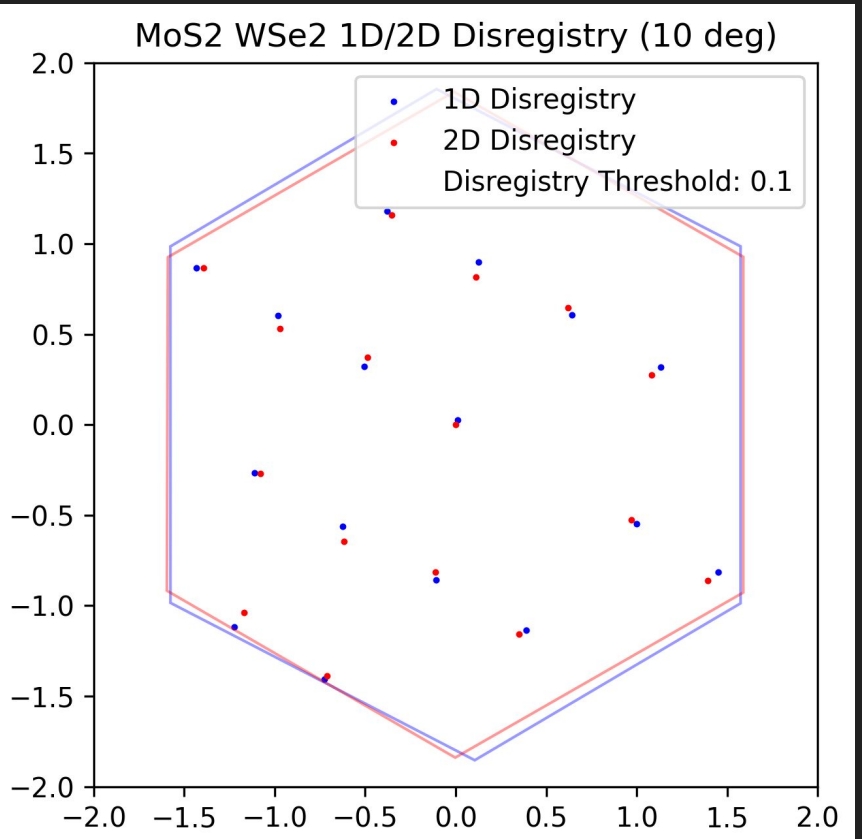
10 deg

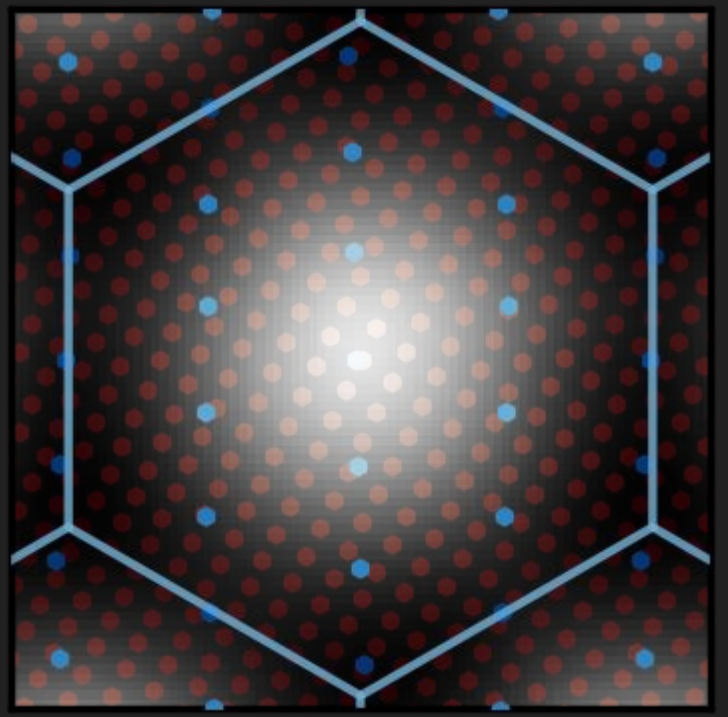


Actual Twist Angle: 9.998113525 03
Total Atoms: 1707
W Atoms (Top Layer): 273
Mo Atoms (Bottom Layer): 296

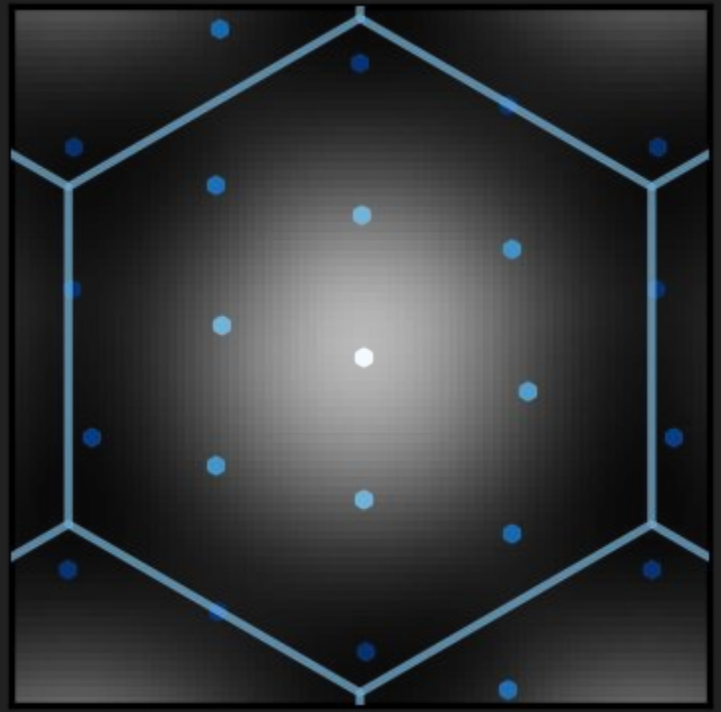

MoS2 WSe2 1D Disregistry (10 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2


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

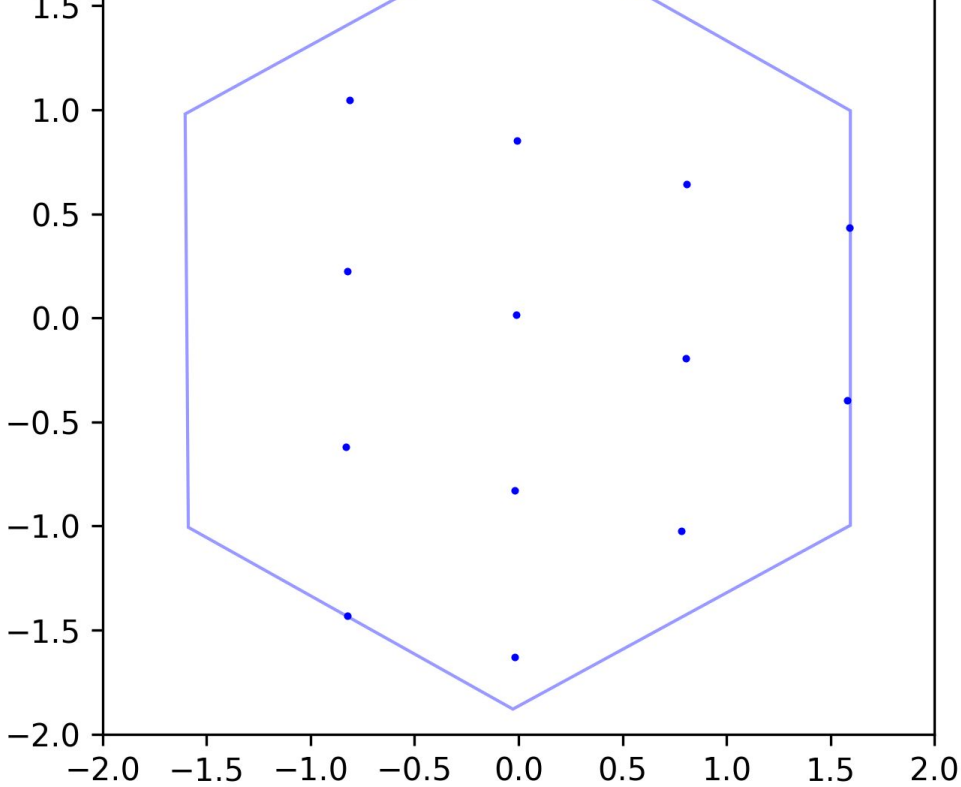

MoS2 WSe2 1D/2D Disregistry (10 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0



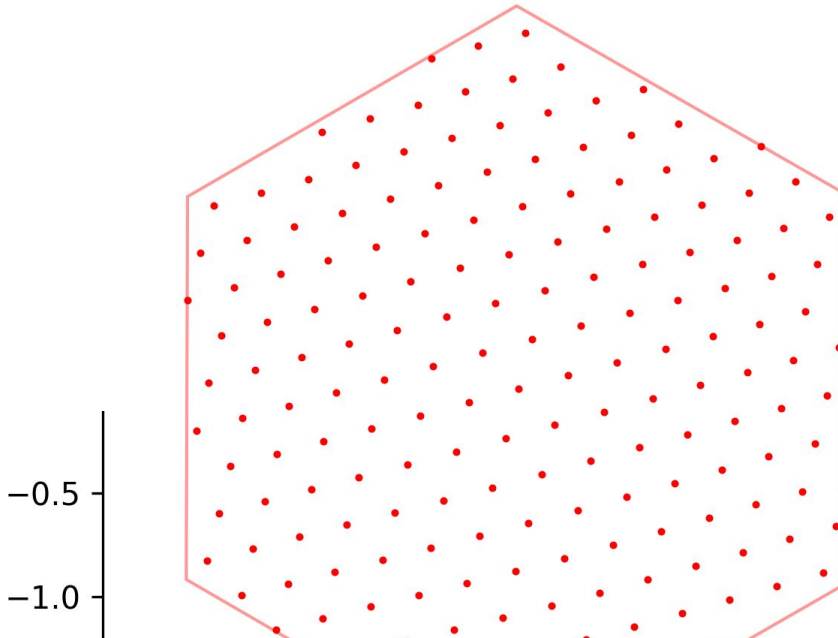
15 deg

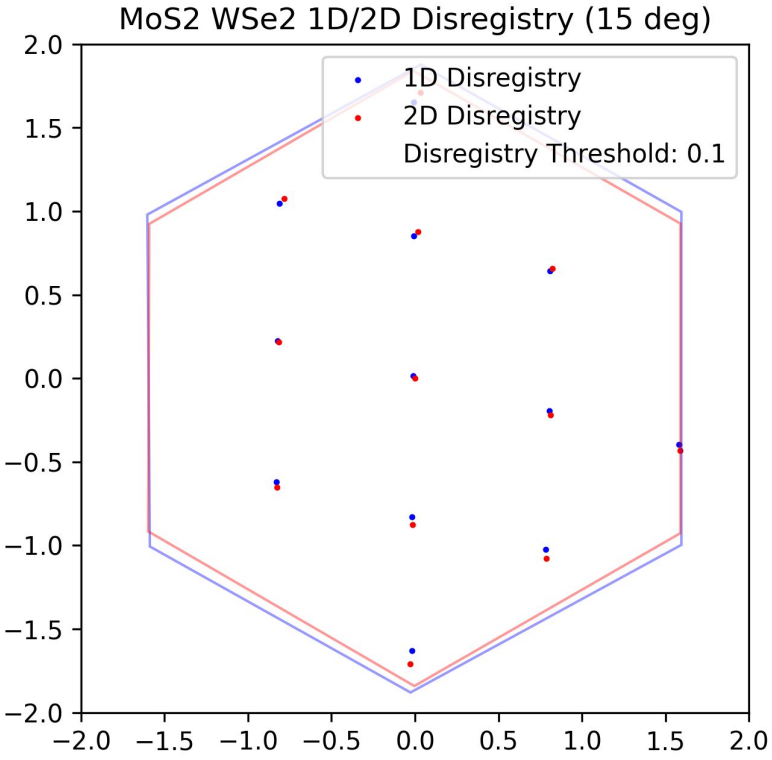


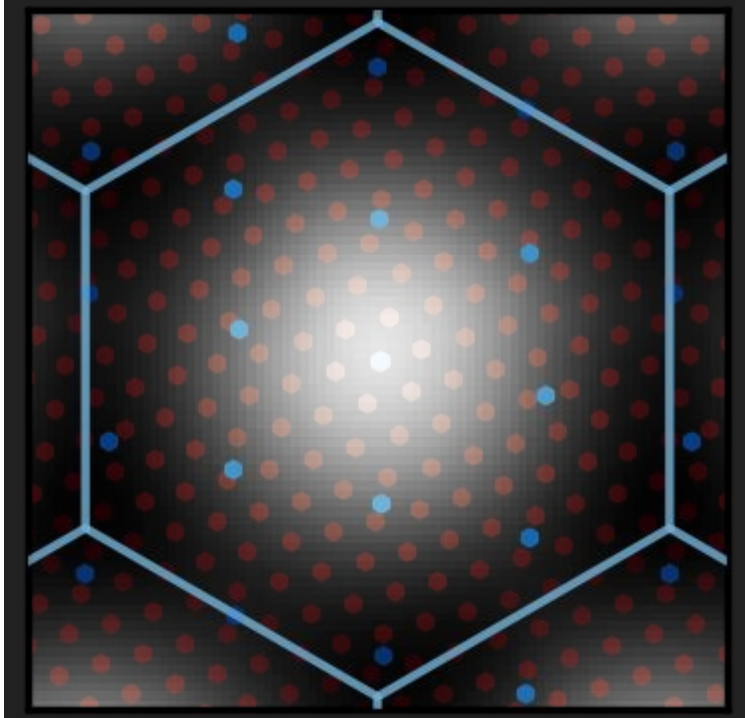
Actual Twist Angle: 15.0172238103
Total Atoms: 1131
W Atoms (Top Layer): 181
Mo Atoms (Bottom Layer): 196



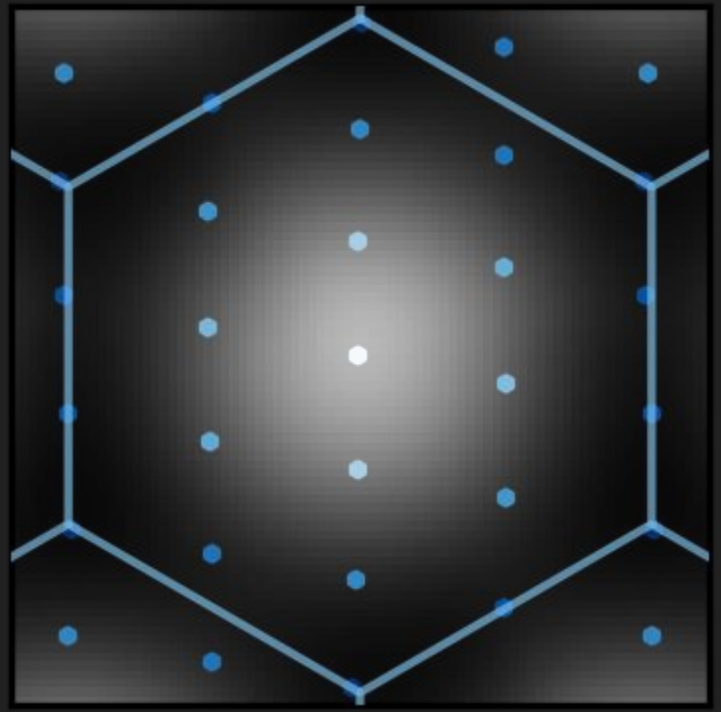
MoS2 WSe2 2D Disregistry (15 deg

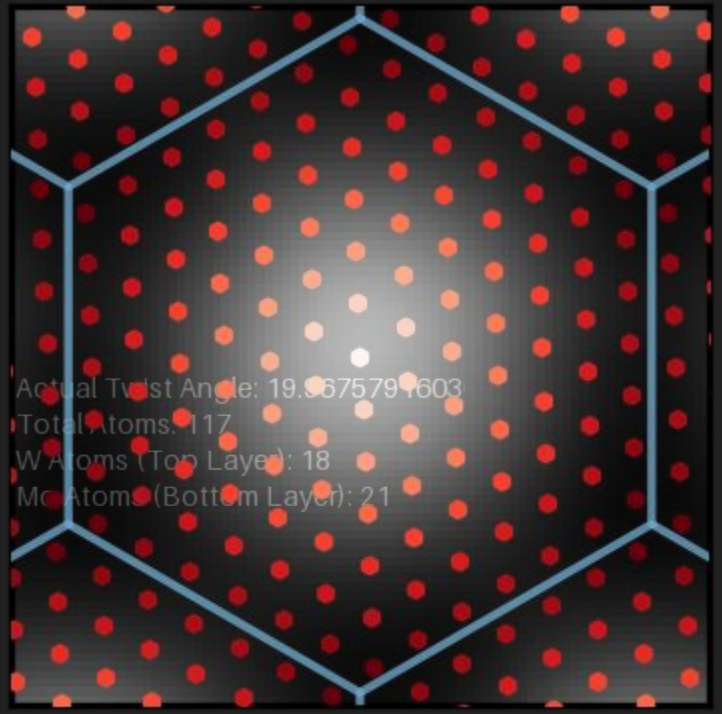



MoS2 WSe2 1D/2D Disregistry (15 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

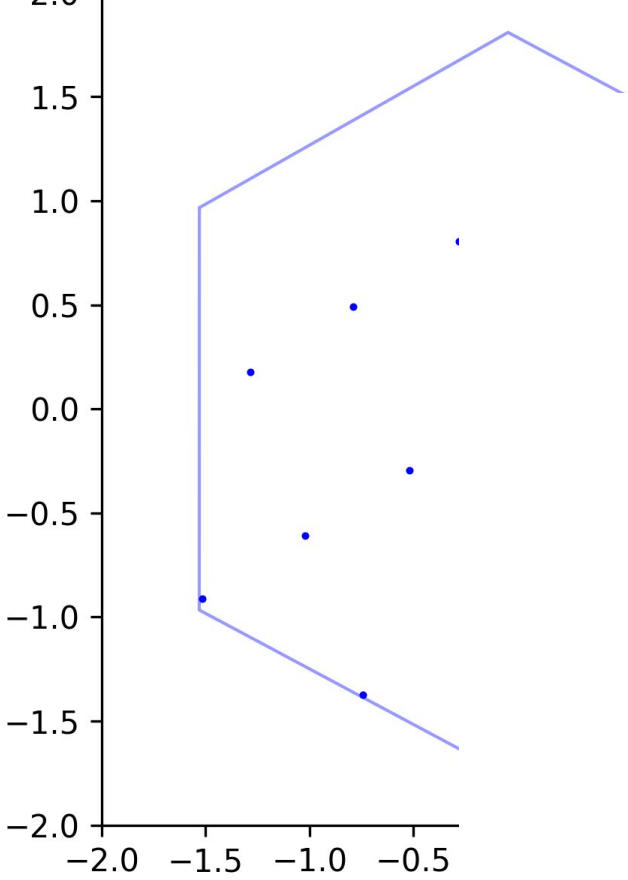


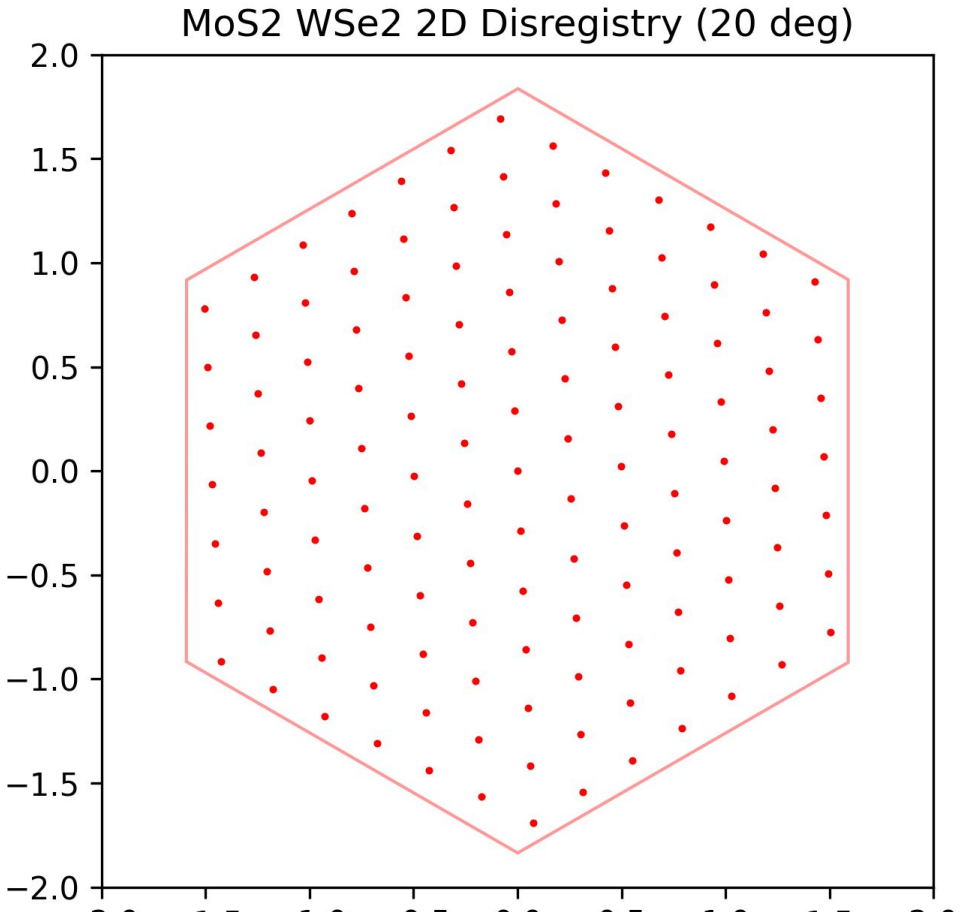
20 deg

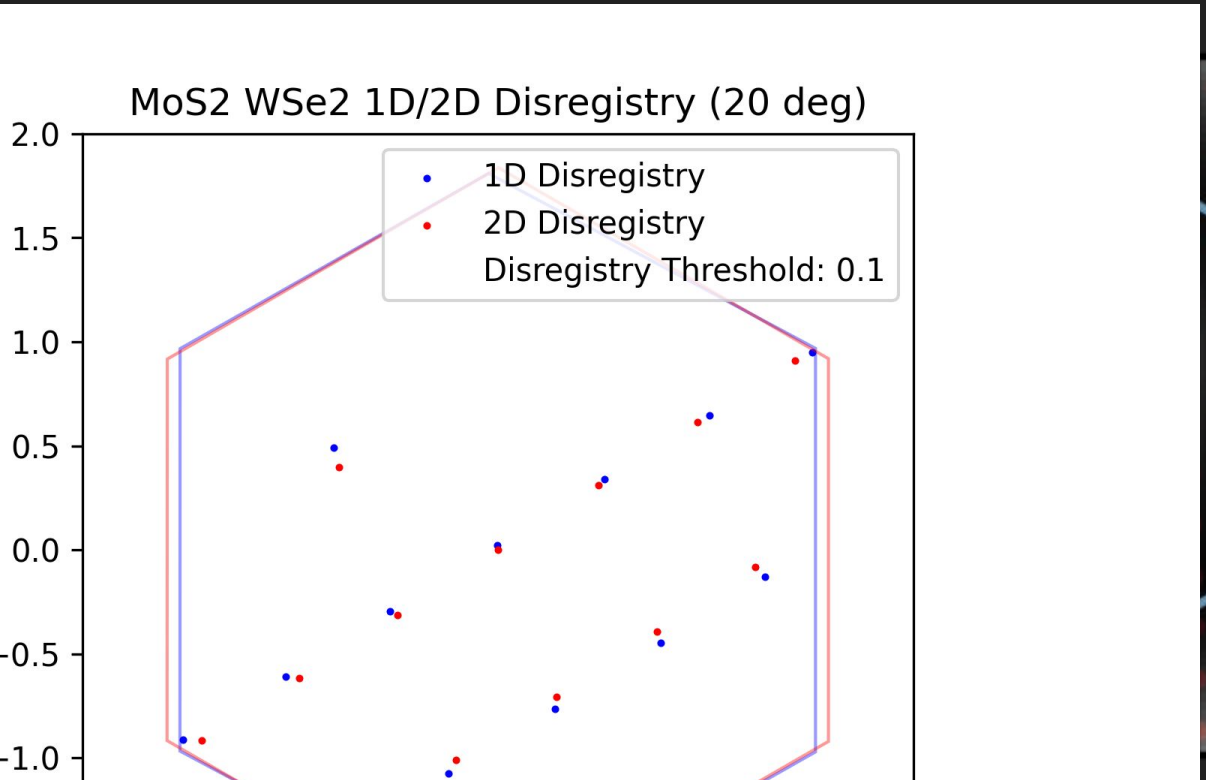


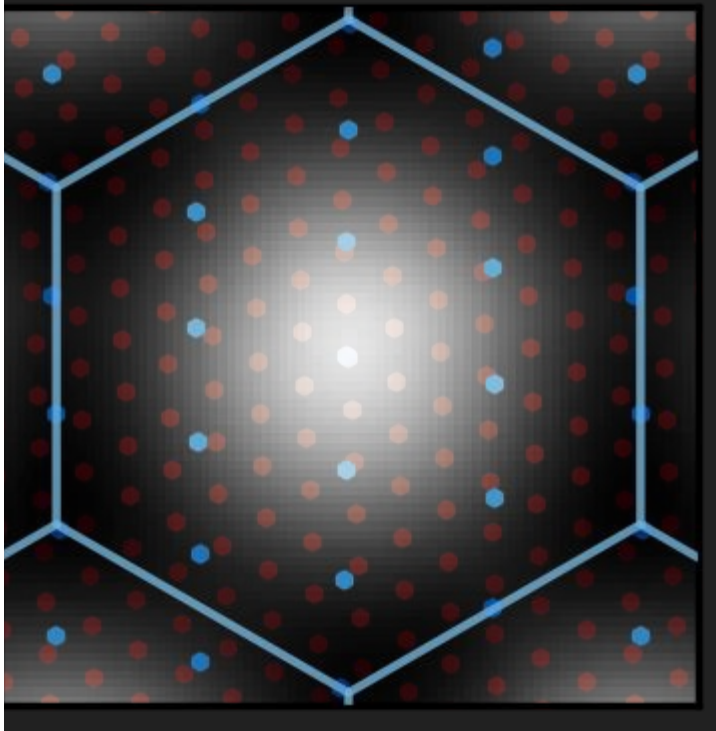


Actual Twist Angle: 19.9790383162
Total Atoms: 798
W Atoms (Top Layer): 127
Mo Atoms (Bottom Layer): 139

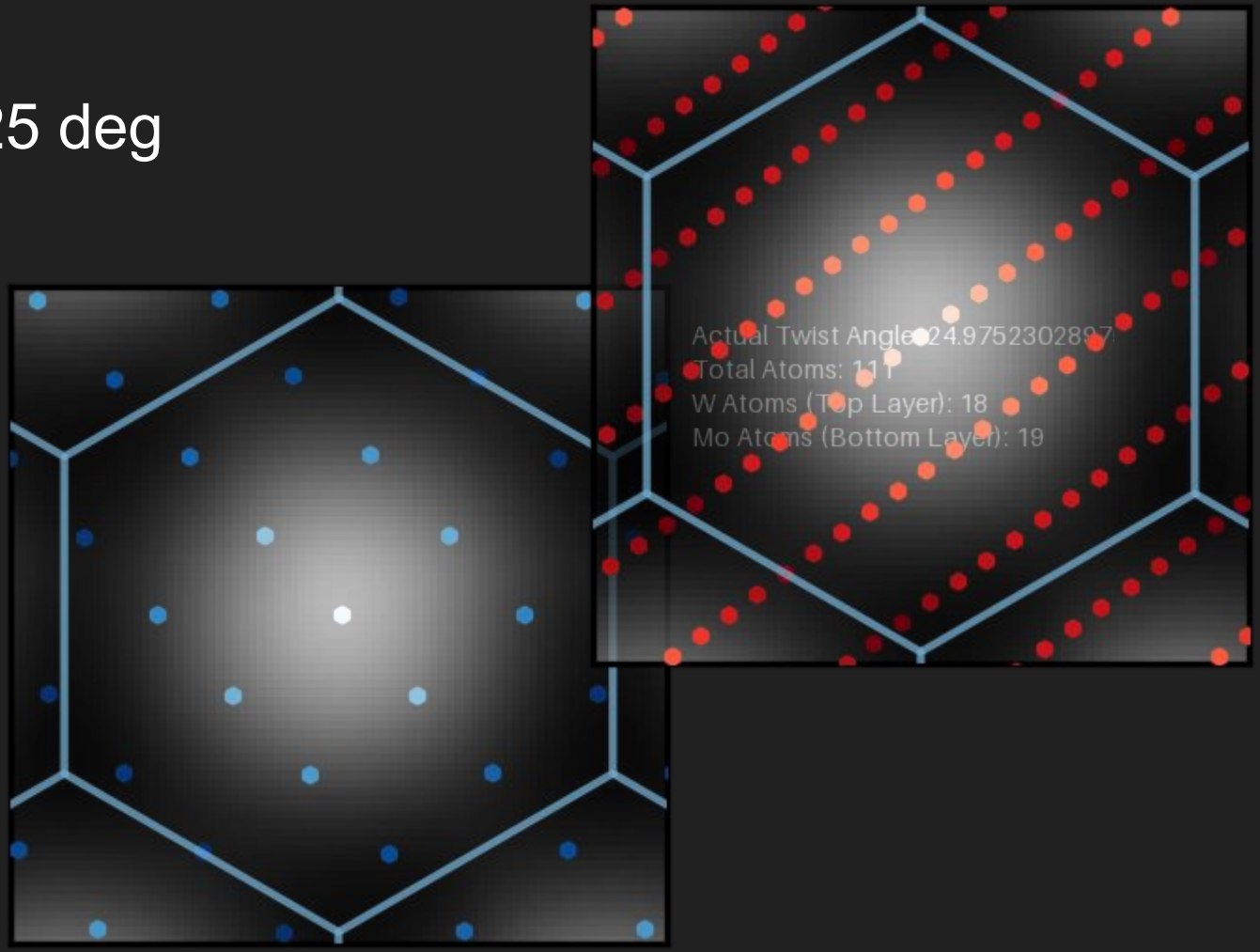

2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5

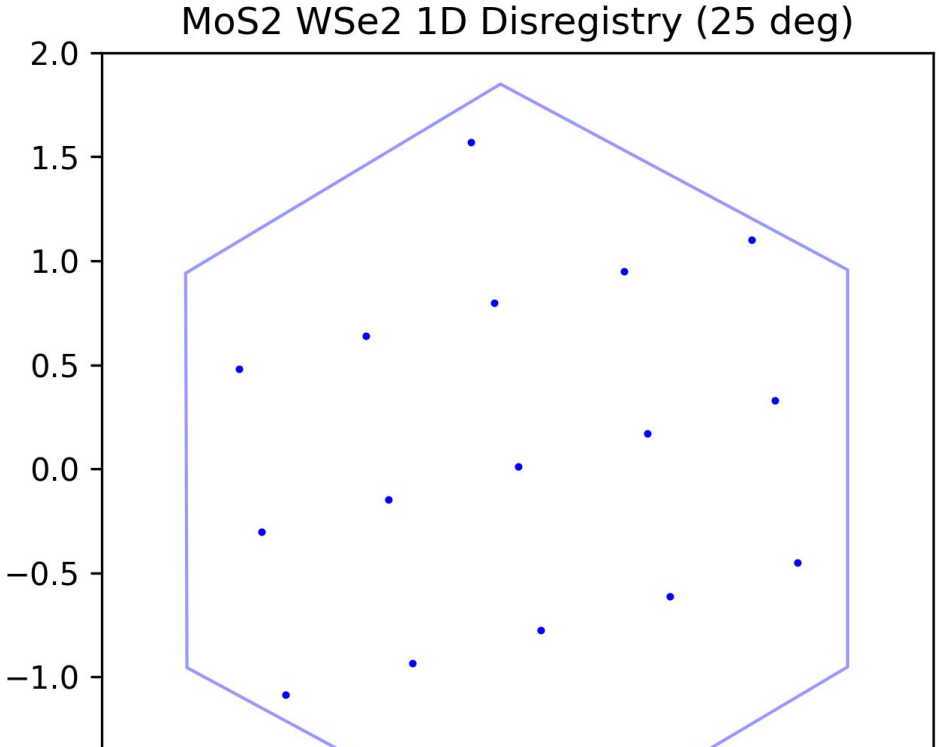

MoS2 WSe2 2D Disregistry (20 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

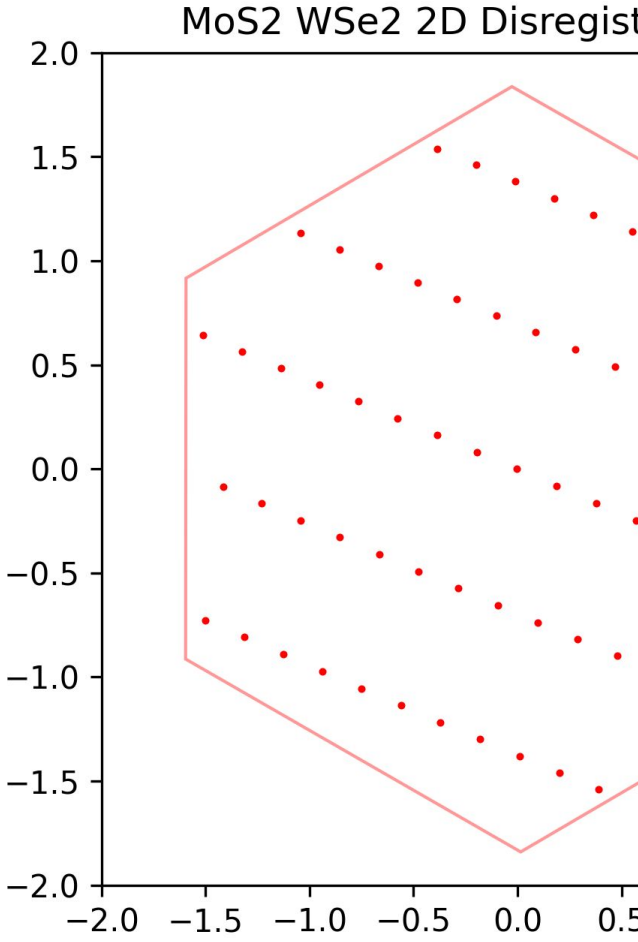

MoS2 WSe2 1D/2D Disregistry (20 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

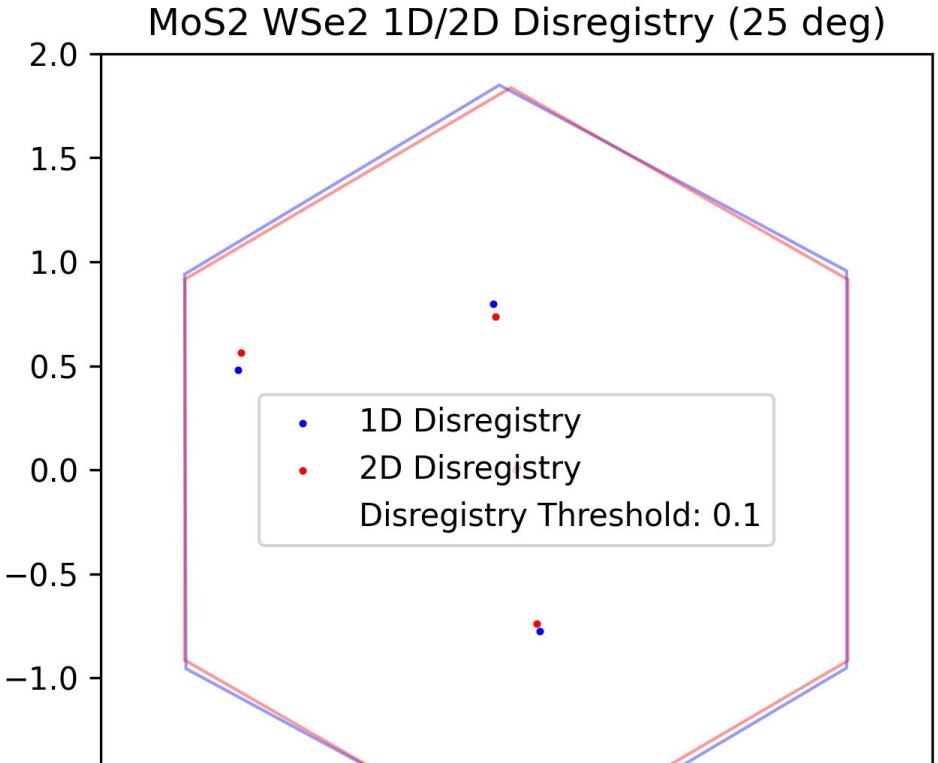


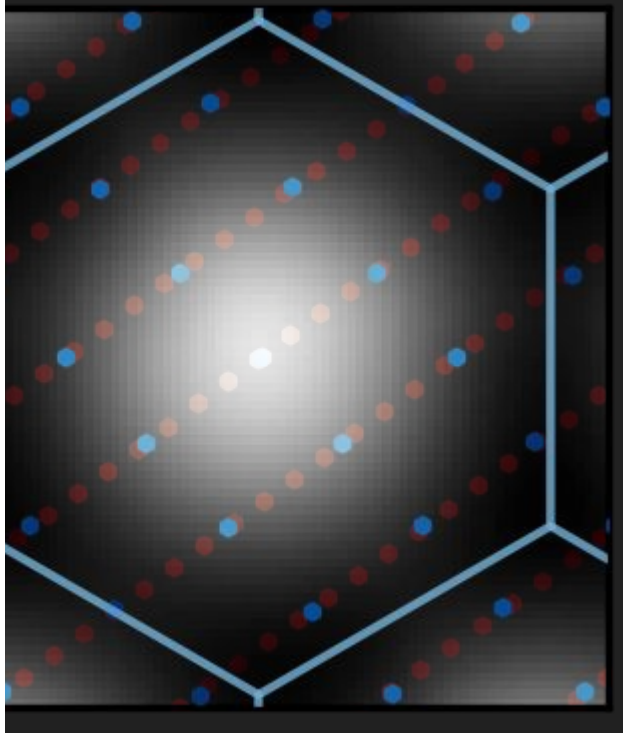
25 deg


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

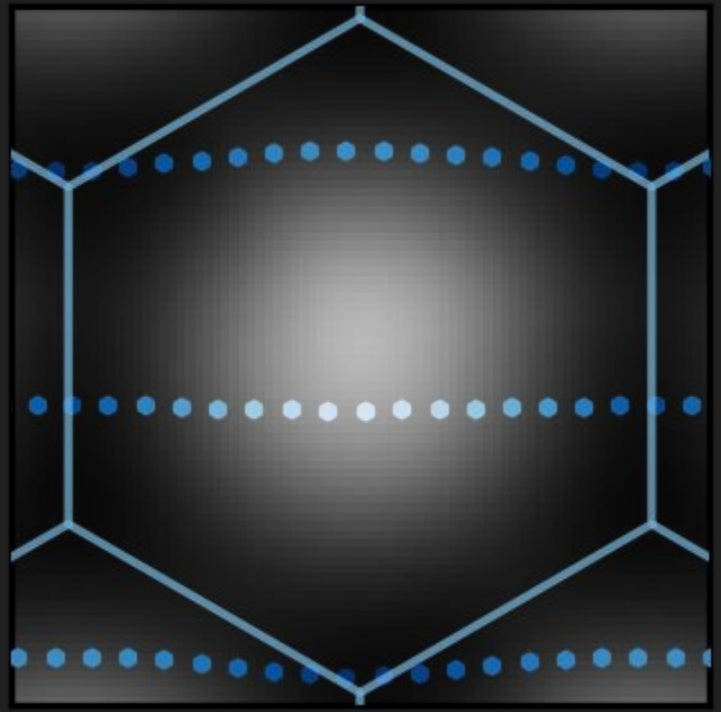

MoS2 WSe2 1D Disregistry (25 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

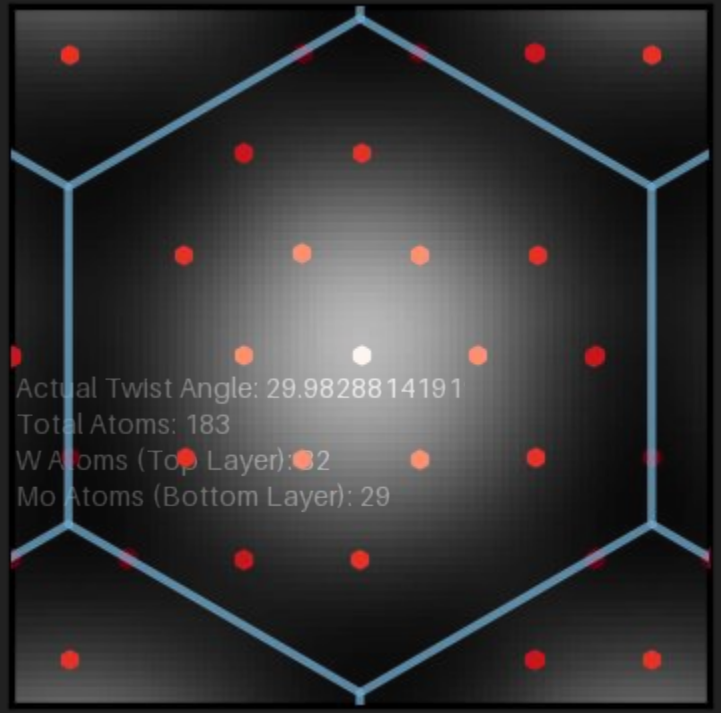

MoS2 WSe2 2D Disregist
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5


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

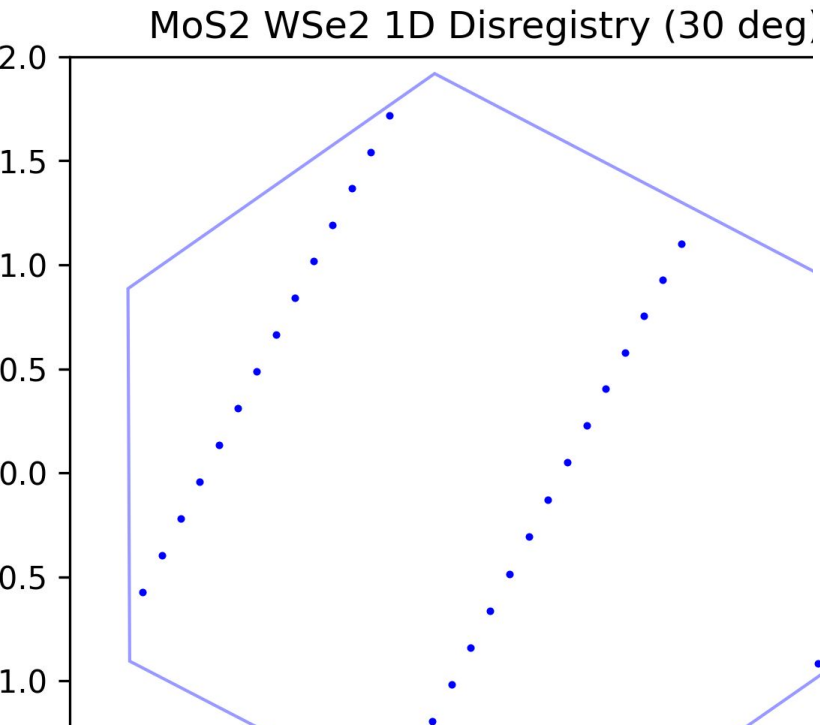


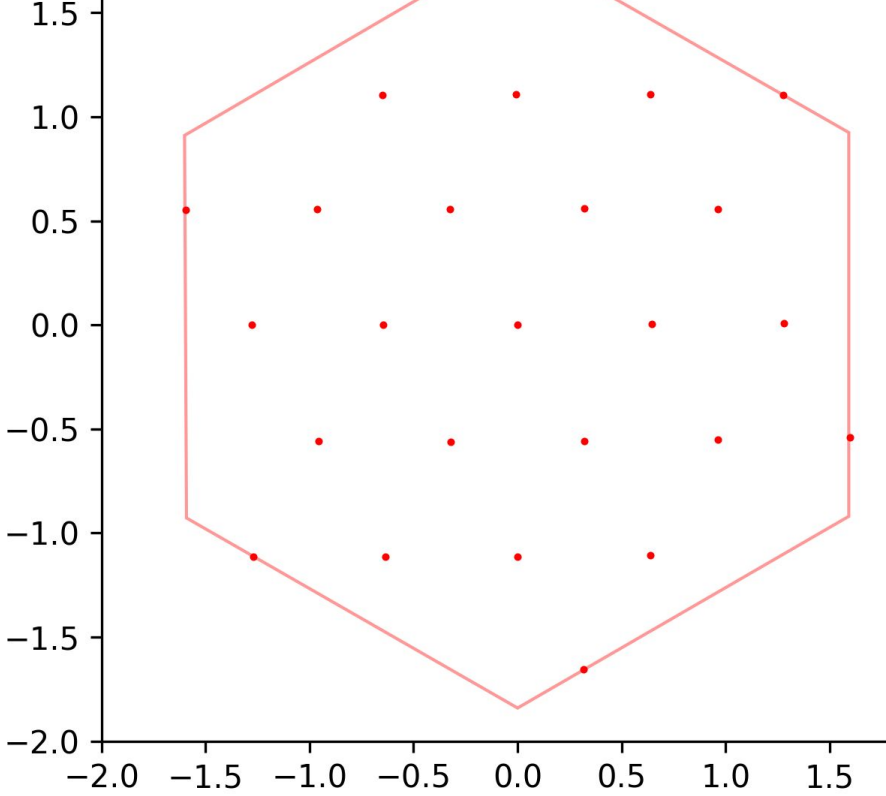
30 deg

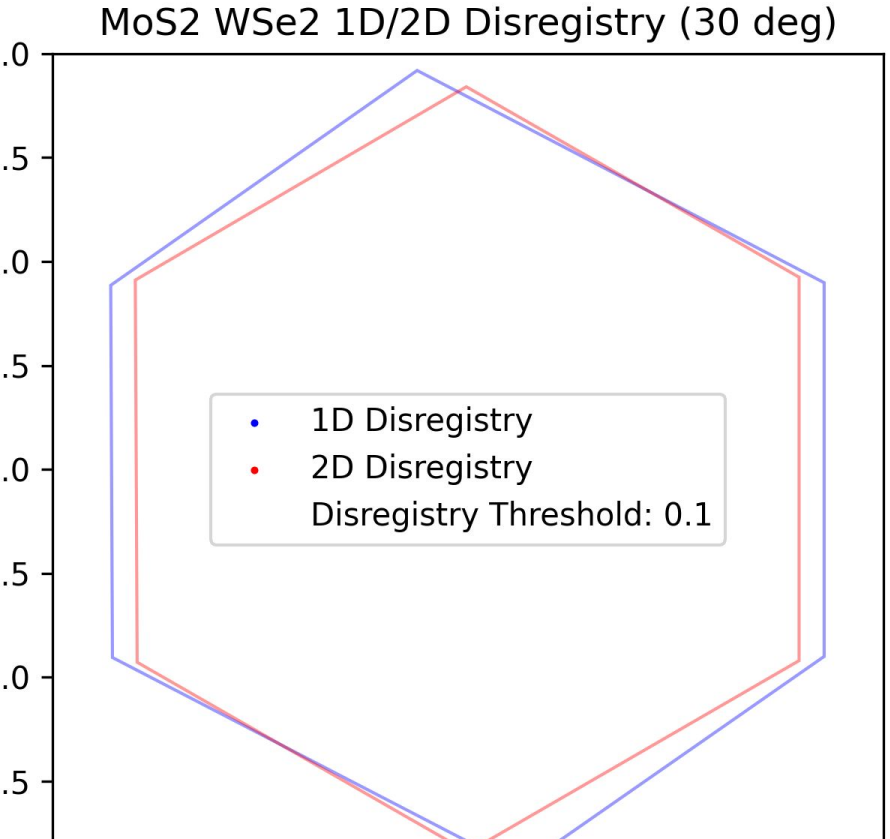


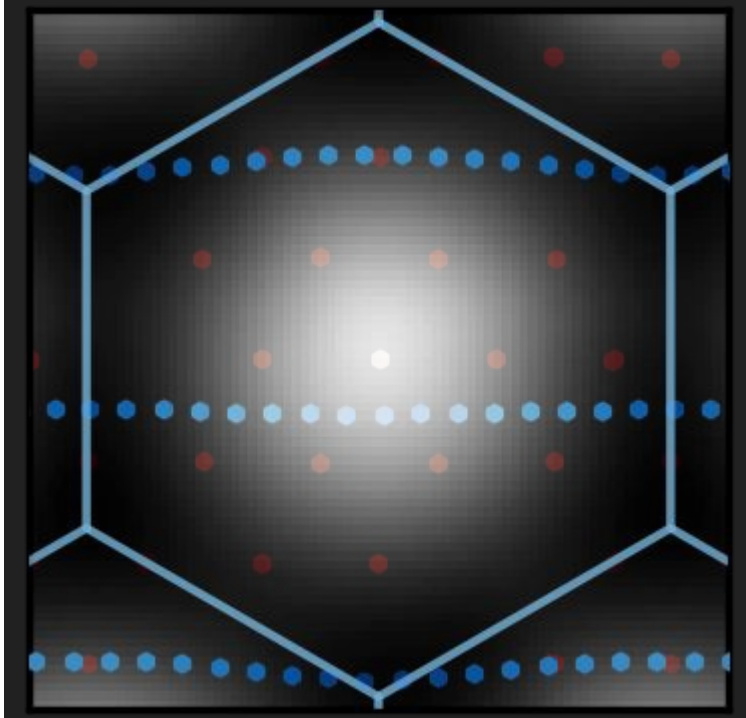


Actual Twist Angle: 30.0172588869
Total Atoms: 156
W Atoms (Top Layer): 25
Mo Atoms (Bottom Layer): 27

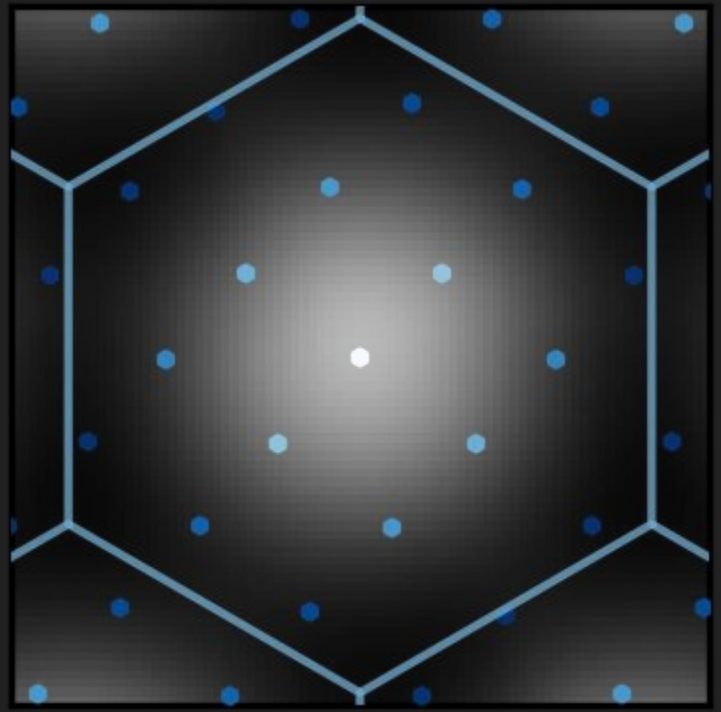

MoS2 WSe2 1D Disregistry (30 deg)
2.0
1.5
1.0
0.5
0.0
0.5
1.0


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

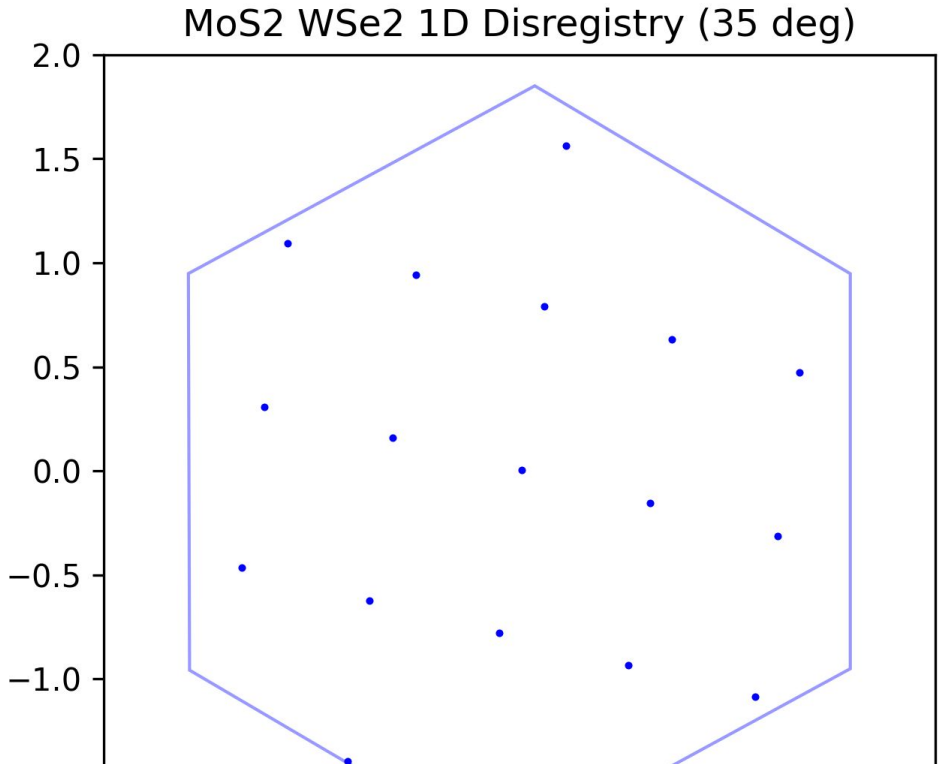

MoS2 WSe2 1D/2D Disregistry (30 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

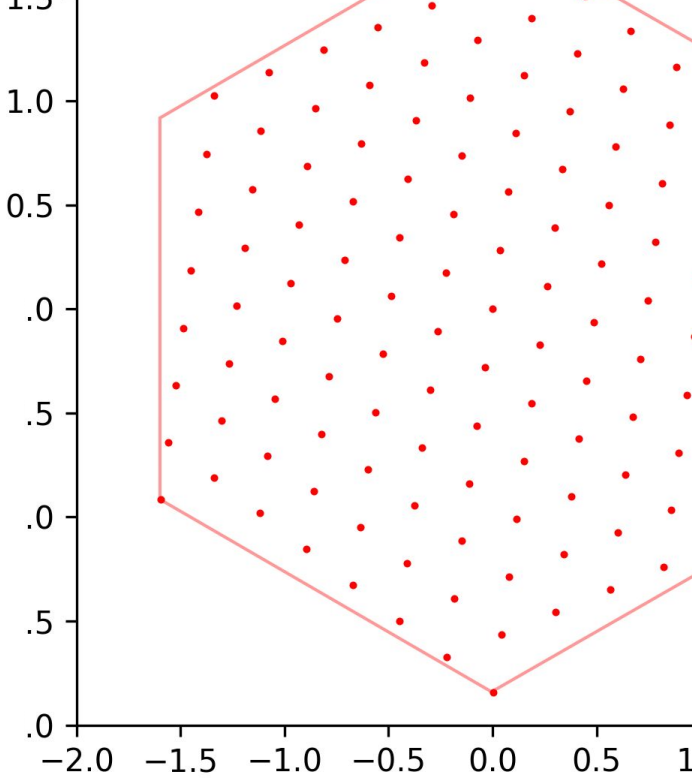


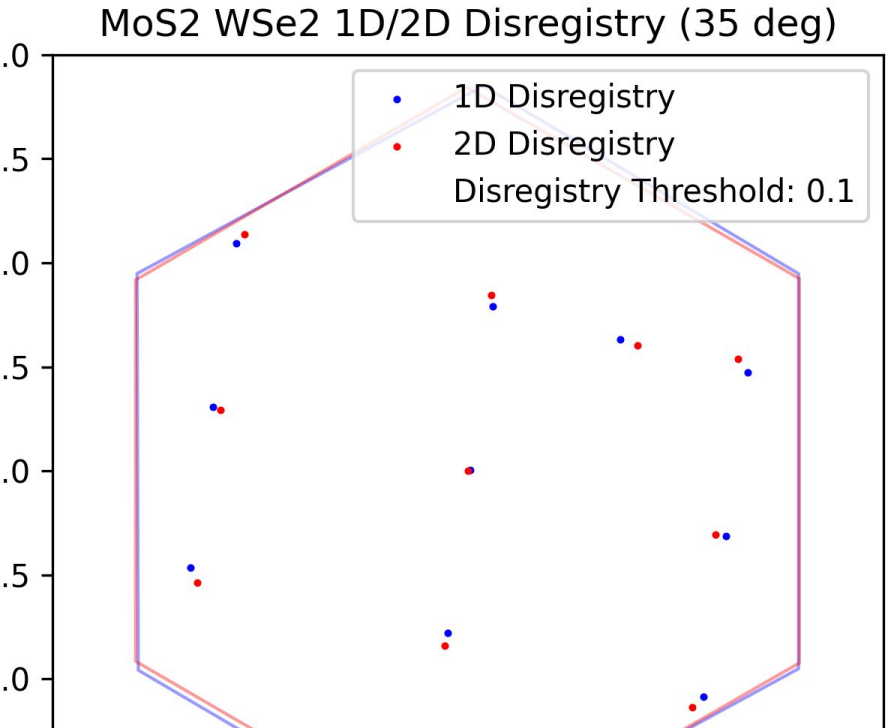
35 deg

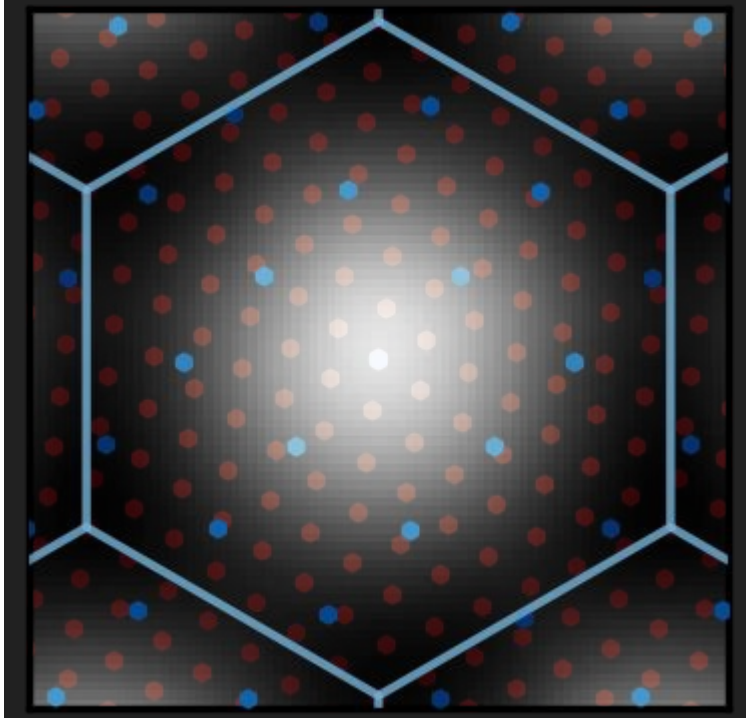


Actual Twist Angle: 34.9790733927
Total Atoms: 804
W Atoms (Top Layer): 129
Mo Atoms (Bottom Layer): 139

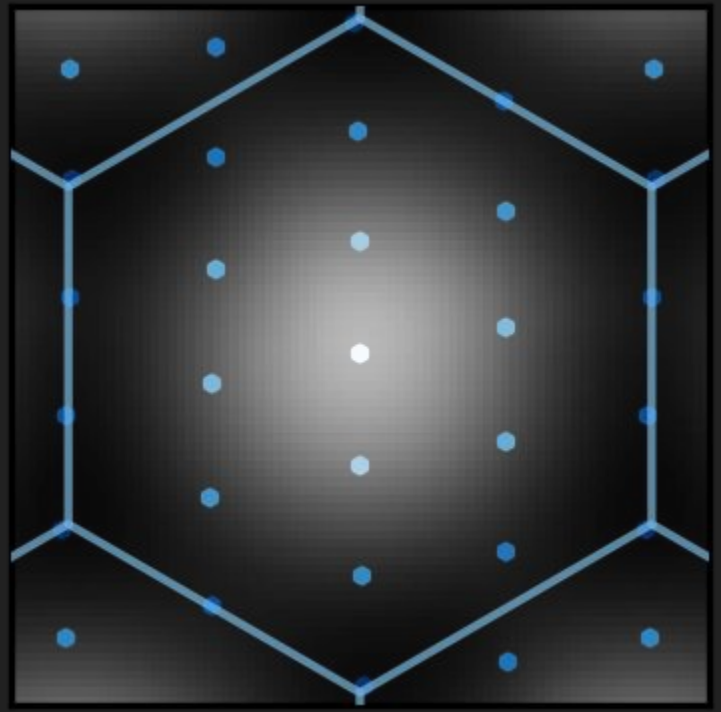

MoS2 WSe2 1D Disregistry (35 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

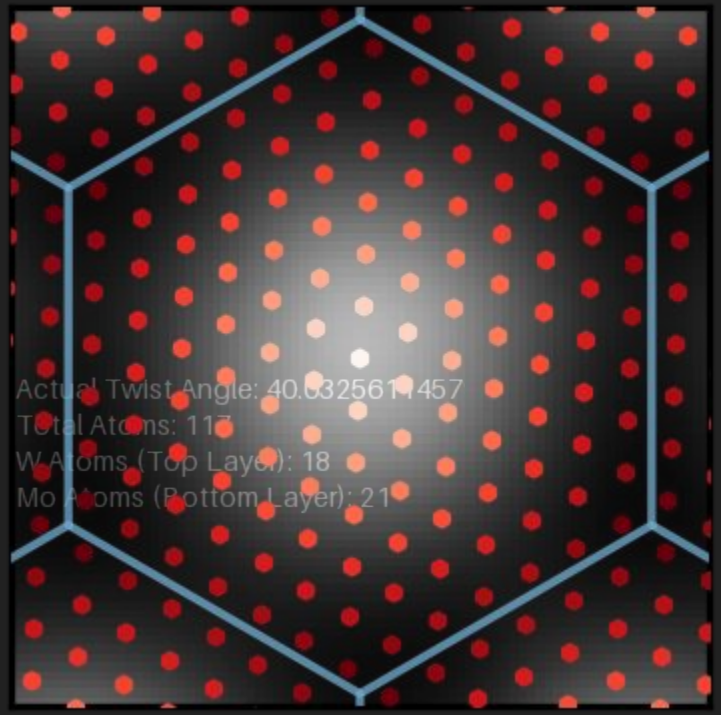

1.0
0.5
.0
.5
.0
.5
.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5


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



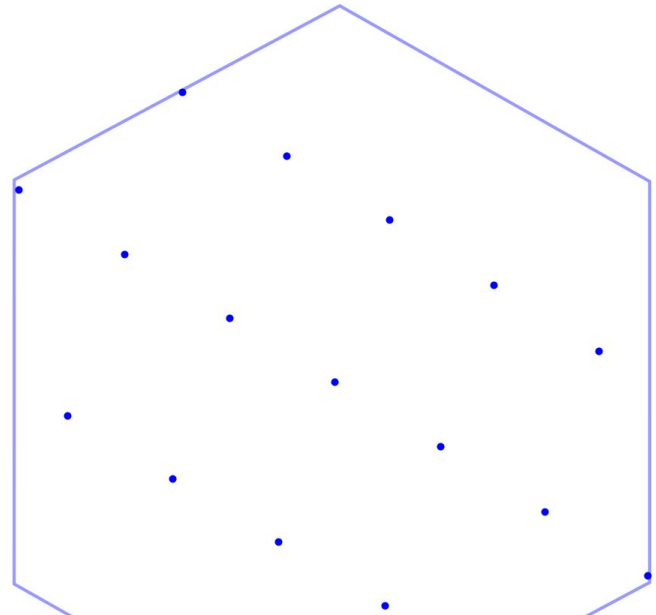
40 deg

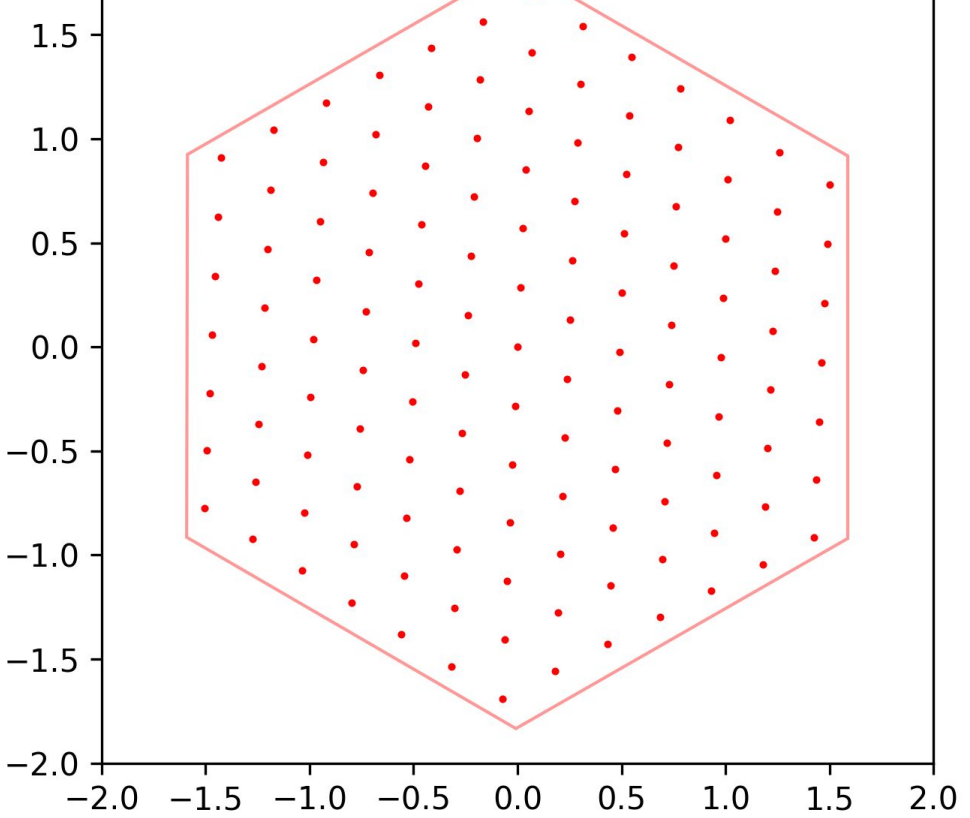


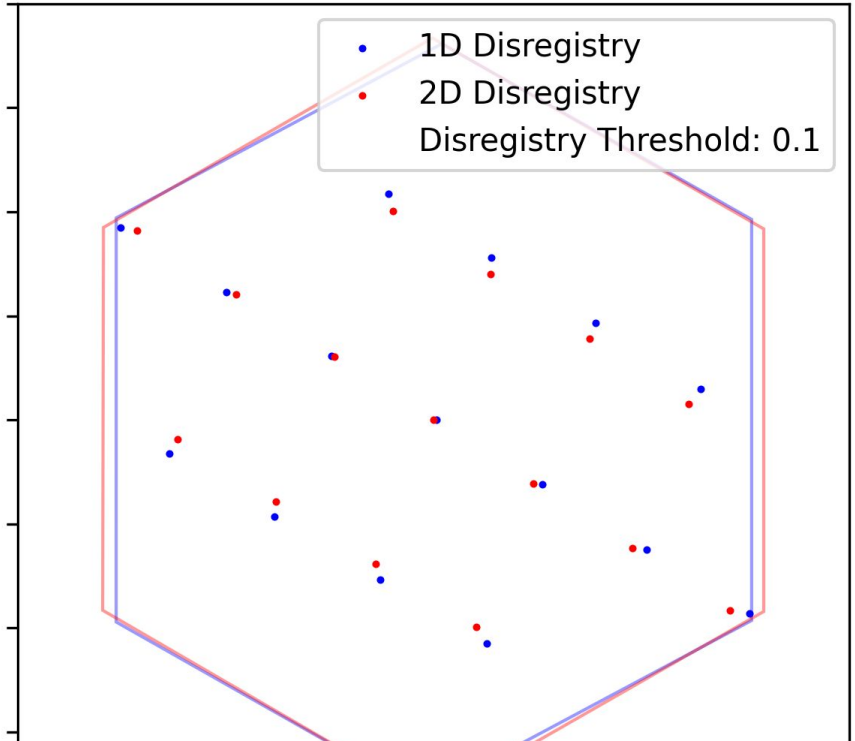


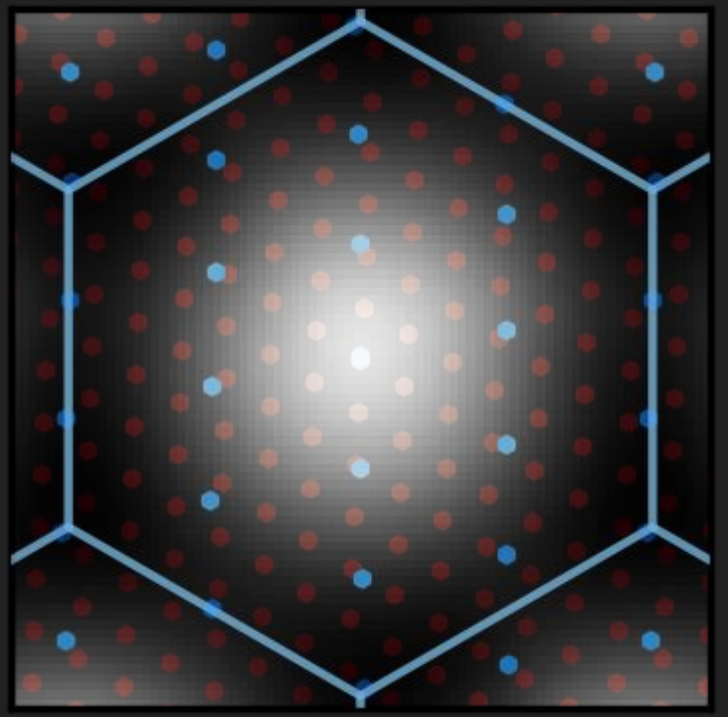
Actual Twist Angle: 40.0153724119
Total Atoms: 798
W Atoms (Top Layer): 127
Mo Atoms (Bottom Layer): 139

MoS2 WSe2 1D Disregistry (40 deg

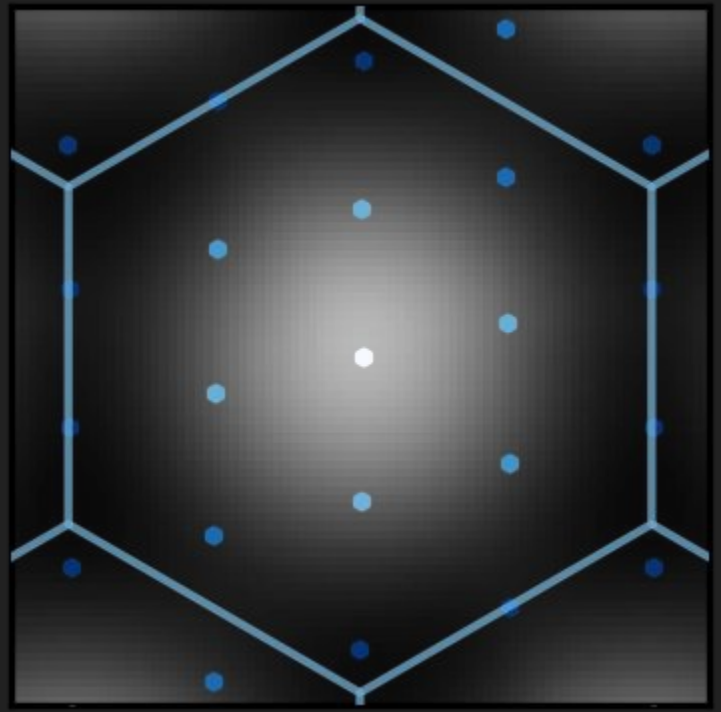


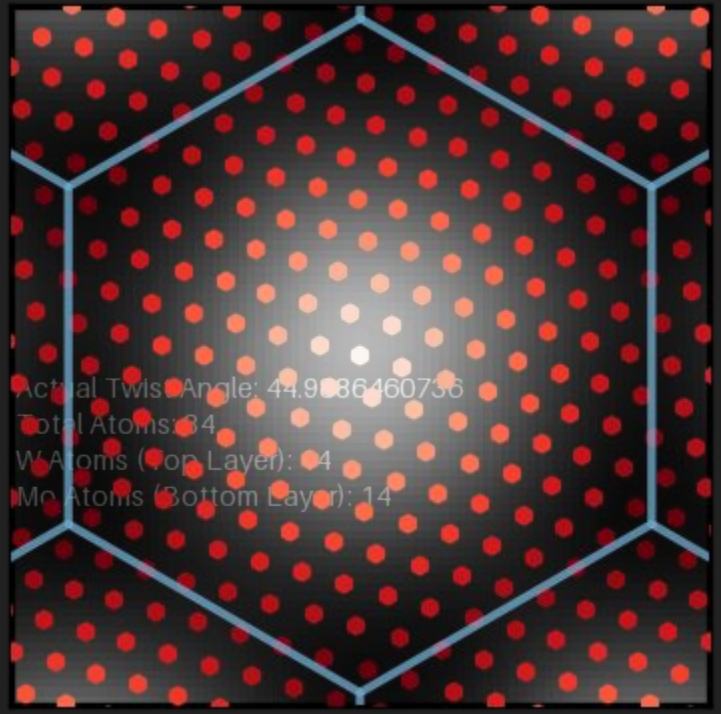


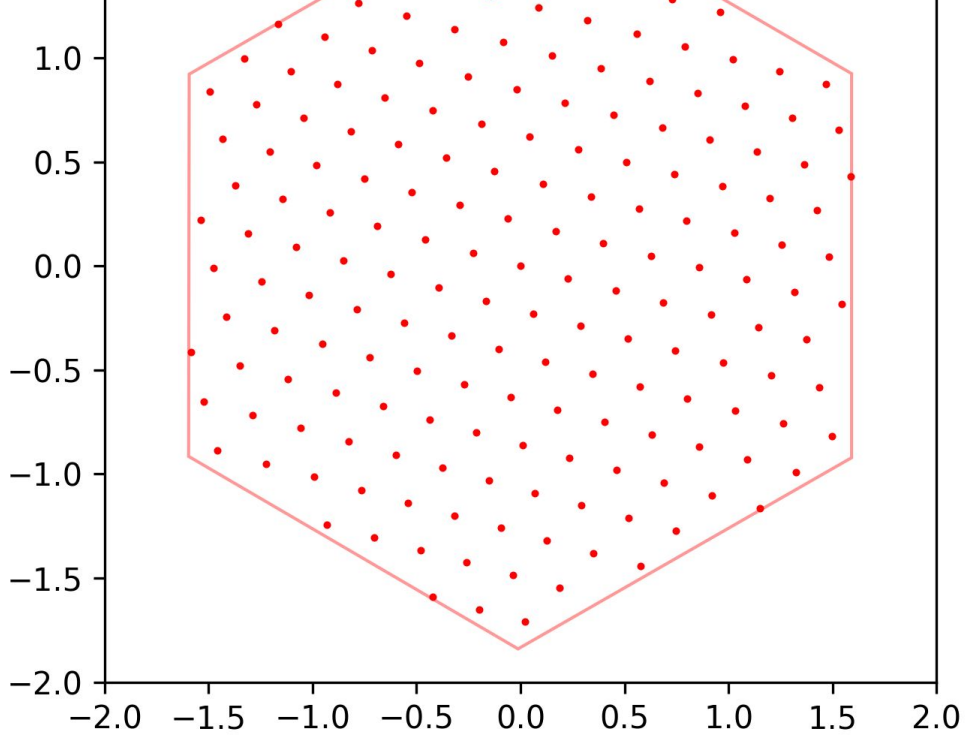

MoS2 WSe2 1D/2D Disregistry (40 deg)
1D Disregistry
2D Disregistry
Disregistry Threshold: 0.1

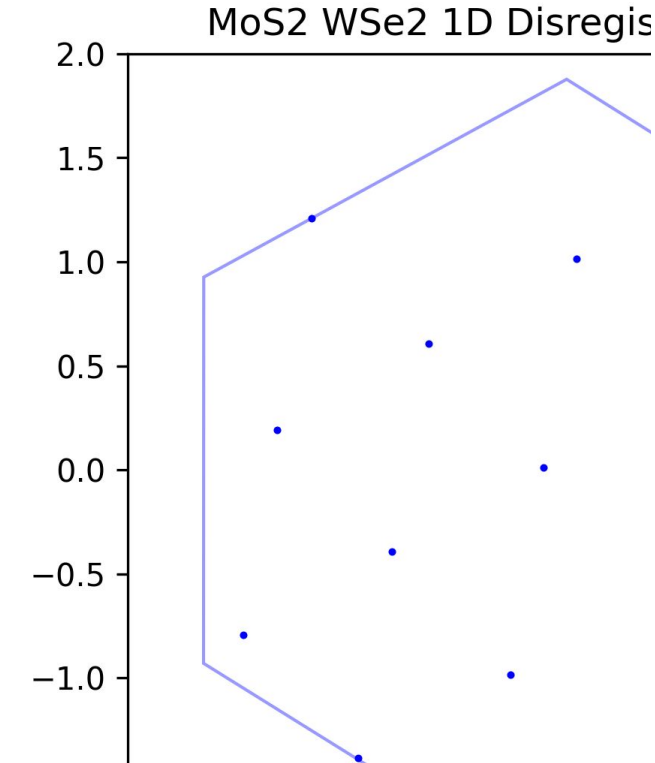


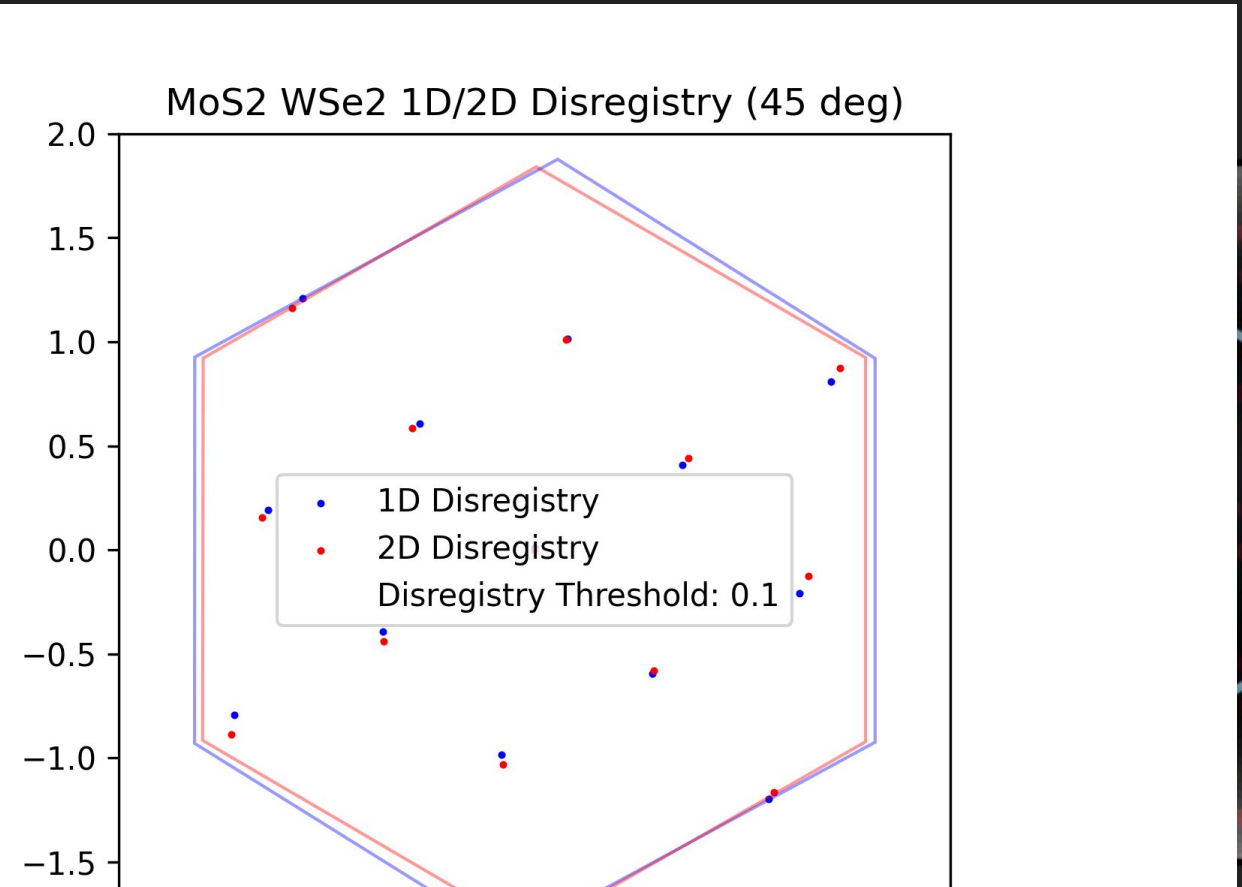
45 deg

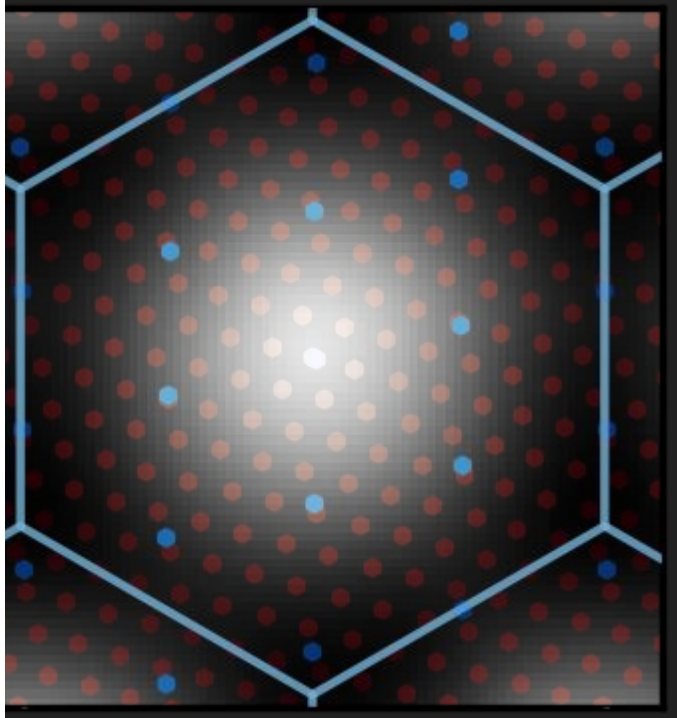



Actual Twist Angle: 44.9829164957
Total Atoms: 1131
W Atoms (Top Layer): 181
Mo Atoms (Bottom Layer): 196

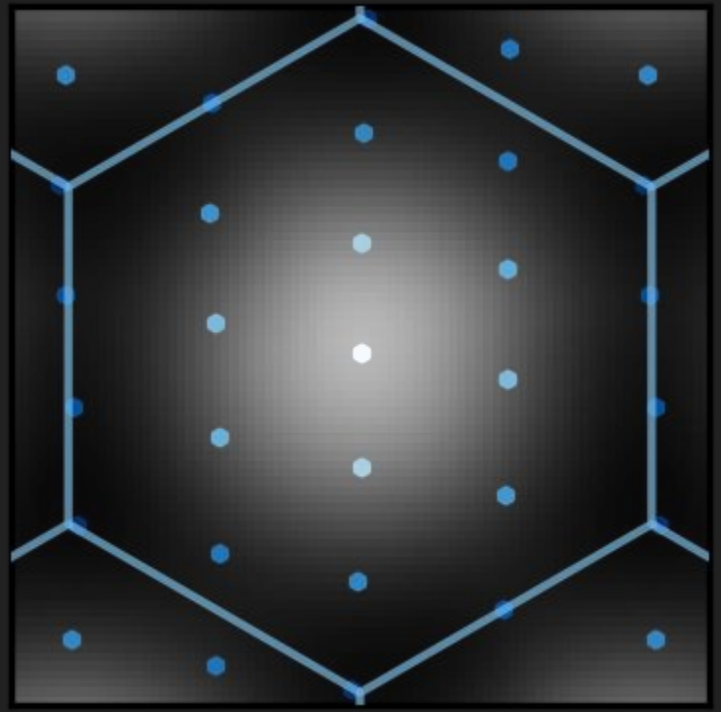

1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

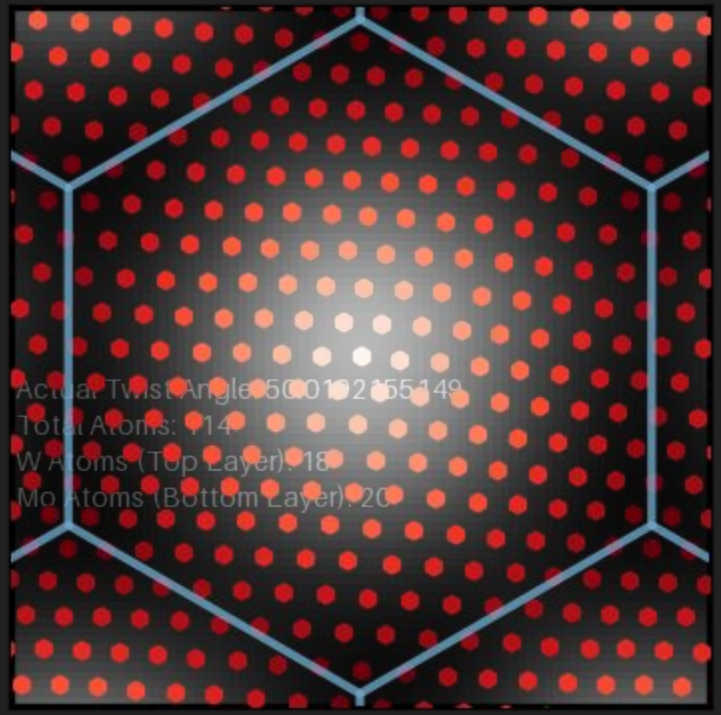

MoS2 WSe2 1D Disregis
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


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

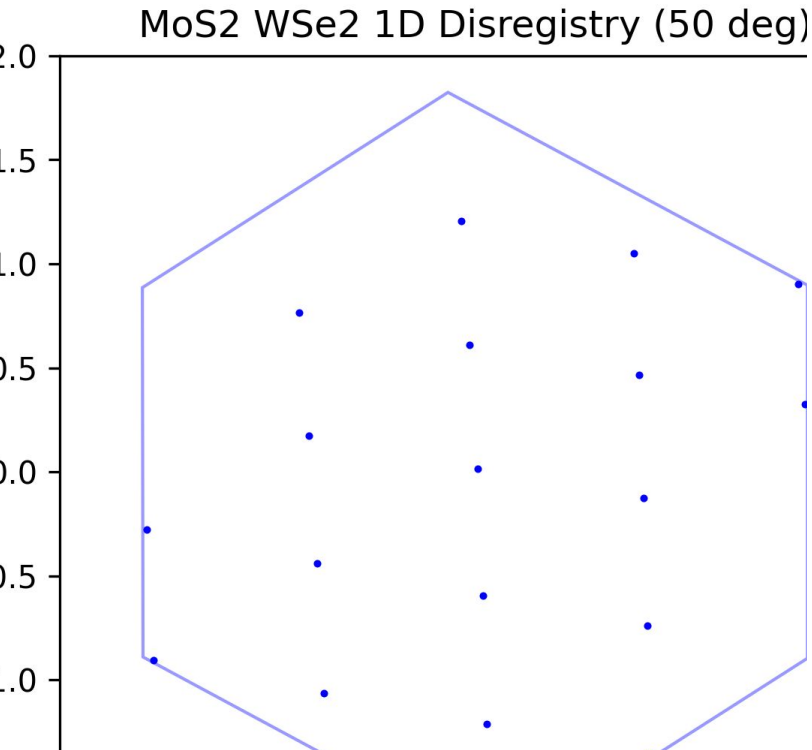


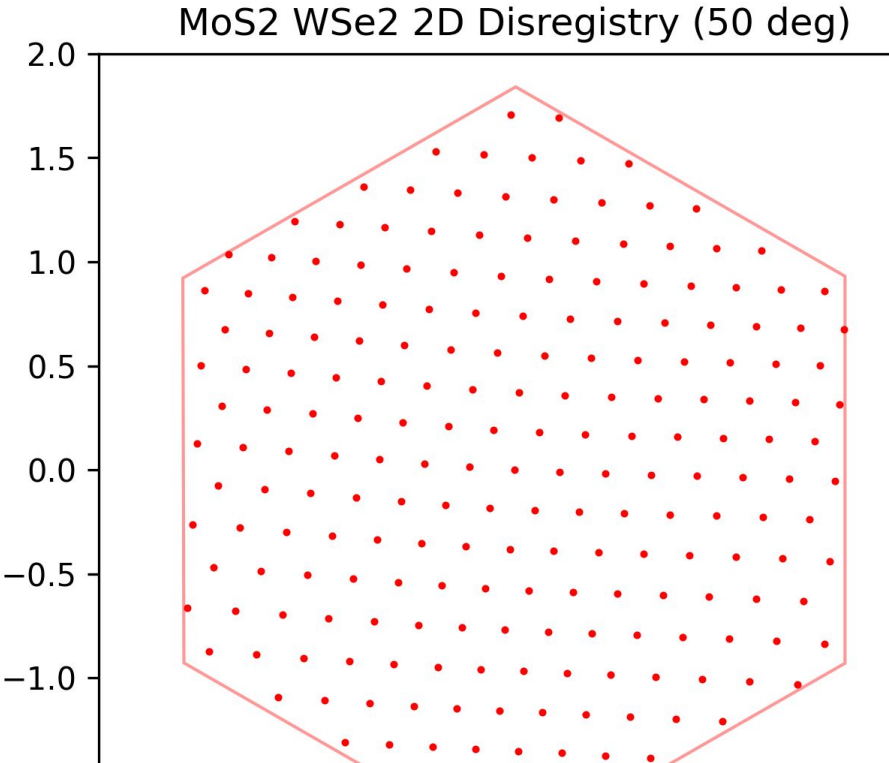
50 deg

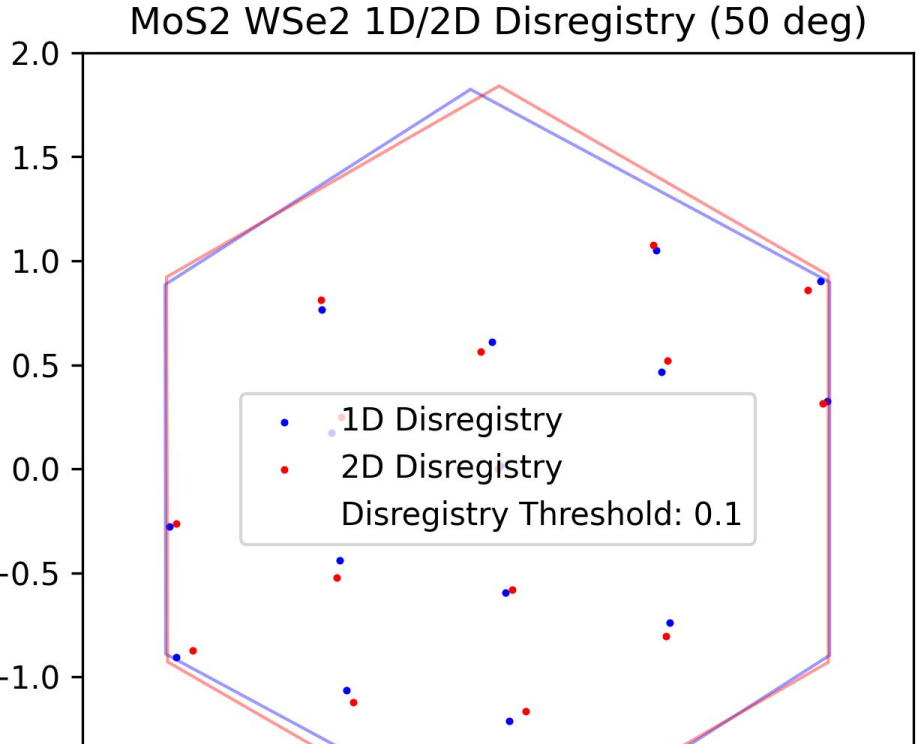


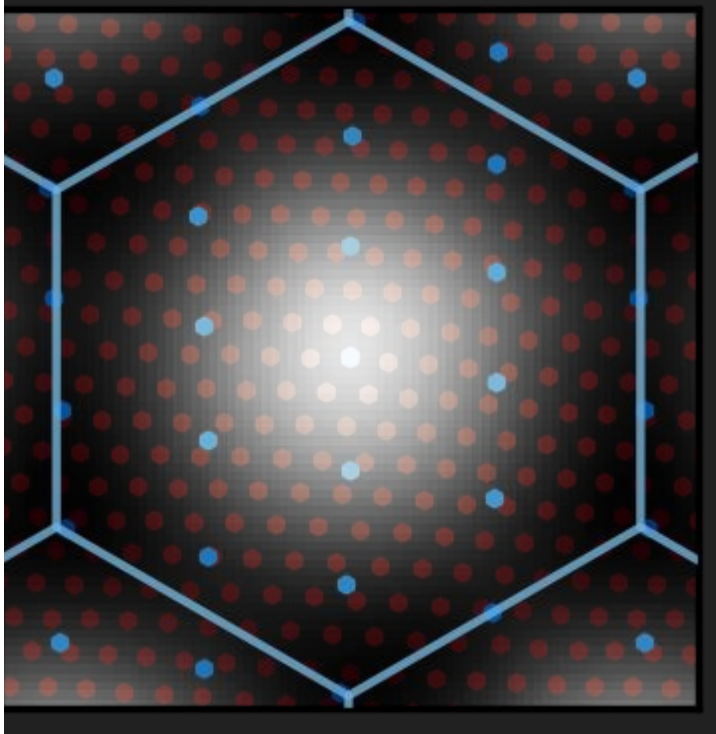


Actual Twist Angle: 50.0192155149
Total Atoms: 1317
W Atoms (Top Layer): 211
Mo Atoms (Bottom Layer): 228

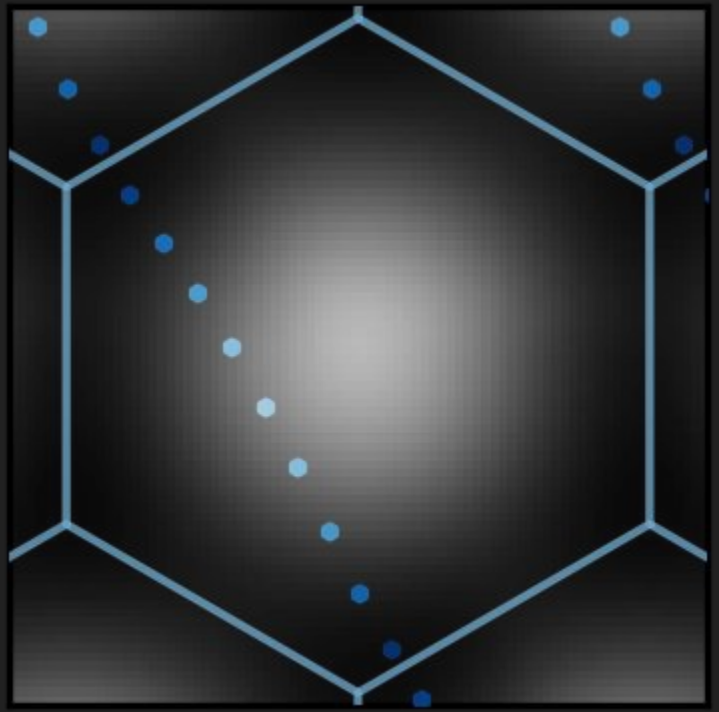

MoS2 WSe2 1D Disregistry (50 deg)
2.0
1.5
1.0
0.5
0.0
0.5
1.0

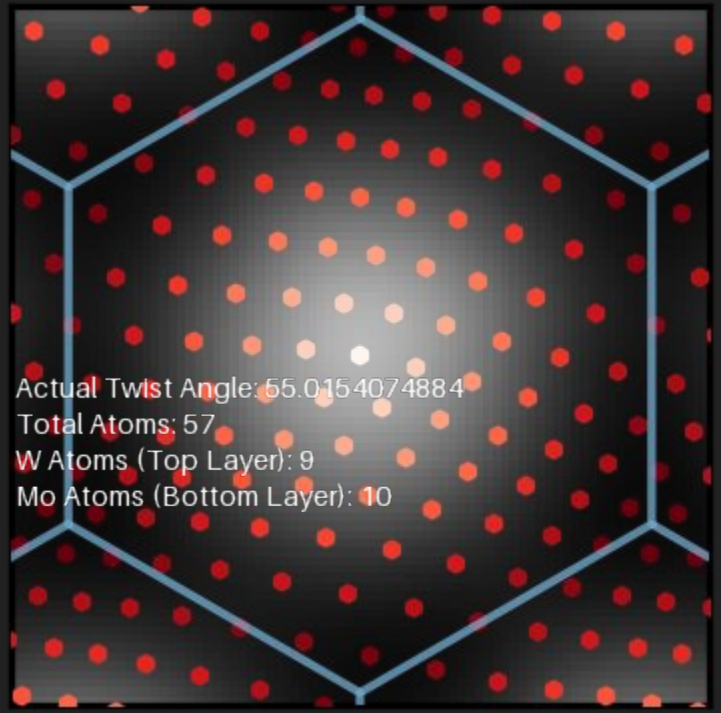

MoS2 WSe2 2D Disregistry (50 deg)
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


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

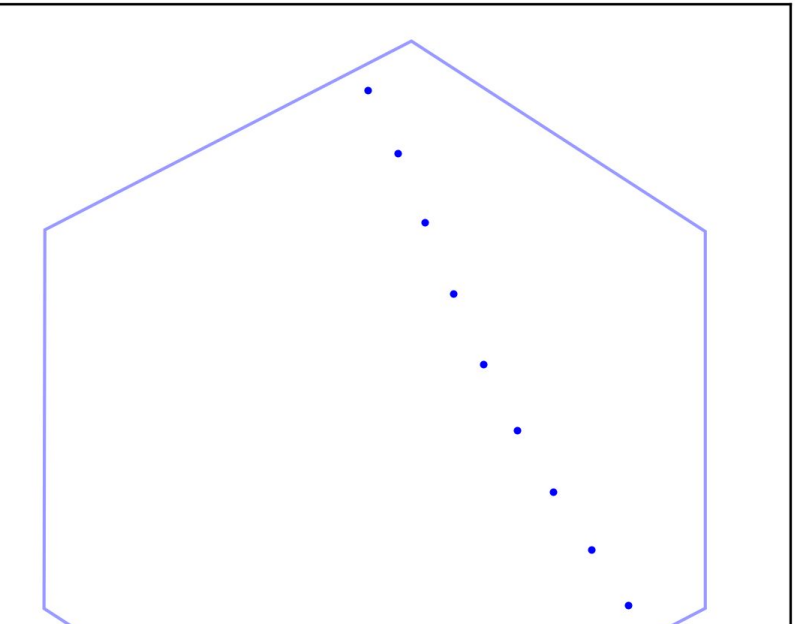


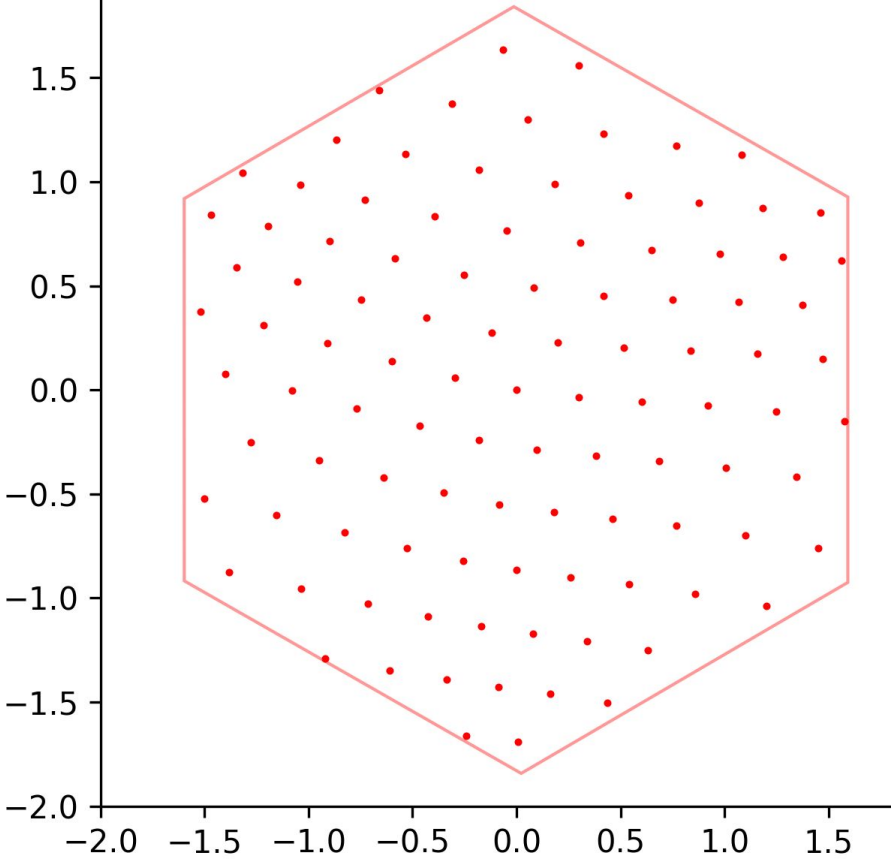


Actual Twist Angle: 55.0154074884
Total Atoms: 642
W Atoms (Top Layer): 103
Mo Atoms (Bottom Layer): 111

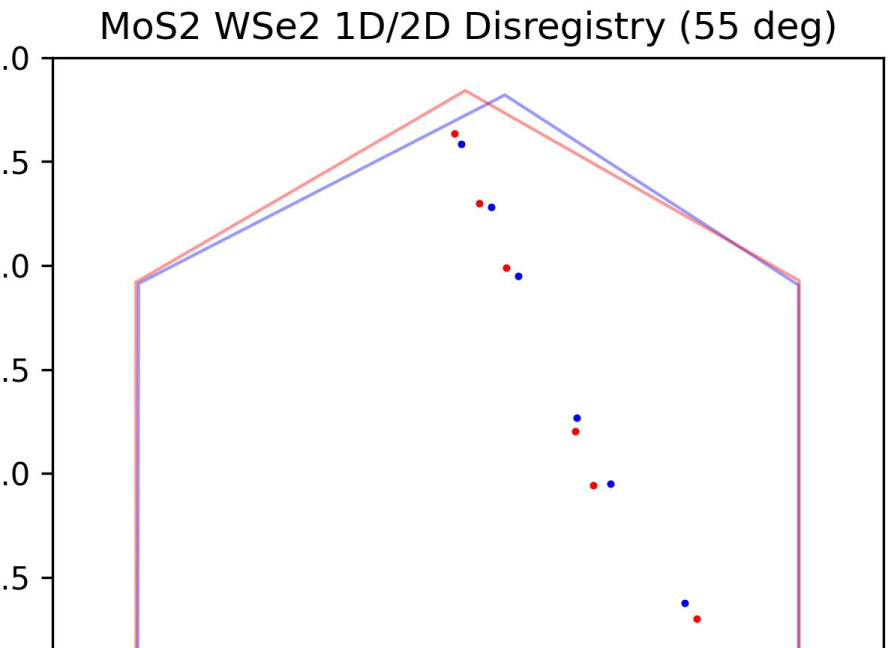
[redacted]

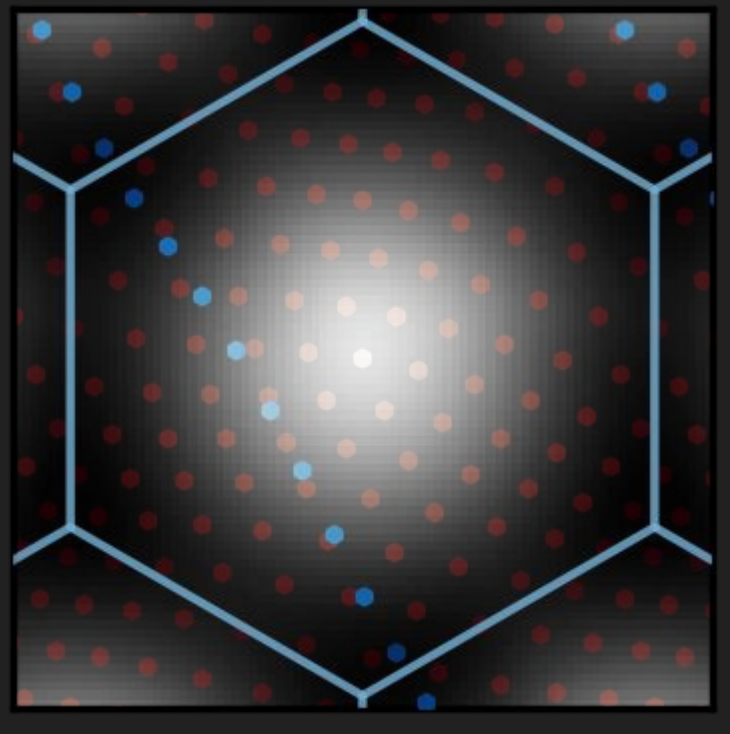
MoS2 WSe2 1D Disregistry (55 deg)



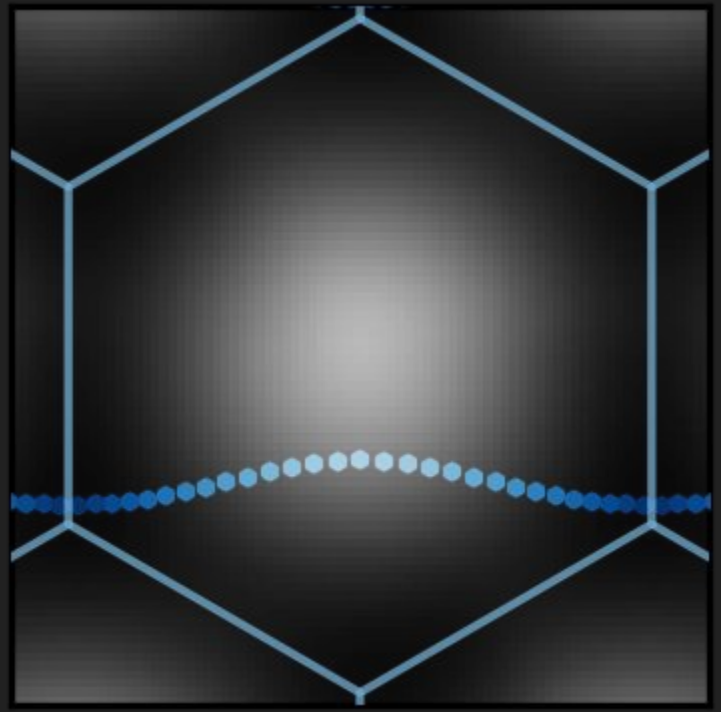


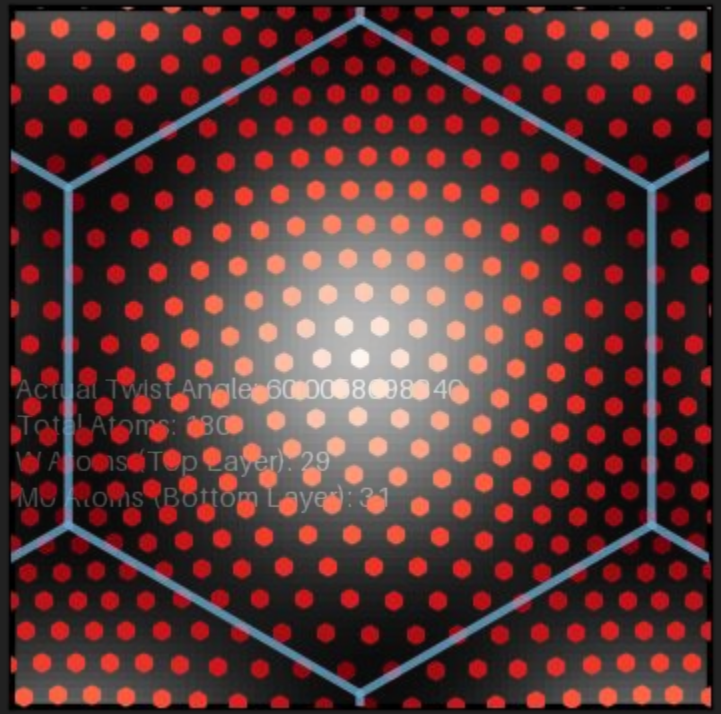
[redacted]


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

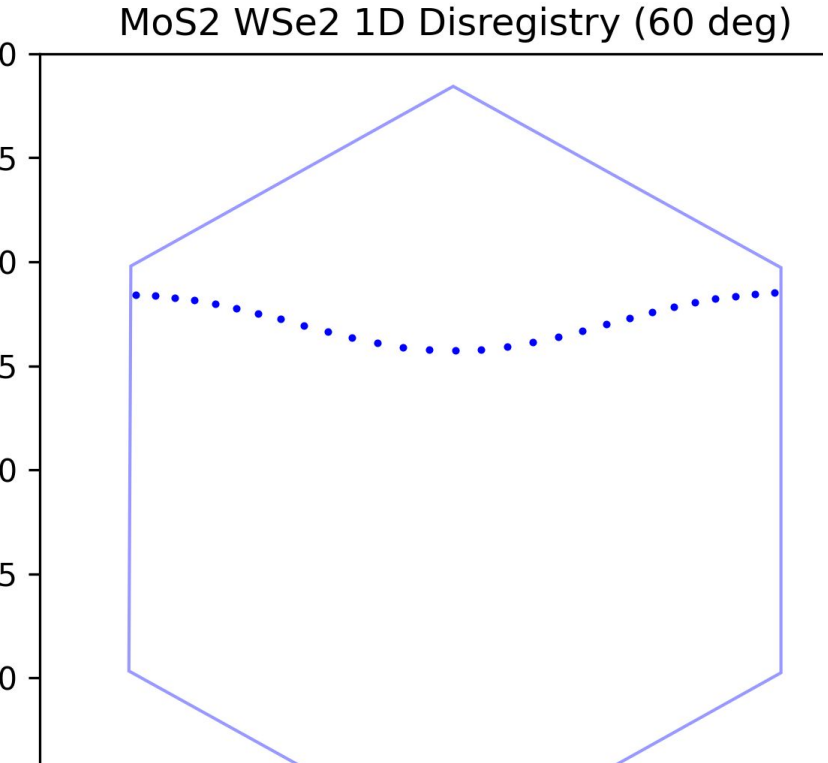


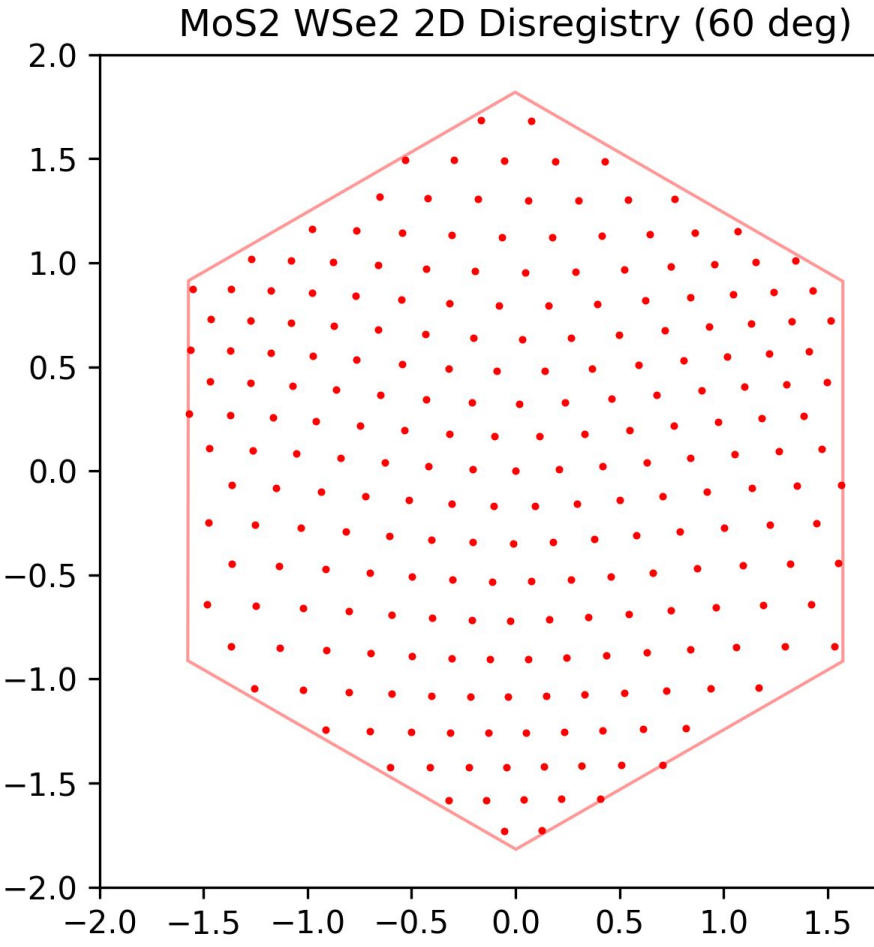
60 deg

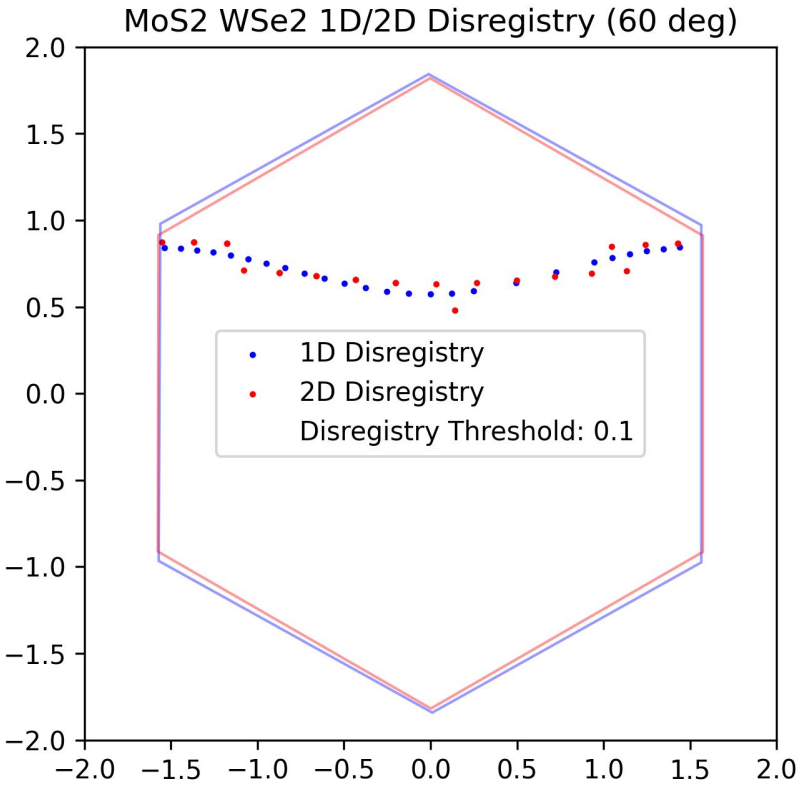




Actual Twist Angle: 59.97722199420
Total Atoms: 1536
W Atoms (Top Layer): 240
Mo Atoms (Bottom Layer): 272


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