

# Results

**Grain boundary:** al\_S5\_0\_N1\_1\_-2\_1\_N2\_-1\_1\_-2

**Number of accepted structures:**

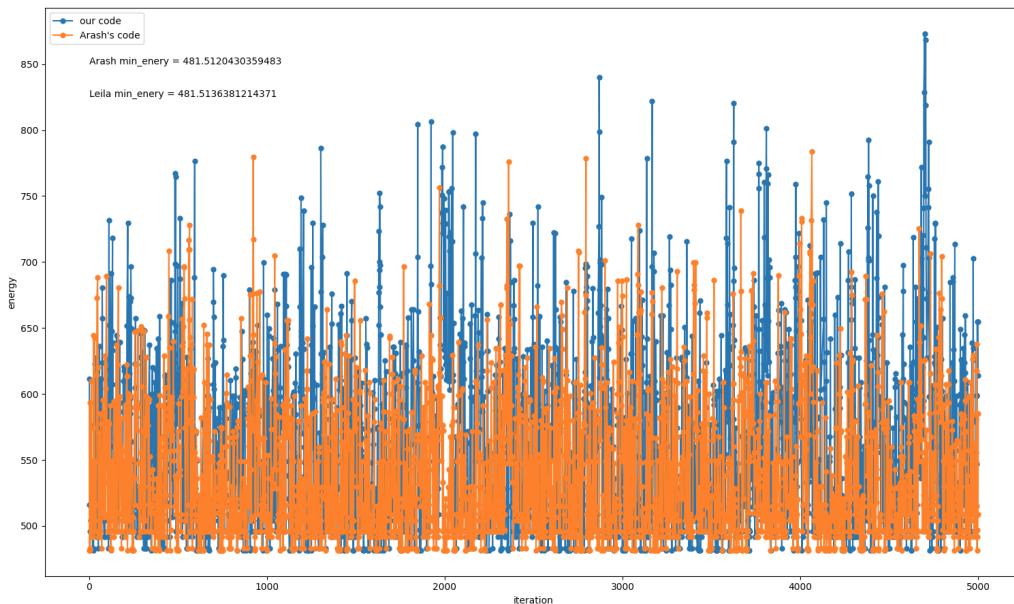
Arash's code: 2621

our code: 2853

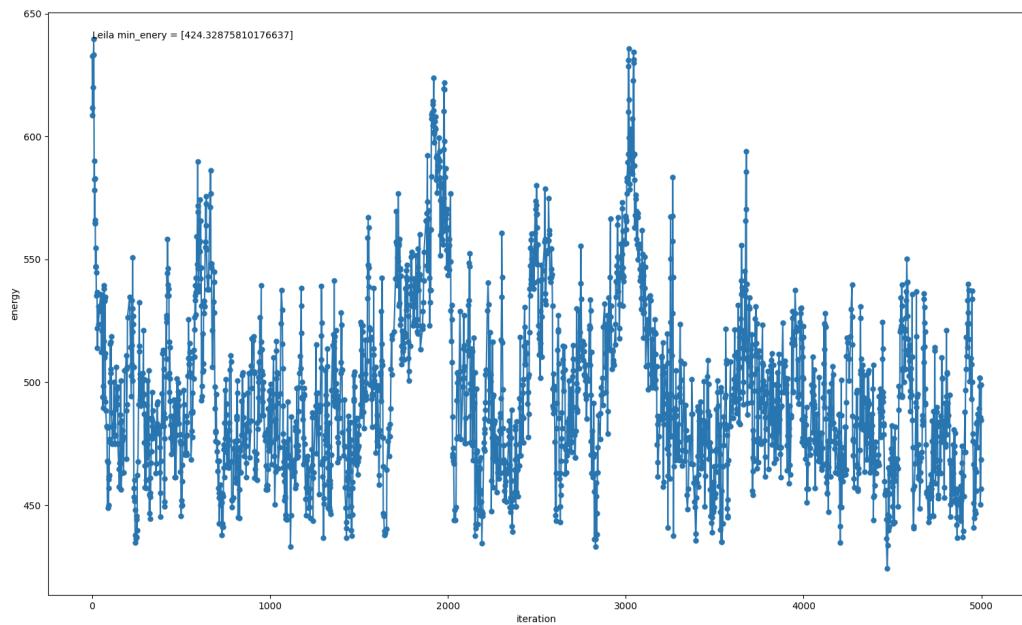
**The Structure with min energy found in**

Arash's code: 481.512043 mj/m<sup>2</sup>

our code: 481.513638 mj/m<sup>2</sup>



Energy vs iteration for the pkl file:



## Heating

Smale id	Change box	equil_dt	fix_reg	
min	heat			
S1	N	.0001	N	N
S2	Y	.0001	N	N
s3	N	.0001	Y	N
s4	Y	.0001	Y	N

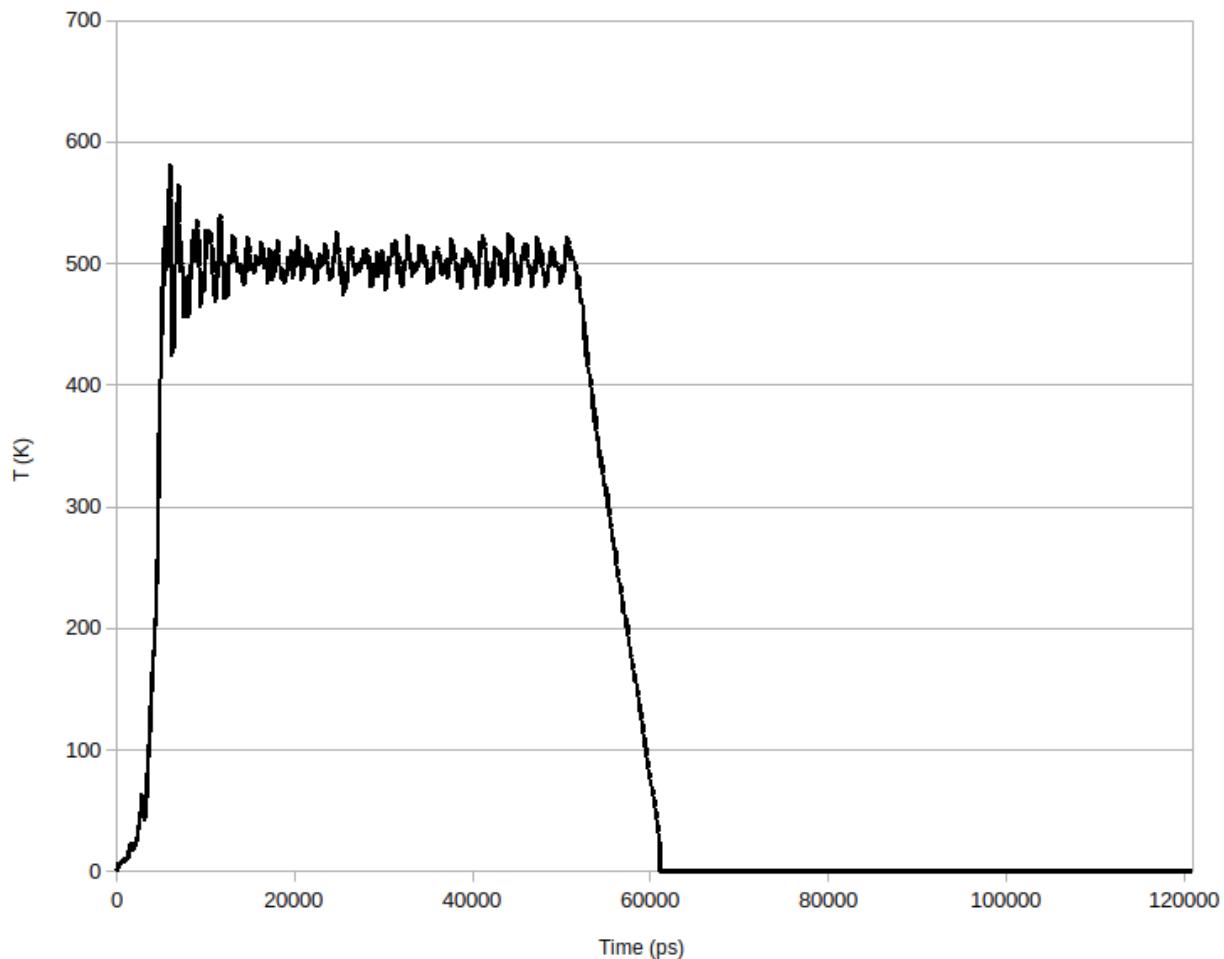
1.  $50000 \times 0.0001 \text{ ps}$
2.  $T = 500K$  ( $T_m = 966 \text{ K}$ )
- 3.

heating fix nvt: 0 - 1000

equilibrium fix nvt: 1000 - 51000

cooling fix nvt: 51000 - 61000

equilibrium fix npt: 111000 - 121000



Temperature versus time:

$T_m = 933.5$

set velocity for  $T=T_m/2 = 466.7$

fix nve: 0-1000

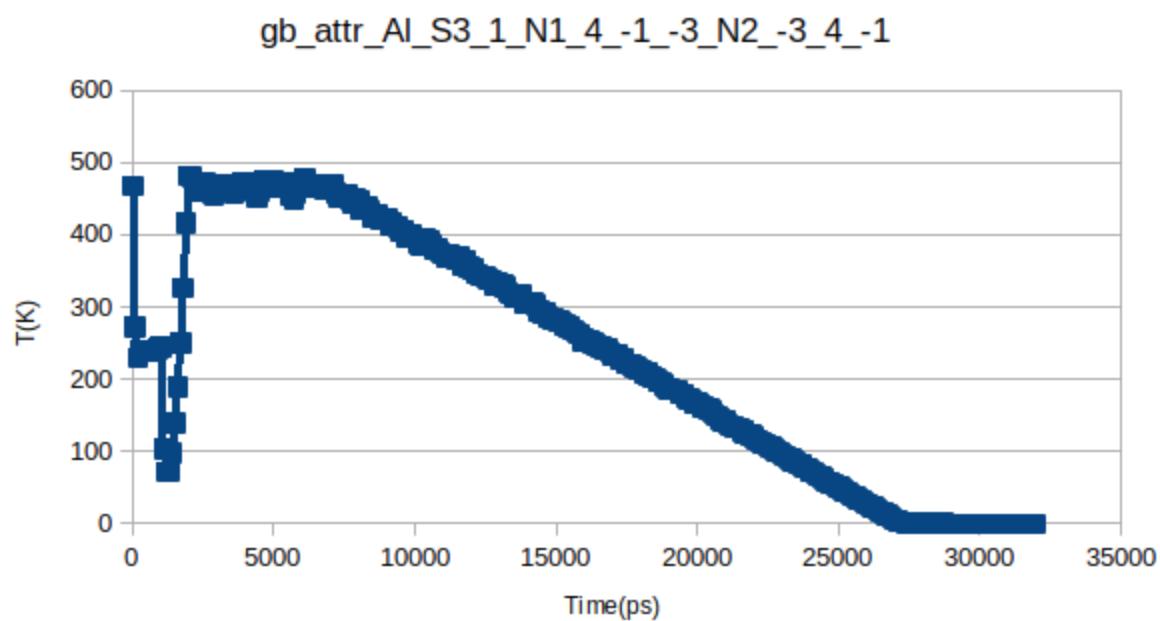
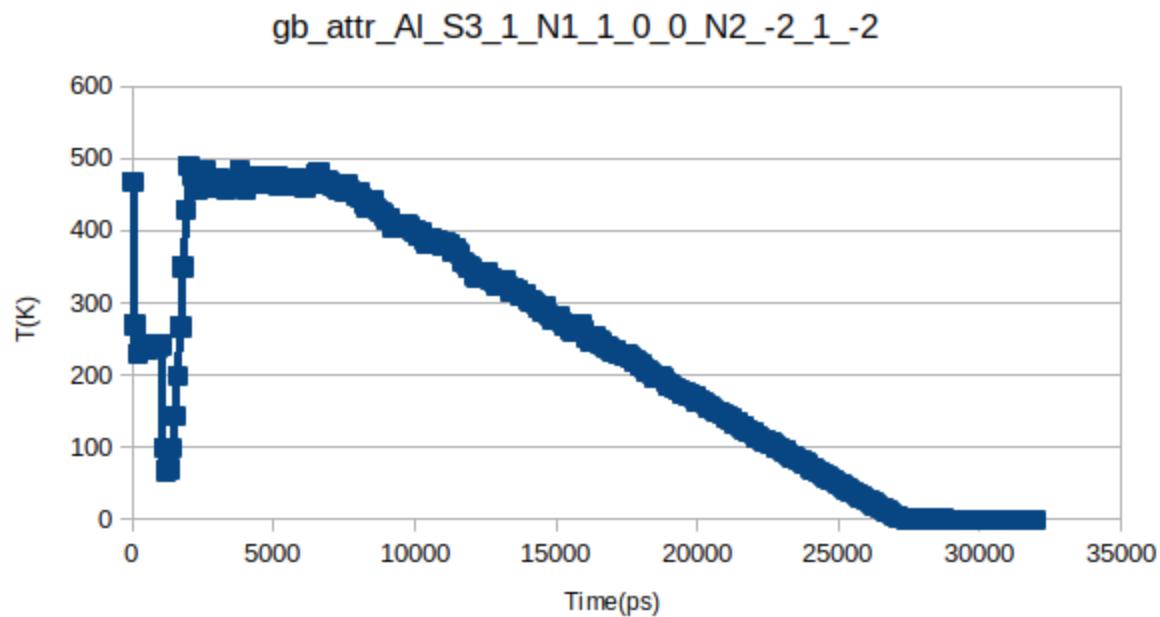
heating ( 0.01 to  $T_m/2$  K) fix nvt: 1000 - 2000

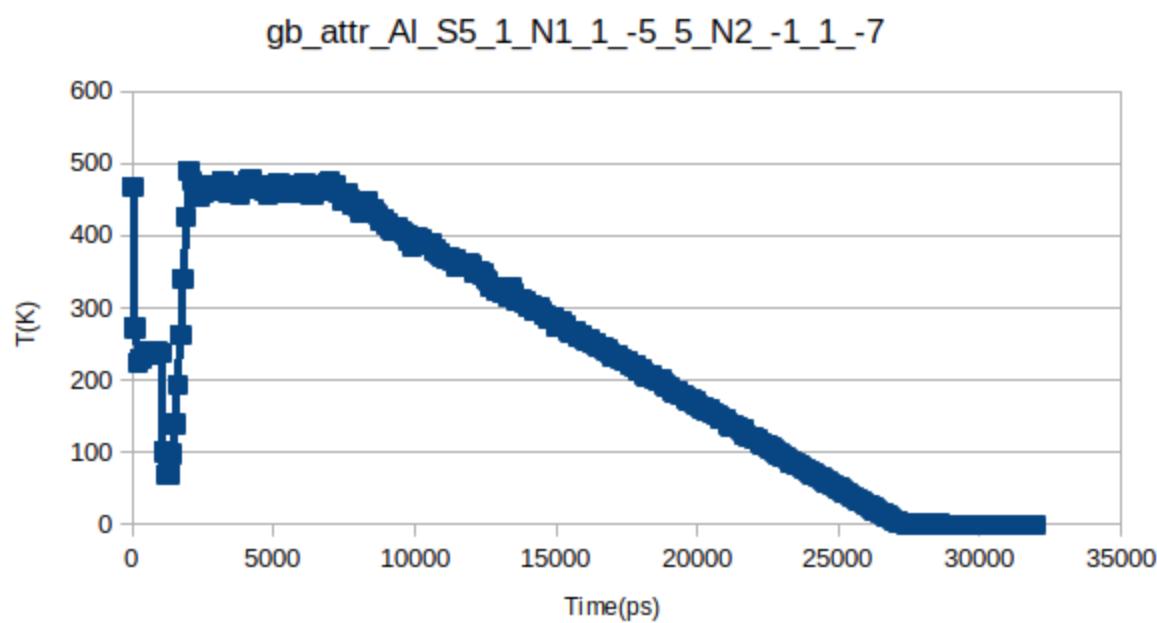
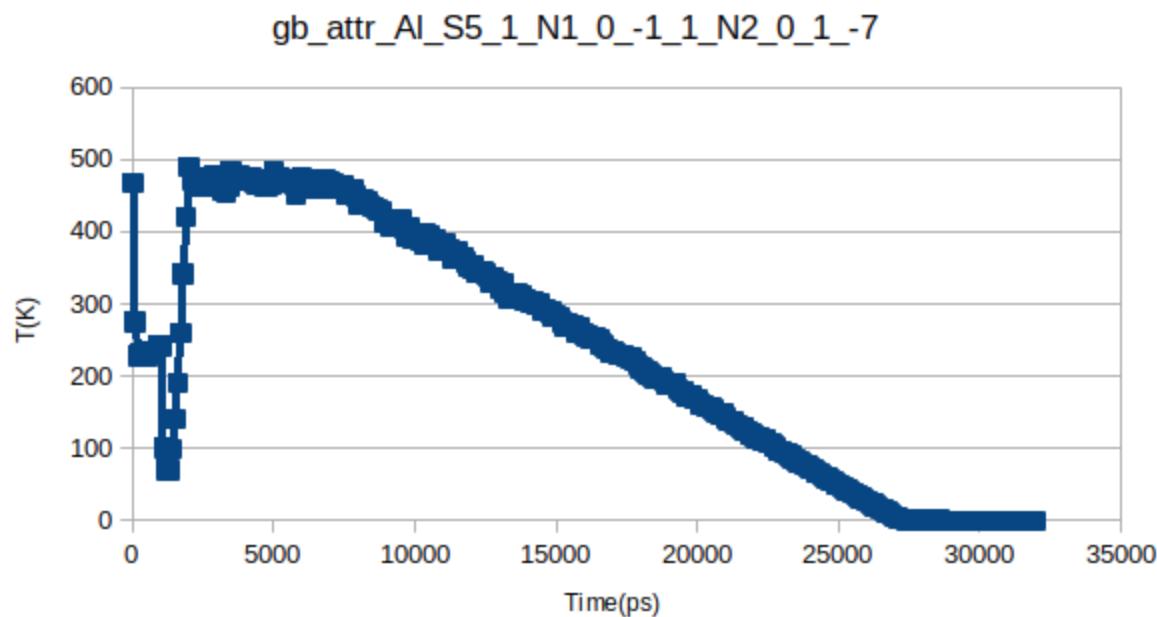
equilibrium (  $T_m/2$  K) fix nvt: 2000 - 7000

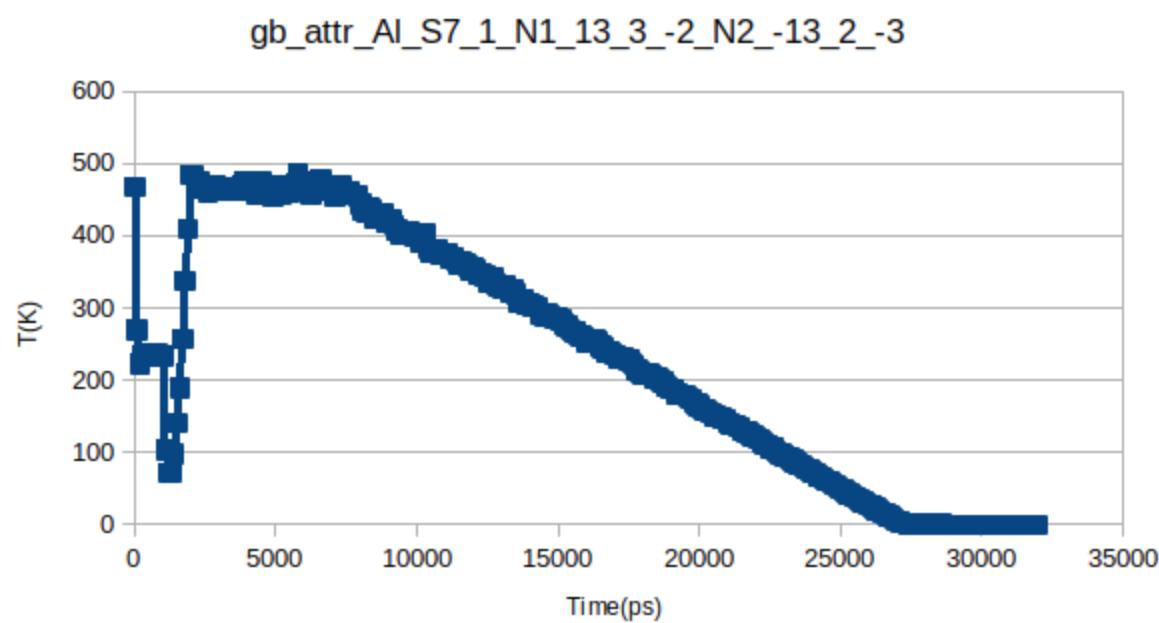
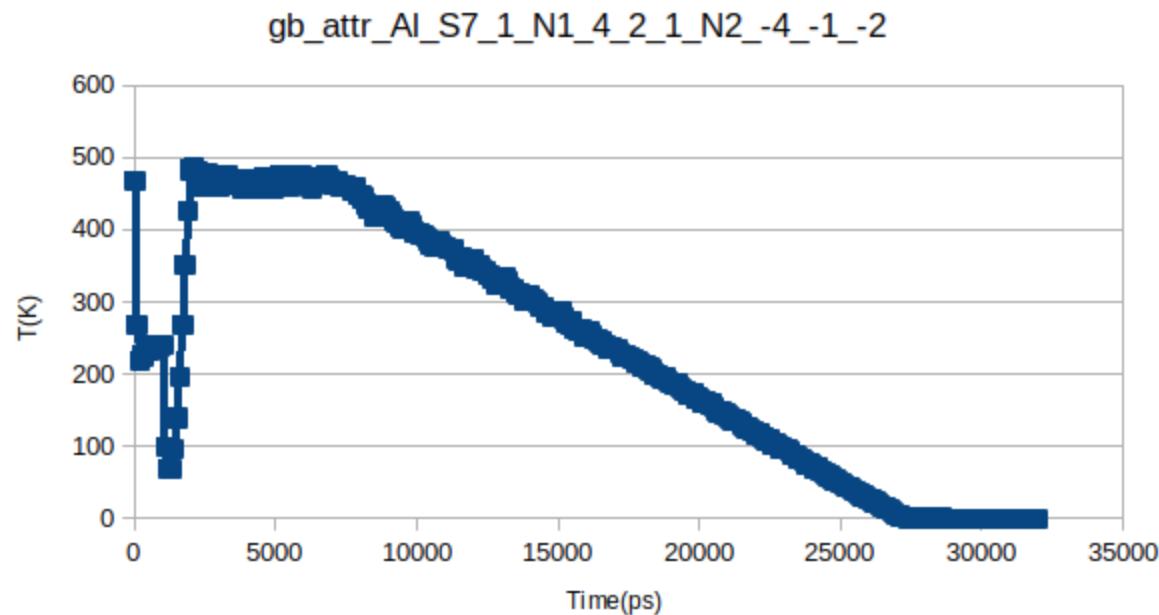
cooling ( $T_m/2$  to 0.01 K) fix nvt: 7000 - 27000

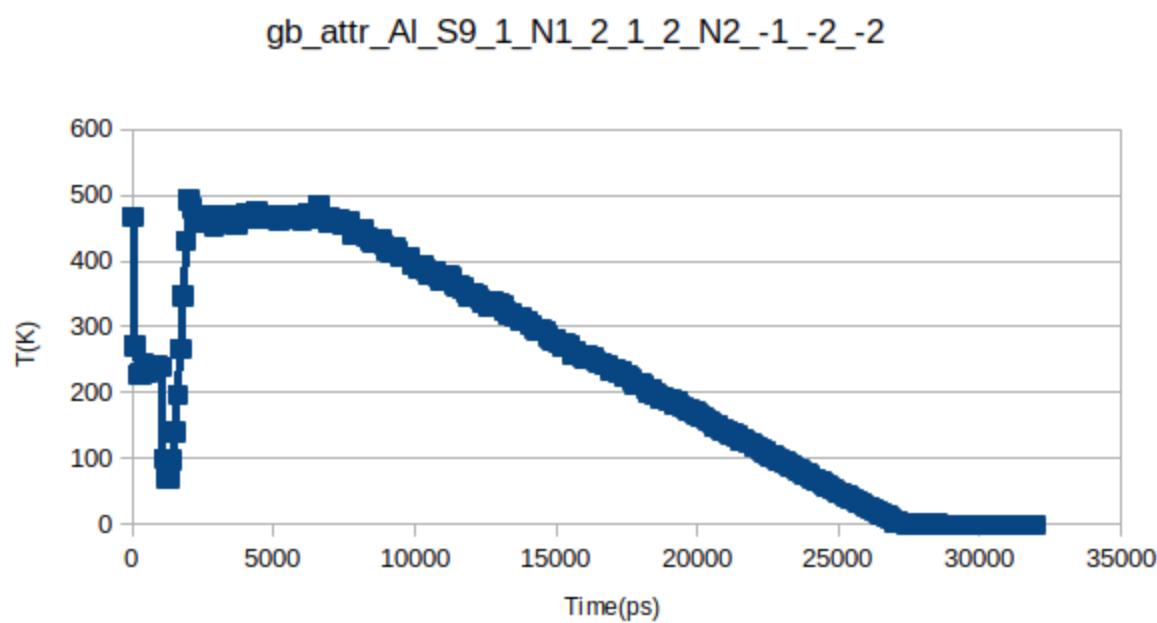
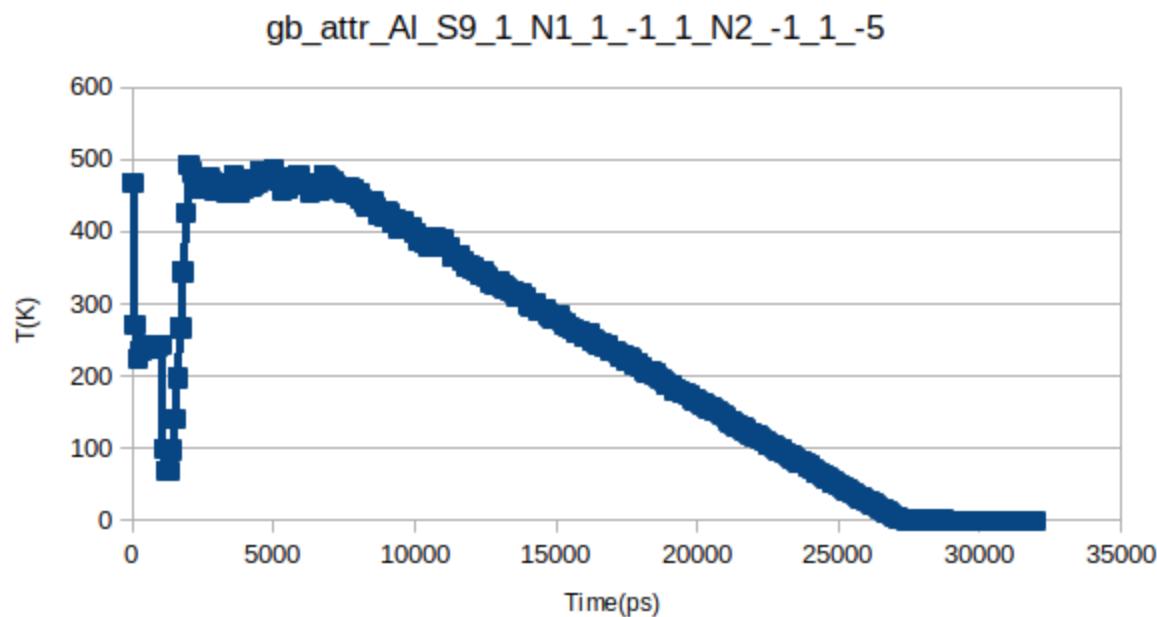
equilibrium ( 0.01 K) fix nvt: 27000 - 27000

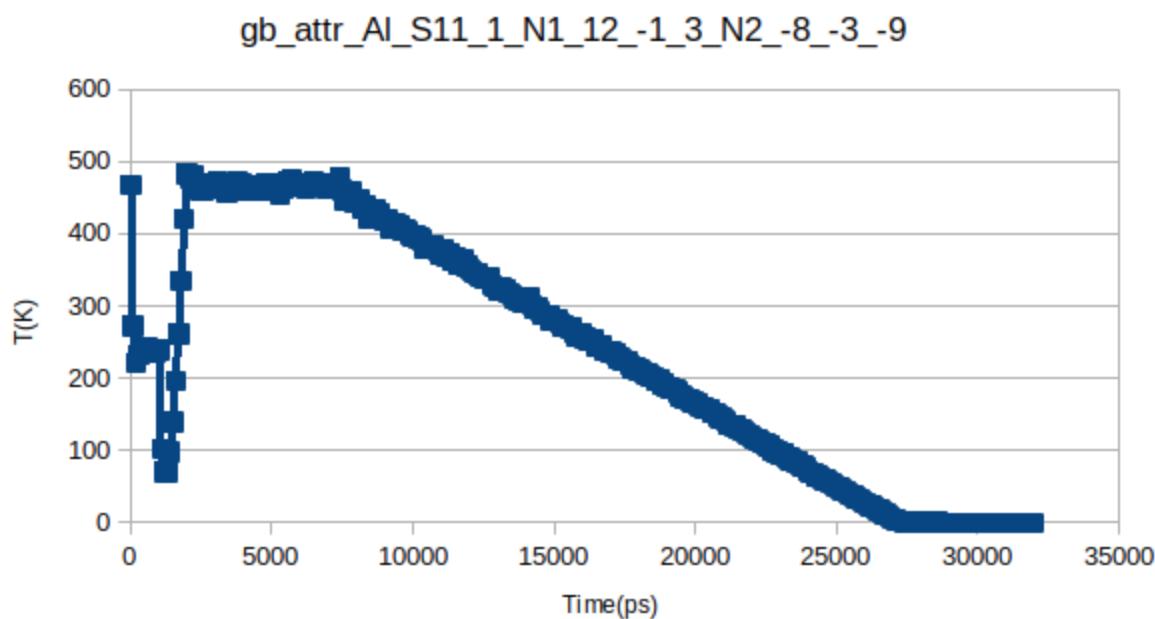
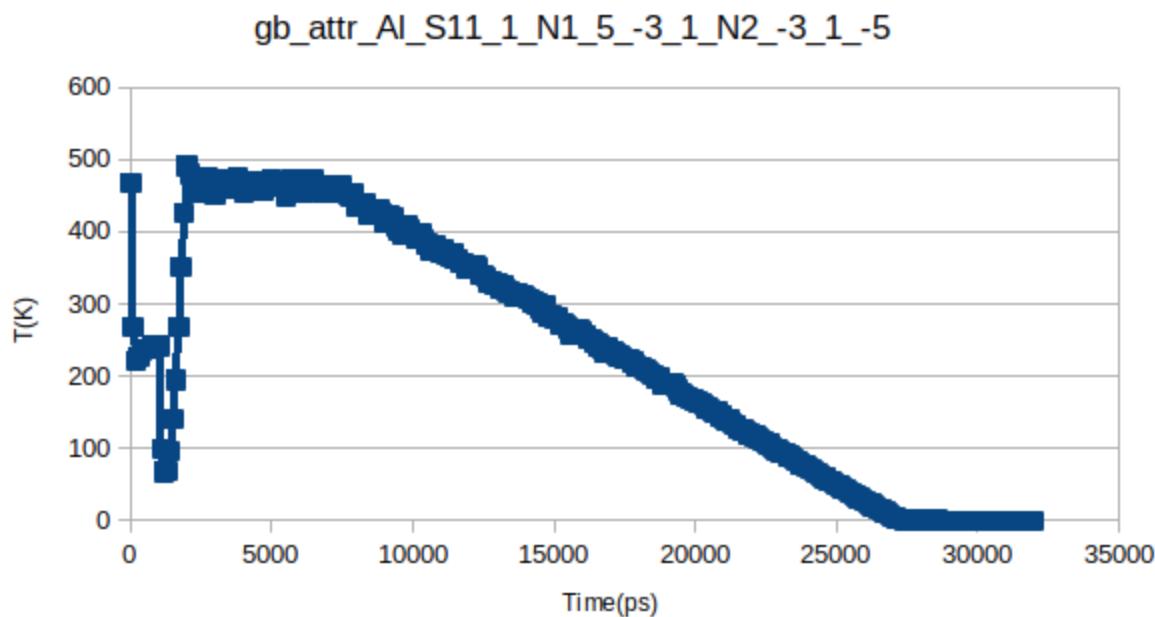
equilibrium ( 0.01 K) fix npt: 27000 - 32000









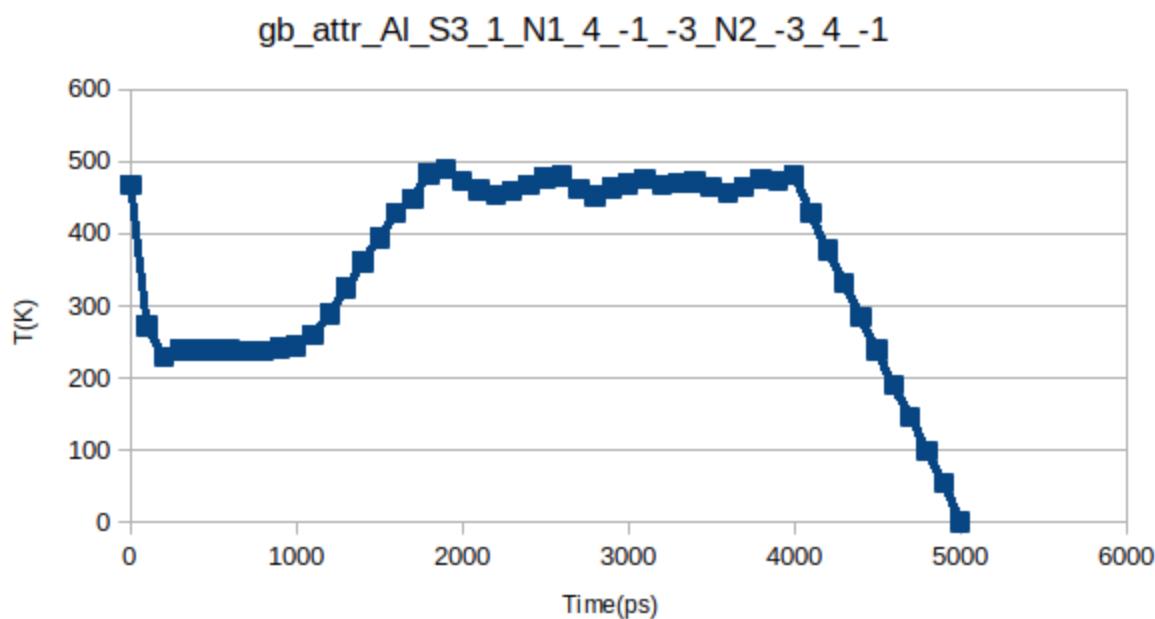
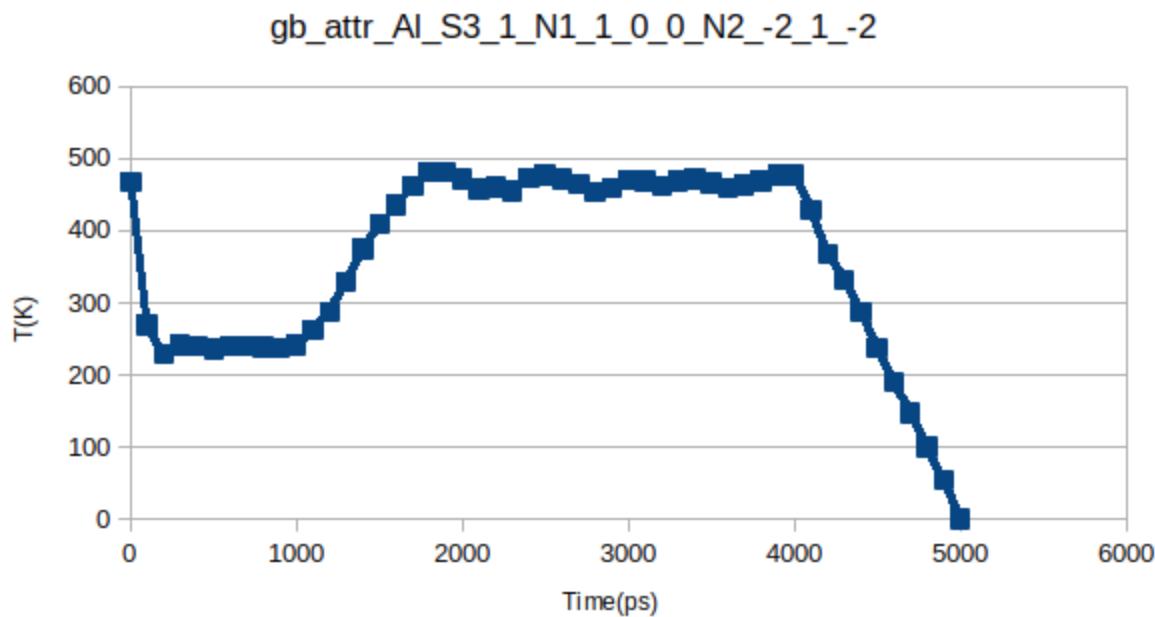


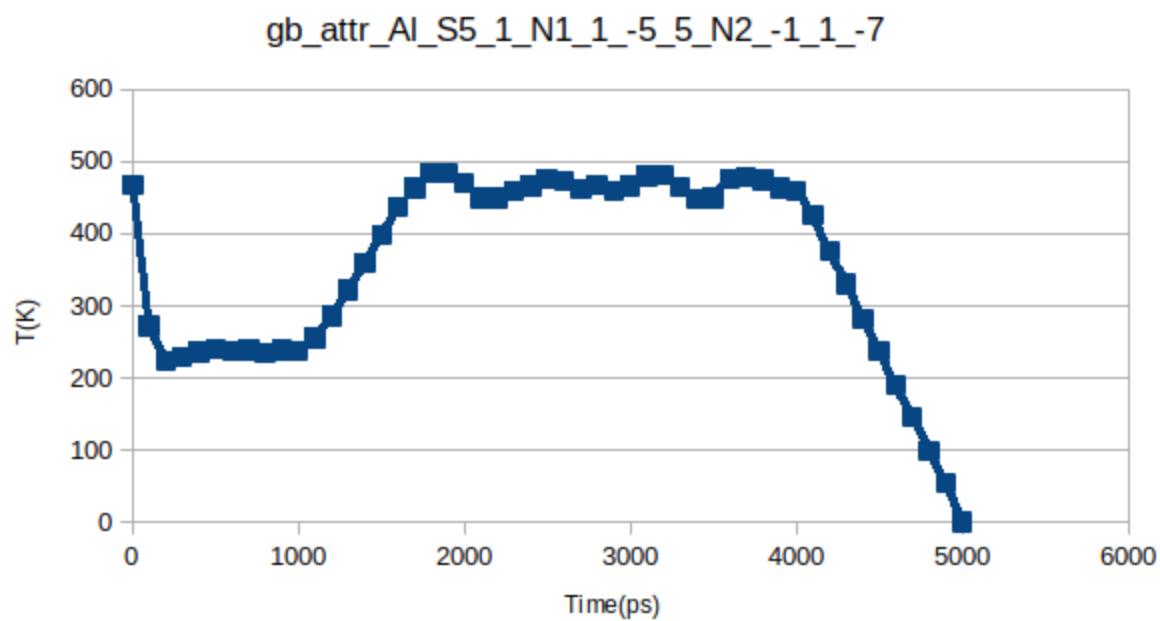
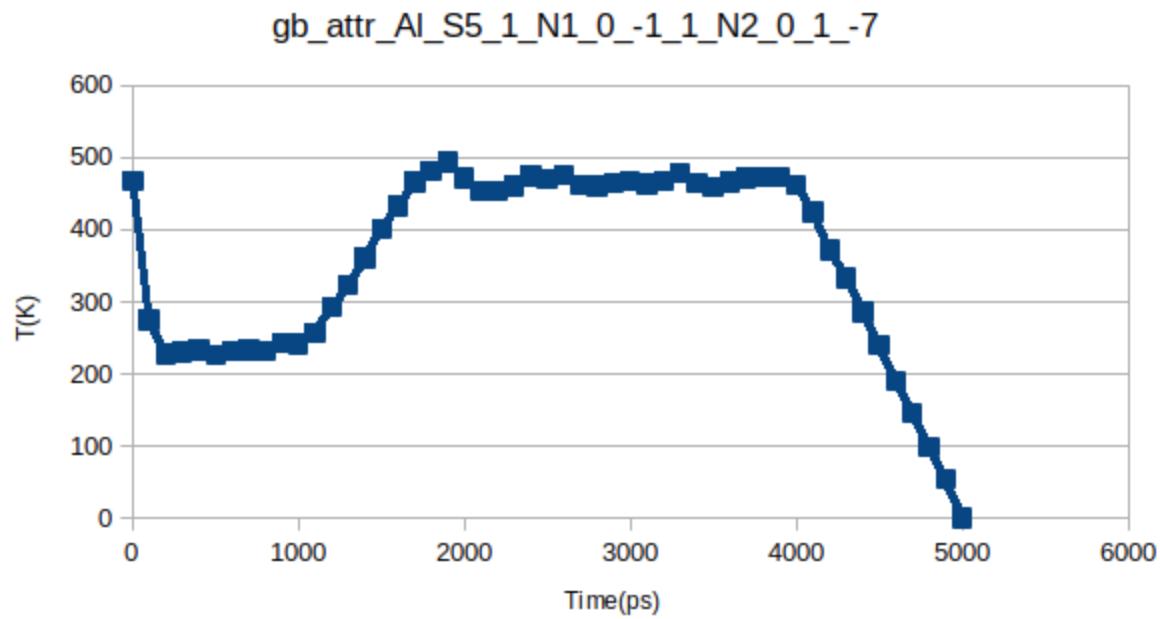
**July 6, 2020**

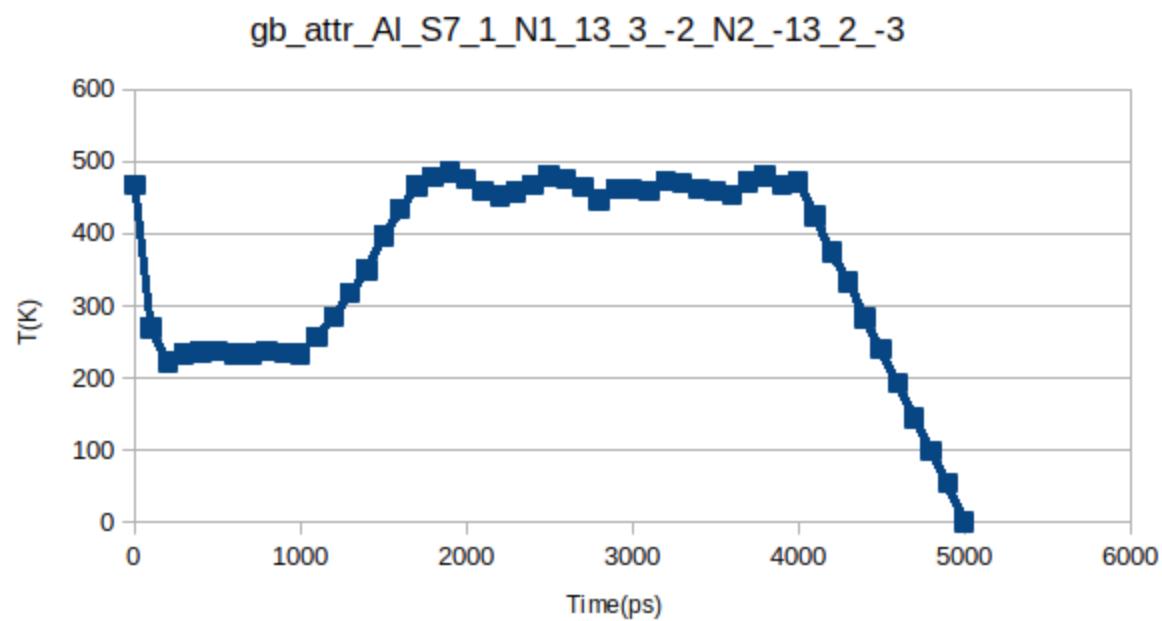
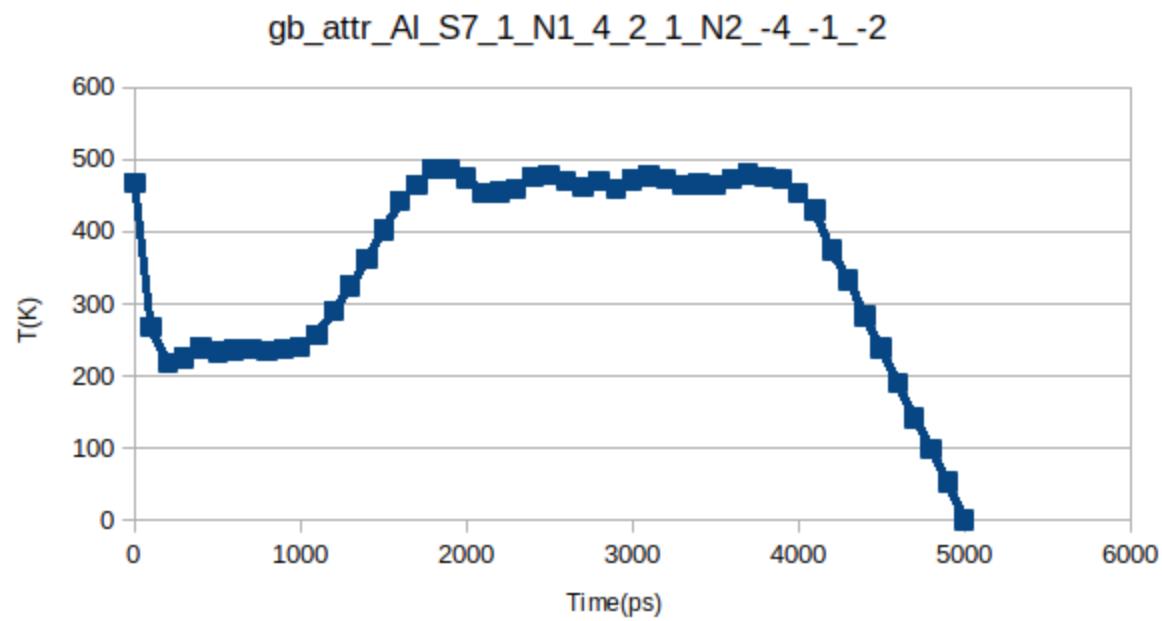
### New protocol

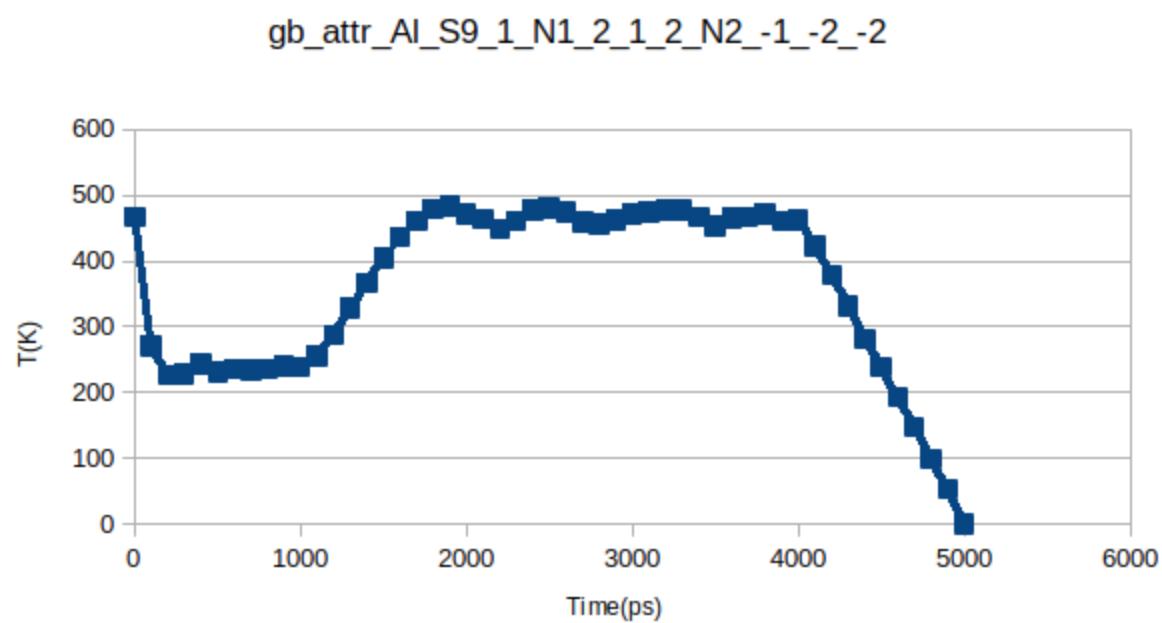
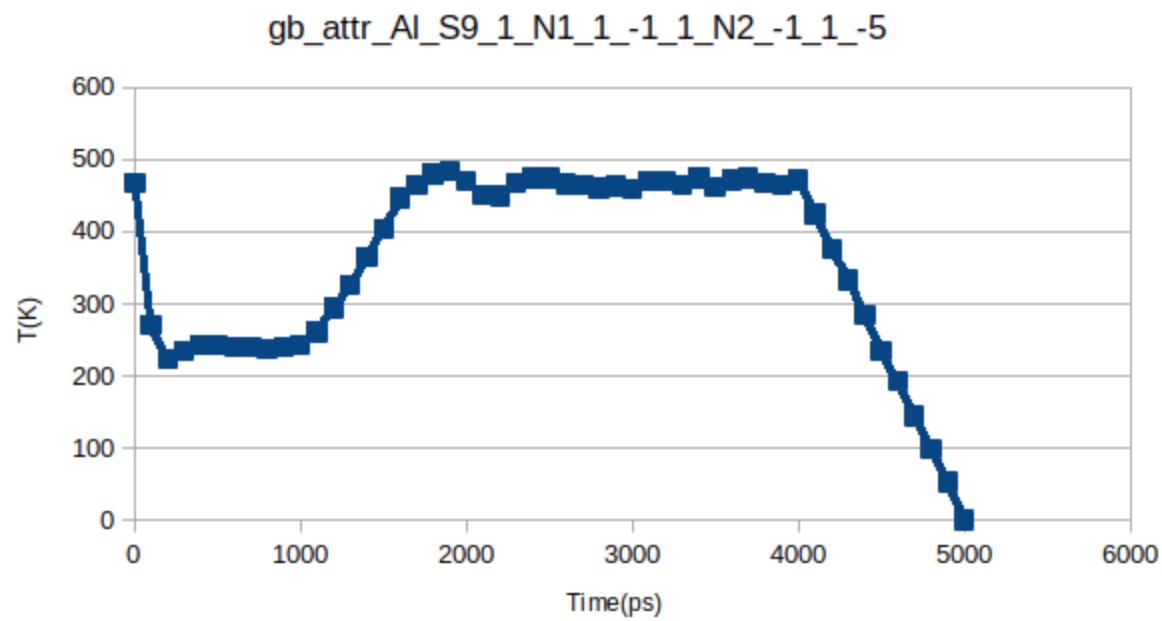
1.  $T_m = 933.5$
2. set velocity for  $T=T_m/2 = 466.7$
3. fix nve: 0-1000

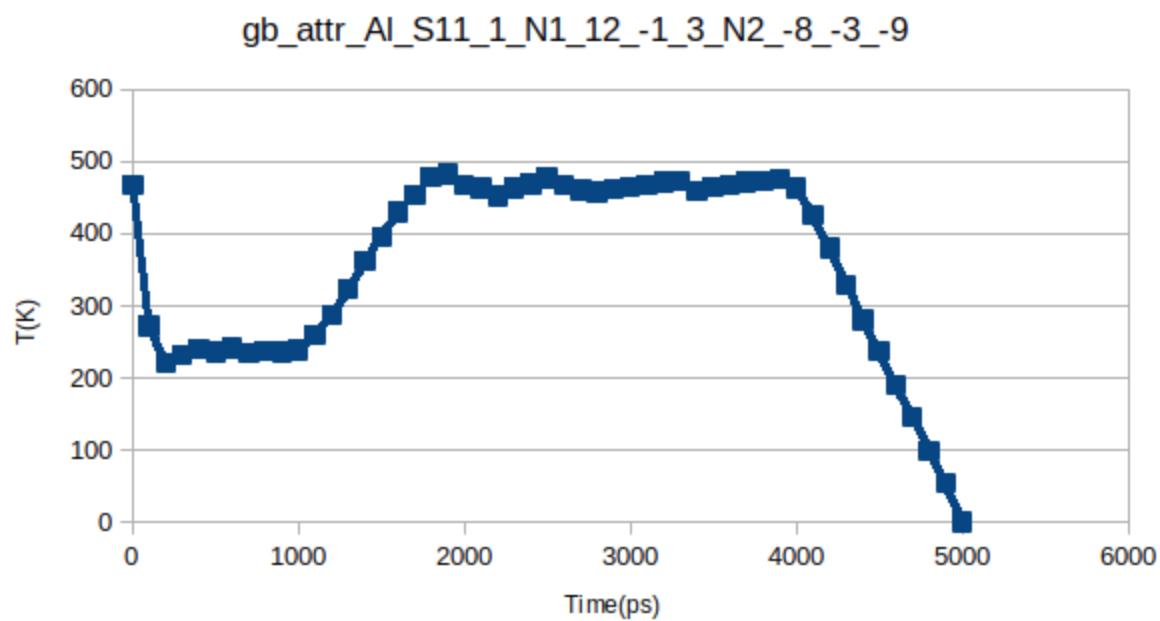
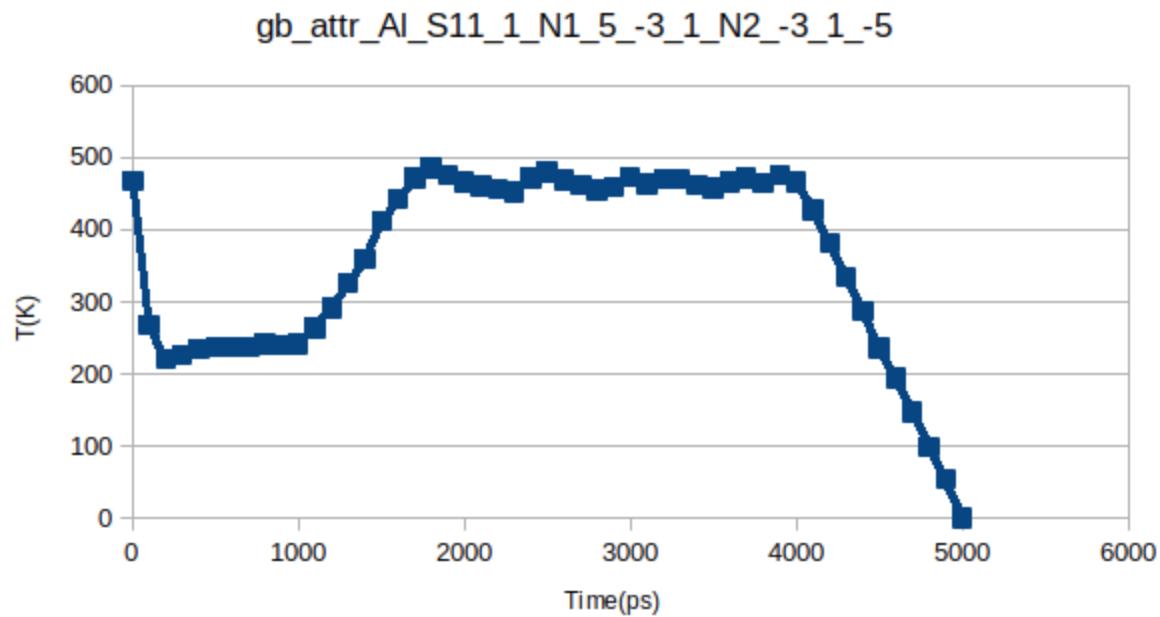
4. equilibrium (  $T_m/2$  K) fix nvt: 1000 - 4000
5. cooling ( $T_m/2$  to 0.01 K) fix nvt: 4000 - 5000
6. Minimize



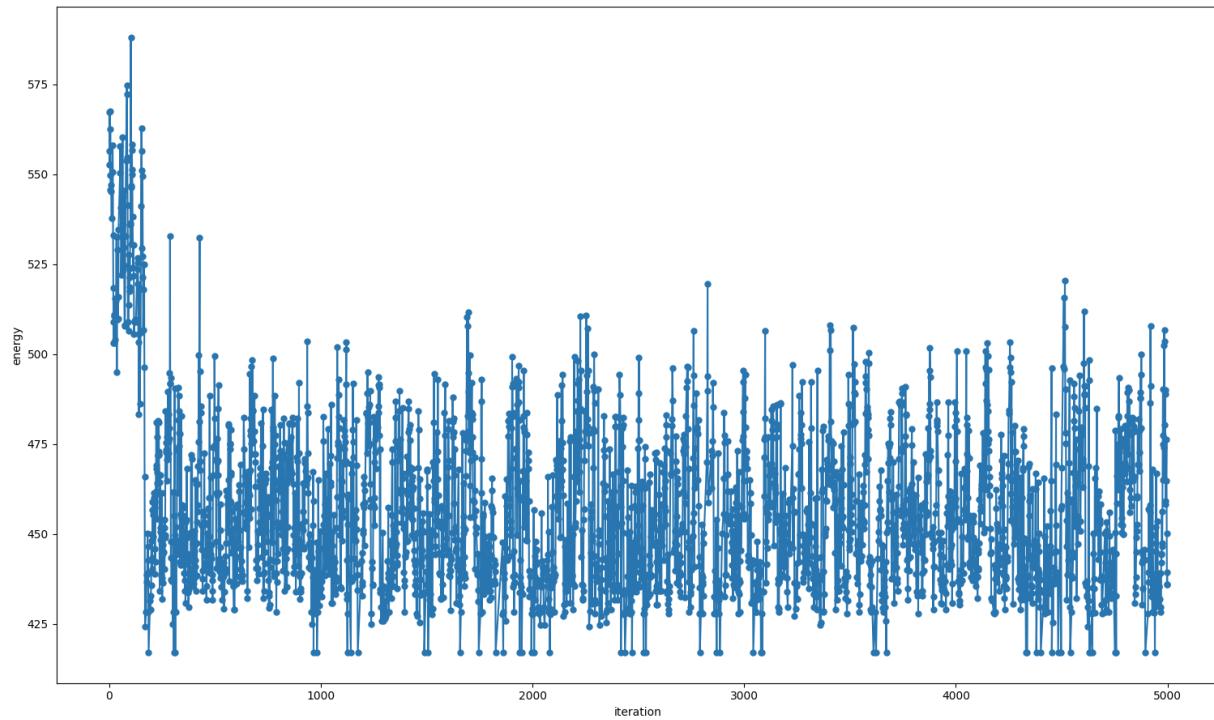
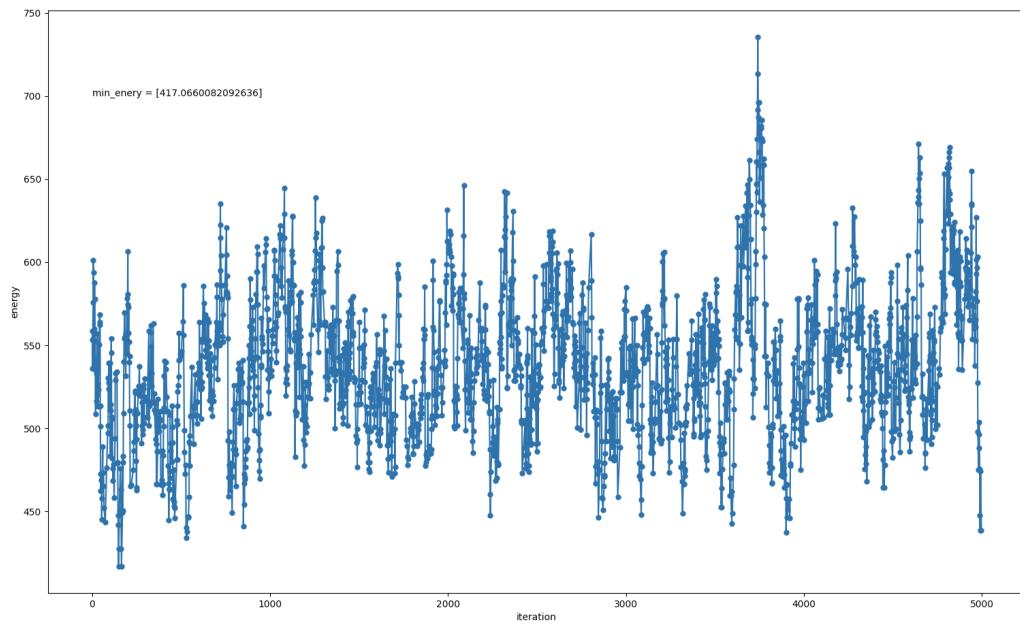








The following results are for the `gb_attr_Al_S3_1_N1_4_-1_-3_N2_-3_4_-1`



## Byxtal

### 1. Figure Edits for Byxtal

#### a. Center and optimize scaling

14 of 28 2. [@Leila k](#) Add Markdown cells content to Jupyter notebooks

8/10/20, 2:07 PM

3. [@Srikanth P](#) To add code content to Jupyter notebooks
4. [@Leila k](#) - Check to see how to add numbered latex equations (that can be cross-referenced) in jupyter notebooks.

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July 20, 2020

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The gcmc code is ran on 6 different situations which are explained in the tabs.

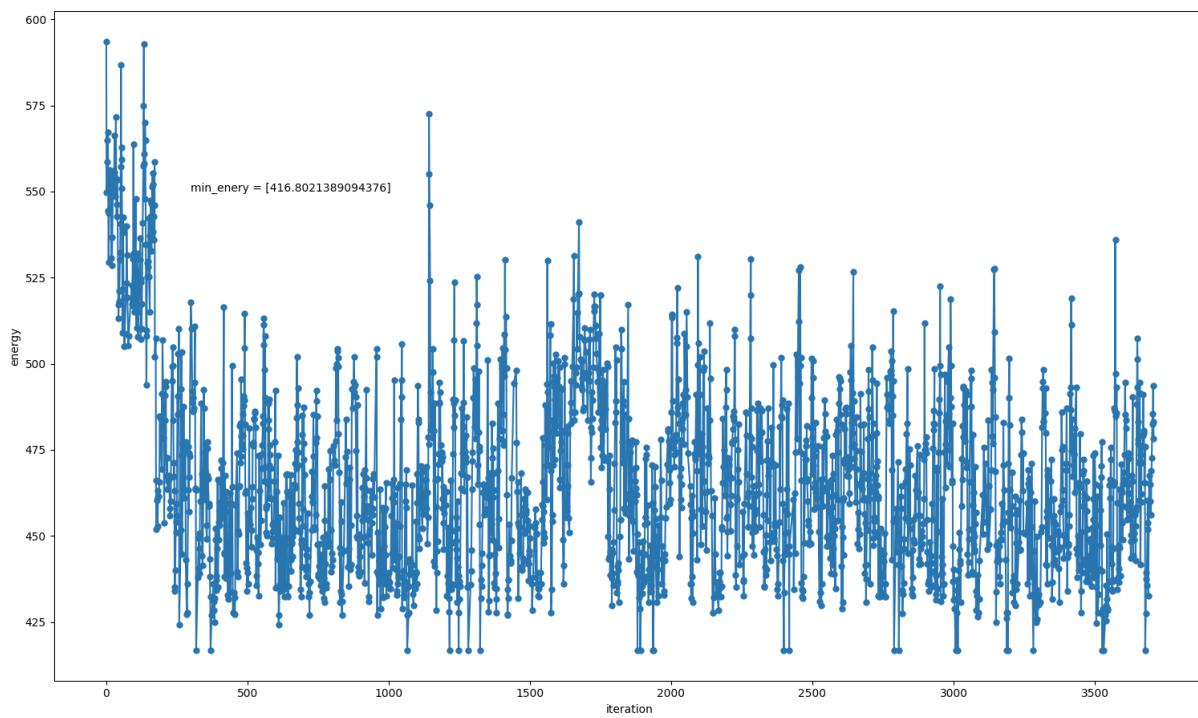
Some explanations about the tables:

- 1st min: the first minimization without applying box /relax
- 2nd min: the second minimization with box/relax
- Fix rigid is NOT applied except the last sample at the last slide

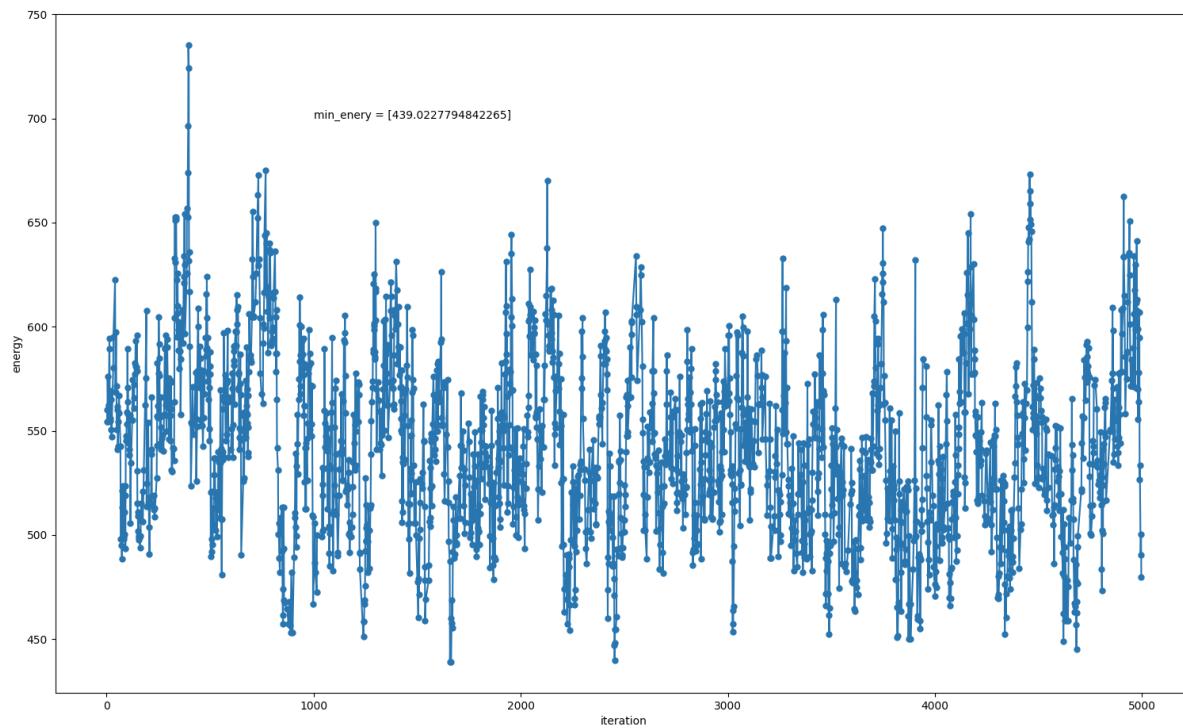
GB: Al\_S3\_0\_N1\_4\_-1\_-3\_N2\_-3\_4\_-1

Energy using brute force: **424.201463096**

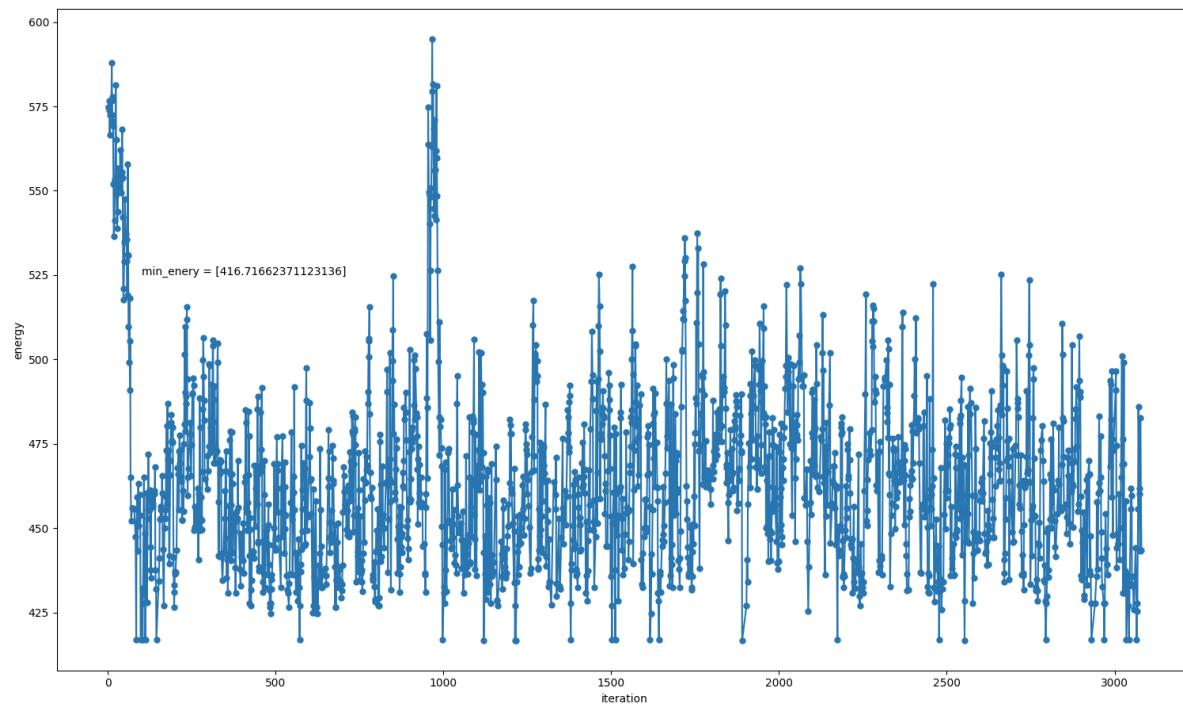
Sample #	Buffer reg.	1st min	2nd min	vmax	heat/cool	E_min
<b>1_h</b>	No	yes	yes	.0001	yes	416.802



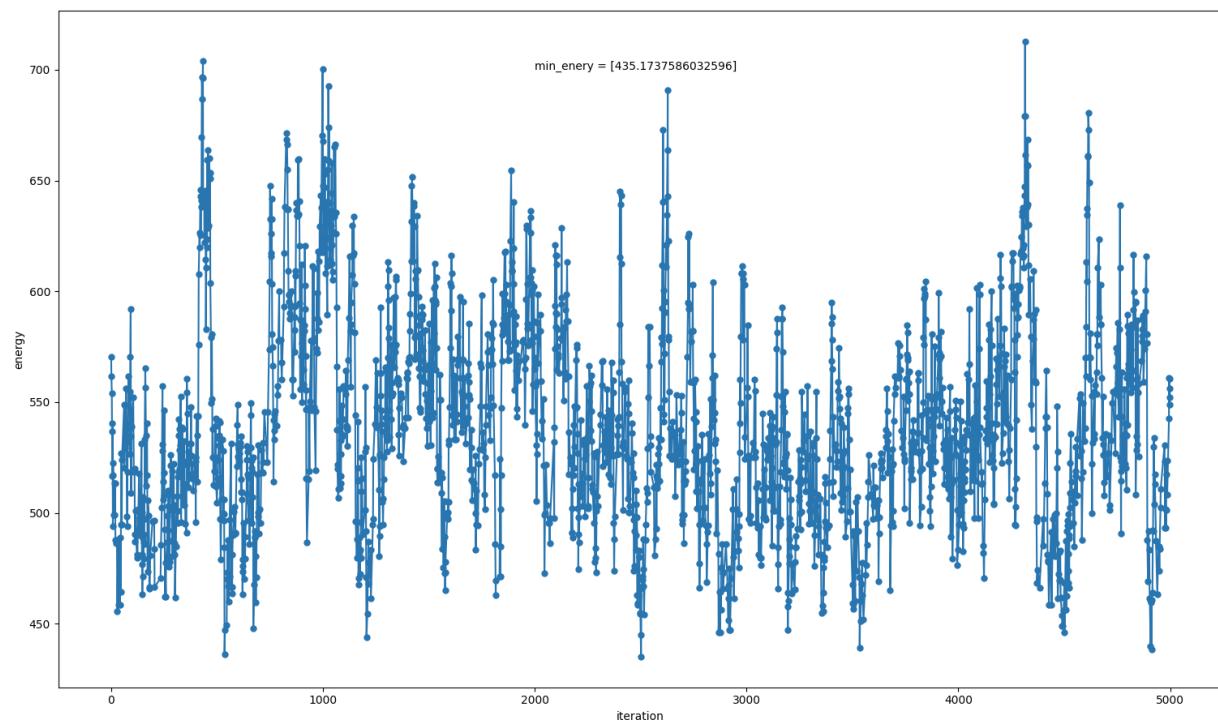
Sample #	Buffer reg.	1st min	2nd min	vmax	heat/c ool	E_min
<b>1_m</b>	No	yes	yes	.0001	no	439.022



Sample #	Buffer reg.	1st min	2nd min	vmax	heat/cool	E_min
2_h	no	yes	yes	.001	yes	416.7166

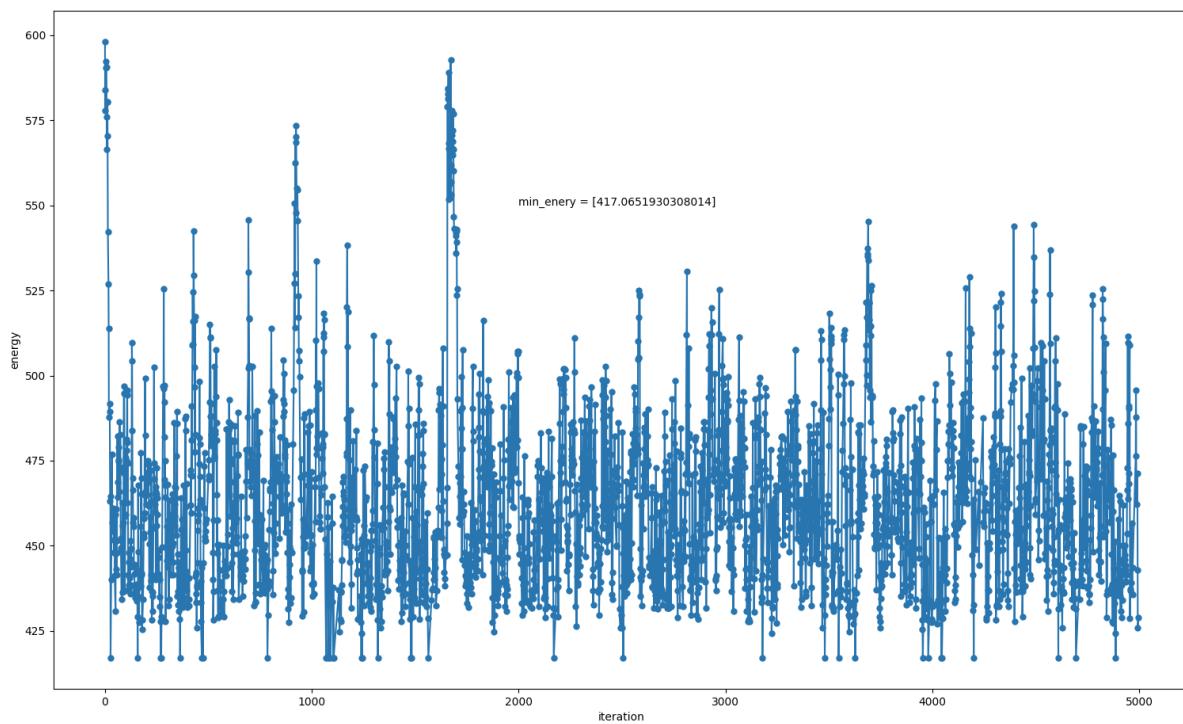


Sample #	Buffer reg.	1st min	2nd min	vmax	heat/cool	E_min
2_m	no	yes	yes	.001	no	435.1737

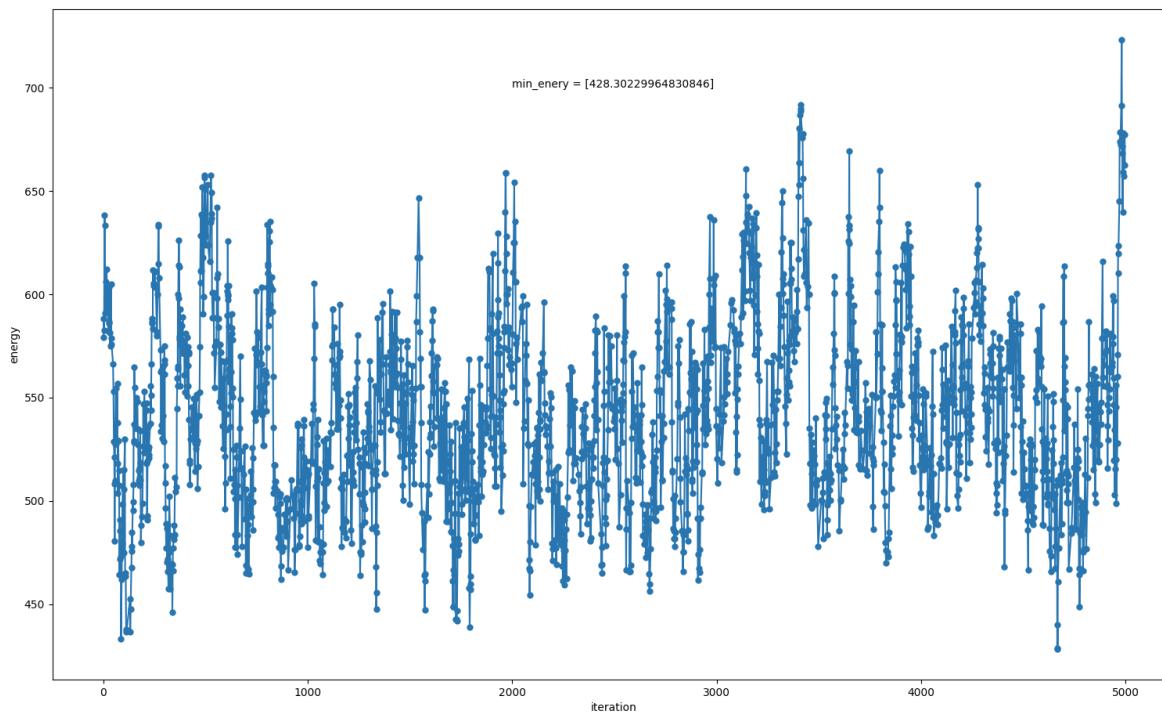


Sample #	Buffer reg.	1st min	2nd min	vmax	heat/cool	E	-	m	in
3_h	no	yes	No	-	yes	4	4	1	1

1	
4	
1	
6	
8	
5	



Sample #	Buffer reg.	1st min	2nd min	vmax	heat/coo	E_min
3_m	no	yes	No	-	no	428.3023



## Tentatively the protocol for simulating GBs

1. **Step 1:** 1st minimization - w/o box-relax (Tol: 1e-5)
2. **Step 2:** 2nd minimization - with box-relax (Tol: 1e-5)
3. **Step 3:** Heating-Cooling
  - a. Describe the steps of heating/cooling here
4. **Step 4:** 3rd minimization - w/o box-relax (Tol: 1e-5)
5. **Step 5:** 4th minimization - with box-relax (Tol: 1e-25, vmax = 0.001)

## July, 22

1. Test the protocol for the 10 grain boundaries
2. Identify how to simulate the GBs on HPC

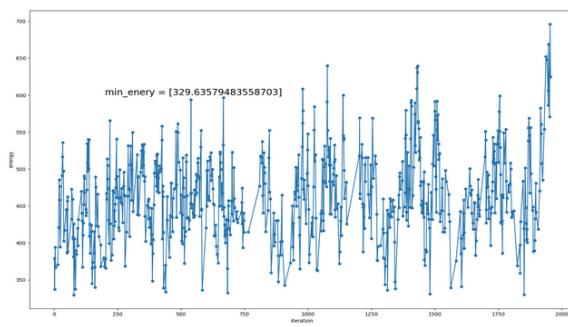
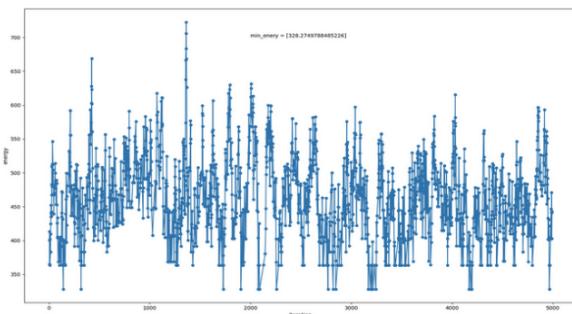
## August 1

The highlighted GBs are gets close to the surface.

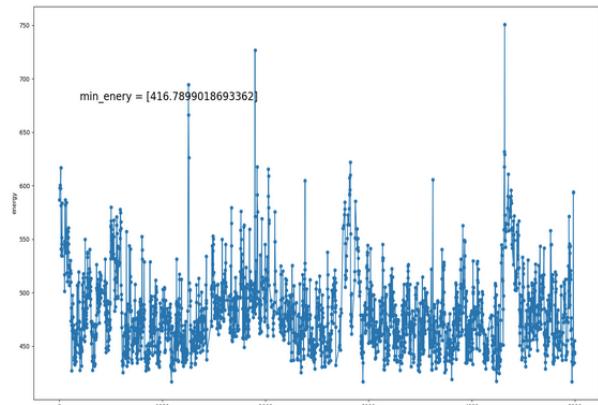
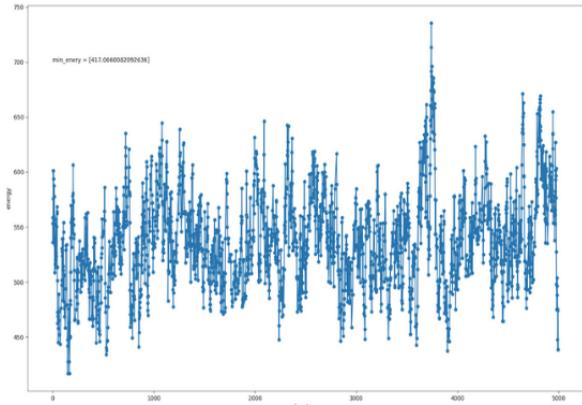
GB_name	Min energy (brute force)	Min energy (GBMC) Just minimiza tion	error (100*(E_bf - E_gbm_m)/E_ bf)	Min energy (GBMC) heating/c ooling	error (100*(E_bf - E_gbm_h c)/E_bf)
Al_S3_0_N1_1_0_0_N2_-2_1_-2	328.289 016257	328.2749 7884852 3	0.0042759299 82994	329.6358	-0.410243 31497758
Al_S3_0_N1_4_-1_-3_N2_-3_4_-1	<b>424.201</b> <b>463096</b>	417.0660 0820926 4	1.6820910599 0782	416.7899	1.747179 9936538
Al_S5_0_N1_0_-1_1_N2_0_1_-7	528.332 728861	518.7325 2750351 3	1.8170748910 7924	522.1303 7	1.173949 39252983
Al_S5_0_N1_1_-5_5_N2_-1_1_-7	522.709 404119	526.5401 3068655 6	-0.7328596993 6058	523.269	-0.107056 78462837 7
Al_S7_0_N1_4_-2_1_N2_-4_-1_-2	359.731 157638	359.7324 6211003 8	-0.0003626241 45918	398.855	-10.87585 59083088
Al_S7_0_N1_13	440.952	445.0420	-0.9274970665	441.8547	-0.204666 8/10/20, 2:07 PM

<u>_3_-2_N2_-</u> <u>13_2_-3</u>	228598 7	4758324 7	75787 1	1	47937565 9
AI_S9_0_N1_1_- 1_1_N2_-1_1_-5	374.391 216221 5	374.3557 9522397 5	0.0094609583 47928	375.8003 6	-0.376366 67687423 6
AI_S9_0_N1_2_- 1_2_N2_- 1_-2_-2	475.928 096933 8	483.3762 2695904 8	-1.5649695981 4853	475.4907	0.091903 99470396 9
AI_S11_0_N1_1_2_-1_3_N2_- 8_-3_-9	475.726 019264 8	476.9439 3169401 8	-0.2560113133 82064	481.9208	-1.302174 04244233
AI_S11_0_N1_5_-3_1_N2_- 3_1_-5	432.130 180133 4	432.1185 2091667 4	0.0026980796 20916		

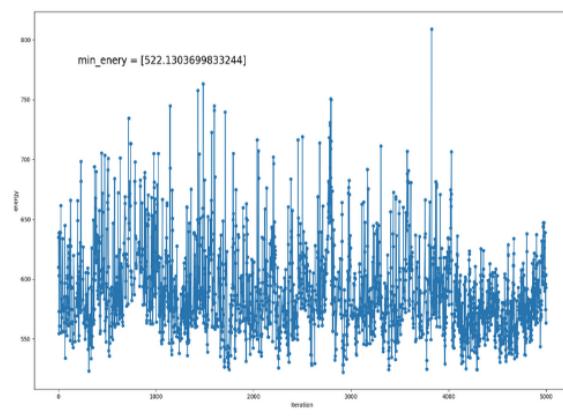
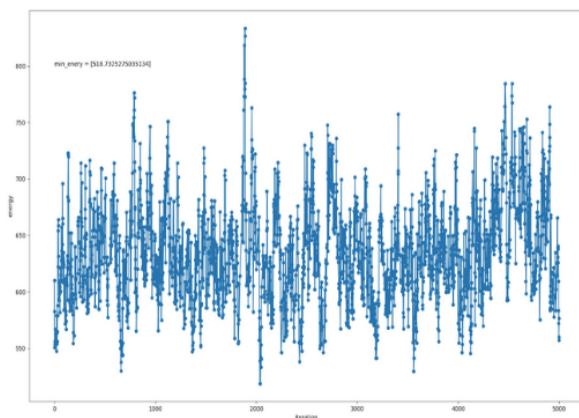
Table for the acceptance ratio



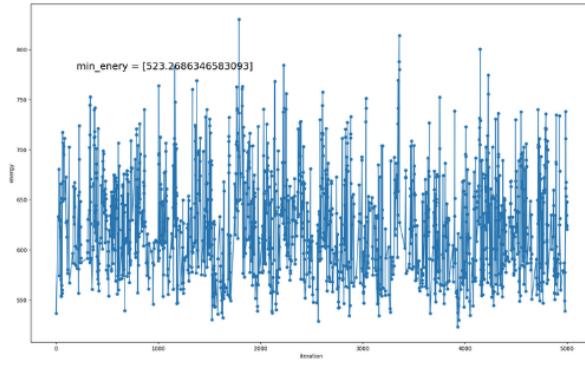
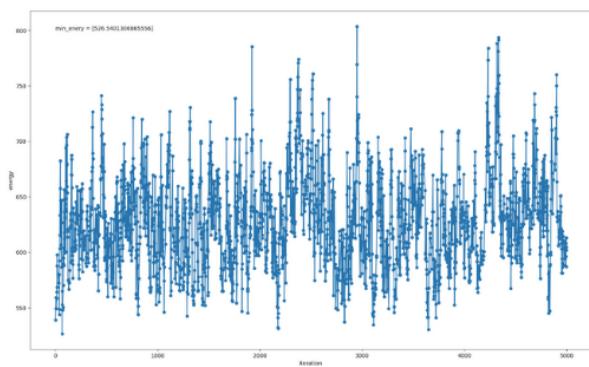
gb\_attr\_AI\_S3\_1\_N1\_1\_0\_0\_N2\_-2\_1\_-2



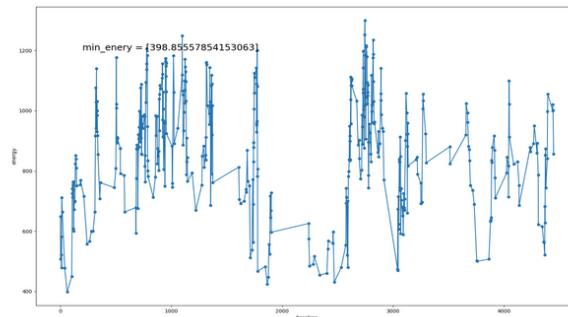
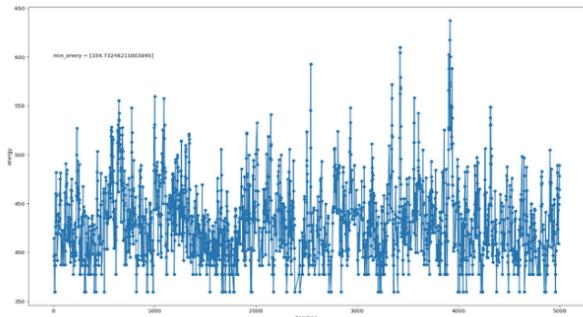
*gb\_attr\_AI\_S3\_1\_N1\_4\_-1\_-3\_N2\_-3\_4\_-1*



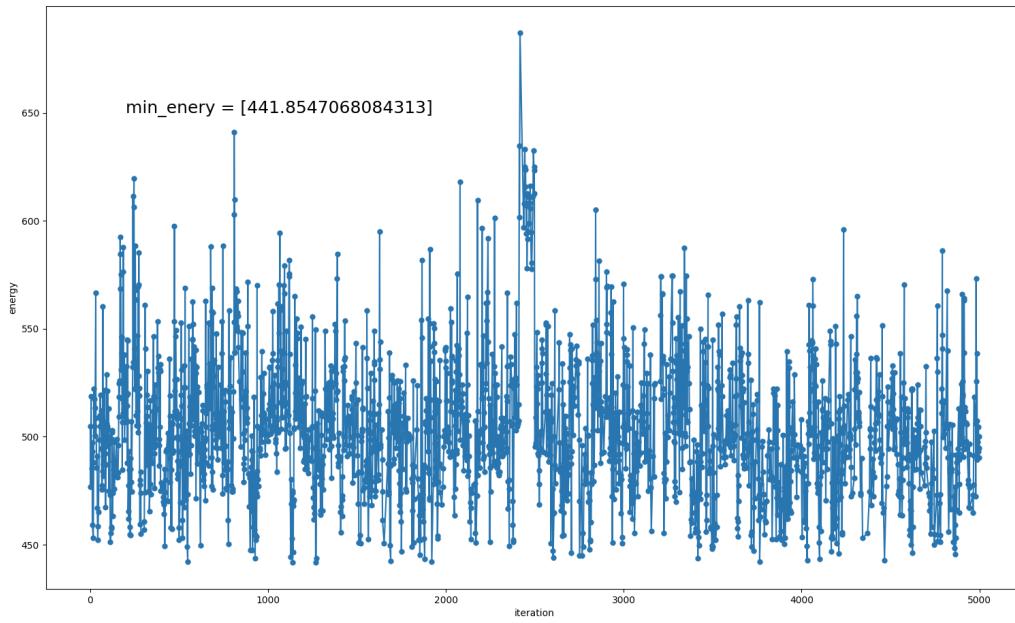
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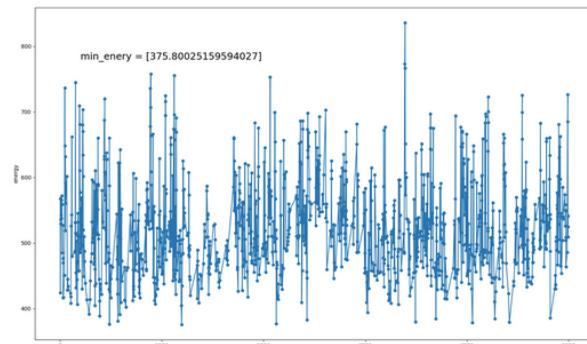
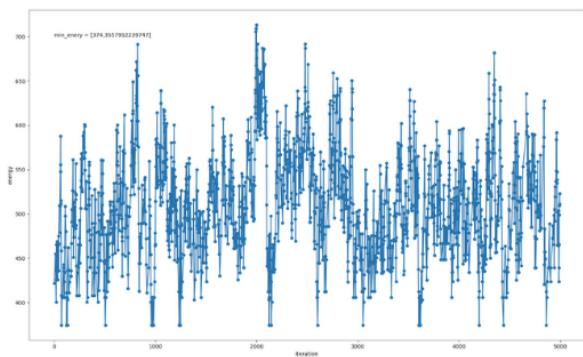
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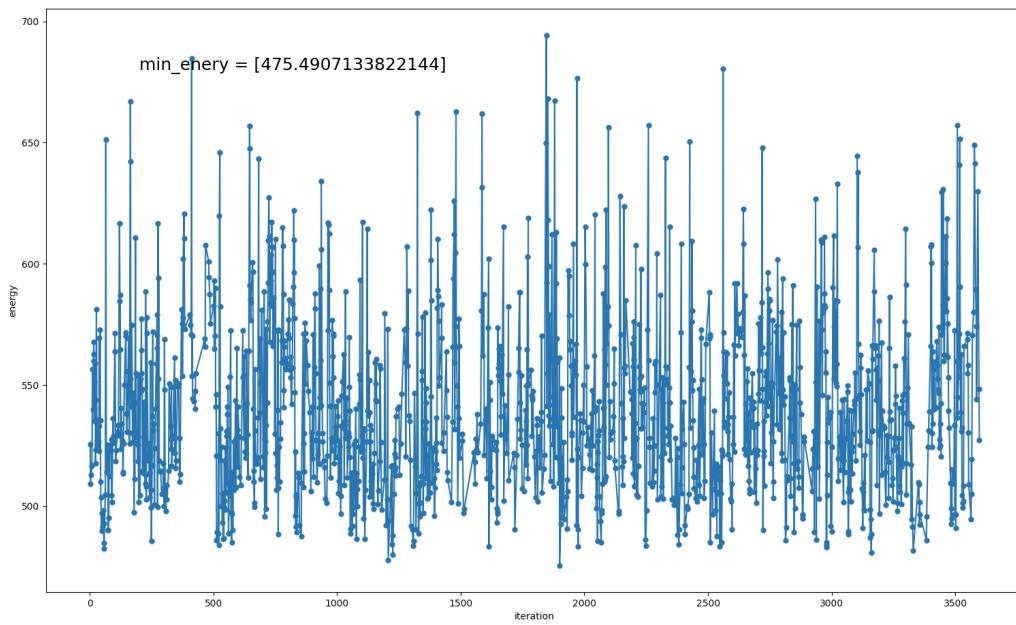
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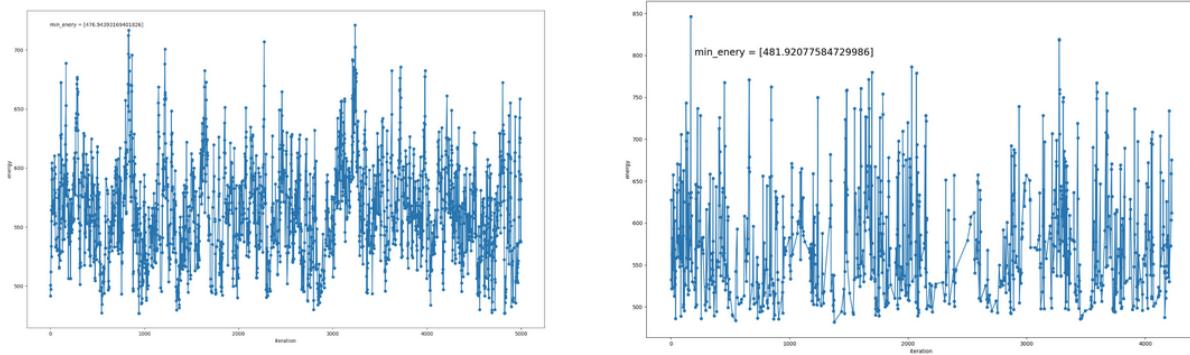
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*gb\_attr\_A1\_S9\_1\_N1\_1\_-1\_1\_N2\_-1\_1\_-5*

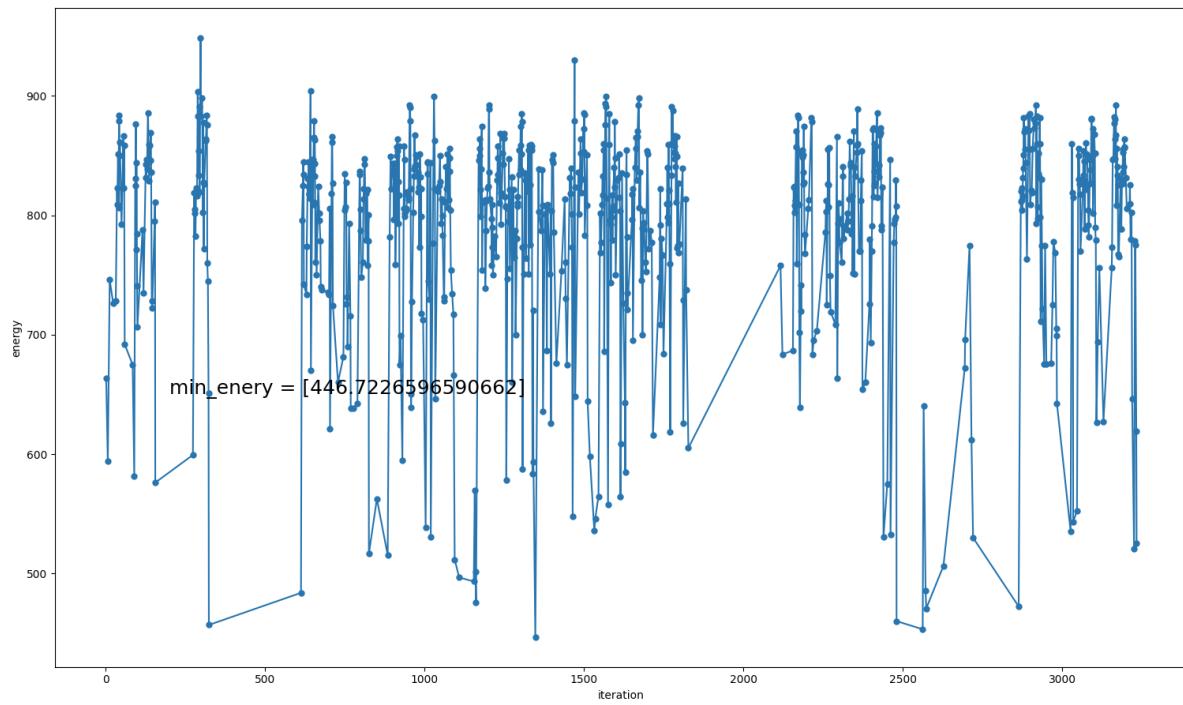


*gb\_attr\_A1\_S9\_1\_N1\_2\_1\_2\_N2\_-1\_-2\_-2*



gb\_attr\_AI\_S11\_1\_N1\_12\_-1\_3\_N2\_-8\_-3\_-9

August 10



AI\_S11\_0\_N1\_5\_-3\_1\_N2\_-3\_1\_-5

