

Theory and Computation Update

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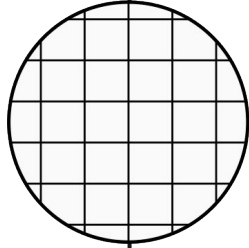


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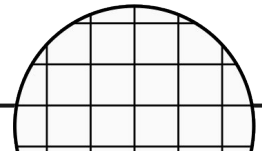
GitHub Updates

02

**Switch Status for
Each Carbon**

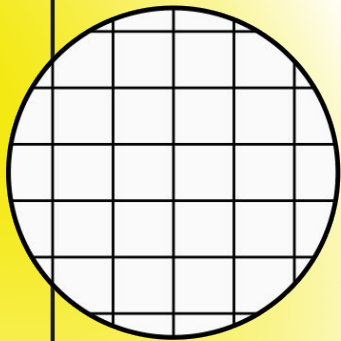
03

**Ethane Radial &
Z Distance
versus Time**

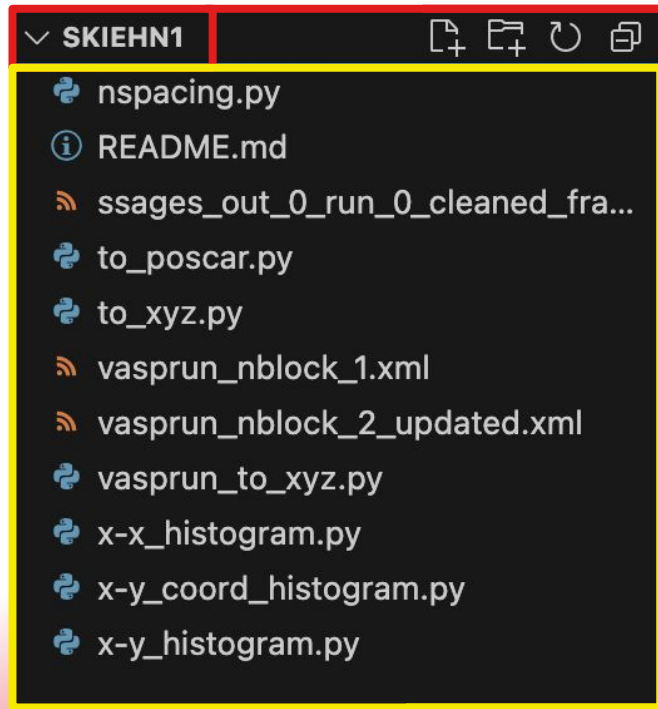


01

GitHub Updates

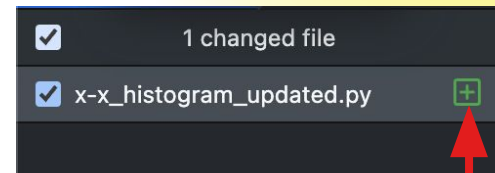


Github Updates



skiehn repository directly
accessible via vscode

content of skiehn
repository directly
pushable from vscode to
github → **realtime updates**

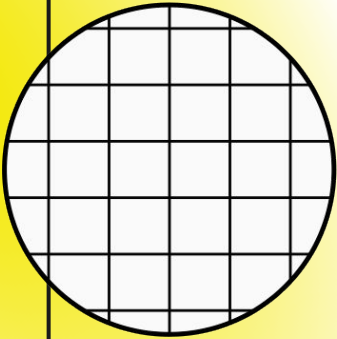


github desktop app
facilitates this
process

+ sign indicating updated
file ready to be pushed

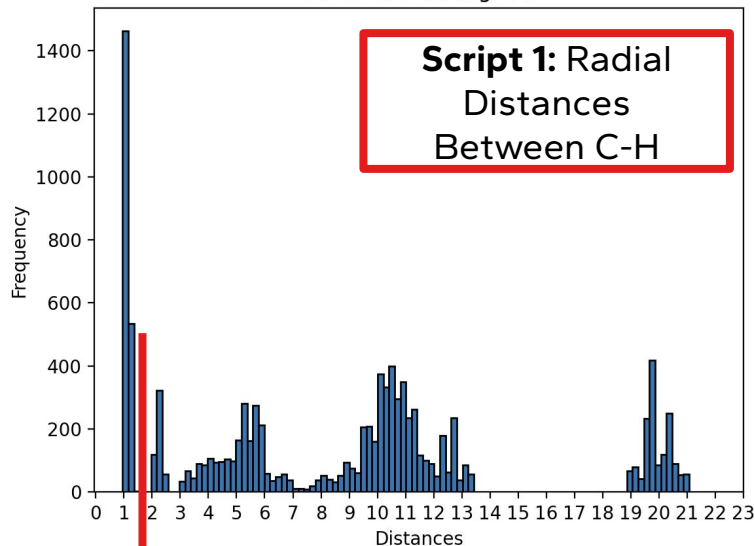
02

Switch Status for Individual Carbons



Distance Histograms

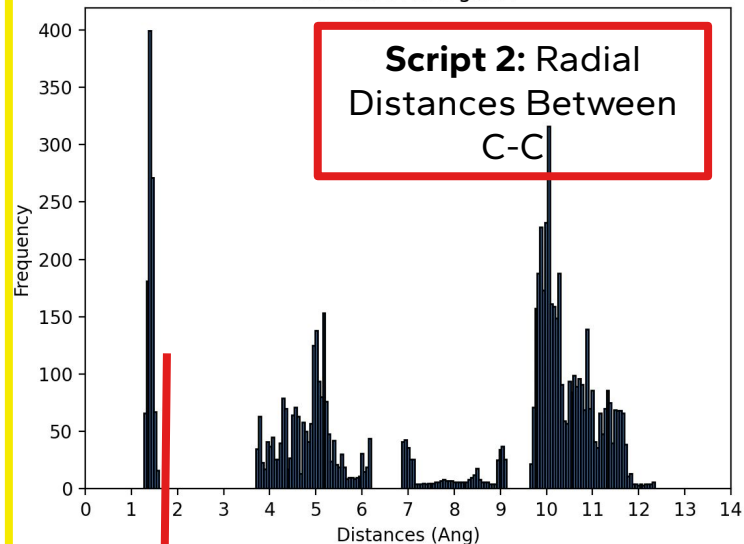
Difference Histogram



**Script 1: Radial
Distances
Between C-H**

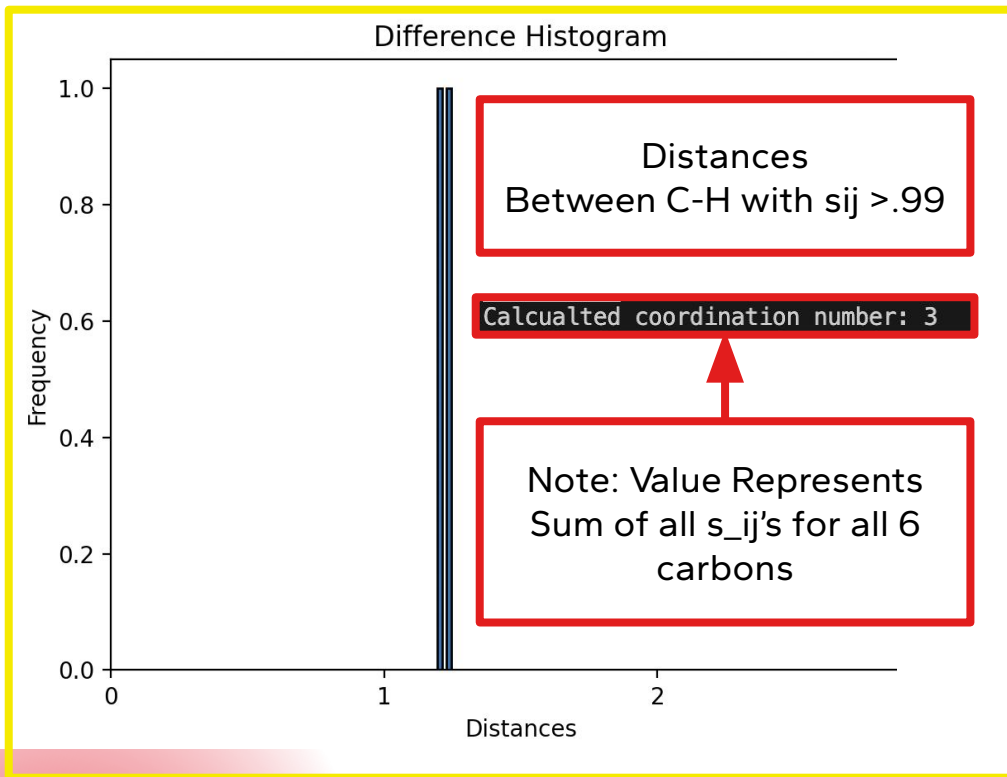
Easily Identifiable Cutoff
Distances: Denote Bond
Length

Distance Histogram



**Script 2: Radial
Distances Between
C-C**

Switch Status for Individual Carbons



Coordination number:
Sum₁ of total bond lengths
 that meets **switching**
criteria₂ for given atom in a
 given iteration

Sum of Bonds

$$\sum_{i \in A} \sum_{j \in B} s_{ij}$$

Switching Criteria

$$s_{ij} = \frac{1 - \left(\frac{r_{ij} - d_0}{r_0} \right)^n}{1 - \left(\frac{r_{ij} - d_0}{r_0} \right)^m}$$

Switch Status for Individual Carbons

```
{ 'C_1': [1.1943361919185764, 2.191329375349721, 4.665030351289955, 3.200335415008365, 10.549649349652714, 10.015768953234396, 9.125304478315154, 8.761160457485756, 5.4864601, 6.172117717444537, 4.035011205526215, 5.516433689709444, 6.240566589343522, 5.965317729585664, 5.6922064892000765, 6.148947582241183, 4.230585130328722, 5.225535338137358, 6.363452221255986, 5.692719547784529, 9.961851390841572, 11.697408193672711, 10.75421412969315, 11.97179614409666, 10.790375333740105, 10.868186358534698], 'C_2': [2.1803519588727855, 1.1402089221244471, 3.622747270928671, 3.7361931258745527, 10.108087868450873, 9.521836349016992, 8.55839801484941, 8.15427295608741, 4.840406, 5.402064892218022, 4.373523137374109, 4.9613612789198385, 6.371370042417722, 6.2108218785015215, 5.194631711230991, 5.587194181840276, 3.025379196308583, 3.0332497614652745, 6.777123884474292, 5.078394270786192, 9.49814081214932, 11.694519977984221, 10.250650776414396, 11.438927196274035, 10.89599176824288, 10.734960138049677], 'C_3': [5.838873458793493, 3.605440674303433, 1.032808868497587, 5.893029524109491, 8.651736525550321, 8.038820175724052, 4.753778895947056, 7.139000637700386, 4.868097, 5.3844352368189226, 3.7007998902411865, 3.8091734312124927, 7.193324277959442, 7.250062435473235, 3.5931820449622034, 3.533052271114177, 3.6322850454714155, 7.231471249927252, 7.123440049009083, 3.480228685342234, 10.351021311684738, 12.455656012437752, 10.50637523790223, 10.97730058766185, 12.311993388846465, 12.319441613207108], 'C_4': [3.674159913623629, 5.363504795333334, 6.155645579645068, 1.2455841677893316, 11.48084430979399, 11.14660793471918375, 10.83899143283892, 8.4399, 9.251137672834057, 7.270803639500807, 6.486597752935449, 6.867715632348923, 6.250027847358067, 5.510764911995945, 5.040163459510187, 7.665293224066315, 5.542424091898415, 3.0894326274140593, 5.305265749902921, 11.5586908001132265, 10.707993607539674, 11.755653461502749, 12.25340119930109, 11.12601139584888, 11.975287407702616], 'C_5': [10.0274666683949987, 10.93951906101135, 11.748232481762829, 10.112830053144771, 19.827600029645875, 19.242380418073008, 18.285483616193222, 17.8758284362568, 7.4487666094, 4.711805355575688, 1.936055972795744, 14.332571861149466, 16.0135382579945, 15.655883463645414, 13.358485121360784, 13.303051907250444, 10.8664905410341, 9.775959491330807, 10.222339727038523, 10.731558065960092, 4.046465396037498, 5.1947023584823935, 4.506957300327614, 6.286222760543716, 1.060696864672026, 2.045808966744297], 'C_6': [10.976798519072216, 10.783191273282322, 11.456203743981227, 10.371512947749125, 19.590309578452026, 18.00728667266238, 17.899630813764688, 17.48886989882507, 7.7737051987, 14.225290384241454, 13.75493477188507, 14.163674979526856, 16.009191949095473, 15.70703987813303, 13.28935895348413, 13.220865200366108, 10.340115573360272, 9.742591035708042, 10.61463666359423, 10.657521630667086, 2.805774661232448, 5.855350521936346, 3.6234169704011157, 5.841322493708271, 2.135138663740331, 1.1261630023627181}]
```

Distances Between Each Carbon-Hydrogen Grouped by Carbon

```
{ 'C_1': [0.9991850892235272, 0.9815736713344207, 0.000993800381646056, 0.039735903141175206, 1.8205755201935582e-06, 2.622138591875928e-06, 5.086917008929537e-06, 6.8299827e-06, 0.0002576362911781607, 0.613368455132861e-05, 0.0006083685568178983, 0.00023815129766168055, 8.10087635122924e-05, 0.00012613366592528485, 0.0001814891335689516, 9.904420875389292e-05, 0.002406684743627284, 0.8433565351891414, 5.4448685744769e-05, 0.0001840539656782104, 2.7239959261823174e-06, 8.89325901196671e-07, 1.5920695755329311e-06, 7.583550719684637e-07, 1.5552484055374376e-06, 1.4793339659235207e-06], 'C_2': [0.9097733093049468, 0.997835486117003, 0.010811582712368584, 0.0079368543802494, 2.457869292313574e-06, 3.7528014107447356e-06, 8.086481989741649e-06, 1.978762e-05, 0.010005423229728218, 0.00028321096279455274, 0.001771319879959576, 0.0005811201879541304, 7.4827240724395608e-05, 9.149137692516177e-05, 0.00039300888054630956, 0.00021446440432689479, 0.0735456688778306, 0.0714691936735985, 4.6301616428412976e-05, 0.0004760625958780177, 3.82006811854467e-06, 9.90838921613663e-07, 2.22718821214796235e-06, 1.03743881625898519, 2.928243e-05, 1.6120894972498367e-06], 'C_3': [0.0001498551605383, 0.011349706930352777, 0.989788589969571, 0.00013910887852888203, 7.47356327596116e-06, 1.79337564720072e-05, 1.671620175112647e-05, 2.2497475e-05, 0.000684316509156242, 0.00021009310890099, 0.00722912390701572, 0.006552478712535849, 2.936211622659813, 2.766639812130589e-05, 0.011749651179961156, 0.01363735665539890, 0.010527665791266362, 2.8209217490244457e-05, 3.162087255864583e-05, 0.016227172634049276, 0.79882390756895e-05, 5.783216121252672e-07, 1.8736952794741628e-06, 1.3799530566690278e-06, 4.774719295386928e-07, 6.156832941071183e-07], 'C_4': [0.009379044706383956, 0.0003005942717333058, 9.819126351307496e-05, 0.9997288890586602, 1.0115698436740849e-06, 1.240792828128573e-06, 1.1240144655757783e-06, 2.511516721e-06, 7.74246291848857e-06, 6.411107986746368e-06, 8.480352745576392e-05, 5.503478860015928e-05, 4.180659944348859e-05, 7.0533036859788e-05, 0.00024019911941967794, 0.000149588036587397, 1.8208311389159427e-05, 0.000229127134088981, 0.005619355082330803, 0.0003292658445244341, 9.654921743566776e-07, 1.6406246512001814e-06, 8.58990573206608e-07, 6.46699931479791e-07, 1.2569593278423232e-06, 7.568398426642696e-07], 'C_5': [1.4243914020880446e-06, 1.4135142123911033e-06, 8.63188035631802e-07, 2.449760731414079e-06, 6.2855546953865744e-08, 3.20574272938957e-08, 4.47091928786057, 1853765473592926e-08, 2.6330777329026704e-07, 1.8802990113704057e-07, 2.703359941931428e-07, 2.2393278072955236e-07, 1.070150666376208e-07, 1.2427336949194073e-07, 3.596044289800756e-07, 3.69857080367941e-07, 1.4809417052209785e-06, 3.1123505814436943e-06, 2.270915766573822e-06, 1.6156573624260001e-06, 0.0036541254529015593, 0.0003929638115412984, 0.0013509812232506916, 8.317760835645516e-05, 0.9933706938890685, 0.9744398880379996], 'C_6': [1.3804780826587058e-06, 1.64576793252486814e-06, 1.0266842541680252e-06, 2.051223412224133e-06, 2.8531459866133292e-08, 3.5102940189330605e-08, 5.14083837435, 5.962990719494934e-08, 3.2583773824403883e-07, 2.3197931002435535e-07, 2.9521189167551194e-07, 2.42460703657798e-07, 1.0718664520837168e-07, 1.2161253746920006e-07, 7.2444203627701285e-07, 3.0569304286531507e-07, 2.095325182686691e-06, 3.188717906411642e-06, 1.7440666440903912e-06, 1.6956317680485104e-06, 0.1678278815364046, 0.00014648655234709716, 0.010791360406243981, 0.00014934918014376163, 0.9383975251983898, 0.9972778637437455]} 
```

S_{ij} values for Each Distance Grouped by Carbon

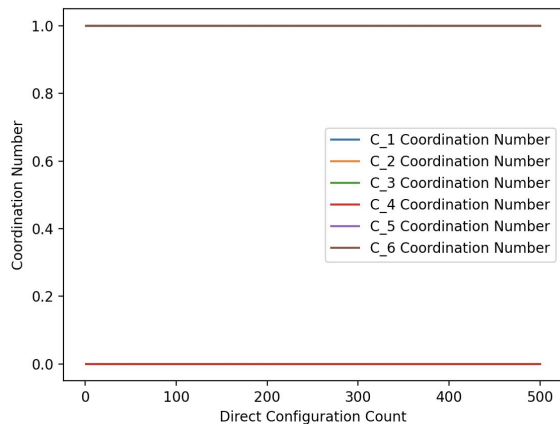
S_{ij} values > .99 for Each Distance Grouped by Carbon



```
{ 'C_1': [0.9991850892235272], 'C_2': [0.997835486117003], 'C_3': [], 'C_4': [0.9997288890586602], 'C_5': [0.9933706938890685], 'C_6': [0.9972778637437455]}
```

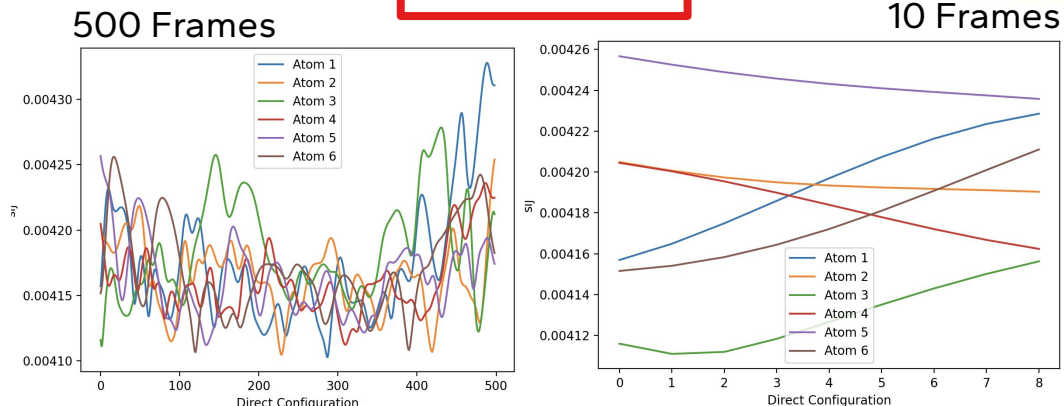

Switch Status for Individual Carbons

1st Iteration



Shows: Only C_6 is bonded:
Incorrect Logic

2nd Iteration



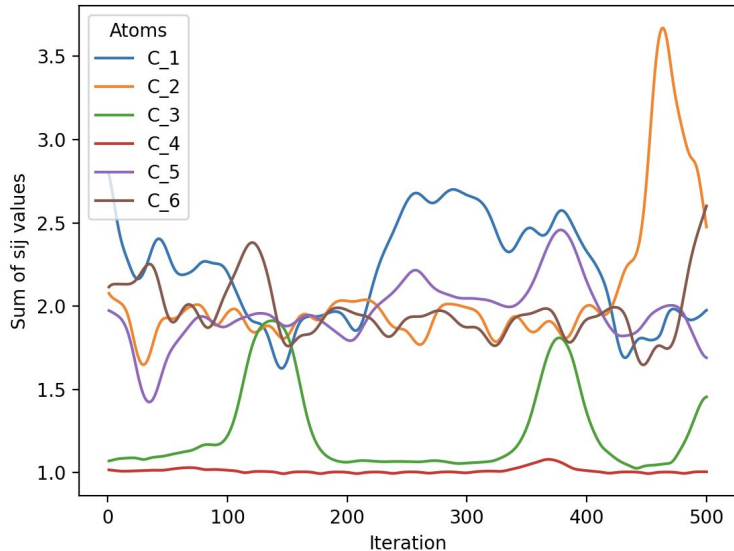
Shows: Atoms never bond as s_{ij} Never Peaks:
Incorrect Logic

Switch Status for Individual Carbons

```
{'C_1': [2.78921330029383], 'C_2': [2.0763401186985444], 'C_3': [1.070259226678582], 'C_4': [1.0163945100792626], 'C_5': [1.9733085221062097], 'C_6': [2.1146524582017445]}
```

3rd Iteration

Coordination Number as a Function of Iteration Between C and H



Sum of s_{ij} Values for Each Carbon (first frame)

Parameters:

$$d_0 = 1.5\text{\AA}$$

$$r_0 = 1\text{\AA}$$

$$n = 6$$

$$m = 12$$

Values are reasonable
and in expected
range

$$s_{ij} = \frac{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^n}{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^m}$$

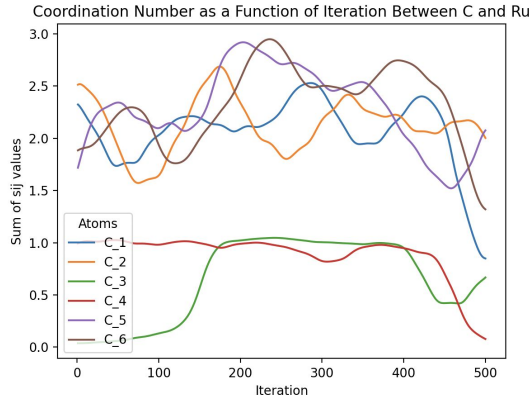
Switch Status for Individual Carbons

Code is completely generalizable: Will work on any XDATCAR file

Select which atoms to find CN
between in arguments

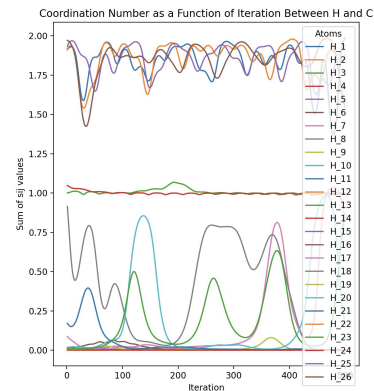
First noninput argument
defines "principle" atom:
corresponding to reference
atomtype.

Ex 1: Carbon and Ruthenium



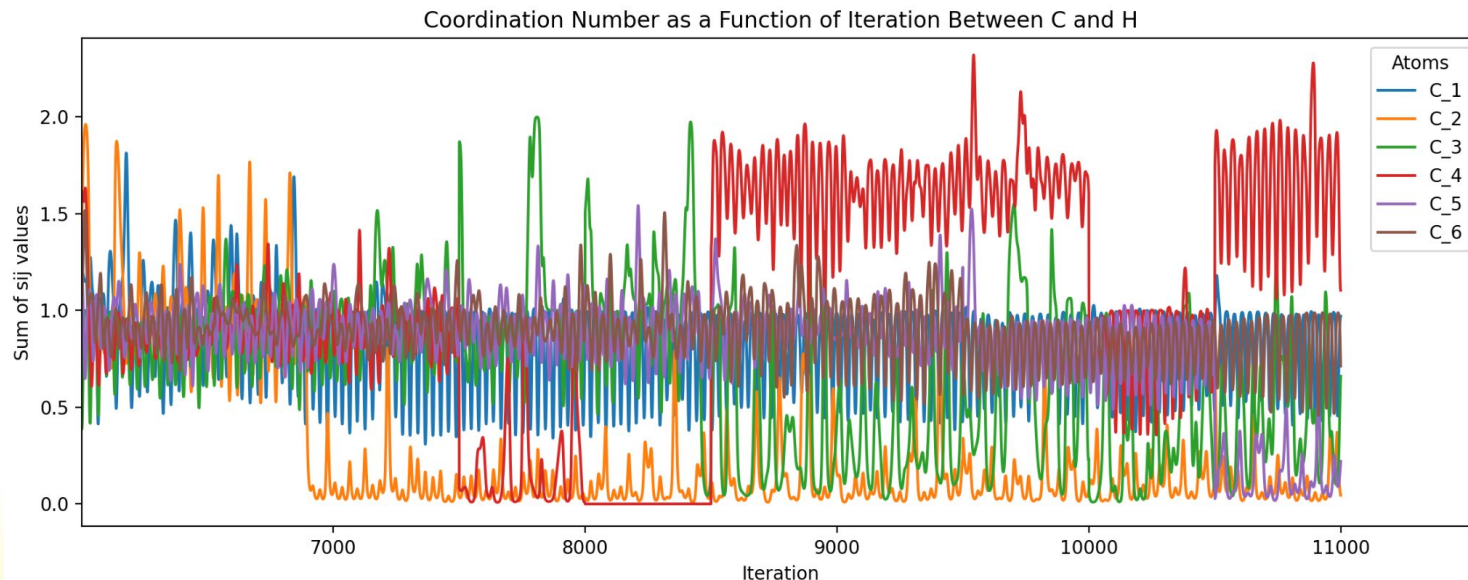
```
parser("XDATCAR_first500", "C", "Ru")
```

Ex 2: Hydrogen and Carbon



```
parser("XDATCAR_first500", "H", "C")
```

Switch Status for Individual Carbons



$d_0 = 1.5\text{\AA}$

$r_0 = .5\text{\AA}$

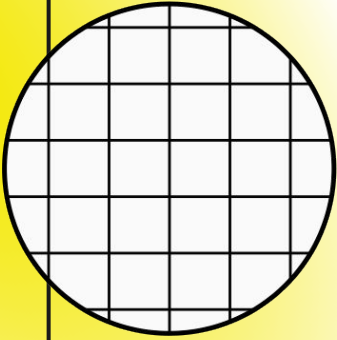
$n = 6$

$m = 12$

XDATCAR_system 2

03

Ethane Radial & Z Distances v. Time



Ethane Z and R Distances: Ethane Isolation

```
{'C_1': [0.991169210879772], 'C_2': [0.991169210879772], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0161513465661207], 'C_2': [1.0161513465661207], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0386738532847584], 'C_2': [1.0386738532847584], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.057902022687999], 'C_2': [1.057902022687999], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0729156004320155], 'C_2': [1.0729156004320155], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0827651871783008], 'C_2': [1.0827651871783008], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0865585845267633], 'C_2': [1.0865585845267633], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0835669921718207], 'C_2': [1.0835669921718207], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0733359553451942], 'C_2': [1.0733359553451942], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0557698130750182], 'C_2': [1.0557698130750182], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0311550337503865], 'C_2': [1.0311550337503865], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}  
{'C_1': [1.0001262284667571], 'C_2': [1.0001262284667571], 'C_3': [], 'C_4': [], 'C_5': [], 'C_6': []}
```

```
Iteration 1:  
Ethane Lists: [['C_1', 'C_2'], ['C_5', 'C_6']]  
Iteration 2:  
Ethane Lists: [['C_1', 'C_2'], ['C_5', 'C_6']]  
Iteration 3:  
Ethane Lists: [['C_1', 'C_2']]  
Iteration 4:  
Ethane Lists: [['C_1', 'C_2']]  
Iteration 5:  
Ethane Lists: [['C_1', 'C_2']]  
Iteration 6:
```

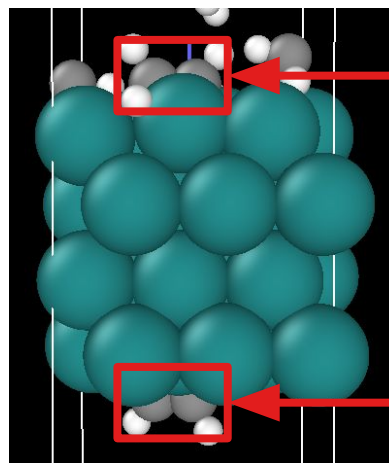
First 5 iterations with $s_{ij} > .5$
bonding condition

Same s_{ij}
values
between
carbons =
ethane
→ Easy to
isolate.

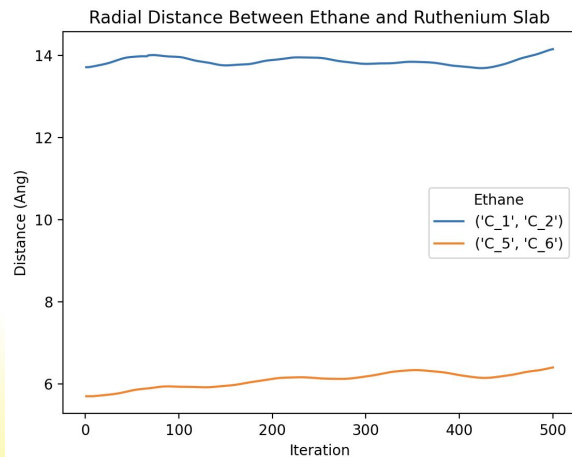
Bonded Carbons
Visible Via s_{ij} values
calculated for each
other: In this case C_1
and C_2.

C_1 and C_2 pair

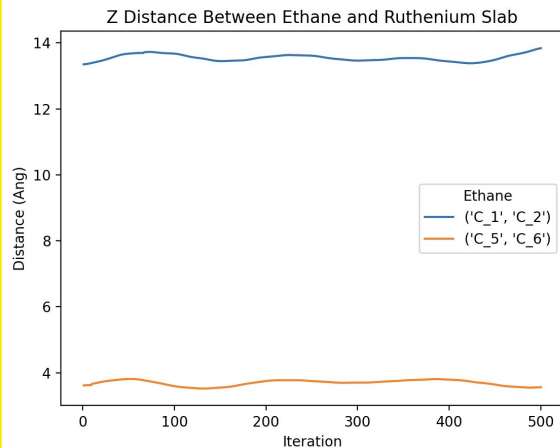
C_5 and C_6 pair



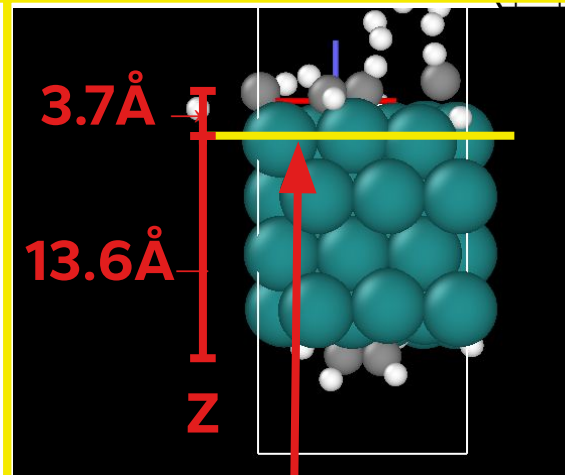
Ethane Z and R Distances: Graphs



Radial Distance Between Ethane and Ruthenium Slab for n Detected Ethanes with $s_{ij} > .3$ bonding condition



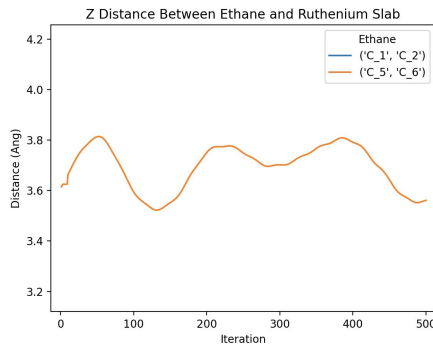
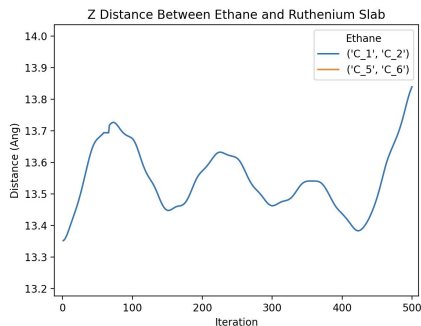
Z Distance Between Ethane and Ruthenium Slab for n Detected Ethanes with $s_{ij} > .3$ bonding condition



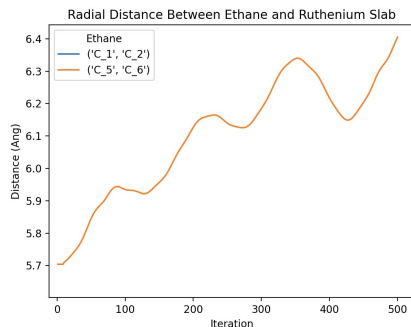
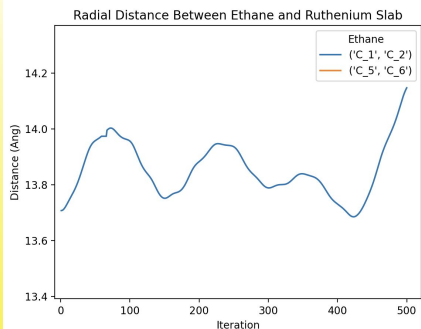
Reference Z Plane for Z Dist. Calculation

Note: Ethane Positions = Average of Component Carbons Positions

Ethane Z and R Distances: Graphs



Z Distances
Plotted
Separately



Radial
Distances
Plotted
Separately

Higher Fidelity
Graphs

Ethane Z and R Distances: Graphs

Notes/Caveats

- 1 Script Will Work on Any Carbon, Hydrogen, Ruthenium System in XDATCAR Format with "C, H, Ru" order in line 6. This means amount of atoms doesn't matter.
- 2 Does Not Work for Non Carbon atoms. Only Ethanes. Cannot find H₂
- 3 Need to Define Slab Size → Inspect System with OVITO
- 4 Ethanes need to be defined for all iterations



Thanks!