Theory and Computation Update

Scott Kiehn

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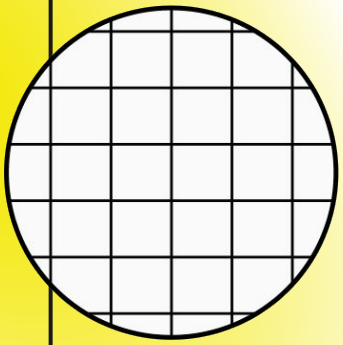
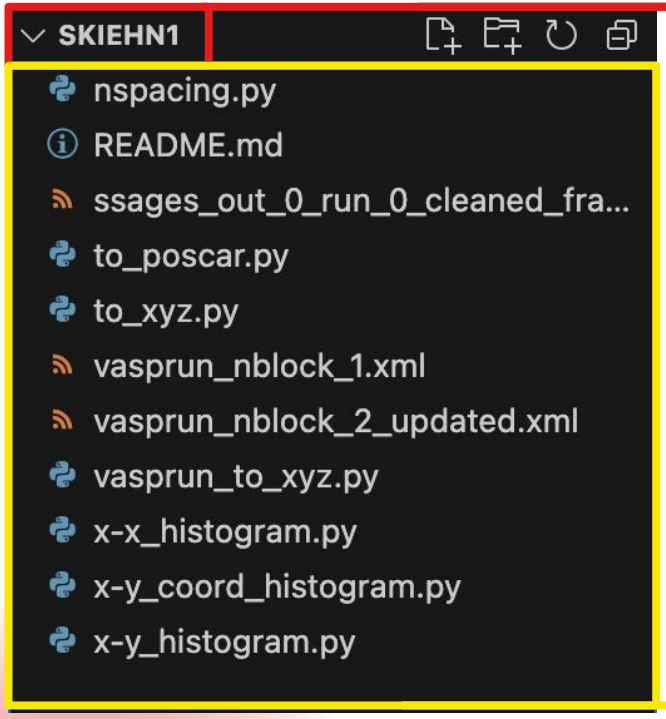
GitHub Updates

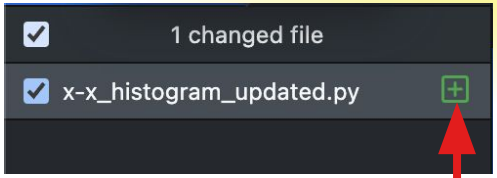


Github Updates



skiehn repository directly accessible via vscode

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

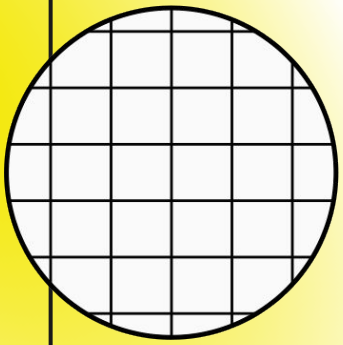


github desktop app facilitates this process

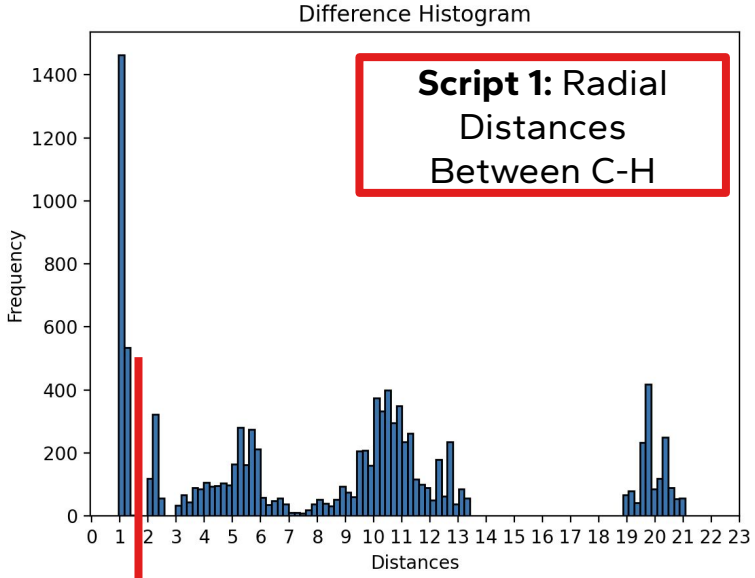
\+ sign indicating updated file ready to be pushed

02

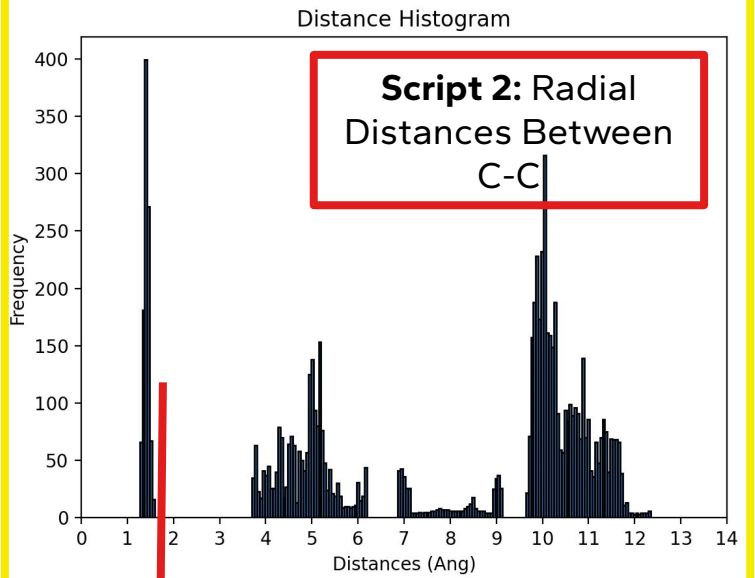
Switch Status for Individual Carbons



Distance Histograms



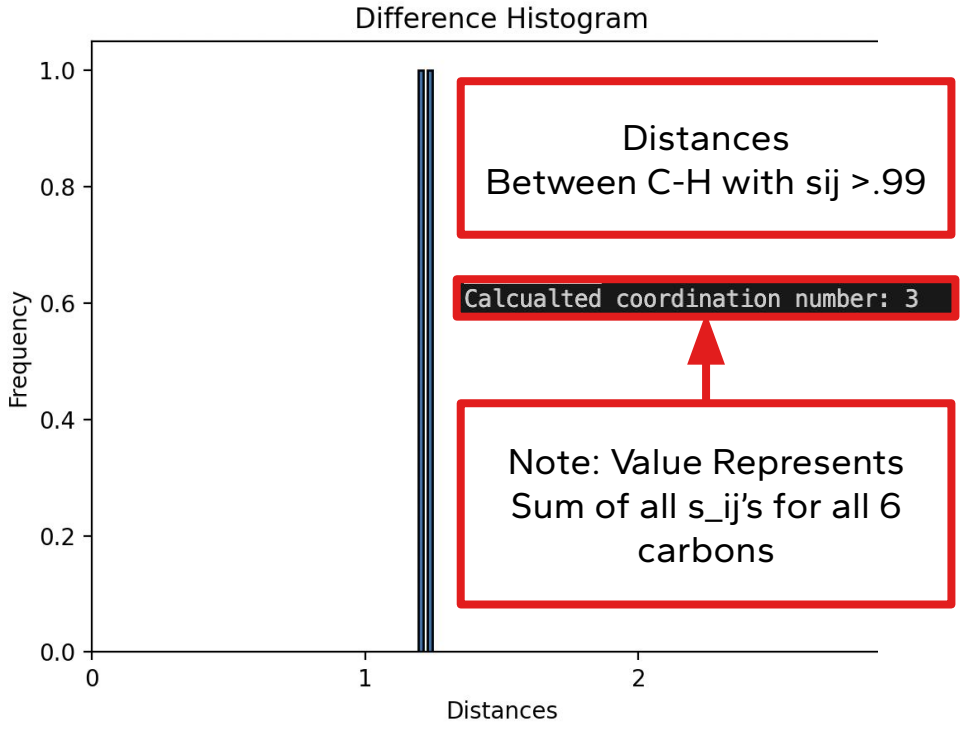
Script 1: Radial Distances Between C-H



Script 2: Radial Distances Between C-C

Easily Identifiable Cutoff Distances: Denote Bond Length

Switch Status for Individual Carbons



Distances
Between C-H with sij >.99

```
Calcualted coordination number: 3
```

Note: Value Represents Sum of all s_ij's for all 6 carbons

Coordination number:
Sum$_1$ of total bond lengths that meets **switching criteria$_2$** for given atom in a given iteration

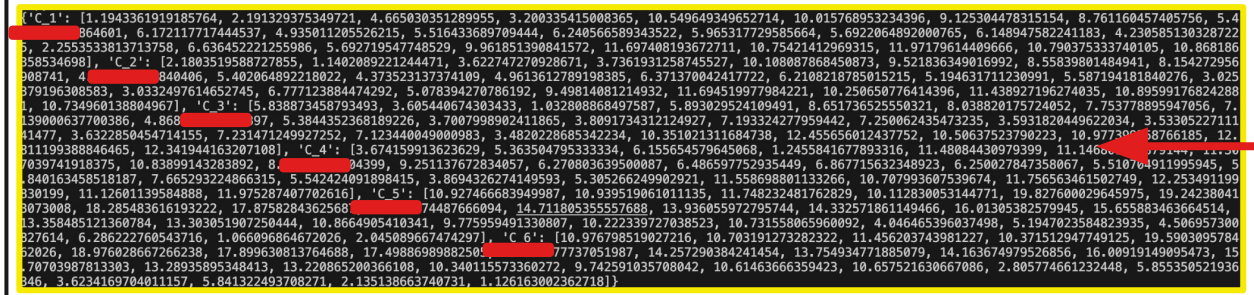
Sum of Bonds

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

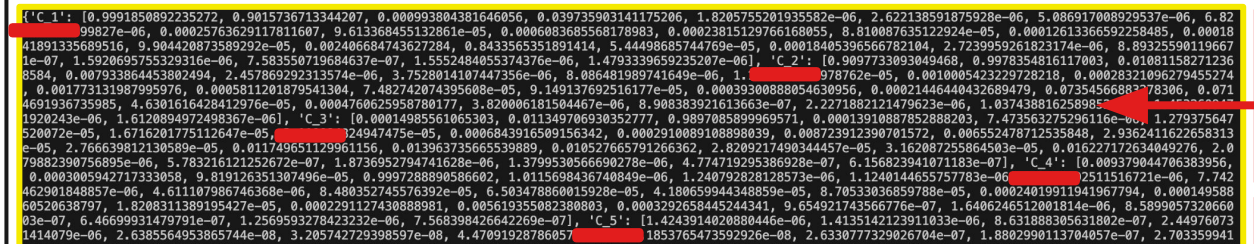
Switching Criteria

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

Switch Status for Individual Carbons



Distances Between Each Carbon-Hydrogen Grouped by Carbon



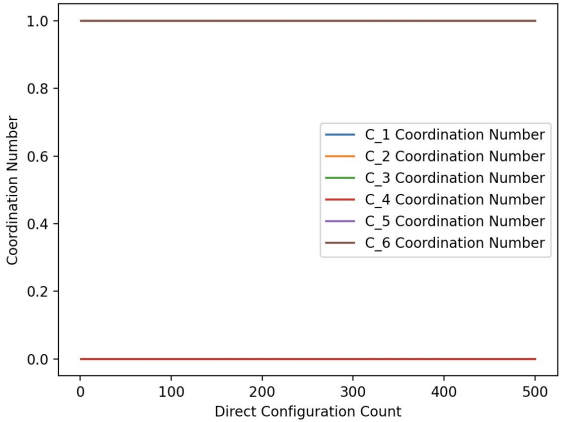
S_ij values for Each Distance Grouped by Carbon

S_ij values > .99 for Each Distance Grouped by Carbon

{'C_1': [0.9991850892235272], 'C_2': [0.9978354816117003], 'C_3': [], 'C_4': [0.9997288890586602], 'C_5': [0.9933706938890685], 'C_6': [0.9972778637437455]}

Switch Status for Individual Carbons

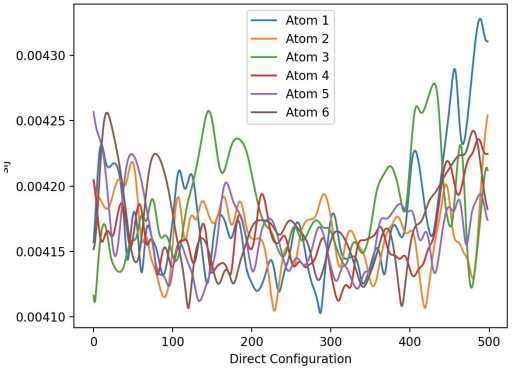
1st Iteration



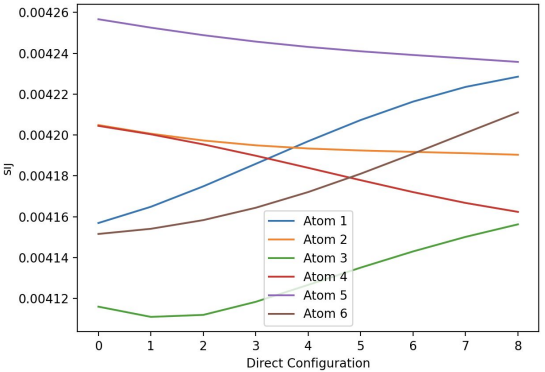
Shows: Only C_6 is bonded: Incorrect Logic

2nd Iteration

500 Frames



10 Frames



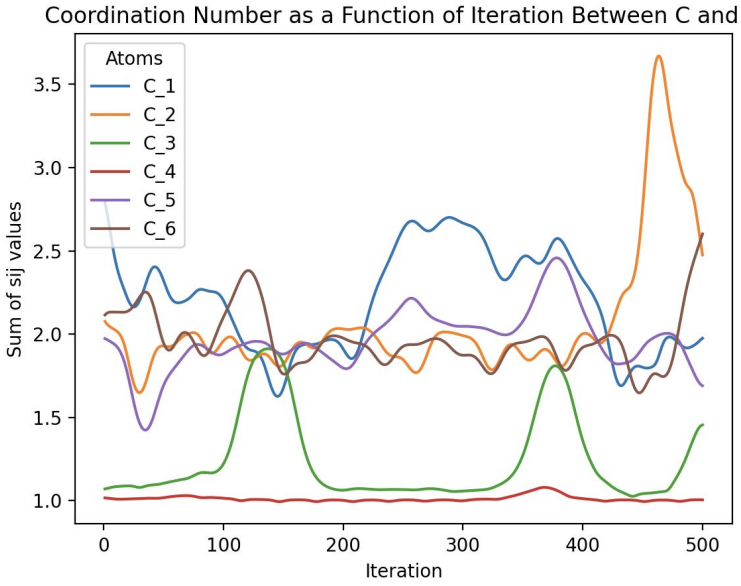
Shows: Atoms never bond as s_ij Never Peaks: Incorrect Logic

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]}

Sum of s_ij Values for Each Carbon (first frame)

3rd Iteration



Parameters:

d_0 = 1.5Å	r_0 = 1Å	n = 6	m = 12

Values are reasonable and in expected range

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

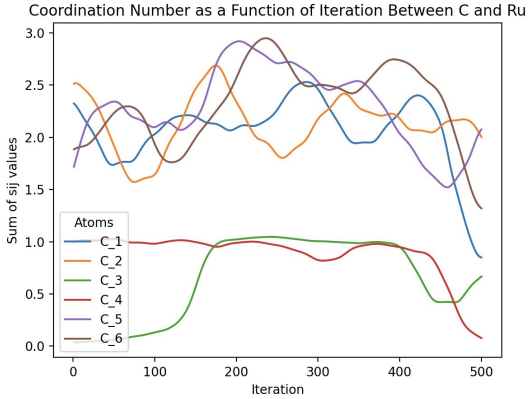
Switch Status for Individual Carbons

Code is completely generalizable: Will work on any XDATCAR file

Select which atoms to find CN between in arguments

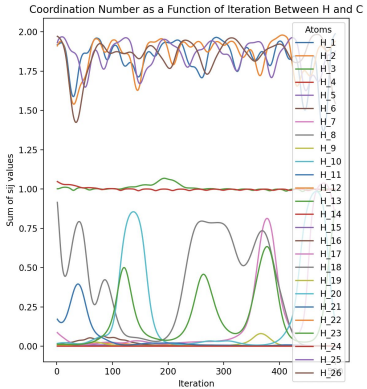
First noninput argument defines “principle” atom: corresponding to reference atomtype.

Ex 1: Carbon and Ruthenium



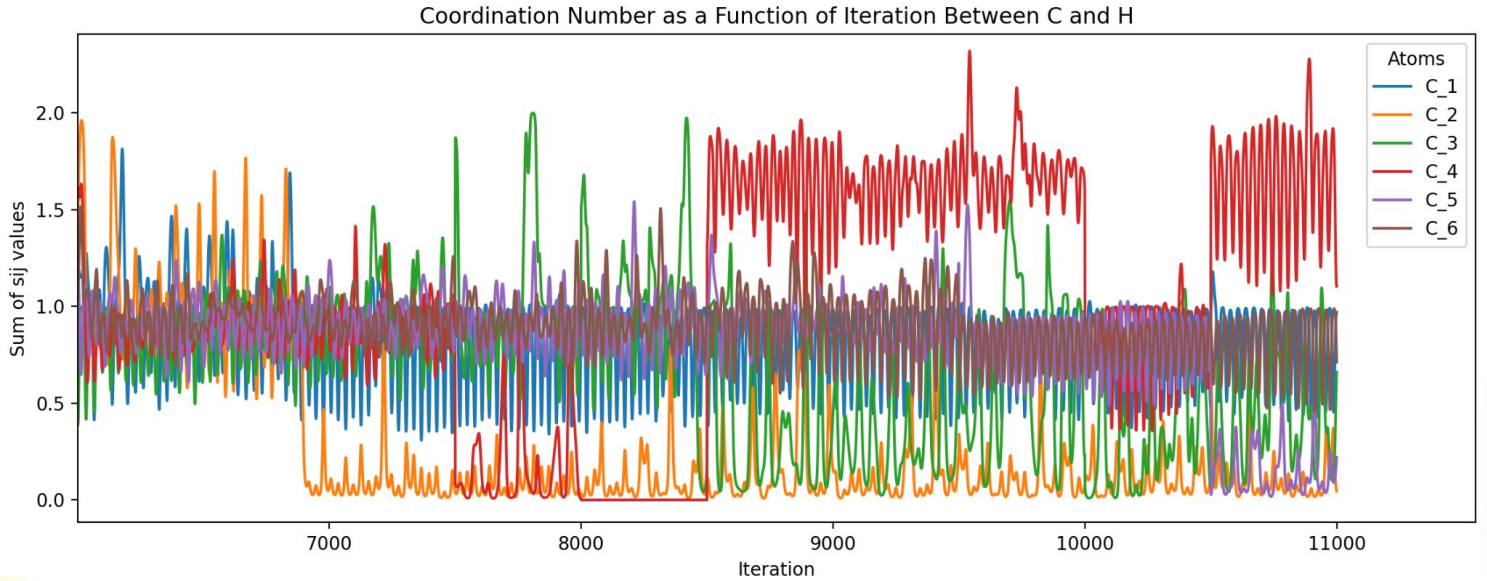

```
parser("XDATCAR_first500", "C", "Ru")
```

Ex 2: Hydrogen and Carbon




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

Switch Status for Individual Carbons



d_0 = 1.5Å	r_0 = .5Å	n = 6	m = 12

XDATCAR_system 2

03

Ethane Radial & Z Distances v. Time

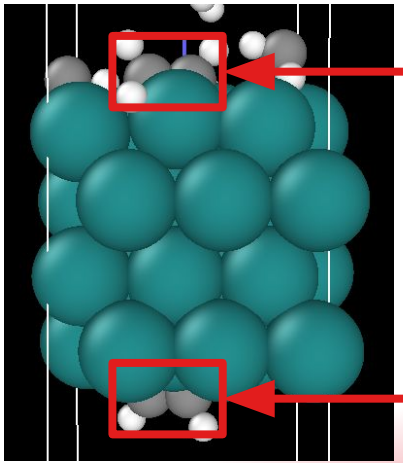
Ethane Z and R Distances: Ethane Isolation

```
{'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']]
```

First 5 iterations with s_ij > .5 bonding condition

Same s_ij values between carbons = ethane → Easy to isolate.

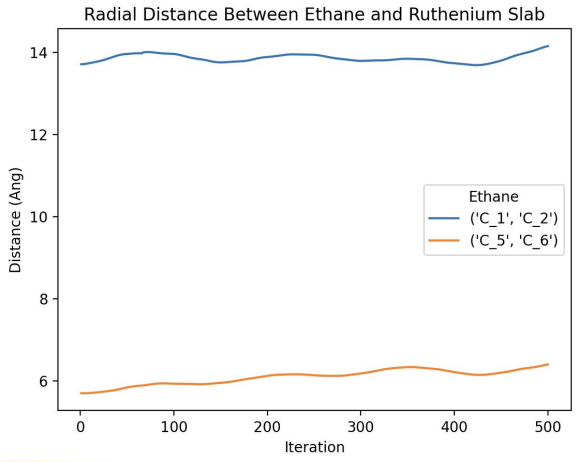


Bonded Carbons Visible Via s_ij values calculated for each other: In this case C_1 and C_2.

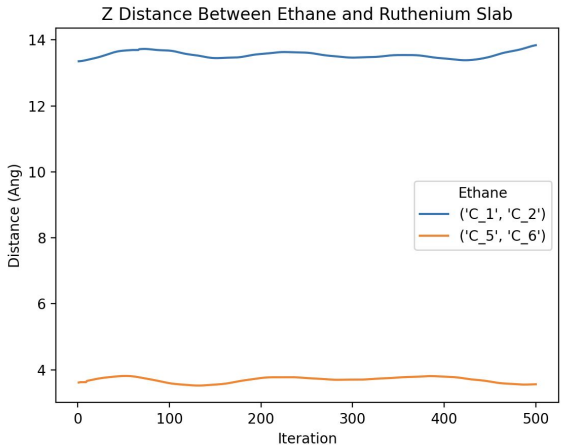
C_1 and C_2 pair

C_5 and C_6 pair

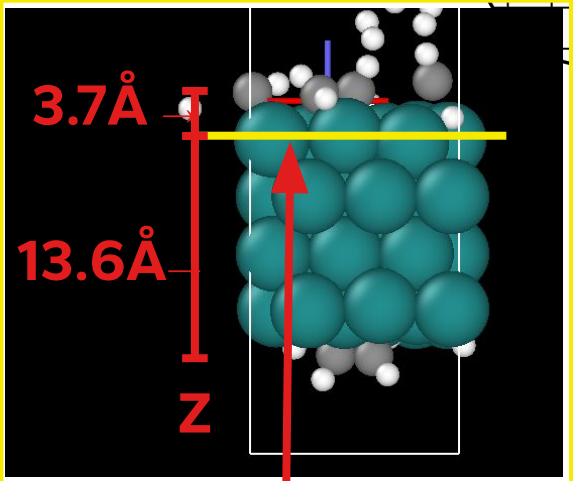
Ethane Z and R Distances: Graphs



Radial Distance Between Ethane and Ruthenium Slab for n Detected Ethanes with s_ij > .3 bonding condition



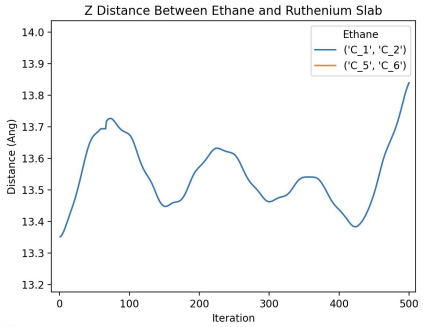
Z Distance Between Ethane and Ruthenium Slab for n Detected Ethanes with s_ij > .3 bonding condition

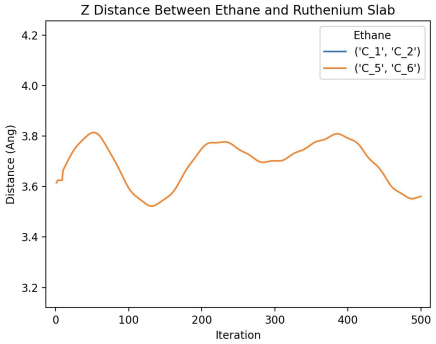


Reference Z Plane for Z Dist. Calculation

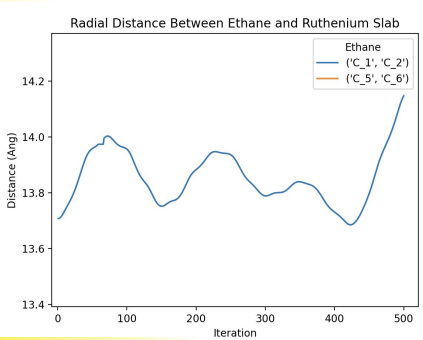
Note: Ethane Positions = Average of Component Carbons Positions

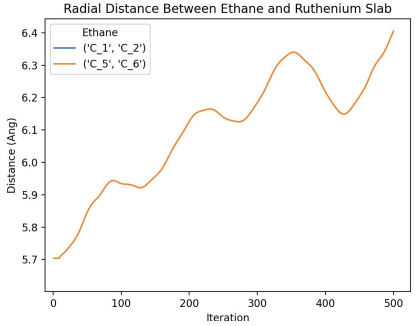
Ethane Z and R Distances: Graphs





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 H_2
3	Need to Define Slab Size → Inspect System with OVITO
4	Ethanes need to be defined for all iterations

Thanks!