

xsf2bonds_ase2

September 9, 2024

```
[1]: import numpy as np
import ase.io
import sys
from ase.geometry.analysis import Analysis
from ase.neighborlist import NeighborList
from ase import Atoms
```

```
[2]: np.set_printoptions(legacy='1.25')
```

```
[105]: def printbonds(A,B,d):
        i = ase.neighborlist.neighbor_list('i', crys,
            {(A, B): d})
        if(len(i)>6):
            coord = int(len(i)/2)
        else:
            coord = int(len(i))
        print("There are {} {}-{} neighbors up to d= {}".format(coord,A,B,d))
        dists = ase.neighborlist.neighbor_list('d', crys,
            {(A, B): d})
        print(dists, "Average:", np.average(dists), "Min:",min(dists))
```

```
[101]: filename='P4mm_80GPa_findsym.cif'
#filename=sys.argv[1]
print(filename)
crys = ase.io.read(filename)
ana = Analysis(crys,cutoffs=[10.]*len(crys))
```

P4mm_80GPa_findsym.cif

```
[102]: printbonds('Pb','O',4)
```

```
There are 12 Pb-O neighbors up to d= 4
[2.64050155 2.64050155 2.64050155 2.5465001 2.5465001 2.47548341
 2.47548341 2.5465001 2.47548341 2.47548341 2.5465001 2.64050155
 2.47548341 2.47548341 2.64050155 2.64050155 2.64050155 2.47548341
 2.47548341 2.64050155 2.5465001 2.5465001 2.5465001 2.5465001 ] Average:
2.554161686475258 Min: 2.4754834051530206
```

```
[103]: printbonds('Ti','O',3)
```

There are 6 Ti-O neighbors up to d= 3
[1.875109 1.80792976 1.80792976 1.80792976 1.80792976 1.754975
1.80792976 1.80792976 1.80792976 1.80792976 1.875109 1.754975] Average:
1.810300503592381 Min: 1.754975000052

```
[106]: printbonds('Pb', 'Pb', 5)
```

There are 6 Pb-Pb neighbors up to d= 5
[3.630084 3.630084 3.601241 3.601241 3.601241 3.601241] Average:
3.6108553333333333 Min: 3.601241

```
[108]: printbonds('Ti', 'Ti', 5)
```

There are 6 Ti-Ti neighbors up to d= 5
[3.601241 3.601241 3.601241 3.601241 3.630084 3.630084] Average:
3.6108553333333333 Min: 3.601241

```
[109]: printbonds('Pb', 'Ti', 4)
```

There are 8 Pb-Ti neighbors up to d= 4
[3.10057088 3.10057088 3.15410949 3.15410949 3.15410949 3.15410949
3.10057088 3.10057088 3.10057088 3.10057088 3.15410949 3.15410949
3.15410949 3.15410949 3.10057088 3.10057088] Average: 3.1273401870375452 Min:
3.1005708830758776