LAMMPS Post Processing Documentation

# Magnolia

Magnoli is a python package to post process the LAMMPS output data. In this document all the modules in the magnolia will be briefly discussed. There are the following modules currently in the package.

1. bondfile\_parser
2. dumpfile\_parser
3. logfile\_parser

# Bond File Parser

The following are the functions in the bond file parser module.

1. parsebondfile
2. get\_molecules
3. get\_molecular\_weight
4. get\_molecular\_formula
5. get\_SpeciesCountAtEveryTimestep
6. stepwise\_species\_count
7. expression\_selector
8. pathway\_tracker
9. step2picosecond
10. get\_nearestindex
11. sort\_molecular\_formula
12. make\_molecular\_formula\_latex
13. compute\_molecular\_weight
14. plot\_species\_heatmap
15. atomic\_weight
16. get\_speciesVStemp
17. get\_onset
18. bondorder\_evolution
19. get\_nbondsVStime
20. species\_to\_molecule
21. cumulative\_nspecies

## parsebondfile