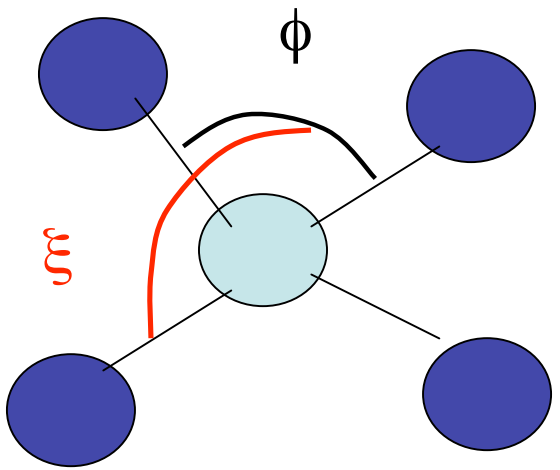
# Practicalities on using MD

- Geometry constraints: Z-matrix
- Equilibration of MD
- Restart of phonon calculations

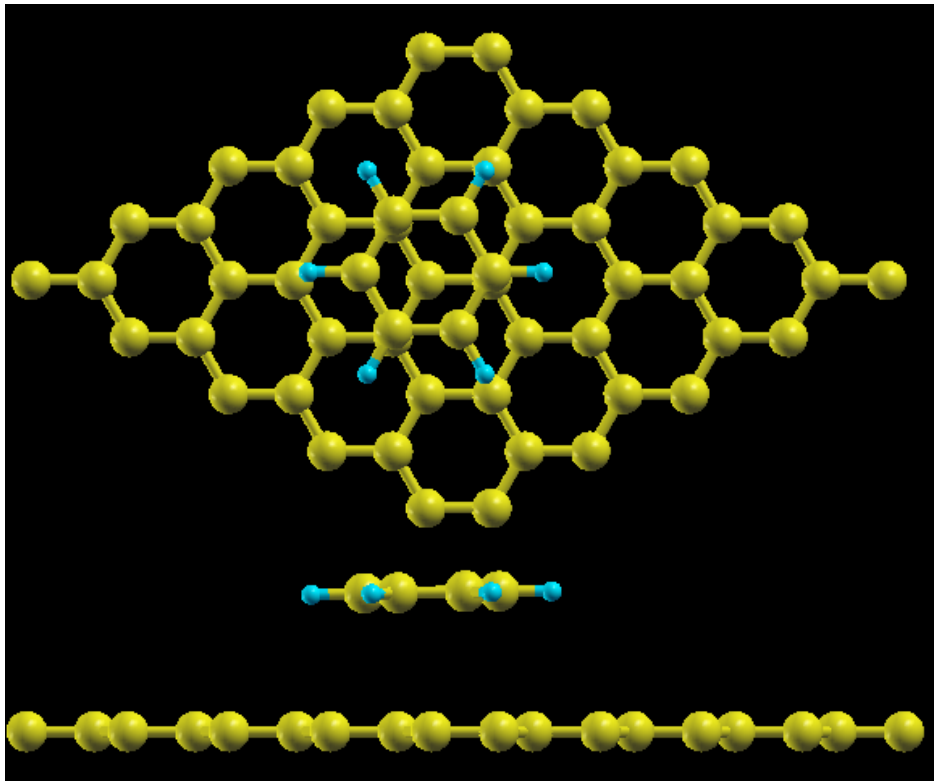
# Z-Matrix coordinate format

- Internal coordinates: Molecules represented by :
  - Bond lengths $\chi_i$
  - Bending angles $\phi_i$
  - Dihedral angles $\xi_i$

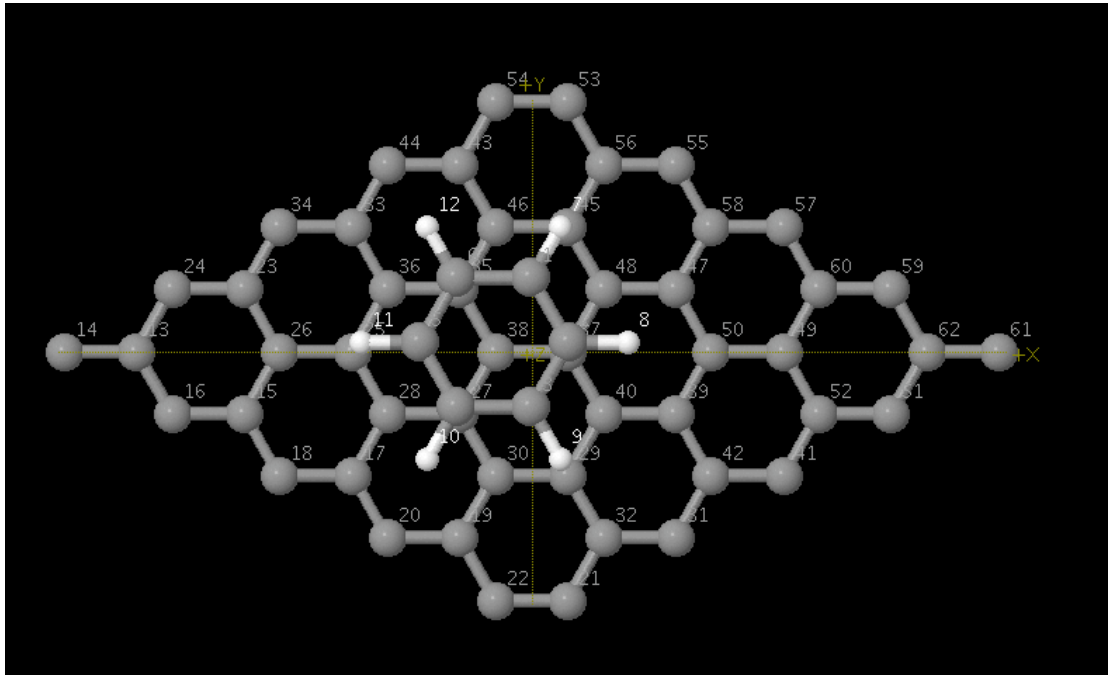


# Z-Matrix

- Allows for mixing of generalised and Cartesian coordinates: Useful for constraint relaxations



Explore the PES by using
A relevant coordinate:
Useful for estimating
barriers




```
%block Zmatrix
molecule
#N(l) i    j    k   rlj     alji      tlkji      ifr    ifa   ift
  1   0    0    0    0.00   1.396      zm1        0      0     1
  1   1    0    0    CC     90.0      -60.0       0      0     0
  1   2    1    0    CC     CCC       90.0       0      0     0
  1   3    2    1    CC     CCC       0.0        0      0     0
  1   4    3    2    CC     CCC       0.0        0      0     0
  1   5    4    3    CC     CCC       0.0        0      0     0
  2   1    2    3    CH     CCH       180.0      0      0     0
  2   2    1    7    CH     CCH       0.0        0      0     0
  2   3    2    8    CH     CCH       0.0        0      0     0
  2   4    3    9    CH     CCH       0.0        0      0     0
  2   5    4    10   CH     CCH       0.0        0      0     0
  2   6    5    11   CH     CCH       0.0        0      0     0
```

```
cartesian
1   -7.79941320326530       0.000000000000000E+000  0.000000000000000E+000   0 0 0
1   -9.21748831324190       0.000000000000000E+000  0.000000000000000E+000   0 0 0
1   -5.67230051370190       -1.22808908925970       0.000000000000000E+000   0 0 0
1   -7.09037562367850       -1.22808908925970       0.000000000000000E+000   0 0 0
1   -3.54518782413850       -2.45617817857230       0.000000000000000E+000   0 0 0
1   -4.96326293411510       -2.45617817857230       0.000000000000000E+000   0 0 0
1   -1.41807513457510       -3.68426726783200       0.000000000000000E+000   0 0 0
1   -2.83615024455170       -3.68426726783200       0.000000000000000E+000   0 0 0
1   0.709037554988300       -4.91235635714460       0.000000000000000E+000   0 0 0
variables
     zm1 2.95
constants
     CC 1.417
     CH 1.112
     CCH 120.0
     CCC 120.0
%endblock Zmatrix
```

Finally, constraints must be specified in a `constraints` block.

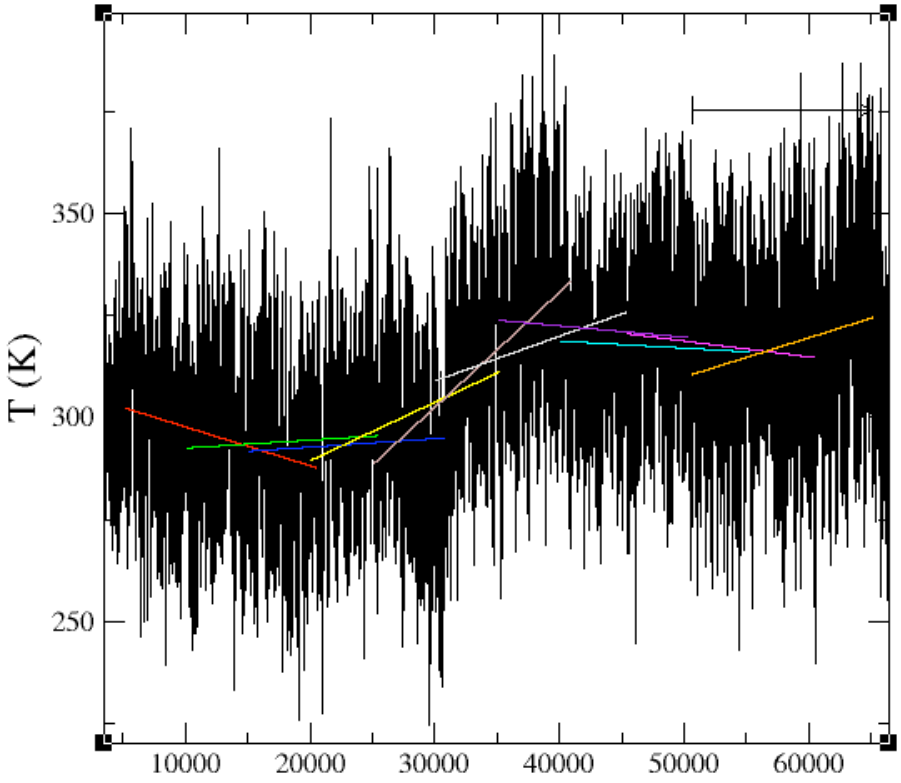
`constraint` This sub-section allows the user to create constraints between symbols used in a Z-matrix:

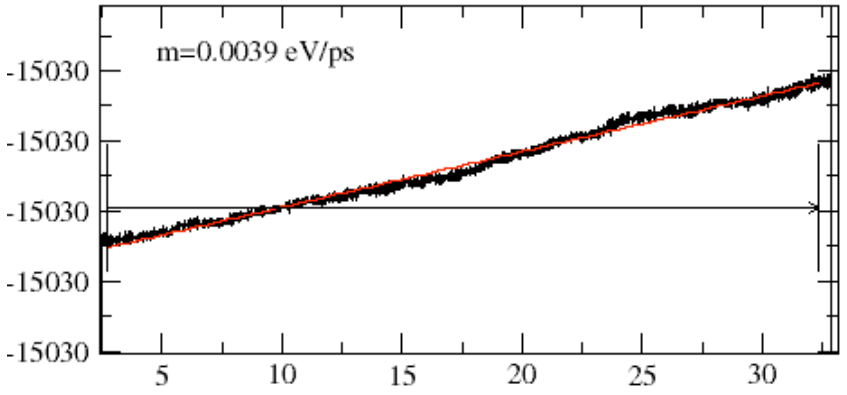
```
constraint
  var1 var2 A B
```

Here var1 and var2 are text symbols for two quantities in the Z-matrix definition, and A and B are real numbers. The variables are related by $var1 = A * var2 + B$.

- Z-matrix Symbol Section -------
- Variables
- zm1 2.55000000000000
- Constants
- cc 1.41700000000000
- ccc 120.000000000000
- ch 1.11200000000000
- cch 120.000000000000
- ---------- End of Z-matrix Information

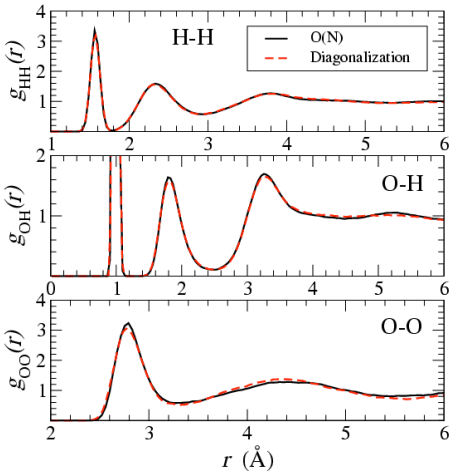
# Equilibration of MD

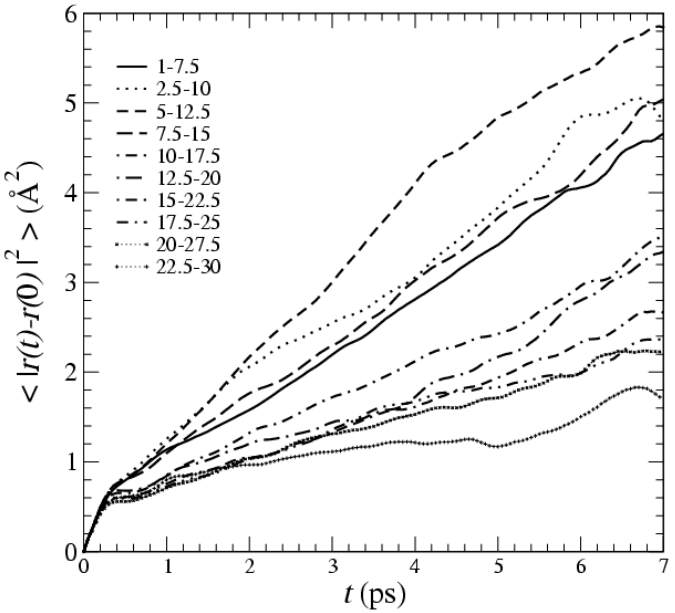


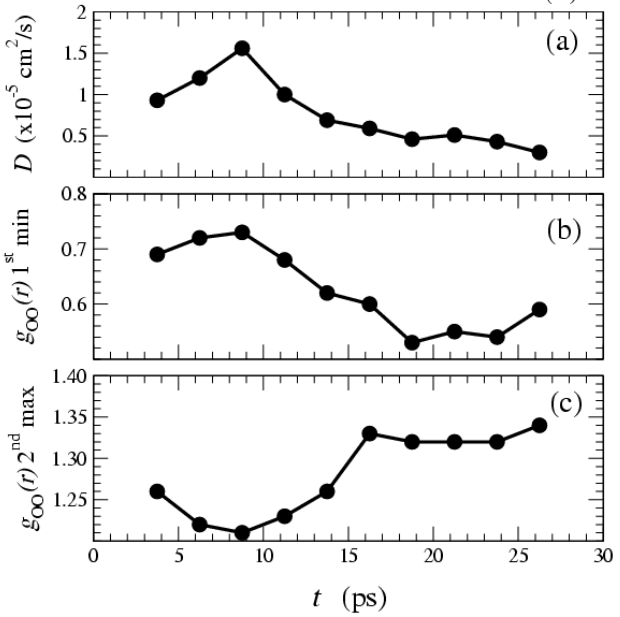



# Moving -windows

Divide the trajectories in overlapping windows of 7.5 ps length and 2 ps interval



# Output files

- SystemLabel.XV  Stores coordinates and Velocities, necessary for restarts (keep always a backup copy!!)
- SystemLabel.MDE

| # Step | T (K) | E_KS (eV) | E_tot (eV) | Vol (A^3) | P (kBar) |
|---|---|---|---|---|---|
| 1 | 300.00 | -854.95859 | -854.68716 | 169.572 | 8.679 |
| 2 | 281.04 | -854.94170 | -854.68741 | 169.572 | 12.576 |

- SystemLabel.MD : Saves positions and Velocities for each time frame, formatted.

# Phonon Calculations

- Easy to parallelize: Each displacement is independent of others. We can parallelize by atoms.
- Care is needed when reassembling the .FC files.
- If calculation crashes we can restart it without loosing information, but doing it with care.