Molecular Dynamics Simulations of Epoxy Resin Systems

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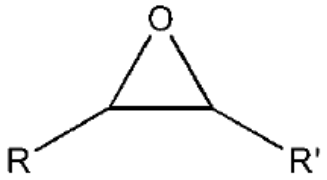
Epoxy Resins

- Epoxy resins are a class of thermoset polymers.
- The epoxy resins can cross-link with amine hardeners, producing cured resins.
- Applications: adhesives, coatings, encapsulates, casting materials, etc.



Basic chemical structure of epoxy group

Objectives:

Midweek Objectives: Create the epoxy systems and run tests in LAMMPS(Large-scale Atomic/Molecular Massively Parallel Simulator).

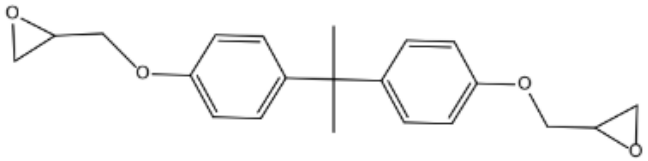
End of Summer Objectives: Run a multitude of tests with openDIEL and prepare another epoxy system and measure its physical properties.

Research Plan

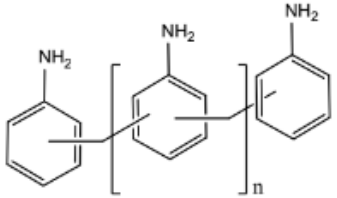
1. Create molecules in VMD
2. Optimize the molecular structure
3. Pack molecules into a simulation box
4. Encode each atom in the simulation box with important information about that atom
5. Create a suitable data and input file for LAMMPS
6. Run LAMMPS on Stampede2
7. Analyze simulation data
8. Create an experiment to confirm glass transition temperature etc. of the epoxy.

PRO-SET® M1002 Resin (Epoxy) and M2046 Hardener (Amine)

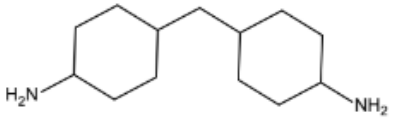
MSDS and Sigma Aldrich



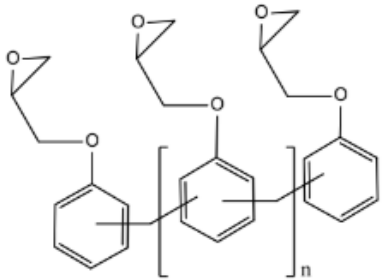
Propane, 2,2-bis[p-(2,3-epoxypropoxy)phenyl [BADGE] (70-100%)



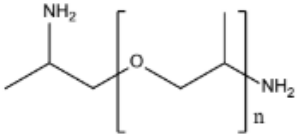
Benzenamine-formaldehyde polymer [Aniline formaldehyde] (15-35%)



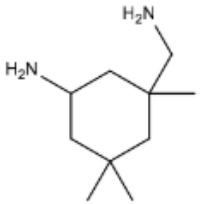
4, 4'-Methylenebiscyclohexanamine [Methylene-BCHA] (10-30%)



Phenol-formaldehyde polymer glycidyl ether [PDGE formaldehyde] (10-20%)

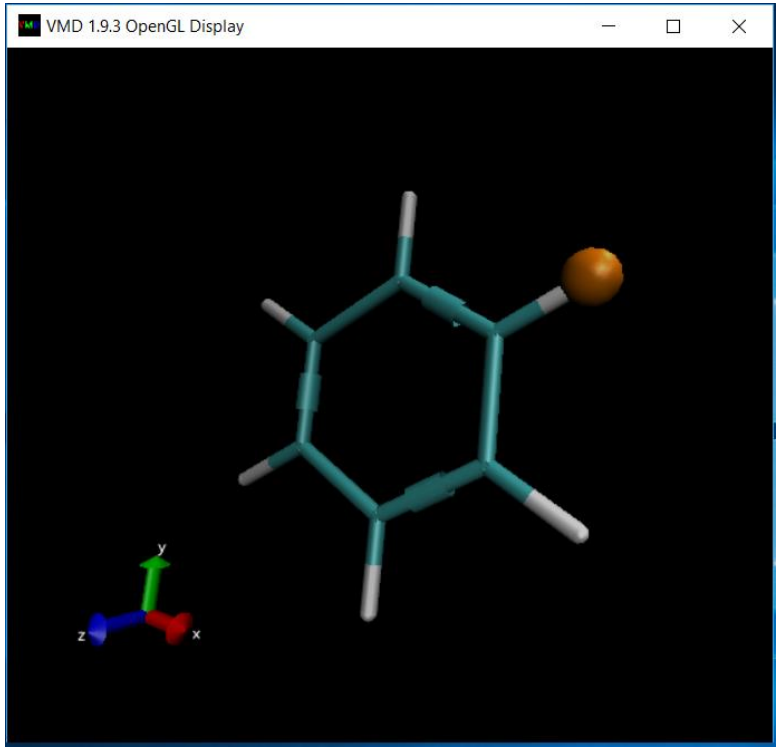


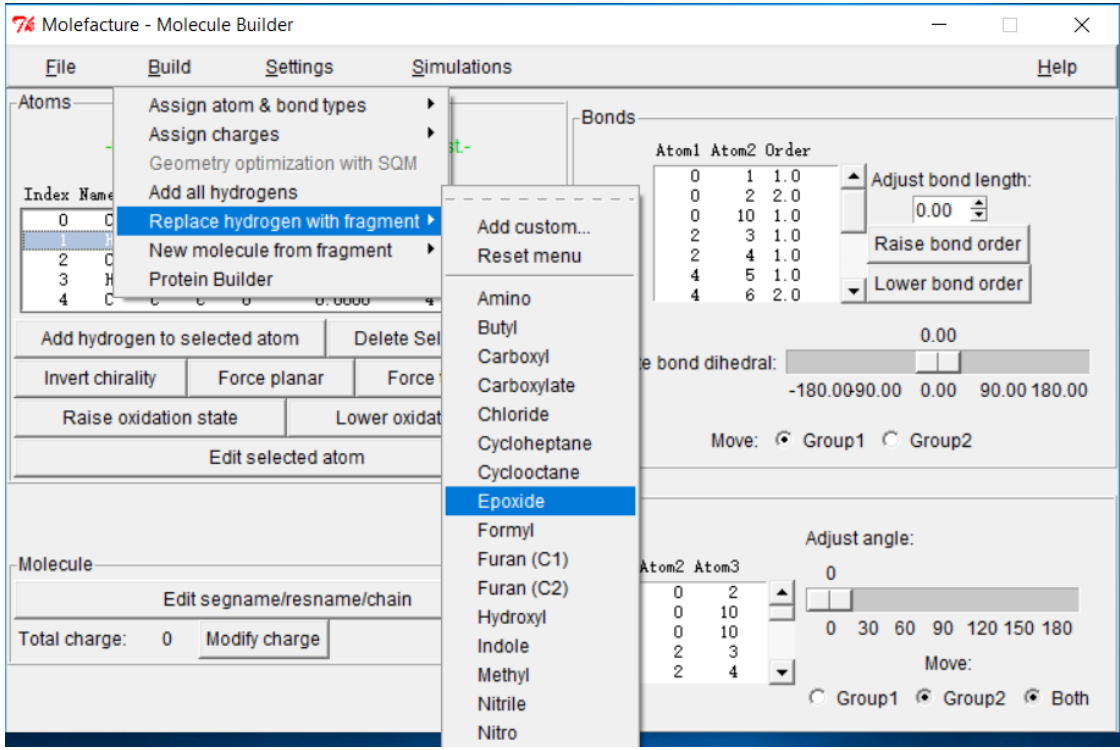
Polyoxyropylenediamine [POPDA] (10-30%)



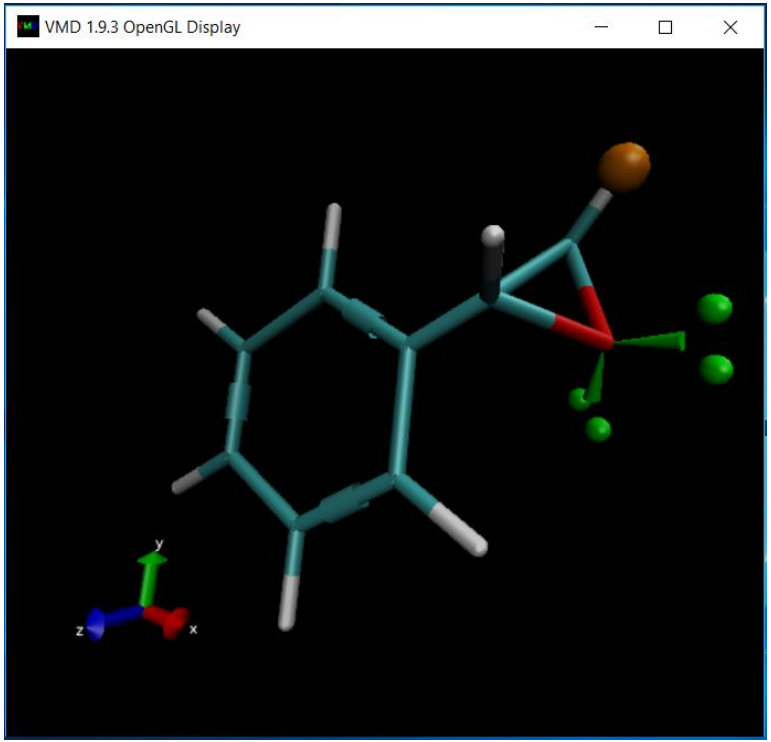
Isophoronediamine [IPDA] (10-30%)

Creating Molecules in VMD





Creating Molecules in VMD



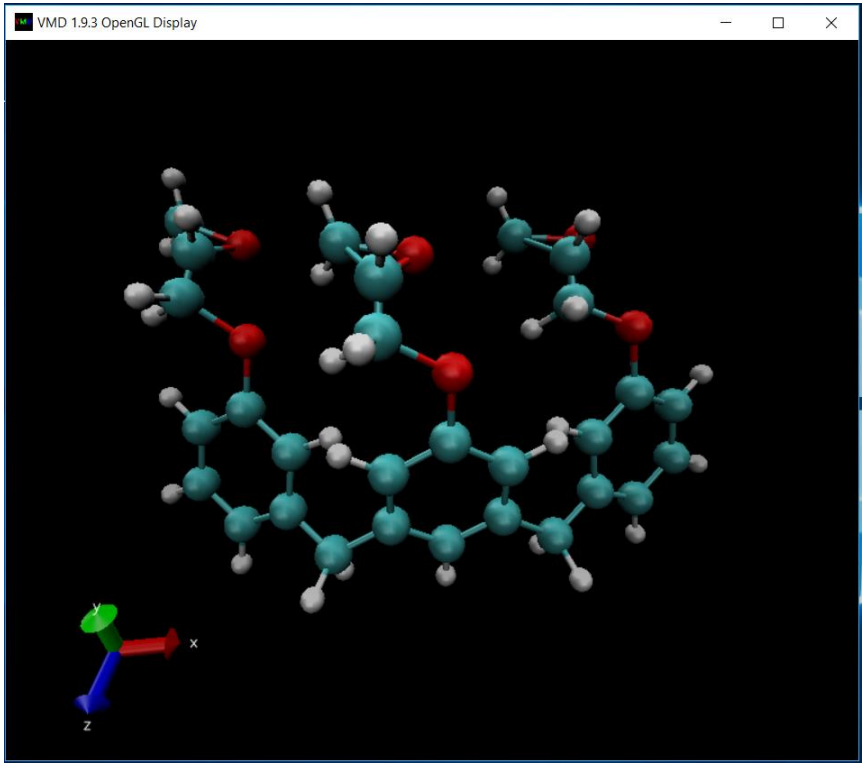
By repeatedly replacing the atoms with functional groups, we can build complicated molecular structure.

Molecular Structure Optimization

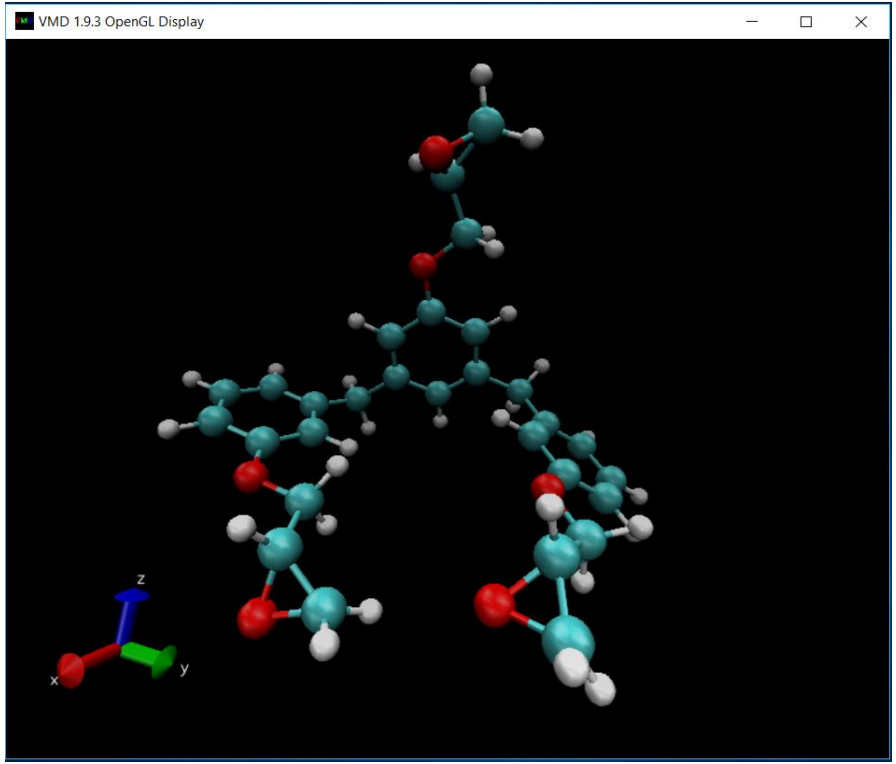
- We adopted the NWChem program to perform structural geometry optimization.
- The optimization is based on density functional theory (DFT), which is a quantum mechanical method widely used in computational chemistry.
- Through the optimization, the molecules will become more stable.

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

Molecular Structure Optimization

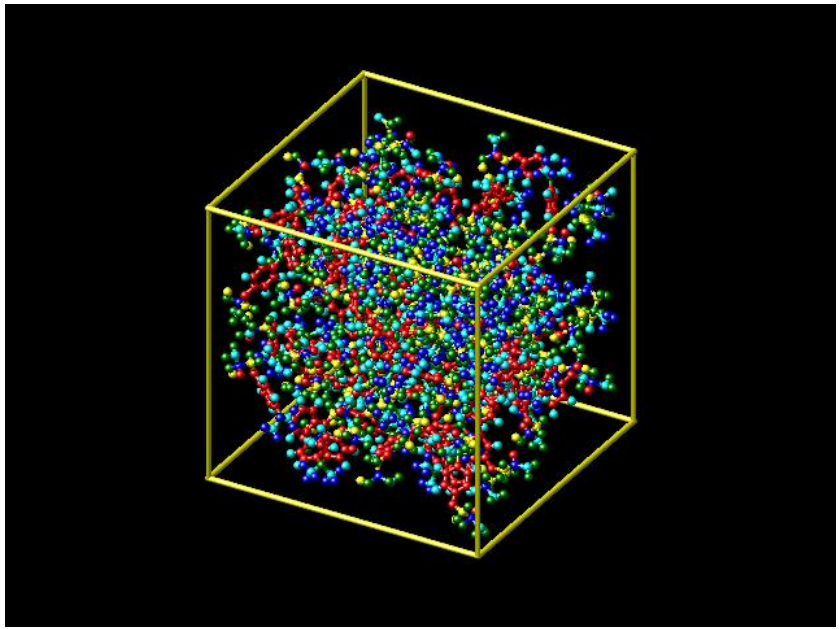


Unoptimized PDGE



Optimized PDGE

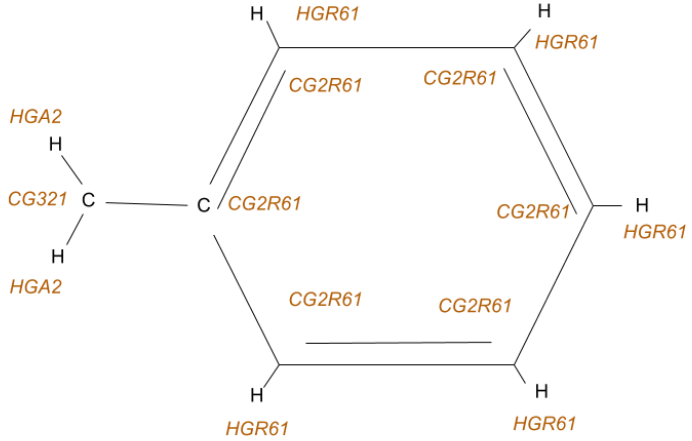
Pack molecules into a box



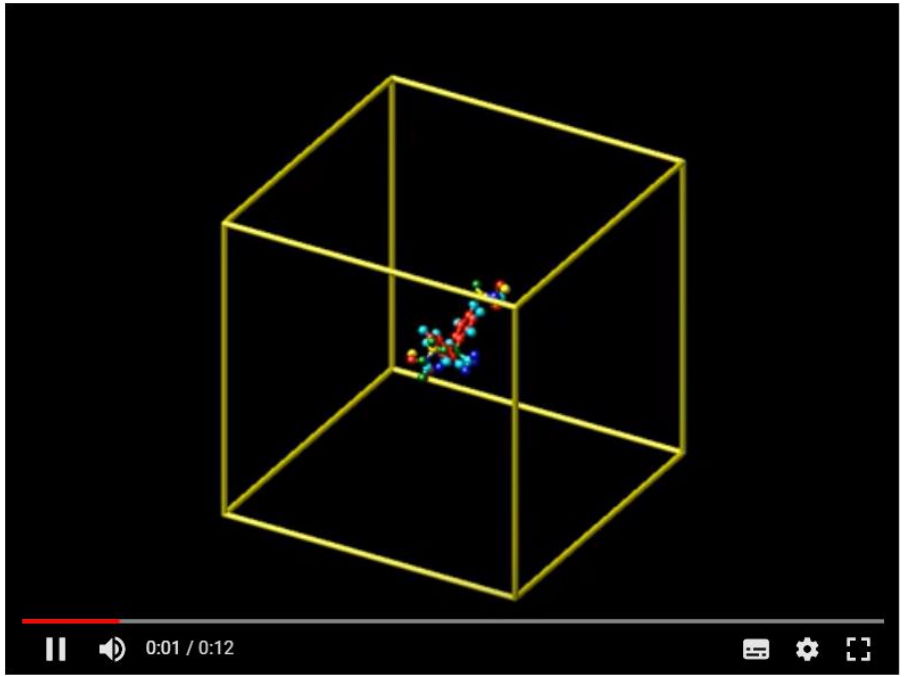
We built a simulation box with Packmol program.

Encode Atoms

- First letter is Atomic element
- Letters and numbers after refer to specific types of each atom.
- Other encoding includes partial charge



LAMMPS input/output



Problems to be Solved in LAMMPS

```
Setting up Verlet run ...
  Unit style    : real
  Current step  : 0
  Time step     : 1
Per MPI rank memory allocation (min/avg/max) = 18.9 | 19.06 | 19.34 Mbytes
Step Temp E_pair E_mol TotEng Press Volume
       0            0   -210.42704    4755.6541    4545.2271    166.67951        32768
       1   0.16385939   -210.62521    4754.6968    4545.1808     144.0002    32768.003
       2   0.56082297   -211.18313    4752.4775    4545.0908    81.150447    32768.011
       3     1.003405   -212.00296    4750.2567    4545.0462   -6.5427877    32768.021
       4    1.3885873   -212.95551    4748.6314    4545.0759   -95.826006    32768.032
       5     1.754868   -213.92039    4747.1627    4545.1218    -161.9299    32768.039
       6    2.1674615    -214.8196     4745.265    4545.1179   -187.77938     32768.04
       7    2.5856028   -215.63588    4743.2073    4545.0745   -170.83369    32768.035
       8    2.8803302   -216.40857    4741.9768    4545.0664   -123.00313    32768.024
       9    2.9823682   -217.21006    4742.1628    4545.1417   -64.153456    32768.008
                                                                          135,1         40%
```

```
     146    62.838354   -480.48297    4676.8385    4621.7347   -1629.9674    32404.479
     147    77.351189   -521.32655      4678.57    4680.8661   -1717.1416    32397.039
     148            0 -8.0056482e+10    4711.5532 -8.0056477e+10 -6.7791618e+11    32389.548
ERROR on proc 7: Out of range atoms - cannot compute PPPM (../pppm.cpp:1941)
Last command: run              500
ERROR on proc 15: Out of range atoms - cannot compute PPPM (../pppm.cpp:1941)
Last command: run              500
ERROR on proc 4: Out of range atoms - cannot compute PPPM (../pppm.cpp:1941)
Last command: run              500
```

References

- Epoxy Resins picture. Retrieved from https://images-fibreglast-com.s3.amazonaws.com/pio-resized/750/System%202000%20Laminating%20Epoxy%20Resin-2.jpg
- L. Martínez, R. Andrade, E. G. Birgin, J. M. Martínez. Packmol: A package for building initial configurations for molecular dynamics simulations. *Journal of Computational Chemistry*, 30(13):2157-2164, 2009.
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- M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, "NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations" *Comput. Phys. Commun*. 181, 1477 (2010).
- S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J Comp Phys*, 117, 1-19 (1995).