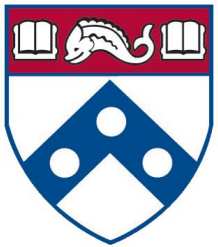
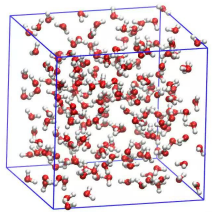
RECSEM REU 2017- Molecular Dynamics of Epoxy Resin Systems

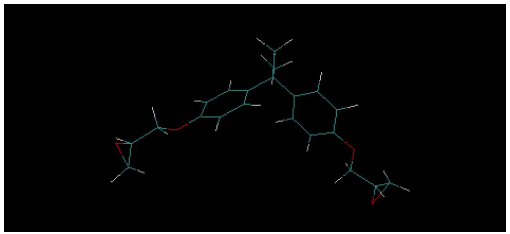
Stephen Wu and Lam Tran
Dr. Lonnie Crosby



Molecular Dynamics

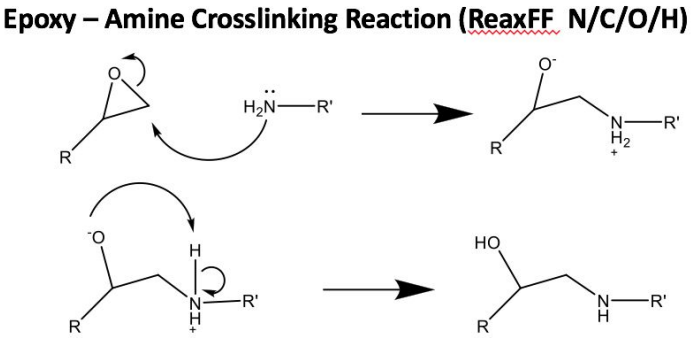
- Molecular Dynamics
  - Simulations that numerically solve the equations of motion for a system of particles as a function of time given a force field describing particle interactions.
  - Microscopic length and time scales (nm/angstrom, ps/ns). Results “can be as accurate as needed”.
  - Relative to actual experiments, MD simulations can save time and money. Furthermore, they can oftentimes more easily reveal physical properties of a system (structure, microscopic interactions, etc.)





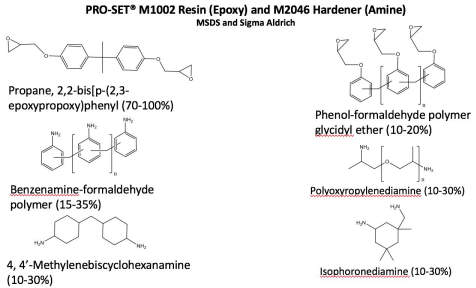
Epoxy Resins

- Epoxy Resins
  - First developed in the 1930s and used today in a wide range of applications.
  - High strength/durability, low shrinkage and excellent adhesive and insulative properties.
  - Composed of a base resin (BADGE, cycloaliphatic, biobased, etc.) and a hardener/curative (amine type, alkali, catalytic) that confers additional properties.



Project Purpose and Goals-Why?

- Use MD simulations to examine the physical properties of the ProSet M1002 base resin/M2046 amine hardener system as a function of the components and the extent of crosslinking.
    - ∂V terms- Thermal expansion coefficient α (~∂V/∂T), Isothermal compressibility κ (~∂V/∂P)
- Are the adhesive properties of the system appropriate for usage in an industrial setting with aluminum surfaces?

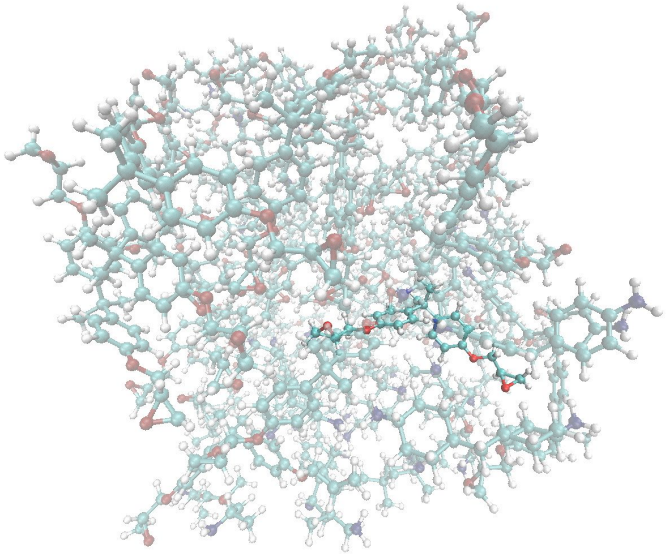


Overview of Steps to Take

- Parameterization
  - Are numerical values (like force constants) associated with charges, bonds, angles, torsions/dihedrals present and correct?
- Nonreactive Force Field Simulations-GROMACS
  - Are individual component molecules of the epoxy resin system behaving as expected? For example, is a molecule remaining compact and its atomic distances staying relatively constant?
  - Are the atoms with positive dipoles in polar solvents attracted to the oxygen with nonbonded electrons?
- Reactive Force Field Simulations-LAMMPS
  - Is the epoxy-amine crosslinking reaction dominant over other unwanted side reactions?
  - How do the properties of the system change depending on the extent of temperature-dependent crosslinking?

Past Progress

- Parameterization on each individual molecules
  - OPLS-AA - topology of molecule
- Use quantum mechanics to optimize molecule structure with NWCHEM
  - Spatial coordinates - Solution to Schrödinger equation
  - Partial charge - Lowdin population analysis
- GROMACS sample test to calibrate and visualize the simulation system:
  - Water-solvated oxirane simulation
  - Methane-solvated oxirane simulation



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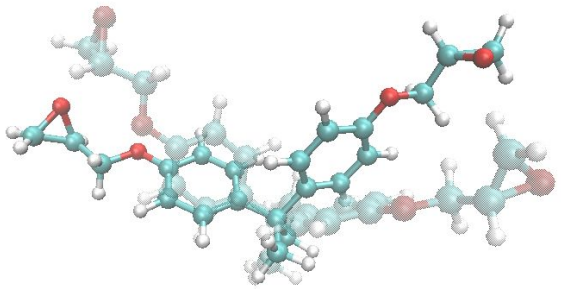

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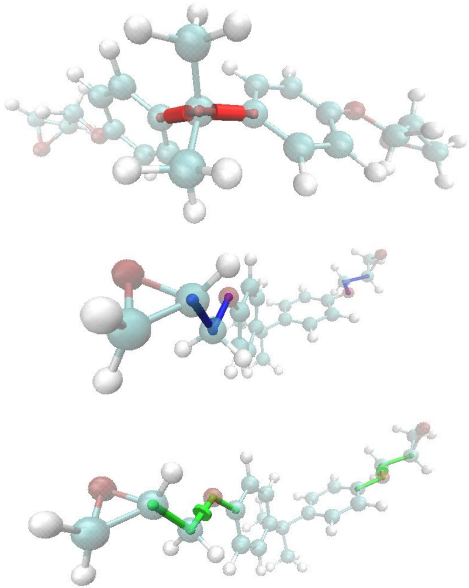
Current Stages

- Parameterization CGenFF
  - VMD plugin fftoolkit - bond, angle, dihedral parameters
- GROMACS sample test data analysis
  - Data analysis on free energy for sample simulation ensemble
- GROMACS Small-scale MD simulation
  - Single epoxy and Single hardener
  - Single epoxy and multiple hardener
  - Multiple epoxy and multiple hardener



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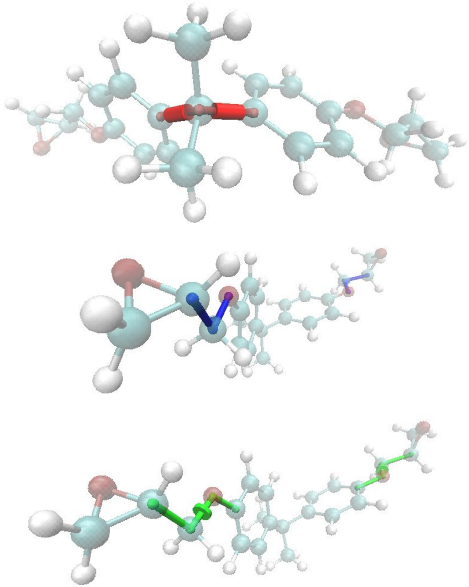

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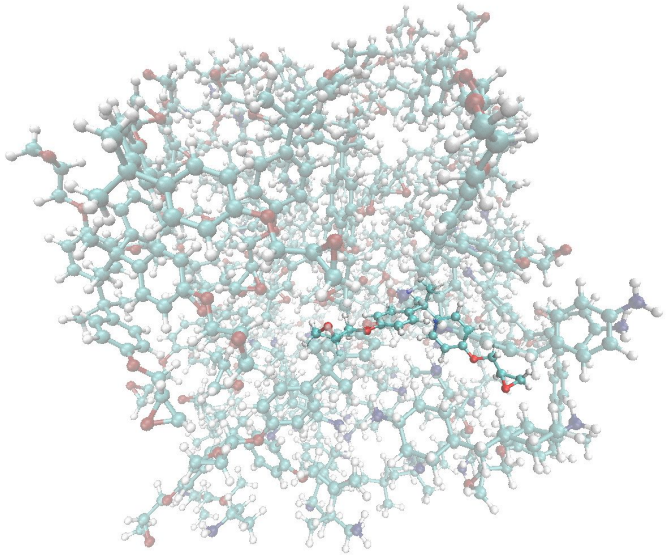
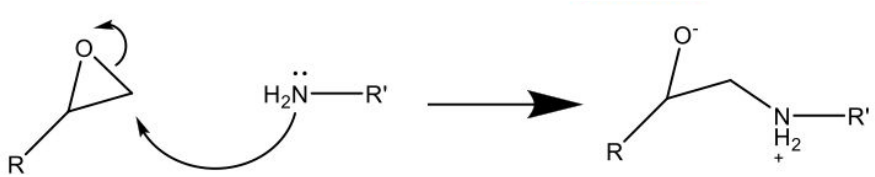


Next Steps

- Small Molecule LAMMPS system construction
  - Translation from GROMACS to LAMMPS
  - Reaction between oxirane and methylamine (N/C/O)



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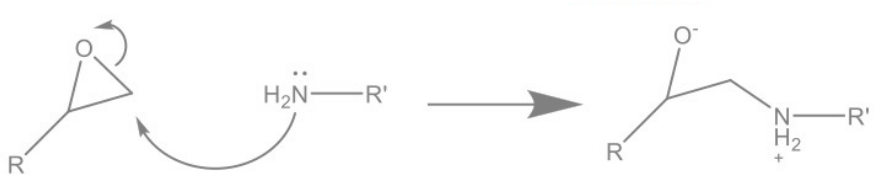

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