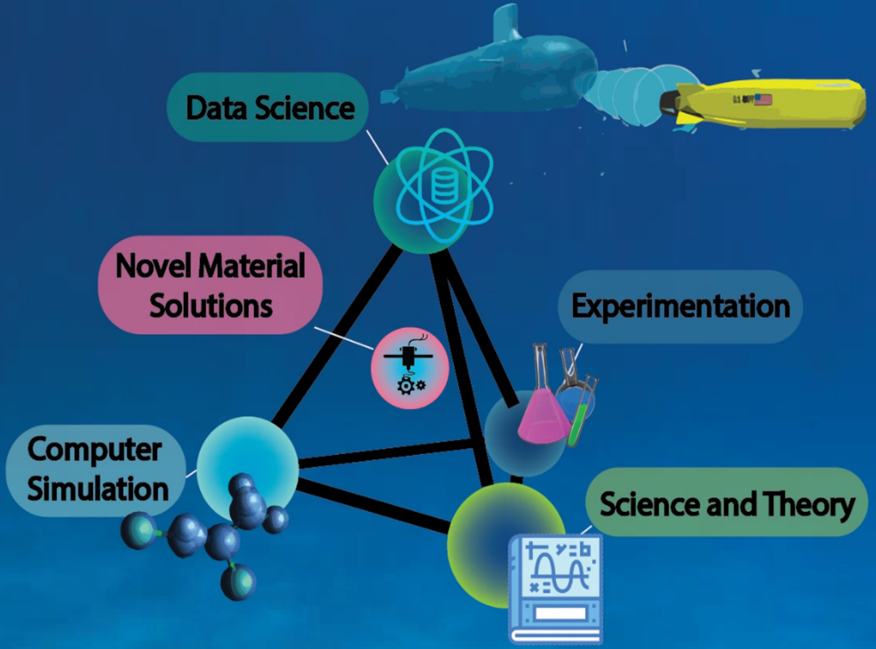
Intelligent Selection and Rational Co-Design of AM Polymers for Marine Applications



Carly Travis
Applied Masters Student
Materials Science and Engineering
University of Washington

Polymer co-design for FDM additive manufacturing

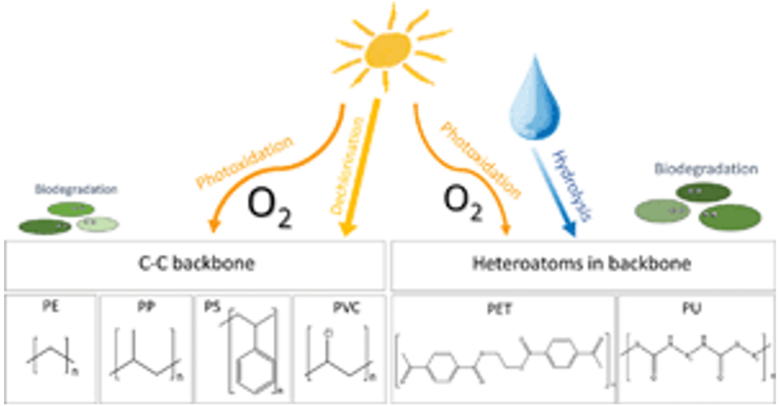
- Goal: **select + design thermoplastic materials for AM that will have superior resistance to marine degradation**
    - Polymers have near-infinite chemical spaces and property variables, making "trial-and-error" approaches ineffective in covering all possibilities

- Solution: **data and simulation-driven approach to selection + design**
    - Screen polymers/monomers within datasets based on property objectives
    - Model chains in simulated marine environments and extract data
    - **Validate model via experiments with accelerated degradation protocol**

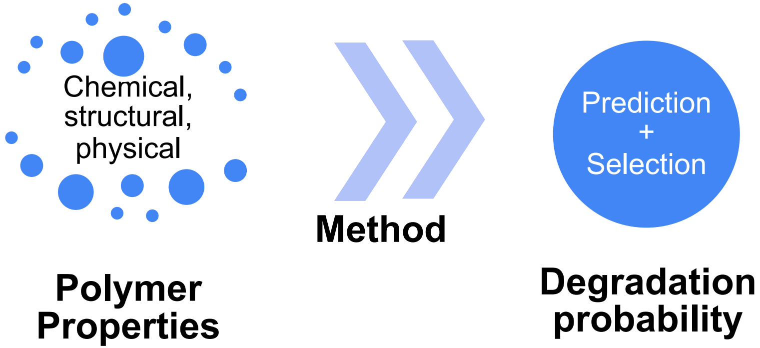
- Why: **Reduce experimental time + resources**
    - Accelerate materials development + Discover unique material solutions
    - Provide framework for future material needs

Polymer marine degradation mechanisms

- Polymer degradation is influenced by chemical sequence
    - Changes at molecular level can reduce functionality of bulk structure (printed part)
- Utilize data science to reveal molecular **structure-property-performance** trends influencing degradation through:
    - **Datasets**
    - **Simulation**
    - **Validation**



Influence of monomer structure on plastic degradation in marine environments



Specific aims for approach:

Aim 1

Construct + screen property datasets to find best candidates

Screen candidates based on property objectives + reveal structure-property-performance trends

Aim 2

Simulate best candidates to reveal molecular-scale degradation mechanisms

Uncover structure-property trends and predict when/why degradation occurs

Aim 3

Validate and guide models via in-person experimentation

Expose polymers to equivalent degradation environments in simulation and laboratory

Aims +

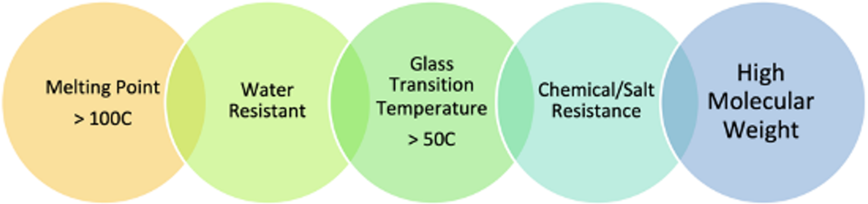
Supplemental Aims

- Incorporate additives (CF/chemical)
- Model UV + biofilm mechanisms
- Simulation-guided design for new properties (i.e. conductivity)

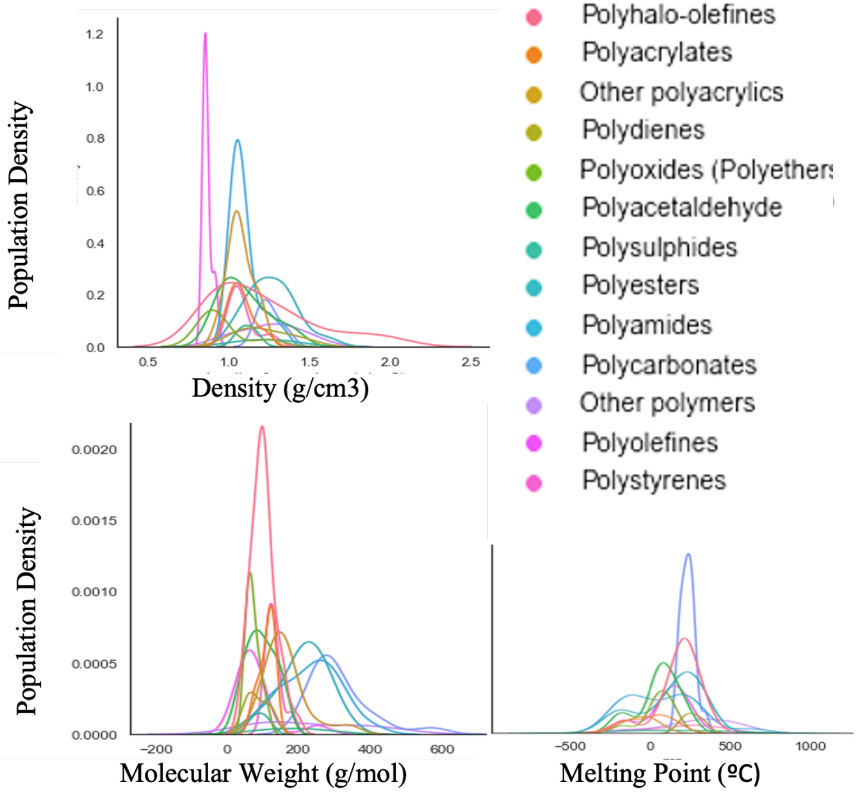
Aim 1 - Data science applied to polymer properties

- Dataset constructed from multiple open-source sets of thermophysical property information
    a. Organized according to monomer unit

- Literature + theory-guided property selection of 5 general parameters for screening:

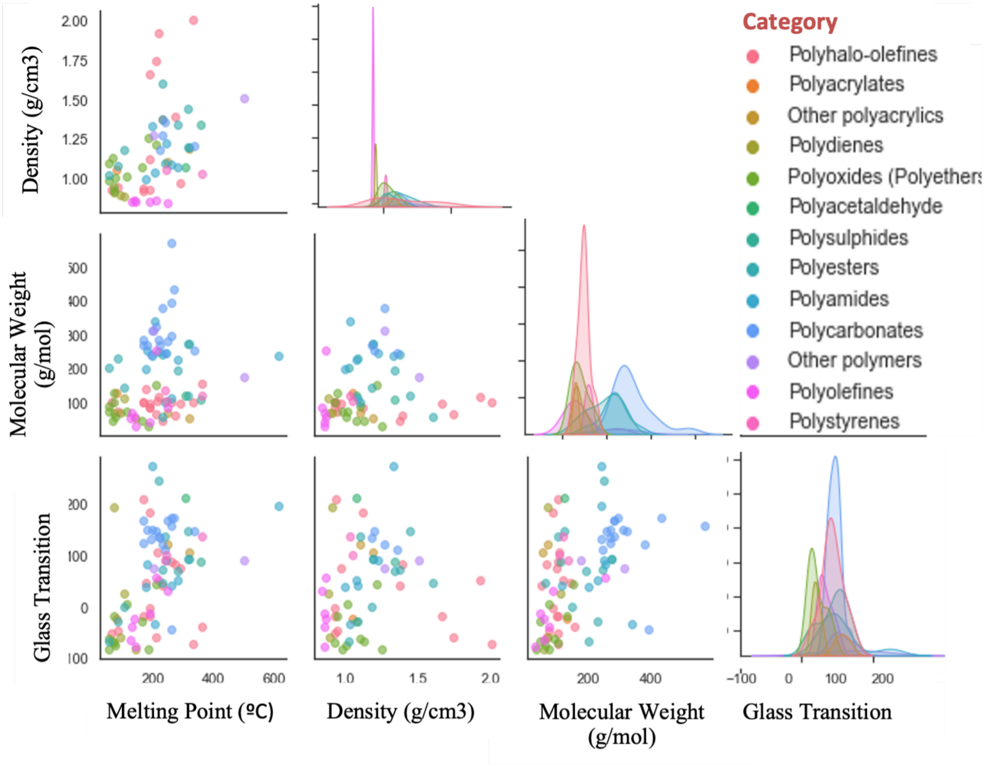


- Aims to reveal structure-property trends in degradation and best candidates for AM



Distribution plots for density, molecular weight, and melting point of select polymers according to their polymer category.

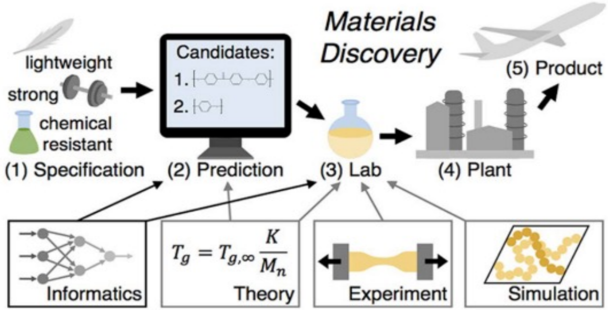
Aim 1 - Data science applied to polymer properties



Distributions of density, molecular weight, melting temperature, and glass transition temperature data in the studied within dataset of interest for marine degradation. Correlation plots between different properties of interest for each category are modeled.

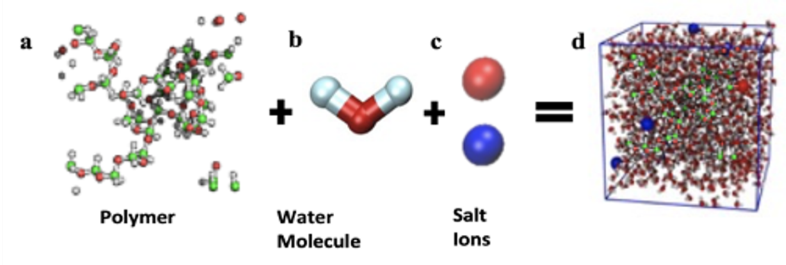
- Polymers with similar monomer structures tend to have similar property distributions

- Chemical sequence coupled with structure and physical behaviors can work together to give predictions of degradation probabilities for a large set of materials



Aim - 2: Simulations of marine degradation - method

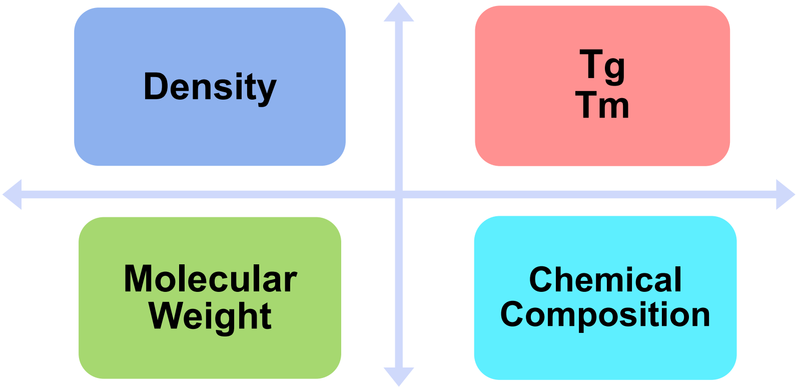
- **LAMMPS** used for simulating marine degradation:
  - **Polymer chain**
  - **Water molecules**
  - **3.5% salt ions**



- Set to accelerated degradation protocol used in laboratory
  - **Temperatures range 20-70C**
  - **Duration of 2 and 4 weeks**

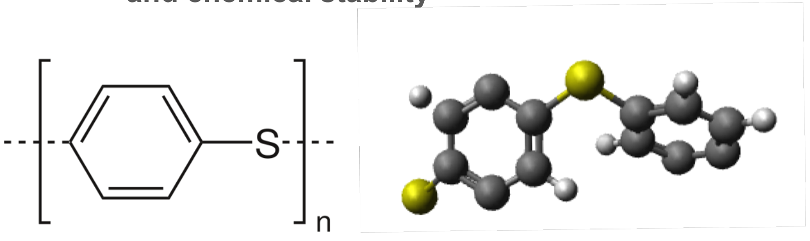
Post-simulation results are compared to initial data to reveal extent of property change and the mechanisms by which they changed

Properties Evaluated in LAMMPS



Aim 3 – Validate models through experimentation

- Perform accelerated aging of AM polymers to guide and validate methods of Aim 1 and Aim 2.
  - **Current work: Polyphenylene Sulfide (PPS)**
    - **Engineering AM polymer with excellent thermal and chemical stability**



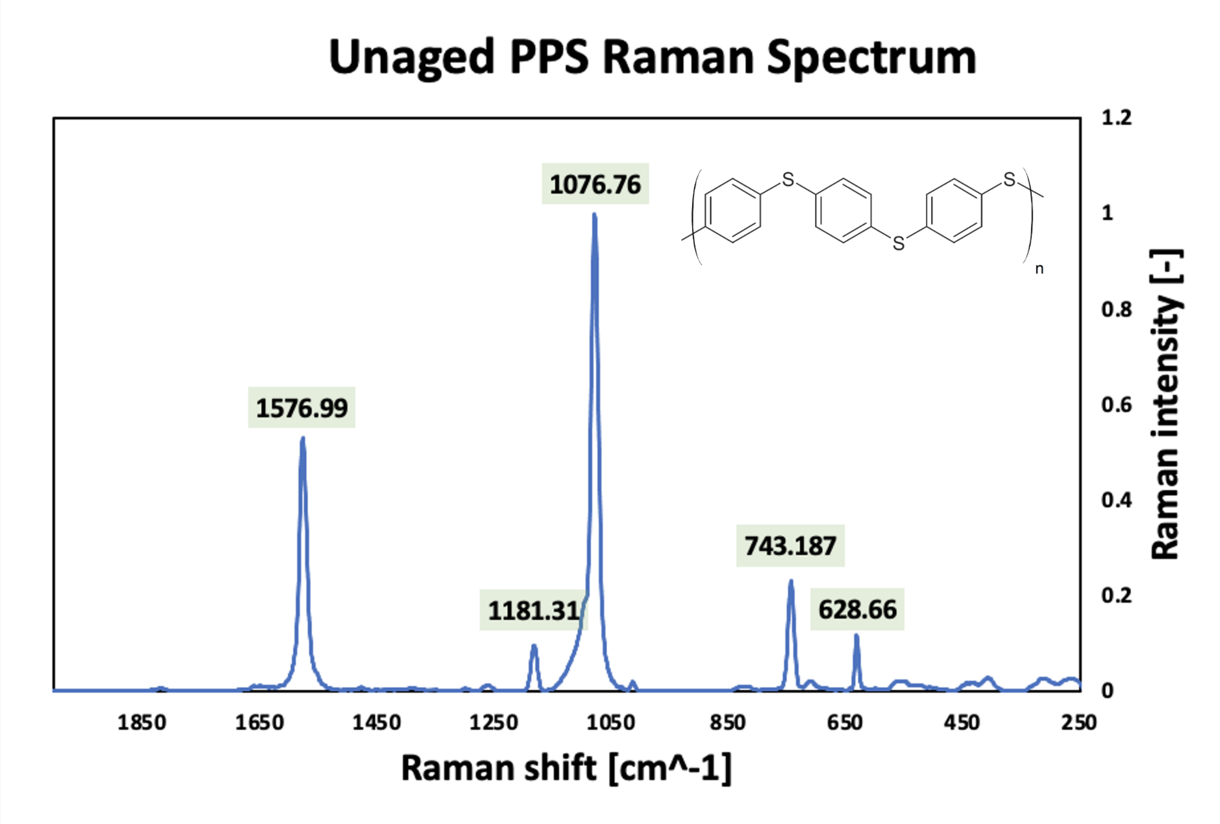
PPS monomer 2D to 3D representation, modeled in Avogadro for LAMMPS

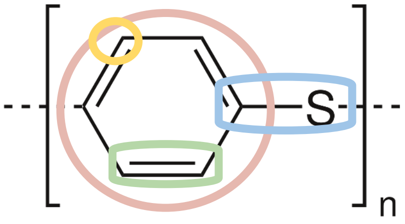
Future candidates: ULTEM, Nylon (PA)

Experiment
- Chemical composition via Raman
- Water absorption via mass gain
- Thermal properties via TGA, DSC
- Bulk property change via tensile test

Simulation
- Chemical composition changes visualized
- Water absorption via surface area change
- Density + volume used to approximate thermal properties

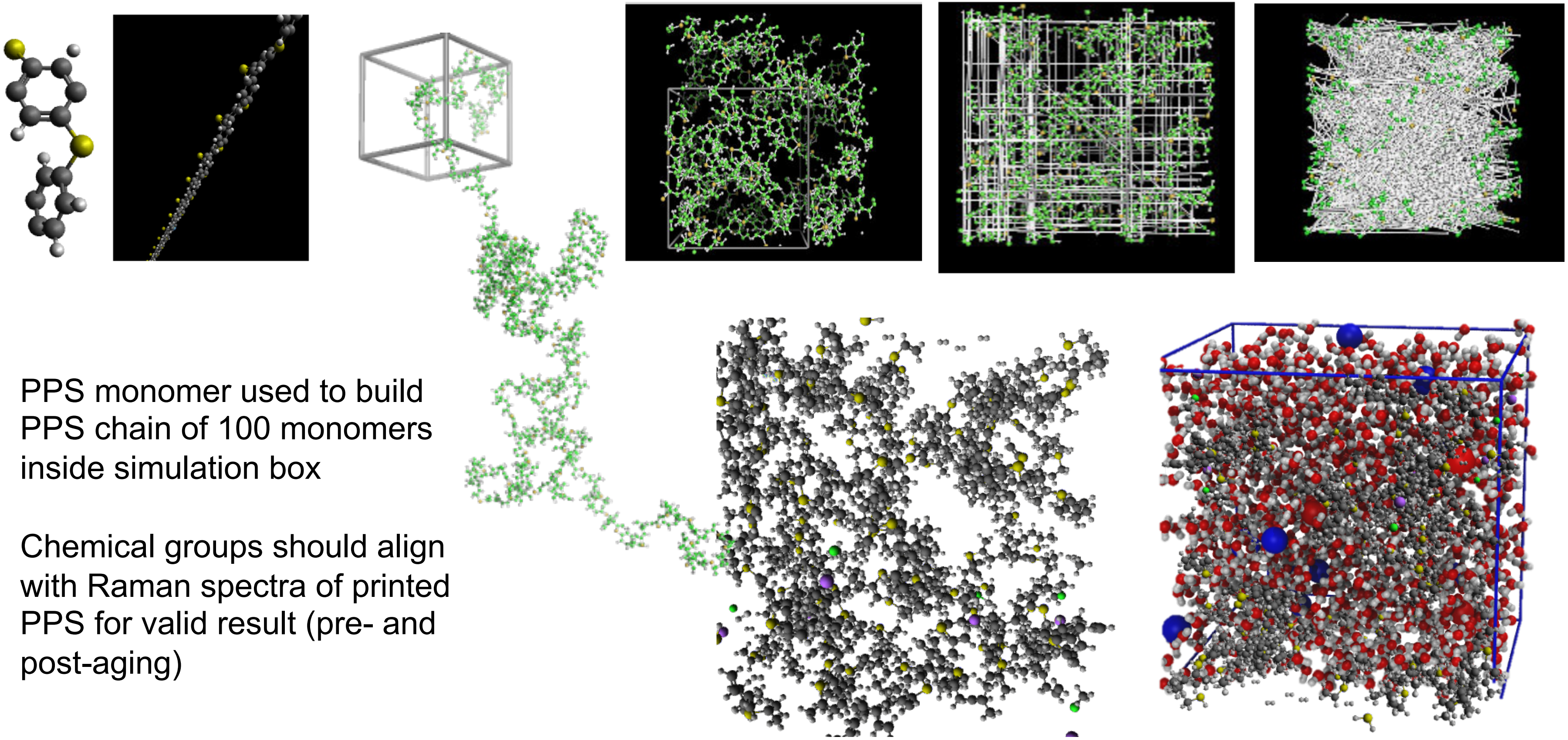
Determining PPS composition via Raman





Peak [cm^{-1}]	Component
1577, 629	C-C (phenyl)
1181	C-H
1077	C=CH (benzene)
743	C-S

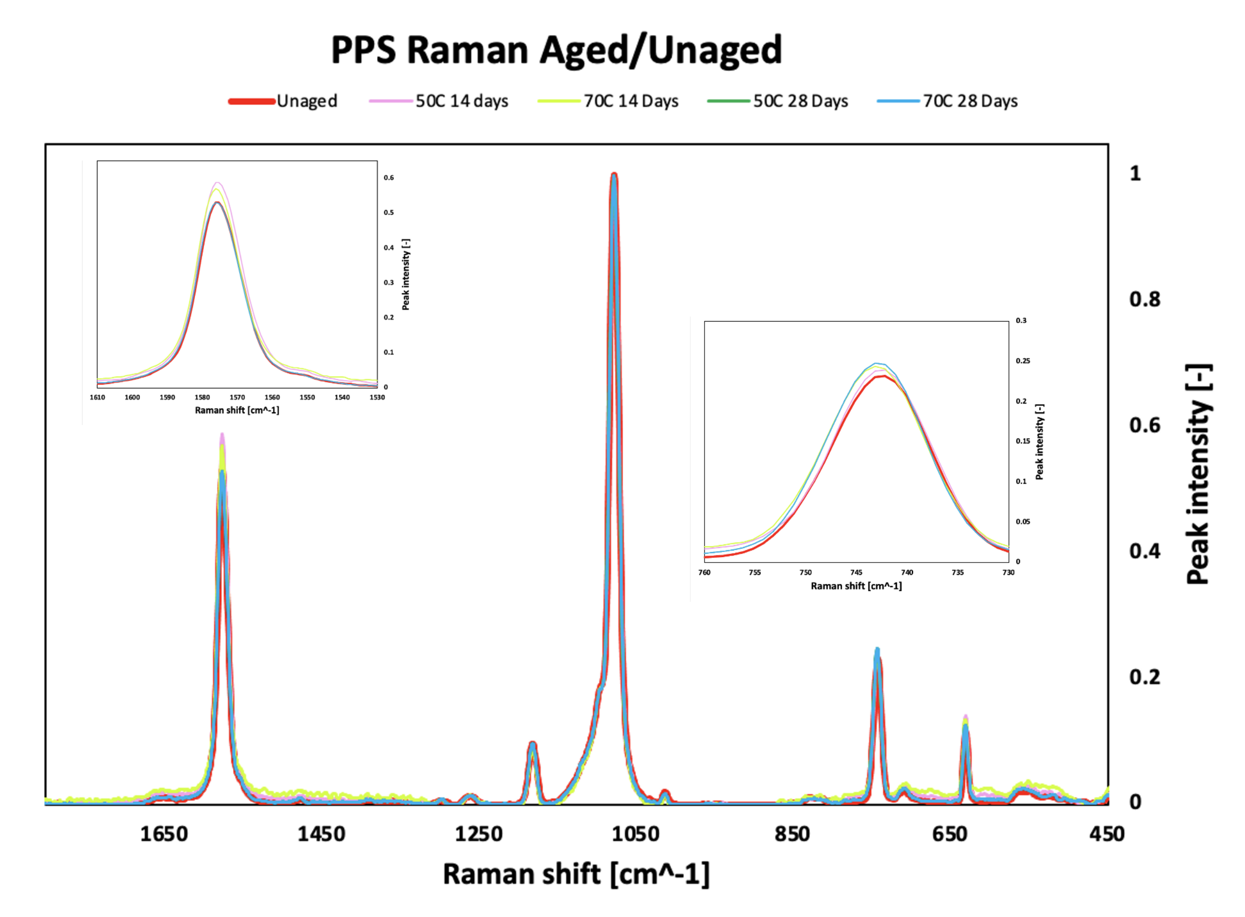
Building and modeling PPS simulation cell



- PPS monomer used to build PPS chain of 100 monomers inside simulation box

- Chemical groups should align with Raman spectra of printed PPS for valid result (pre- and post-aging)

PPS composition after aging



PPS aged in seawater at temperatures of 50, 70C for 14 and 28 days

- Marine exposure at these temperatures has little influence on chemical composition over 14/28 day periods

- Minor change for:
  - **C-C phenyl group** (1577 cm^{-1})
  - **C-S bonds** (743 cm^{-1})

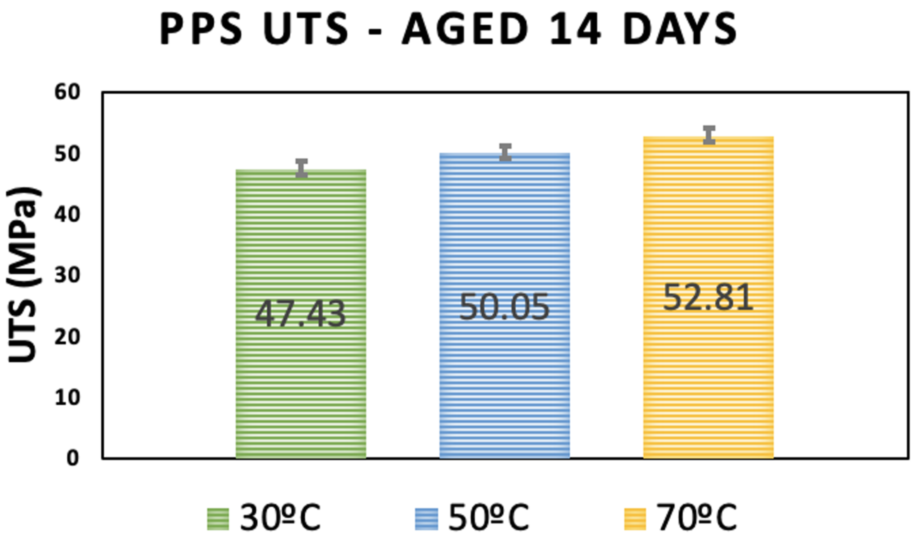
- **No change** for **C=C benzene ring** (1077 cm^{-1})

- We should expect to see minimal change in chemical groups during simulation

Thermal properties PPS

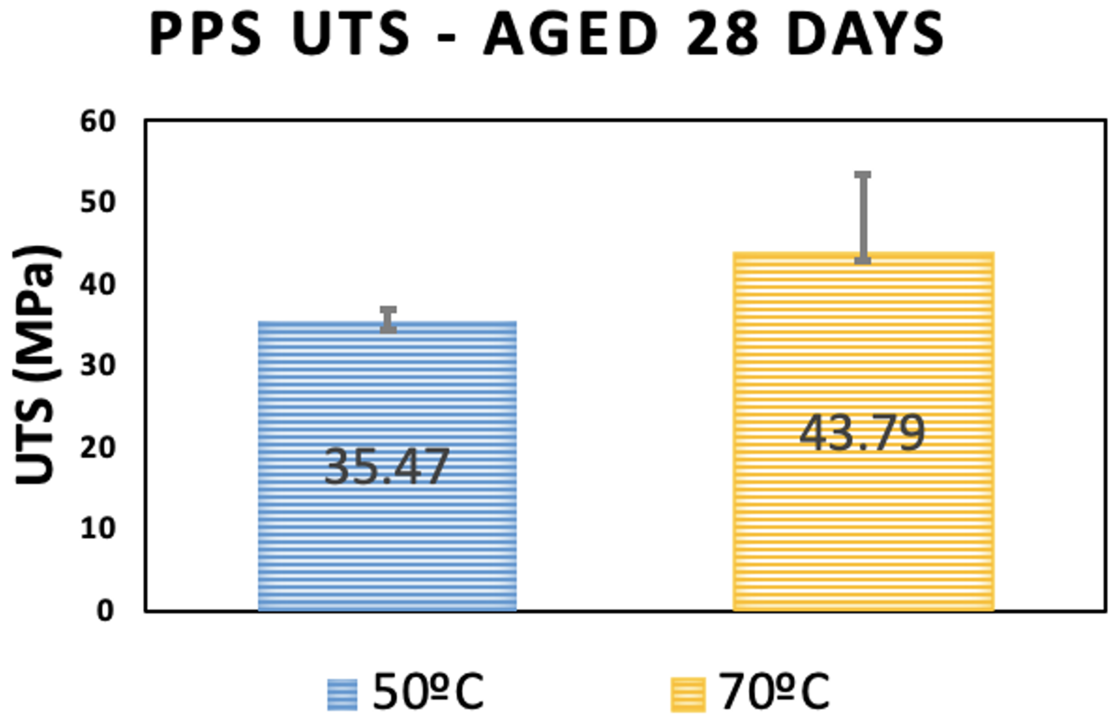
- ** Need to analyze DSC for PPS aged samples
- This is getting too long
- Mechanical?

UTS PPS - Aged 14 Days



Temp (℃)	30	50	70
UTS (MPa)	47.37	50.05	52.81
STDEV	1.23	1.13	1.31

UTS PPS - 28 Days



Temp (℃)	50	70
UTS (MPa)	35.47	43.79
STDEV	1.41	9.56

Overall Comparison UTS