Finite Element Modeling to Optimize Degradation Properties on Polymeric Materials

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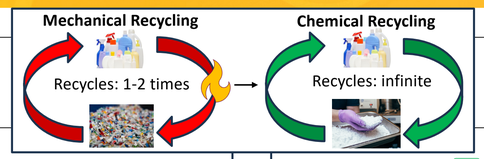
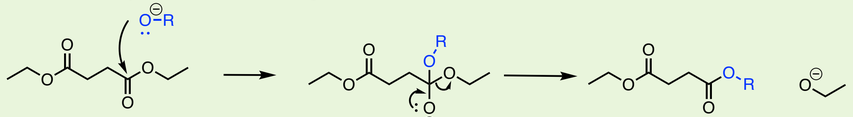
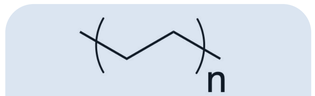
What if we add recyclable sites along the polyethylene chain and incorporate intermolecular interactions through the diol?



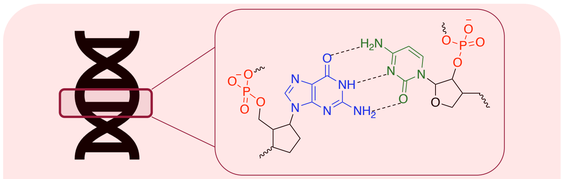
Polyesters are **chemically recyclable** due to the hydrolysis of the ester bond

Base-catalyzed ester cleavage

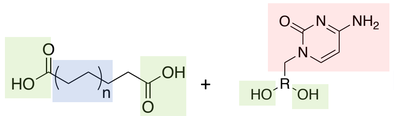


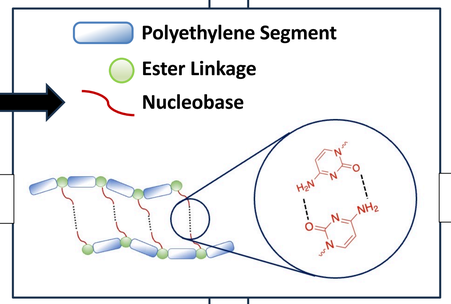


polyethylene - No reactive sites

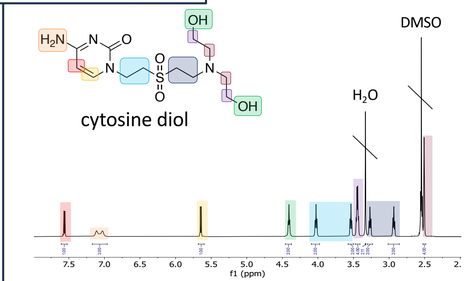


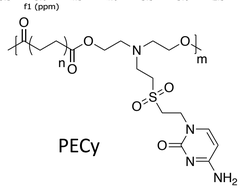
Incorporation of the desirable properties of each component:



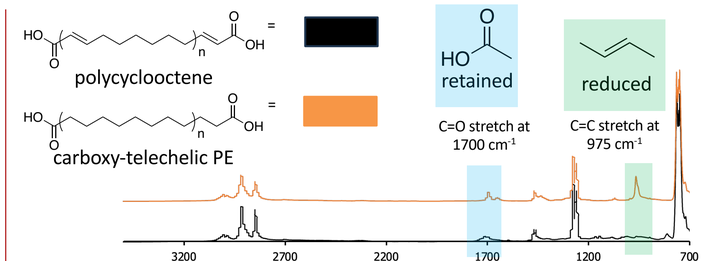


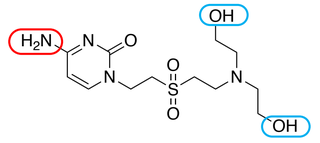
Confirmation of synthesized components and determination of polymer properties





Film **unable** to be **melted**, **crosslinked**?

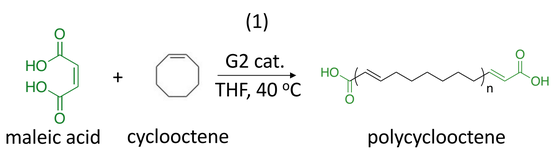


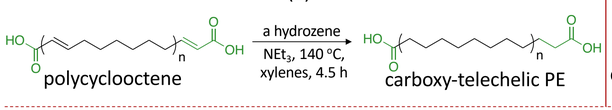


F = 3 functionality from transamidination

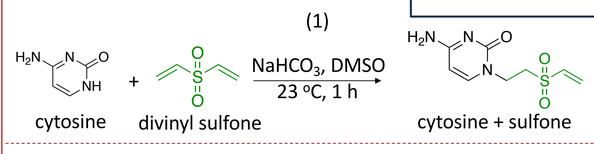
What are the steps to synthesizing this product?

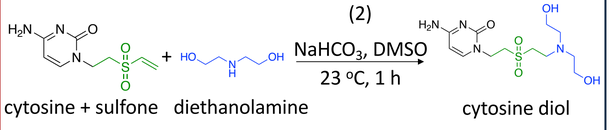
Carboxy-telechelic PE synthesis

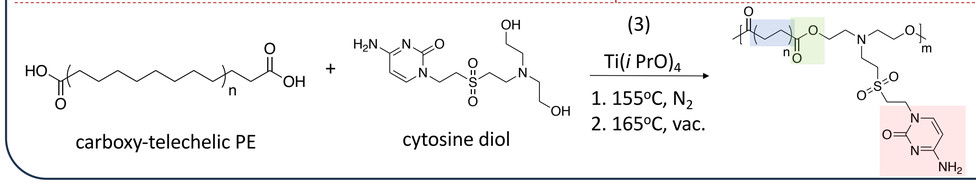




Cytosine Diol Synthesis



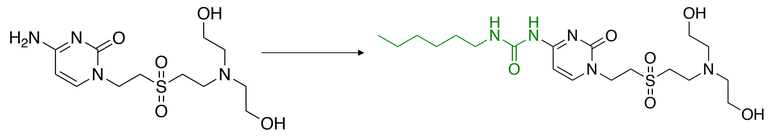




ester-linked polyethylene with **H-bonding** capabilities (PECy)

What are the future steps to this project?

Modification of the **diol**:

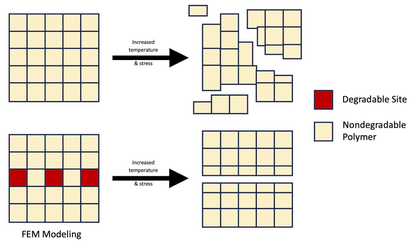


Benefits:

- Complimentary quadruple hydrogen bonding
- Ensures F=2 functionality of the diol

Utility in **Selective Additive Manufacturing** Applications:

- What if we incorporated depolymerizable sites into plastics?
- Allow for predictable and clean fracture
- Usage of computational strategies (i.e. FEM) to determine most effective site placement



Liu, B.; Long, T. E.; et al. *Molecules* **2021** *26*(15), 4705. Arrington, A. S.; Long, T. E. *Polymer* **2022**, *259* (125319), 125319.

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