Homework 5
Polymer Physics 2024
Due Tuesday February 13 at noon
(**pdf** file should be called: **HW 4 Group x Last Name_Name_Name_Name.pdf**)

Ralph Colby wrote a polymer physics book with Rubenstein that is a suggested reading for this class. In 2020 he published a Nature paper on the glass transition of conjugated polymers (polymers that can conduct electricity), Xie R, Weisen AR, Lee Y, Aplan MA, Fenton AM, Masucci AE, Kempe F, Sommer M, Pester CW, Colby RH, Gomez ED *Glass transition temperature from the chemical structure of conjugated polymers* Nat. Com. **11** 893 (2020). Stretchable electronics require flexible conductors which can be achieved by conjugated polymers above their glass transition temperature so it is of some importance to have the ability to predict T_g to design new conjugated polymers.

a) Xie mentions that the glass transition can depend on the Debye-Waller factor, or the free volume using the Lindemann criteria. He also mentions the quantitative structure-property relationships (QSPR) method, group contributions approaches, and machine learning. Give one line descriptions of each of these five methods and the Lindemann criteria.

b) Figure 2 shows plots of G' and G" vs temperature. T_g is determined by the peak in G". Why does G" drop above the glass transition temperature? Why does it drop below T_g? What happens at T_g that causes the peak? How is temperature related to frequency? How is T_g determined from a DSC measurement in Supplementary Figure 5?

c) Supplementary Figure 8 shows fairly good agreement between T_g and the packing length, p. Explain the origin of the packing length using block copolymers as was done in class. Why would T_g decrease with increasing packing length with a power law of about $T_g \sim p^{-3.3}$?

d) Figure 3 shows that the T_g follows a modified Flory-Fox behavior based on the weight fraction of alkyl side chains. Explain the theoretical basis for the Flory Fox equation. Why is the weight fraction used (vs. the molar fraction).

e) Explain Xie's method to determine the "mobility" of the chains. Does this make sense to you? Why might you expect T_g to be proportional to the negative of mobility? Why is it a linear dependence and not a power-law or exponential relationship?