**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.

1. 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.
2. 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?
3. 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 ~ *p*-3.3?
4. 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).
5. 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?