Equilibrium and nonequilibrium gelation in TPR protein/linker mixtures\textsuperscript{1} TIANQI SHEN, ROBERT S. HOY, COREY S. O’HERN, Yale University — Using simulations we model gelation in two-component systems consisting of tetratricopeptide repeat (TPR) proteins and peptide cross linkers. These have recently been shown [1] to form strong, mechanically stable gels with remarkable shape recovery - but only within narrow parameter regimes. Within our minimal, coarse grained model, we elucidate the effects of the packing fraction $\phi$, temperature $T$ and concentration ratio $r$ of TPR and cross linkers on the gel transition. Two gelation mechanisms are identified. At low $\phi$ and $T$, nonequilibrium microphase-separated gels may be formed by rapid temperature quenches. At higher $\phi$ and $T$, homogeneous equilibrium gelation occurs. At low $r$, gelation is suppressed due to depletion of linkers, while at high $r$ gelation is suppressed due to the “coating” of proteins by linkers. The gel transition line in the $(r,T)$ plane has an unusual, asymmetric form. We also briefly compare these results to those for a more realistic “patchy” model which incorporates the directional TPR-linker binding present in the experimental systems.


\textsuperscript{1}T. S. acknowledges support from NSF grant no. PHY-1019147.