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Equilibrium and nonequilibrium gelation in TPR protein/linker mixtures[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 ϕ, temperature T and concentration ratio r of TPR and cross linkers on the gel transition. Two gelation mechanisms are identified. At low ϕ and T, nonequilibrium microphase-separated gels may be formed by rapid temperature quenches. At higher ϕ 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.

[1] T. Z. Grove *et. al.*, JACS, **132**, 14024 (2010).

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