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Coarse-Grained Models of Entropic Allostery in Proteins RHODA HAWKINS, TOM MCLEISH, IRC in Polymer Science and Technology, School of Physics and Astronomy, University of Leeds — Allosteric proteins are involved in many signalling processes in molecular biology. As an alternative to conformational change in the mean static structure, it has been suggested that the information of ligand binding may be transmitted to a distant site across an allosteric protein by changes to the pattern of the internal dynamics of the protein. We explore how ligand binding may change the intramolecular vibrational entropy and free energy through coarse-grained models of this "entropic allostery". We consider coarse-grained models of various repressor proteins such as the lac repressor. We also investigate allostery in alpha helical coiled-coils, found in proteins such as the dynein molecular motor and bacteria chemotaxis receptors.

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