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Mechanostability of Proteins and Virus Capsids[1]

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Molecular dynamics of proteins within coarse grained models have become a useful tool in studies of large scale systems. The talk will discuss two applications of such modeling. The first is a theoretical survey of proteins' resistance to constant speed stretching as performed for a set of 17134 simple and 318 multidomain proteins. The survey has uncovered new potent force clamps. They involve formation of cysteine slipknots or dragging of a cystine plug through the cystine ring and lead to characteristic forces that are significantly larger than the common shear-based clamp such as observed in titin. The second application involves studies of nanoindentation processes in virus capsids and elucidates their molecular aspects by showing deviations in behavior compared to the continuum shell model. Across the 35 capsids studied, both the collapse force and the elastic stiffness are observed to vary by a factor of 20. The changes in mechanical properties do not correlate simply with virus size or symmetry. There is a strong connection to the mean coordination number $< z >$, defined as the mean number of interactions to neighboring amino acids. The Young's modulus for thin shell capsids rises roughly quadratically with $< z >$ - 6, where 6 is the minimum coordination for elastic stability in three dimensions.

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