Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

The Role of Secondary Structure on the Mechanical Properties of Titin RAVI KAPPIYOOR, DANIEL DUDEK, ISHWAR PURI, Virginia Tech — Elastomeric proteins are characterized by high resilience and low stiffness. Recent work suggests that charge interactions between the proteins and water have a large role in these mechanical properties. However, some elastomeric proteins are nonpolar, and, as such, do not have high charge interactions with the surrounding water. This indicates that there are also other factors at work. We consider the role of secondary structure (i.e. alpha helices and beta sheets) on the mechanical properties of one such elastomeric protein, titin. Molecular dynamics simulations are performed on four different configurations: (i) the PEVK domain of titin (little secondary structure in its natural state), (ii) an immunoglobulin-like domain of titin (high secondary structure in its natural state), (iii) the same immunoglobulin-like domain with all of its secondary structure artificially removed, and finally (iv) the PEVK domain linked to the immunoglobulin-like domain in its natural state. These simulations will provide key insight on the role of secondary structure on mechanical properties, which can be used to more efficiently design smart materials.

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Date submitted: 09 Nov 2012

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