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Abstract for an Invited Paper for the MAR11 Meeting of the American Physical Society

## Unfolding proteins with mechanical forces: From toy models to atomistic simulations<sup>1</sup> DMITRII MAKAROV, University of Texas at Austin

The remarkable combination of strength and toughness, displayed by certain biological materials (e.g. spider silk) and often unmatched by artificial materials, is believed to originate from the mechanical response of individual load-bearing protein domains. Single-molecule pulling experiments carried out during the last decade showed that those proteins, when loaded, respond in a non-equilibrium fashion and can dissipate large amounts of energy though the breaking of sacrificial bonds. In my talk, I will discuss what structural properties correlate with mechanical strength and toughness at the single-molecule level, how thermodynamic stability is related to the mechanical stability, and why both atomistic simulations and simple models seem to fail to reconcile the mechanical responses of the same proteins measured under varied loading regimes. I will further discuss whether it is easier to unfold a protein mechanically by pulling at its ends or by threading it through a narrow pore. The latter process is believed to commonly occur in living organisms as an intermediate step in protein degradation.

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