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Determination of the equilibrium free energy for pulled single molecules from nonequilibrium work measurements[1] LIAO CHEN, University of Texas at San Antonio — The Jarzynski equality (JE) is widely accepted for extracting equilibrium free energy from non-equilibrium work measured in single-molecule pulling experiments, even though questions remain on its validity and applicability. In this talk, I will show that the JE is actually inapplicable outside the near-equilibrium regime. I will also present a new fluctuation-dissipation theorem (FDT) that is derived within the context of Brownian dynamics. The new FDT agrees with the JE in the near equilibrium regime but it is valid in far nonequilibrium regime where the JE does not stand. *In silico* experiments of unfolding polypeptides show that the new FDT is indeed accurate for far non-equilibrium processes.

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