

Molecular Mechanisms of Extreme Mechanostability in Microbial Adhesion

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Life is based on interactions between molecules. A large number of these molecular complexes are optimized for adequate resilience to mechanical stress e.g. to allow for adhesion, motility, and structural integrity in cells and tissues. In prokaryotic cells or in tissue of higher organisms the typical forces stabilizing these protein complexes peak in the range of tens of piconewtons. However, certain prokaryotic adhesion complexes were recently found to provide significantly higher mechanical stability beyond nanonewton values, reaching the limit of covalent bonds. We combined AFM-based SMFS with all-atom steered MD simulations to investigate the molecular mechanisms governing this extraordinary stability. This hybrid *in-vivo* and *in-silico* single molecule force spectroscopy reveals details of the force propagation paths and the delicate balance of unbinding and unfolding processes of the protein complexes under load. In this talk, an overview on recent discoveries on the high resilience complexes of cellulosomal constituents of different cellulolytic microbes and on the adhesion complexes of various staphylococcus strains will be given.

- 1) Molecular mechanism of extreme mechanostability in a pathogen adhesin

Lukas F. Milles, Klaus Schulten, Hermann E. Gaub, Rafael C. Bernardi
Science, March 2018, DOI: 10.1126/science.aar2094

- 2) Direction matters: Monovalent Streptavidin/Biotin complex under load

Steffen M. Sedlak, Leonard C. Schendel, Marcelo C. R. Melo, Diana A. Pippig, Zaida Luthey-Schulten, Hermann E. Gaub, and Rafael C. Bernardi,
Nano Lett., October 2018, doi:10.1021/acs.nanolett.8b04045

- 3) Calcium stabilizes the strongest protein fold

Lukas F. Milles, Eduard M. Unterauer, Thomas Nicolaus, Hermann E. Gaub
Nature Communications, November 2018, DOI: 10.1038/s41467-018-07145-6