

**Colloquium**  
**Dahlem Center for Complex Quantum Systems**

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**Stretching proteins - how macromolecules propagate mechanical forces**

**Location: Hörsaal A (1.3.14)**

**Time: Monday, January 9, 2012, 14:00 c.t.**

**Abstract:**

The talk will give insight into the impact of force on biosystems at different length and time scales, from small molecules using quantum and molecular mechanics to complex biomaterials, using continuum mechanics.

The mechanics of complex structures like proteins is determined by the way force distributes through the structure. We recently developed a technique termed Force Distribution Analysis (FDA), based on standard Molecular Dynamics simulations, to reveal the propagation of stress through a molecular structure. FDA is the atomistic-scale analogue of Finite Element Analysis for macroscopic structures.

I will describe the concept of FDA, and recent applications to different protein systems with mechanical function, most importantly silk fibers. In addition, on the small molecular scale, the effect of stretching forces onto the quantum mechanics of chemical bonds will be discussed.