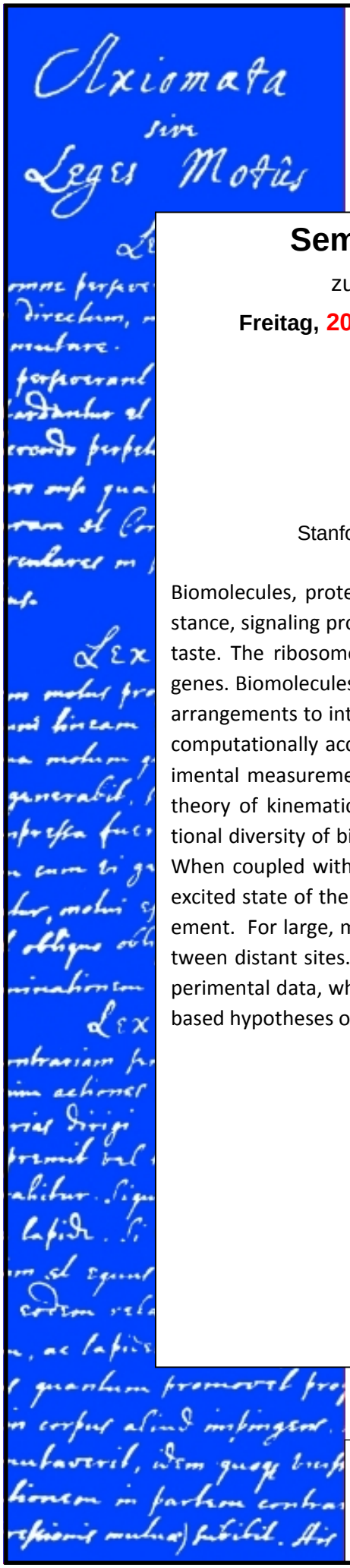

Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Freitag, 20.06.2014, 10:00 Uhr, Haberstraße 1, Raum 01.025

Molecular-scale Kinematics in Computational Structural Biology

Dr. Henry van den Bedem

Stanford University, SLAC National Accelerator Laboratory

Biomolecules, proteins and non-coding RNA, are the workhorses of the cell. For instance, signaling proteins mediate cellular response to sensory input such as vision or taste. The ribosome, a large protein/RNA complex, synthesizes new proteins from genes. Biomolecules are highly dynamic, sampling a wide range of conformational rearrangements to interact with binding partners and perform their function. However, computationally accessing conformational substates, and connecting them to experimental measurements, remains challenging. I will present techniques based on the theory of kinematically redundant manipulators to efficiently probe the conformational diversity of biomolecules, ranging from small RNAs to large protein complexes. When coupled with experimental data, our procedure revealed a 'hidden' transient excited state of the apical binding loop of the RNA HIV1 trans-activation response element. For large, multi-protein complexes we observed conformational coupling between distant sites. Our computational procedure enables an integrative view of experimental data, which can provide the tools to formulate and test dynamic, motion-based hypotheses of functional mechanisms in protein and RNA.

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