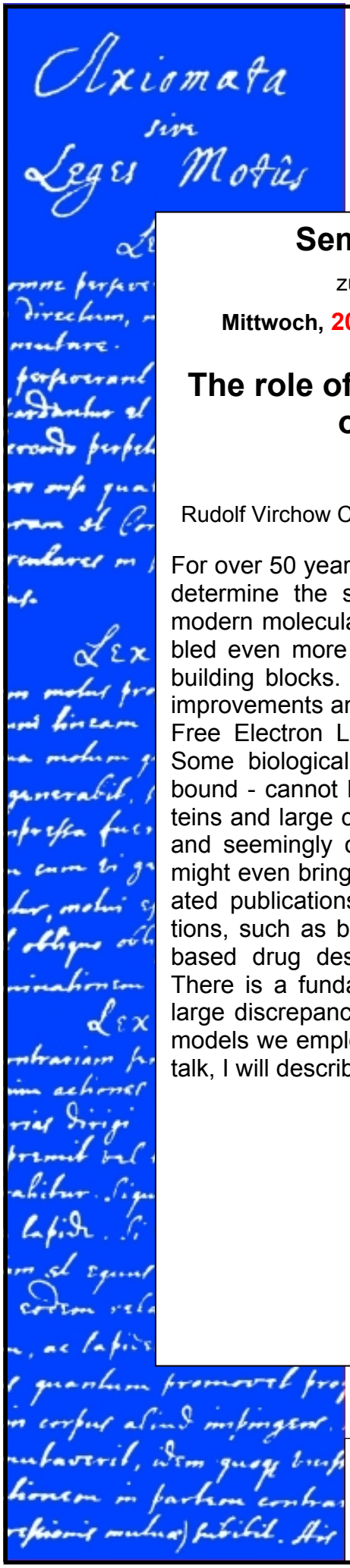

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Mittwoch, 20.11.2019, 09:30 Uhr, Immerwahrstr. 1, Raum 01.025

The role of models in the structure determination of biological macromolecules

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For over 50 years, X-ray crystallography has been the primary method to determine the structures of biological macromolecules, thus defining modern molecular biology. NMR and more recently, Cryo-EM have enabled even more insight into these fascinating molecular machines and building blocks. But even with over 14000 known structures, countless improvements and investments such as the 3.4 km long European X-Ray Free Electron Laser (EuXFEL) in Hamburg, there are still limitations: Some biological questions - for example whether a certain ligand is bound - cannot be answered; some structures, such as membrane proteins and large complexes, cannot be solved; and worst of all, published and seemingly correct structure solutions can have integral flaws that might even bring about complete retraction of a structure and the associated publications. The problem is aggravated as downstream applications, such as biophysical calculations, molecular dynamics and target-based drug design, depend on crystallographic models as a basis. There is a fundamental problem underlining all of these problems: the large discrepancy between the measured X-ray diffraction data and the models we employ to interpret these data. What causes this gap? In this talk, I will describe our search for an answer to this question.

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