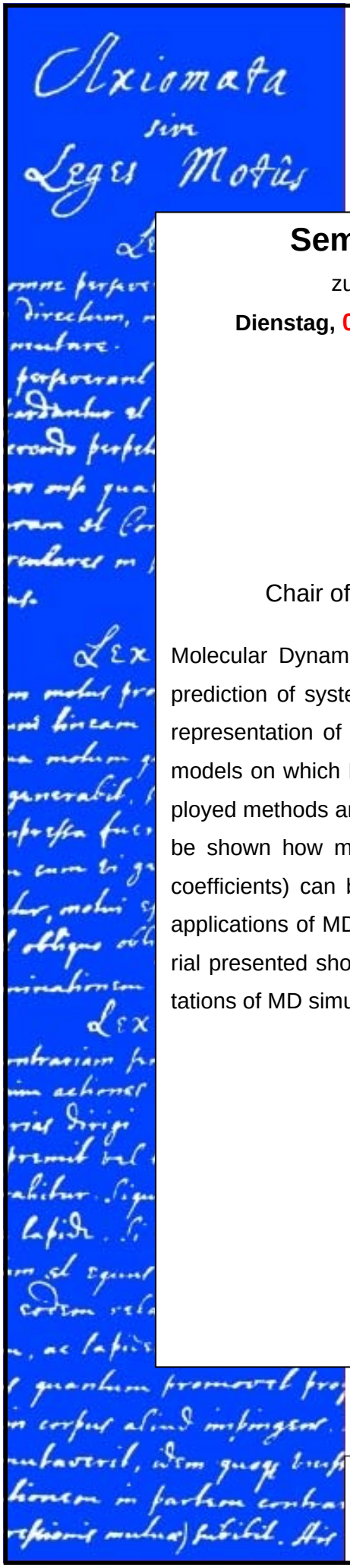

Friedrich-Alexander-Universität
Erlangen-Nürnberg

Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Dienstag, 02.03.2010, 11:30 Uhr, Egerlandstr. 5, Raum 0.044

Introduction to Molecular Dynamics simulations

Dr. Enrico Riccardi

Chair of Theoretical Physical Chemistry, TU Darmstadt

Molecular Dynamics (MD) is a computational technique for the quantitative prediction of system properties from basic physical principles and “atomistic” representation of matter. In the first part of the presentation, the constitutive models on which MD is based will be discussed and the most commonly employed methods and algorithms will be described. In the second part it will then be shown how microscopic and macroscopic system properties (i.e. elastic coefficients) can be calculated by MD simulations. An overview on possible applications of MD by actual research examples will also be given. The material presented should allow non-specialists to estimate the capability and limitations of MD simulation techniques.

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