MAX-BORN-INSTITUT FÜR NICHTLINEARE OPTIK UND KURZZEITSPEKTROSKOPIE IM FVB E.V.

Institutskolloquium

Am **26. Oktober 2005, 16:00 Uhr** spricht:

Prof. Dr. Dominik Marx
Ruhr-Universität Bochum, Lehrstuhl für Th. Chemie

über

Nonadiabatic ab initio Molecular Dynamics: Coupled Proton-Electron Transfer in Solution

The theoretical treatment of photoinduced dynamical processes in condensed phase molecular systems such as hydrogen-bonded liquids is a challenge to Theoretical Chemistry. Here, a recent extension of Car-Parrinello ab initio molecular dynamics which allows to include approximately electronically nonadiabatic effects is presented. This technique makes possible simulations of systems of similar complexity to those typically studied by ground-state Car-Parrinello methods. Using this technique the influence of solvation and hydrogen-bonding on coupled proton-electron transfer involving the nucleobase Guanine will be investigated within a unified framework including gas phase, microsolvation, and full liquid solvation environments.

Ort: **Max-Born-Saal,**
MBI, Max-Born-Str. 2a

Interessenten sind herzlich eingeladen.

Prof. Dr. Th. Elsässer