Program Hünfeld Workshop

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2002"

Friday, April 12th, 2002

12.00 – 13.30 Arrival, registration, and lunch

13.30 – 13.55 Ute Röhrig (ETH Zürich)
Early Steps of the Rhodopsin Photocycle Explored by Molecular Dynamics Simulations

13:55 – 14:20 Nicoleta Bondar (Deutsches Krebsforschungszentrum, Heidelberg)
Computer simulations of proton transport pathways in bacteriorhodopsin

14:20 – 14:45 Martin Zacharias (Institut für Molekulare Biotechnologie, Jena)
Simulation of the structure and dynamics of nucleic acid motifs

14:45 – 15:10 Heiko Carstens (Ludwig-Maximilians Universität München)
Conformational Dynamics of Photoswitchable Cyclic Peptides

15:10 – 15:35 Marcus Elstner (Deutsches Krebsforschungszentrum, Heidelberg)
New approaches for the description of biomolecules in their ground and excited states

15:35 – 15:55 Coffee break

15:55 – 16:20 Florian Müller-Plathe (MPI für Polymerforschung, Mainz)
Systematic Coarse - graining of Macromolecules : Recent Developements and Future directions

16:20 – 16:45 Gunnar Schröder (MPI für Biophysikalische Chemie, Göttingen)
Simulation of Fluorescence Anisotropy Experiments

16:45 – 17:10 Rainer Böckmann (MPI für Biophysikalische Chemie, Göttingen)
Nanoseconds molecular dynamics simulation of primary mechanical energy transfer steps in F_1-ATP synthase

17:10 – 17:35 Jürgen Schlitter (Ruhr-Universität Bochum)
Simulation of activated processes - Formation and breakup of an insulin phenol complex

17:35 – 18:00 Christian Kandt (Ruhr-Universität Bochum)
Dynamics of internal water molecules in bacteriorhodopsin

18:05 – 19:00 Dinner

19:00 – 21:00 Poster Sessions

Saturday, April 13th, 2002

8:00 – 8:40 Breakfast

8:40 – 9:05 Torsten Becker (IWR, Universität Heidelberg)
Resolution effects in elastic incoherent neutron scattering of biomolecules

9:05 – 9:30 Matthias Schmitz (Ludwig-Maximilians Universität München)
Using QM vibrational analysis to monitor DNA repair by Photolyase

9:30 – 9:55 Heinz Sklenar and Remo Rohs (Max-Delbrück-Centrum, Berlin)
Monte Carlo Simulations of nucleic acid structures

9:55 – 10:20 Matthias Ullmann (IWR, Universität Heidelberg)
Electrostatic calculations for understanding proton and electron transfer in proteins.

10:20 – 10:40 Coffee break

10:40 – 11:05 Tomaso Frigato (MPI für Biophysik, Frankfurt)
Proton Transport in H2O and in D2O simulated with Q-HOP molecular dynamics

11:05 – 11:30 Christian Gorba (MPI für Biophysik, Frankfurt)
Diffusional Dynamics of Cytochrome c Molecules close to a charged surface

11:30 – 11:55 Yuguang Mu (J. W. Goethe Universität, Frankfurt)
Conformational dynamics of trialanine in water: Comparison with different force fields and experiments

12:00 Lunch

13:00 Departure