

# Physics Colloquium

## Michigan Technological University

March 2 (Thursday) 2006, 4:00 to 5:00 pm  
Room 139, Fisher Hall

### Solvation by means of Poisson-Boltzmann Methods in Biomolecular Simulation

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#### Abstract

Poisson Boltzmann Methods are frequently employed in simulations of biomolecular matter. They account for the modulating effect of the solvent when some biomolecule becomes dissolved in medium, i.e. water in the majority of cases. In the present seminar we want to discuss basic principles of Poisson Boltzmann methods, outline technical limitations, and show a non-conventional implementation and present recent results.

#### Biography

Siegfried Hoefinger received his PhD degree in Theoretical Chemistry from the University of Vienna in 1998. Subsequently, he was postdoctoral fellow at the Institut de Genetique et de Biologie Moleculaire et Cellulaire in Strasbourg and at the University of Bologna and research assistant at the University of Vienna. In 2001 he became a research associate at the Novartis Institutes for Biomedical Research, Vienna. In late 2005 he joined the group of Prof. U.H.E Hansmann and thus has found his way into the Department of Physics at the Michigan Technological University. His research includes various aspects of the solvation effect, quantum chemistry, high performance computing and the simulation of biomolecular systems.