

## EINLADUNG

zum Vortrag von

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über

**Conical intersections of potential-energy  
surfaces and ultrafast deactivation of excited  
electronic states in biomolecules**

am

**Dienstag, dem 6. Dezember 2005, um 17.30 Uhr**

im Großen Hörsaal des Instituts für Experimentalphysik der Universität Wien  
1090 Wien, Strudlhofgasse 4 / Boltzmannngasse 5, 1. Stock

### Abstract:

It is nowadays well established that conical intersections of electronic potential-energy surfaces are ubiquitous in polyatomic molecules and that they play a decisive role in photochemistry. Ultrafast excited-state deactivation is an essential aspect for the photostability of the building blocks of life. The talk gives a nontechnical overview of generic aspects of time-dependent quantum wave-packet dynamics at conical intersections for representative *ab initio* based models. A simple qualitative picture is developed which allows us to rationalize how conical intersections can effect internal-conversion processes within less than 100 femtoseconds. Evidence is presented that only few degrees of freedom are needed to describe ultrafast internal-conversion dynamics at femtosecond time scales, even in large systems. This opens the perspective of an *ab initio* treatment of elementary photochemical processes, provided that the few active degrees of freedom can be identified by *ab initio* calculations. The basic mechanisms which ensure the exceptional photostability of DNA and proteins are revealed by calculations on DNA bases, base pairs and peptides.