

- c hemisch
- p hysikalische
- g esellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz,  
J. Loschmidt, J. Petzval und J. Stefan



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Fakultät für Chemie

## EINLADUNG

zum Vortrag von

**Prof. Dr. Wolfgang Domcke**

Department of Chemistry, Technical University of Munich

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 / Boltzmanngasse 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.

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Präsident 2004/05: Ao.Univ.Prof. Dr. Harald F. Kauffmann, Institut für Physikalische Chemie, Universität Wien