

## **EINLADUNG**

zum Vortrag

von

**Dr. Sebastian Mai**

Loschmidt-Preisträger 2017

Institut für Theoretische Chemie, Universität Wien

über

### **Excited-state dynamics of nucleobase analogues**

am

**Dienstag, 17. April 2018, um 17:30 Uhr**

**Ort:** Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,  
1090 Wien, Strudlhofgasse 4 / Boltzmannngasse 5, 1. Stock

*Barrierefreier Zugang: Boltzmannngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals*

#### **Abstract:**

The DNA, carrier of the genetic information, possesses several protection mechanisms against damage induced by absorption of UV light. One of these protection layers is given by the ability of the DNA nucleobases to relax to the electronic ground state within only a few picoseconds after absorption. The efficiency of this relaxation depends sensitively on the molecular structure. Therefore, the so-called nucleobase analogues - molecules structurally similar to DNA nucleobases and used in a number of medical therapies and in molecular biological research - are not well protected against UV radiation. In order to study from a computational viewpoint how molecular structure affects photostability in nucleobase analogues, during my dissertation in the AG González I significantly developed the SHARC molecular dynamics method. In my talk, I will present this dynamics method, together with the results I obtained for the investigated nucleobases and nucleobase analogues.

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#### **CHEMISCH-PHYSIKALISCHE GESELLSCHAFT**

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