

SFB  
1078



Protonation Dynamics  
in Protein Function

Wed, **October 19,**  
2016

**10:00 – ca. 16:00**

**TU Berlin**

**PC Building**

**Library – Room PC 305**

Straße des 17. Juni 135  
10623 Berlin-Charlottenburg

## ➤ **Workshop**

### **IR Spectroscopy of Peptides and Proteins**

➤ The workshop will address topics related to the qualitative and quantitative analysis of IR spectroscopy of peptides and proteins. Special focus will be laid on protein secondary structure changes.

➤ The idea is to have sufficient time for discussion, such that the lectures that will be presented should be kept as short as possible. Instead, all participants (not only those listed below) are encouraged to contribute to discussion, also by presenting one or two slides, if appropriate.

#### **Introduction – 10:00**

#### **Peptides – Contributions**

**Prof. Timothy A. Keiderling** (University of Illinois, Chicago, USA)  
*Calculation of amide modes*

**Dr. Jacek Kozuch / Prof. Maria Andrea Mroginski** (TU Berlin)  
*Peptide-membrane interactions – a theoretical approach*

**Dr. Marius Horch** (TU Berlin)  
*Side chain modes*

#### **Proteins – Contributions**

**Prof. Karin Hauser** (University of Konstanz, Germany)  
*Protein dynamics and amide band changes*

**Dr. Francisco Velazquez Escobar** (TU Berlin)  
*Secondary structure changes in phytochromes*

**Prof. Maria Andrea Mroginski / Dr. Tillmann Utesch** (TU Berlin)  
*MD approaches towards secondary structure changes*

**Jan Daldrop** (FU Berlin)  
*Theoretical approach towards the IR continuous bands of hydrogen-bonded water*

Lunch break will be at ca. 13:00.

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