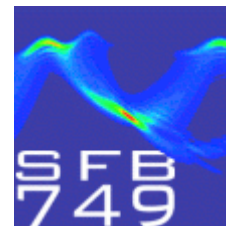


2nd SFB 749 workshop in Wildbad Kreuth: 30.03.-01.04 2009



Montag, 30.03.2009

12:00 - 13:30

lunch

13:55

welcome

14:00

Tatiana Domratcheva, Max Cryle, Thomas Barends (A6):
Structure function analysis of 6-4 photolyase

14:30

Andreas Glas (A4): News from the (6-4) photolyase

15:00

Wolfgang Zinth (A5): Thymine dimerization in different DNA
model systems: the CPD photolesion is predominantly formed via
the singlet channel

15:30 – 16:00

coffee break

16:00

Hendrik Zipse: Thermodynamic aspects of radical reactions

16:30

Irmgard Frank: First principles simulation: news from Hannover

17:00- 18:00

Theorie: Nomenklatur, Konzepte und Methoden (part I)

Kleines ABC der Quantenchemie: Basissatz, Elektronenstrukturmethoden und
Nomenklatur

(R. de Vivie-Riedle)

Methoden zur Berechnung thermochemischer Daten

(H. Zipse)

18:00-19:00

dinner

19:00-20:00

Theorie: Nomenklatur, Konzepte und Methoden (part II)

Was ist QM/MM und wie funktioniert es?

(T. Domratcheva)

Was sind eigentlich Replica-Exchange Simulationen

(R. Denschlag)

Vorteile und Grenzen von Replica-Exchange: Ausgewählte Anwendungen

(M. Lingenheil)

Dienstag, 31.03.2009

9:00

Benjamin Fingerhut (C2): Photoreactions: isomerization in the 6-
4 photodamage and light induced S_{N1} dynamics

9:30

Christian Sailer (B5): Bimolecular reactions from nanoseconds
down to the rotational limit and below

10:00

Mayr and co-workers (B1): Kinetics of polar organic reactions;
progress of last year

11:00 – 11:30

coffee break

11:30

Mikhail Mikhailau (B5): First insights into the ultrafast dissociation
dynamics of diphenylallyl systems

11:45

Konrad Koszinowski (B7): Surprising complexity of seemingly
simple organometallic reagents and intermediates

12:15-14:00 **lunch**

14:00 Tobias Thaler (B2): Organometallics - synthesis, selectivity and dynamics

14:30 Thomas Bein (B6/A2): Dynamics of single molecules in mesoporous host systems

15:30 – 16:00 **coffee break**

16:00 Simone Draxler (A5): Fulgides and fulgimides - dynamics and yields tuned by vibrational excess energy

16:30 Artur Nenov (C2): Characterization of the conical intersection seam for trifluoromethyl-pyrrolylfulgid

17:00 Igor Pugliesi (B5): Novel transient spectroscopy based on supercontinuum fiber lasers: a fast arising chance for the investigation of slow charge recombination in solar cells

17:15 Andrzej Sobolewski (C1): Photochemical water splitting with visible light

18:00-19:00 **dinner**

19:30 Mitgliederversammlung

Mittwoch, 01.04.2009

9:00 Thomas Böttcher (A3): The S.aureus Clp system - dynamic regulation of virulence

9:30 Paul Tavan (C4): What the amide bands in the IR spectra of proteins and peptides can tell us: new computational methods and first applications

10:30 – 11:00 **coffee break**

11:00 Andreas Reiner (A8): Conformational dynamics of alpha helices and small proteins

11:30 Matthias Feige (A1): How antibodies fold

12:00 Martin Sikor and Nikolaus Naredi-Rainer (A2): Single molecule investigations of heat shock proteins: HSP70 and HSP90

12:30-14:00 **lunch**

end of workshop

14:00 Vorstandssitzung