

Deutsche
Forschungsgemeinschaft

DFG

Department of Science & Technology

Joint Indo-German Workshop

**Electronically Excited Molecules:
Structure and Dynamics**

Neuss (near Düsseldorf)
6th - 8th September 2009

*Telekom Tagungshotel
Humboldtstr. 2, 41468 Neuss*

Preliminary Programme

Sunday, 6 Sept. 2009

Location: Foyer, TBA

18:00 –

Dinner & social get-together

Monday, 7 Sept. 2009

Location: Meeting room in the Tagungshotel

8:45 - 9:00

Welcome and opening

9:00 - 9:30

D. Mukherjee (Kolkata)

Aspects of Spin-Adaptation in Multi-Reference Coupled Cluster Formalisms using Multi-exponential Type Cluster Ansatz: State-universal and State-specific Approaches

9:30 - 10:00

A. Dreuw (Frankfurt)

Development of quantum chemical methods for the investigation of excited states of large molecules

10:00 - 10:30

Coffee Break

10:30 - 11:00

S. Pal (Pune)

Coupled-cluster approach for spectra, resonance and properties

11:00 - 11:30

C. Marian (Duesseldorf)

Calculating spin-dependent properties by means of multi-reference configuration interaction methods

11:30 – 12:00

M. Pernpointner (Heidelberg)

Relativistic ADC: a powerful tool for quantum chemistry

12:00 - 14:00

Lunch Break

14:00 - 14:30

N. Sathyamurthy (Chandigarh)

Atoms and molecules in a confined environment

14:30 - 15:00

P. Saalfrank (Potsdam-Golm)

Correlated dynamics of laser-pulse excited electrons

15:00 - 15:30

K. D. Sen (Hyderabad)

Exact Relations for Confined One-Electron Systems

- 15:30 - 16:00** Coffee Break
- 16:00 - 16:30** **W. Domcke** (Munich)
Vibronic coupling by the spin-orbit operator in molecules and clusters
- 16:30 - 17:00** **B. Maiti** (Varanasi)
Importance of Intersystem Crossing in Chemical Reactions
- 17:00 - 17:30** **S. Mahapatra** (Hyderabad)
Quantum Dynamics of Electronically Excited Molecules: Current Developments and Future Challenges
- 17:30 - 18:00** **H. Köppel** (Heidelberg)
TBA

Tuesday, 8 Sept. 2009

Location: Meeting room in the Tagungshotel

- 8:30 - 9:00** **W. Eisfeld** (Bielefeld)
Accounting for strong anharmonicity and dissociation in vibronically coupled systems
- 9:00 - 9:30** **S. Kumar** (Chennai)
Non-adiabatic Collision Dynamics in the Ion- and the Electron-Molecule Reactions
- 9:30 - 10:00** **J. Manz** (Berlin)
Effects of molecular symmetry on quantum reaction dynamics via conical intersections
- 10:00 - 10:30** Coffee Break
- 10:30 - 11:00** **S. Adhikari** (Kolkata)
On the theoretical treatment of multi-state Born-Oppenheimer system with ab-initio and dynamical calculations
- 11:00 - 11:30** **M. Durga Prasad** (Hyderabad)
Coupled cluster approaches to wave packet dynamics
- 11:30 - 12:00** **M. K. Mishra** (Mumbai)
Laser Assisted Control of Bond Cleavage using Repulsive Excited States

12:00 - 14:00	Lunch Break
14:00 - 14:30	R. de Vivie-Riedle (Munich) Structure, dynamics and control of complex chemical systems
14:30 - 15:00	O. Kühn (Rostock) Nonadiabatic Quantum Dynamics and Laser Control of Br₂ in Solid Argon
15:00 - 15:30	V. Bonacic-Koutecky (Berlin) Analysis and Control of Nonadiabatic Dynamics in Complex Systems
15:30 - 16:00	E. D. Jemmis (Thiruvananthapuram) Design of stuffed fullerene-like boron nanoclusters
16:00 - 16:30	Round table discussion on future prospects of Indo-German science collaborations in the field
16:30 - 17:00	Further discussion / END of workshop
17:00 - 17:30	Beginning of STC2009 (Coffee)
17:30	Opening of STC2009

