PROGRAM

MCBR4 Scientific Meeting

Venue: IWH, Hauptstrasse 242, D-69117 Heidelberg

February 23 – 25, 2015

Institute of Inorganic Chemistry (ACI) and the Interdisciplinary Center for Scientific Computing (IWR)

Financial Support by the University of Heidelberg, the Heidelberg Graduate School MathComp (IWR), the Heidelberg Center of South Asia (HCSA) and the BASF

Welcome to MCBR4

The MCBR meetings were initiated by Profs. H. Zipse (LMU) and G.N. Sastry (IICT). MCBR1 was held in 2007 in Hyderabad, followed by MCBR2 (2009) in Wildbad Kreuth and MCBR3 (2013) in Chandigarh. In 2014, G.N. Sastry organized the 1st MCBR-related School in Hyderabad. MCBR4 in Heidelberg is the first to combine a School for PhD students with the scientific meeting and also includes PhD student exchange to strengthen the collaboration between Indian and German research groups. Moreover, it is the first MCBR meeting to extend the Indo-German collaboration to an Indo-German-Japanese network of scientists interested in the physics and modeling of chemical activity, specifically also of biological systems. We hope that MCBR meetings will continue to attract scientists from India, Germany and Japan, interested in the various aspects of fundamental theory, modeling and simulation of structure, electronics, interaction and reactivity of molecular systems, in particular in relation to biology, and that these meetings will continue to combine applied theory and modeling and will continue to be a platform for fundamental and applied research, in particular also for young scientists.

The 3 modules of MCBR4 include:

A 6 day School on electronic structure theory that includes ca. 50% theory and 50% hands-on computation by the 20 students from India and Germany. Part of the time at the computer is used for mini-research projects.

The 3 day MCBR4 scientific meeting with over 20 established scientists from India, Japan and Germany as well as the 20 participants of the school will include scientific lectures, flash presentations by the participants of the School and a poster session.

An exchange program for 5 of the Indian and 5 of the German participants of the School. The selected Indian PhD students will stay on for 2 months with one of the participating German groups and one student each of these German groups will then spend 2 months in India.

The expectation is that the three modules will help to strengthen the links between Indian and German research in this area and therefore help to further advance the MCBR idea and also promote it in Japan.

We are indebted to the strong support from the University of Heidelberg, the Heidelberg Graduate School MathComp of the Interdisciplinary Center for Scientific Computing (IWR) and the Heidelberg Center of South Asia (HCSA).

We wish you a good time at the International Academic Forum Heidelberg (IWH) and at the University of Heidelberg.

MCBR4 Meeting February 23 – 25

Monday, February 23

9:15	Welcome
9:30	*A Journey Through Three-Membered Rings*, E. D. Jemmis, Indian Institute of Science, Bangalore
10:00	*Coffee Break*
10:30	*Computational Mutation and Control of Enzymatic Reaction*, Kazunari Yoshizawa, Kyushu University
11:10	*Hypervalent and Planar Tetravalent Carbon in Grubbs and Schrock Type Metallacycles*, Cherumuttathu Suresh, CSIE-NIIST Trivandrum
11:50	*Radicals in Enzymatic Catalysis*, Hendrik Zipse, University of Munich
12:30	*Lunch*
14:00	Poster Flash Presentations
	(20 students, each 5 minutes per project)
15:30	*Coffee Break*
16:00	Poster Session
18:00	*Dinner*

Tuesday, February 24

8:40	*Density Based Adaptive QM/MM methods for Complex (Bio-)Chemical Systems*, Mark Waller, University of Münster
9:20	*XYZ*, Sourav Pal, CSIR, Pune
10:00	*Coffee Break*
10:30	*Property predictions based on quantum-chemically derived empirical descriptors*, Bodo Martin, University of Heidelberg
11:10	*Dispersion and stacking interactions contribute to protein unfolding in aqueous urea*, Deva Priyakumar, IIIT, Hyderabad
11:50	*Analyzing the transition states of ethylene polymerization catalysts to develop a QSAR model for catalyst design,* Evans Coutinho, Bombay College of Pharmacy, Mumbai
12:30	*Lunch*
14:00	*The algebraic-diagrammatic construction for the polarization propagator - a versatile approach to excited electronic states,* Andeas Dreuw, University of Heidelberg
14:40	*Role of Molecular Modeling on the Development of Molecule Based Magnetic Materials,* Rajaraman Gopalan, IIT Mumbai
15:20	*Molecular Property and Reactivity of Transition Metal Complex: Theoretical Understanding and Prediction*, Shigeyoshi Sakaki, Kyoto University
16:00	*Coffee Break*
16:30	*Interplay of structural stability and dynamics: Control of gene expression by RNA*, Holger Gohlke, University of Düsseldorf
17:10	*Mechanism-Based Inhibition of CYP450 by Reactive Metabolites: A Quantum Chemical study*, Prasad V. Bharatam, NIPER, Nagar
17:50	*Theoretical studies on isocyanate oligomerization*, Yohei Oe,
19:30	*Conference Dinner at Haus Buhl*

Wednesday, February 25

8:40	*Crucial Role of Protein Flexibility in Enzymatic Catalysis*, Shigehiko Hayashi, Kyoto University
9:20	*Fully quantal approach to nonadiabatic molecular photodynamics, H*orst Köppel, University of Heidelberg
10:00	*Coffee Break*
10:30	*XYZ,* Paolo Carloni, FZ Jülich
11:10	*Exploring the mechanistic insights of Ru(II)-Mediated CO2 Insertion Reactions and Ni(II)-Catalysed Alkane Hydroxylation – A DFT study*, Prahba Vadivelu, CSIR-NIIST, Trivandrum
11:50	*Semiempirical excited-state dynamics,* Walter Thiel, MPI Mülheim
12:30	*Lunch*
14:00	*Are there (yet) untapped protein kinases for drug development - a druggability assessment of ATP-binding* sites, Simone Fulle, BioMedX Heidelberg
14:40	*Non-Covalent Interactions: Contrasting Perspectives of Quantum Chemistry, Chemoinformatics and Molecular Dynamics,* G. N. Sastry, Indian Institute of Chemical Technology, Hyderabad
15:20	*Interaction of Biomolecules with Carbon Nanomaterials*, V. Subramanian, CSIR, Chennai
16:00	*Coffee Break*
16:30	*Some Exercises in Modern Chemical Bonding Theory*, Gernot Frenking, University of Marburg
17:50	Wrap-up discussion
19:00	*Dinner, Drinks from 18:30h*

Delegates list

Bharatam, Prasad V.	NIPER Email: : pvbharatam@niper.ac.in
Carloni, Paolo	Forschungszent Jülich Email: p.carloni@fz-juelich.de
Comba, Peter	University of Heidelberg Email: peter.comba@aci.uni-heidelberg.de
Coutinho, Evans	Bombay College of Pharmacy Email: evans@bcpindia.org
Deva Priyakumar	Indian Institute of Information Technology Hyderabad, Email: deva@iiit.ac.in
Dreuw, Andreas	University of Heidelberg Email: dreuw@uni-heidelberg.de
Frenking, Gernot	University of Marburg Email: frenking@chemie.uni-marburg.de
Fulle, Simone	BioMedX, Heidelberg Email: fulle@bio.mx
Gohlke, Holger	University of Düsseldorf Email: gohlke@uni-duesseldorf.de
Hayashi, Shigehiko	Kyoto University Email: hayashig@kuchem.kyoto-u.ac.jp
Jemmis, E. D.	Indian Institute of Science, Bangalore Email: jemmis@ipc.iisc.ernet.in
Köppel, Horst	University of Heidelberg Email: horst.koeppel@pci.uni-heidelberg.de
Martin, Bodo	University of Heidelberg Email: bodo.martin@aci.uni-heidelberg.de
Mewes, Jan	University of Heidelberg Email: jan.mewes@iwr.uni-heidelberg.de
Rajaraman, Gopalan	Indian Institute of Technology Bombay Email: rajaraman@chem.iitb.ac.in
Sakaki, Shigeyoshi	Kyoto University Email: sakaki.shigeyoshi.47e@st.kyoto-u.ac.jp
Sastry, G. Narahari	Indian Institute of Chemical Technology Hyderabad, Email: gnsastry@iict.res.in
Schäfer, Ansgar	BASF SE Email: ansgar.schaefer@basf.com
Sourav Pal	CSIR-National Chemical Laboratory, Pune Email: s.pal@ncl.res.in
Subramanian V	Central Leather Research Institute , CSIR Chennai , Email: subbu@clri.res.in
Suresh, Cherumuttathu H	CSTD,CSIR-NIIST, Trivandrum Email: sureshch@gmail.com
Thiel, Walter	Max-Planck-Institut für Kohlenforschung Email: thiel@kofo.mpg.de
Vadivelu, Prahba	CSTD,CSIR-NIIST, Trivandrum Email: prabha.vadivelu@niist.res.in
Waller, Mark	University of Münster Email: m.waller@uni-muenster.de
Wormit, Michael	University of Heidelberg Email: michael.wormit@iwr.uni-heidelberg.de
Yohei Oe	Doshisha University Gastprofessor bei Zipse, University of Munich Email: yooech@cup.uni-muenchen.de
Yoshizawa, Kazunari	Kyushu University Email: kazunari@ms.ifoc.kyushu-u.ac.jp
Zipse, Hendrik	LMU, Munich Email: zipse@cup.uni-muenchen.de