



UNIVERSITÄT  
HEIDELBERG  
ZUKUNFT  
SEIT 1386

## PROGRAM

### MCBR4 Winter School

Venue: IWH, Hauptstrasse 242, D-69117 Heidelberg and Otto-Meyerhof-Zentrum (OMZ), Im Neuenheimer Feld 350, 69120 Heidelberg (maps see last page)

February 17 – 22, 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



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SOUTH ASIA



## 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 1<sup>st</sup> 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 Winter School

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### Tuesday, February 17 (IWH)

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8:30 – 8:45	<i>Welcome</i>
8:45 – 10:00	Basic electronic structure theory (Jan Mewes, Michael Wormit) <i>Coffee Break</i>
10:30 – 12:00	Basic electronic structure theory (Michael Wormit, Hendrik Zipse) <i>Lunch Break</i>
14:00 – 15:30	Analysis tools & properties; NBO, AIM, charges (Bodo Martin) <i>Coffee Break</i>
16:00 – 17:30	QM/MM and large systems (G.N. Sastry) <i>Dinner</i>

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### Wednesday, February 18

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8:30 – 10:00	Applications in organic chemistry (Hendrik Zipse) <i>Coffee Break</i>
10:30 – 12:00	Applications in biological systems (G. N. Sastry) <i>Lunch Break</i>
14:00 – 15:30	Applications in bioinorganic chemistry (Rajaraman Gopalan) <i>Coffee Break</i>
16:00 – 17:30	Applications to excited states (Michael Wormit) <i>Dinner</i>

<b>Thursday, February 19</b>		<b>Saturday, February 21</b>	
8:30 – 10:00	Hands-on Tutorials <i>Coffee Break</i>	8:30 – 10:00	Student projects <i>Coffee Break</i>
10:30 – 12:00	Hands-on Tutorials <i>Lunch Break</i>	10:30 – 12:00	Student projects <i>Lunch Break</i>
14:00 – 15:30	Hands-on Tutorials <i>Coffee Break</i>	14:00 – 15:30	Student projects <i>Coffee Break</i>
16:00 – 17:30	Hands-on Tutorials <i>Dinner</i>	16:00 – 17:30	Student projects <i>Dinner</i>
<b>Friday, February 20</b>		<b>Sunday, February 22</b>	
8:30 – 10:00	Applications in molecular magnets and computational spectroscopy (Rajaraman Gopalan) <i>Coffee Break</i>	8:30 – 10:00	Student projects <i>Coffee Break</i>
10:30 – 12:00	Dynamics, including no BO effects I (Horst Köppel) <i>Lunch Break</i>	10:30 – 12:00	Student projects <i>Lunch Break</i>
14:00 – 15:30	Dynamics, including no BO effects II (Horst Köppel) <i>Coffee Break</i>	14:00 – 15:30	Student projects <i>Coffee Break</i>
16:00 – 17:30	Presentation of student projects <i>Dinner</i>	16:00 – 17:30	Wrap-up discussion <i>Dinner</i>

## Participants list

Mr. Harish Jangra	University of Munich
Ms. Sandhiya Lakshmanan	University of Munich
Johannes Straub	University of Heidelberg
Markus Rössler	University of Heidelberg
Dennis Müller	University of Heidelberg,
Jie Han	University of Heidelberg
Jörg Eisele	University of Heidelberg
Daniel Ciupka	University of Düsseldorf
Gulia Pagani	University of Düsseldorf
Suzanne McAnanama- Brereton	University of Münster
Min Zheng	University of Münster
Azaj Ansari	Indian Institute of Technology Bombay
Mohammad Hussain	Indian Institute of Chemical Technology Hyderabad
Bhaskar Sharma	Indian Institute of Chemical Technology Hyderabad
J. Vijaya Sundar	Central Leather Research Institute Chennai
Ms. Bai Anjali	CSTD,CSIR-NIIST, Kerala
Mr. Chaitanya Kr. Jaladanki	NIPER, Punjab
Ms. Priyakumari	Indian Institute of Science Bangalore
Siladitya Padhi	International Institute of Information Technology Gachibowli Hyderabad
Sudip Pan	Bombay College of Pharmacy