



Modeling Chemical and Biological (Re)activity

Indian Institute of Chemical Technology, Tarnaka, Hyderabad - 500007

<http://203.199.182.73/gnsmmg/MCBR/index.html>

Topics

Large Molecular Systems - Methodology
Non-Covalent Interactions
Catalysis
Organic Reaction Mechanisms
Reactivity Descriptors
Biological Activity
Drug-Receptor Interactions
Molecular Dynamics

Objective

To have an Indo-German initiative for the discussion of the emerging trends in computational modeling of chemical reactivity and biological activity. The emphasis of the meeting will be on problems of experimental relevance and on getting the right answers for right reasons from theoretical modeling. Thus, there is a necessity to expand the realm of first principle calculations to medium sized and larger molecules. Drug design and catalyst design were identified as two important topics, where there is high activity in contemporary computational and experimental research. Germany is in the forefront of this activity and India, which made significant straits in information technology and with a talented pool of scientists, is an emerging force. Moreover, the barriers between various branches of chemistry and biology are looking more superfluous now than ever.

Speakers

I. Antes	S. Balasubramanian
T. Becker	S. Bandyopadhyay
P. Comba	P. V. Bharatam
G. Frenking	P. K. Chattaraj
H. Gohlke	E. Coutinho
S. Grimme	S. R. Gadre
G. Klebe	E. D. Jemmis
J. Sauer	S. Mahapatra
P. R. Schreiner	S. Pal
W. Sippl	K. Roy
B. Straub	N. Sathyamurthy
W. Thiel	V. Subramanian
R. C. Wade	R. B. Sunoj
M. Zacharias	C. H. Suresh
H. Zipse	P. Venuvanalingam

Contact

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Registration

- Corporate: Rs. 12,000/-
Academia: Rs. 3000/-
Rs. 4000/- (with accommodation)
Doctoral students and postdoctoral fellows:
Rs. 2000/-
Rs. 3000/- (with accommodation)
Accompanying person: Rs. 1500/-
- Invited speakers are registered.
- *Fee includes meals (breakfast, lunch and dinner including banquette).*
- 1 Euro \cong Rs. 55/-

Abstract & Poster Details

- Participants are requested to submit their abstract on or before **31st August 2007**.
- Abstract format is available in the conference website (<http://203.199.182.73/gnsmmg/MCBR/abstract.html>).
- Poster specifications can also be obtained from the conference website. The poster session will be held on the 28th September.
- The scientific advisory committee will select few outstanding posters and the best poster award will be announced on the 28th evening. Three of them will be given an opportunity to give oral presentation on 29th September.

All participants are requested to present a poster !

Local Organizing Committee

- Dr. J. S. Yadav (Chief Patron)
- Dr. A. C. Kunwar
- Dr. J. M. Rao
- Dr. M. Vairamani
- Dr. U. S. N. Murthy
- Dr. G. V. M. Sharma
- Dr. S. Chandrasekhar
- Dr. T. K. Chakraborty
- Dr. K. Bhanuprakash
- Dr. B. Jagannath
- Dr. Y. Soujanya
- Mr. D. Krishna Rao (Symposium Secretary)
- Dr. G. N. Sastry (Convener)

Scientific Advisory Committee

- Prof. Dr. P. K. Chattaraj
- Prof. Dr. P. Comba
- Prof. Dr. G. Frenking
- Prof. Dr. S. R. Gadre
- Prof. Dr. S. Grimme
- Prof. Dr. E. D. Jemmis
- Prof. Dr. D. Mukherjee
- Dr. S. Pal
- Dr. G. N. Sastry
- Prof. Dr. N. Sathyamurthy
- Prof. Dr. P. R. Schreiner
- Prof. Dr. W. Thiel
- Dr. J. S. Yadav
- Prof. Dr. H. Zipse

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