



S.A.S. NAGAR



3<sup>rd</sup> CONFERENCE ON



# MODELING CHEMICAL AND BIOLOGICAL (RE)ACTIVITY



THE 3<sup>rd</sup> INDO-GERMAN CONFERENCE ON

## MODELING CHEMICAL AND BIOLOGICAL (RE)ACTIVITY

26<sup>th</sup> Februry - 1<sup>st</sup> March 2013



## 3<sup>rd</sup> CONFERENCE ON MODELING CHEMICAL AND BIOLOGICAL (RE)ACTIVITY

26<sup>th</sup> February - 1<sup>st</sup> March, 2013 - NIPER & IISER Mohali, India



The goal of 3<sup>rd</sup> Indo-German conference is to interconnect the concepts in computational modeling of chemical reactivity and biological activity. Both fields have in common the challenge to work with large systems at molecular resolution as well as the goal to match existing experimental data with high accuracy. Theoretical methods are expected to provide quantitative models for the rationalization of existing data and for the prediction of the properties of new systems in pharmaceutical and catalysis research.

### Major Objectives

- ✓ Biological Activity Catalysis
- ✓ Drug-Receptor Interactions
- ✓ Macromolecular Modeling
- ✓ Molecular Dynamics
- ✓ Non-covalent Interactions
- ✓ Property Design
- ✓ Reaction Mechanisms
- ✓ Reactivity Descriptors

### Invited Speakers

- A. Schaefer, BASF, Ludwigshafen
- B. Ganguly, CSMCRI, Bhavnagar
- B. Jayaram, IIT, New Delhi
- B. Kirchner, Univ. Leipzig
- C. Suresh, NIIST, Thiruvananthapuram
- D. Bhattacharyya, Saha Institute, Kolkata
- E.D. Jemmis, IISER, Thiruvananthapuram
- G. Rajaraman, IIT, Mumbai
- G.N. Sastry, ICT, Hyderabad
- G.P.S. Raghava, IMTECH, Chandigarh
- G. Frenking, PU, Marburg
- H. Zipse, LMU, Munchen
- H. Gohlke, HHU, Dusseldorf
- J. Rademann, Univ. Leipzig
- L. Guruprasad, Univ. Hyderabad
- M.R. Reddy, Rational Labs, Hyderabad
- M. Ullmann, Univ. Bayreuth
- P. Parameswaran, NIT, Calicut
- P. Comba, Univ. Heidelberg
- P. R. Schreiner, JLU, Giessen
- R. Berger, TU, Darmstadt
- S. Pal, NCL, Pune
- U.D. Priyakumar, IIIT, Hyderabad
- V. Subramanian, CLRI, Chennai
- W. Thiel, MPI, Muelheim
- W. Sippl, MLU, Halle-Wittenberg

### Important Dates

Last date of registration: 31<sup>st</sup> December, 2012  
Abstract submission: 31<sup>st</sup> December, 2012

### Satellite Conference

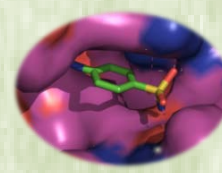
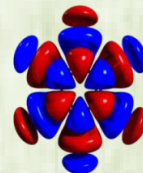
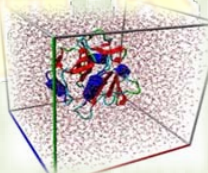
3-4<sup>th</sup> March 2013 : IIS Univ. Jaipur

### Registration + Accommodation Fees

Student:	4000 + 600	INR
Faculty:	6000 + 1200	INR
Industry Delegate:	8000 + 1200	INR
German Participant:	100 + 40	EUR

### Payment Details

Please Send a Bank Draft in Favor of 'The Director, NIPER' Payable at State Bank of Patiala, NIPER Branch, Sector-67, S.A.S. Nagar - 160062, Punjab, India



Prof. Prasad V. Bharatam

Department of Medicinal Chemistry  
National Institute of Pharmaceutical Education & Research (NIPER)  
Sec-67, S.A.S. Nagar - 160 062 Punjab, India

☎: +91-172-2292018, ☎: +91-9417503172, ☎: +91-172-2214692

✉: mcb3@niper.ac.in



Visit us at: <http://www.niper.gov.in/mcb3/index.html>