EDITORIAL

Fourth Indo−U.S. Workshop on Mathematical Chemistry, January 8−12, 2005, Pune, Maharashtra, India

The Fourth Indo−U.S. Workshop on Mathematical Chemistry with applications in drug design, risk assessment of chemicals, chemoinformatics, bioinformatics, computational biology, and toxicology was held on January 8−12, 2005, in Pune, Maharashtra, India, under the joint sponsorship of the Natural Resources Research Institute (NRRI) of the University of Minnesota, Duluth, U. S. A., and the University of Pune. This issue of the Journal of Chemical Information and Modeling contains papers presented at the workshop.

The concept of the Indo−U.S. workshop series was originally conceived by Subhash Basak, a senior scientist at NRRI, and received enthusiastic support from Dilip K. Sinha, a mathematician and educator from India. Together, Basak and Sinha have remained the chairpersons of the biennial, international Indo−U.S. Workshop series from the U. S. A. and India, respectively. The first event of the series was held in 1998 at Visva Bharati University, India, where Dilip Sinha was the vice chancellor at that time; the second and third workshops were organized by NRRI on the campus of the University of Minnesota, Duluth. The success of the Fourth Indo−U.S. Workshop, with the participation of over 125 participants from five continents, shows that the workshop series has established itself as one of the most important conferences in the field. The quality of the presented papers published in this volume after peer review demonstrates the high standard of scientific discourse taking place at the workshop.

Discrete mathematical chemistry has made important advances in the past 25 years. This has been fueled primarily by two factors: (a) the formulation of new concepts and (b) easy access to high-speed computers. Methods developed in this field have found applications in pharmaceutical drug design and hazard assessment of environmental pollutants. Interestingly, discrete mathematical concepts, originally developed for the characterization of chemical systems, are being extended to deal with the explosion of data in "omics" science, namely, genomics, proteomics, and so forth. A few of the 17 papers from the Fourth Indo−U.S. Workshop presentations published in this issue of JCIM are outstanding examples of this expanding chemo−bioinformatics continuum.

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We appreciate the diligent and excellent work of Paty Morales de Tirado of JCIM/Yale University in the publication of the special issue containing papers presented at the Fourth Indo−U.S. Workshop on Mathematical Chemistry.

Dilip K. Sinha, Chairperson (India)
Indo−U.S. Workshop on Mathematical Chemistry Series

Subhash C. Basak, Chairperson (U. S. A.)
Indo−U.S. Workshop on Mathematical Chemistry Series and President,
International Society of Mathematical Chemistry

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