



**INSTITUTE COLLOQUIUM**  
**INDIAN INSTITUTE OF SCIENCE**

**Prof. S Ramasesha**

Solid State and Structural Chemistry Unit  
Indian Institute of Science, Bangalore 560 012

will deliver a lecture  
on

**Quantum Chemistry in the Age of the Second Coming  
of Plastics**

on

**Tuesday, 16<sup>th</sup> November 2004  
at 4.00 PM in the Faculty Hall**

**The Director**  
will preside

**All are cordially invited**  
Coffee/tea: 5.00 p.m.  
Venue: Reception Hall

**ABSTRACT**

The discovery of molecular materials, which exhibit electronic and magnetic properties that were the preserve of simple inorganic solids, in the last few decades, has offered a grand challenge to quantum chemists. Theoretical studies of these systems, which require inventing new models and new techniques, have provided a paradigm shift in quantum chemistry. In this colloquium, the focus will be on the electronic and magnetic properties of  $\pi$  - conjugated and other molecular materials. A brief outline of the new developments in numerical quantum many-body techniques to deal with molecular systems, with particular emphasis on contributions from our group, will be presented. Application of these methods to some of the most important issues in the electronic structure of conjugated materials such as, higher harmonic generation in molecules, ordering of energy levels in conjugated systems, exciton binding energy in conjugated systems, singlet-triplet branching ratio in electron-hole recombination and quantum resonant tunnelling in molecular magnets will be discussed.