

Theoretical Models for Molecular Structure, Properties and Dynamics

Foreword

This volume is an outcome of a suggestion by the editorial board of the Proceedings (Chemical Sciences) to bring out a special issue on modern developments in theoretical chemistry. We have here a collection of forty invited articles encompassing three major areas of theoretical chemistry, viz. electronic structure, properties and dynamics. We believe that the volume is an indicator of the present theoretical chemistry scenario within India. Further, it also contains articles from thirteen eminent scientists from abroad.

This volume is loosely organized in the following manner. A treatment on atoms is followed by semiempirical method-based contributions. Articles on density functional theory and *ab initio* molecular energetics and properties follow. Finally, we have publications on post Hartree–Fock methods, highly correlated systems, dynamics and other miscellaneous topics.

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Last, but not the least, I am grateful to the authors for their valuable contributions to this issue.

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Guest Editor