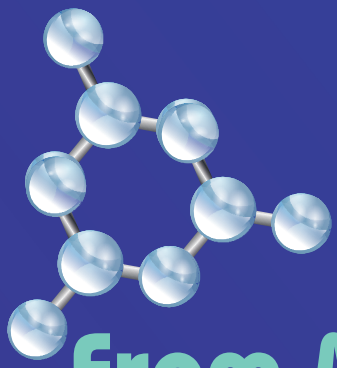

From Molecules to Materials

Unlocking new synergies in Theory, Computations and Experiments

I am delighted to write this foreword for the thematic issue of BARC Newsletter on "Theoretical & Computational Chemistry at BARC" to be published on the important occasion of National Science Day. The research on theory, computations and simulations has been an integral component of all scientific and technological research, of late. With the advent of newer and efficient theoretical methods and availability of high performance supercomputing machines, importance and scope of theory and computations have expanded many folds, as real life challenges can be tackled now very efficiently and accurately in a highly economical way. With the need to understand the structure and energetics of the complex molecules as well as materials and their behavior under extreme conditions, the quantum and classical mechanical methods have now become the most indispensable tools not only in chemistry but in chemical, biological and material sciences as well. In recent years, the cutting edge research in theoretical and computational modeling of materials at different length and time scales have provided an in-depth understanding and rationalization of various chemical processes. Moreover, the capability for discovering and designing new materials, predicting the unknown structure and tailor-made properties of materials that cannot be probed directly by the experiments has made the theoretical and computational methods even more beneficial. This has been possible solely due to the development of advanced theoretical methods, simulation tools and high performance supercomputing machines. The discovery of the state-of-the-art techniques such as machine learning and high-throughput screening methods has further empowered the theoretical and computational methods to tackle real-life problems with greater complexity. Two Noble prizes awarded in the years 1998 and 2013 have demonstrated the increasing importance and vast spread of this branch of research in Chemistry.

In this regard, this issue of BARC Newsletter provides a glimpse of theoretical and computational research in BARC relating to the development of sophisticated theoretical methods, energy storage materials, catalysis, health care etc. Interestingly, the design of newer fuels for advanced nuclear reactors, the evaluations of the physicochemical properties of nuclear fuels and structural materials under extreme conditions and suitable ligand and solvent design for the reprocessing of the spent nuclear fuels have been covered in this issue.

I sincerely hope this collection of research articles will provide a brief idea of the role of theoretical and computational methods in chemistry. It will definitely motivate and encourage the researchers from different areas of scientific field, in particular those involved in experimental studies in DAE related problems to use theoretical methods through collaboration to understand the fundamental concepts from the ab initio level.

I take this opportunity to thank all the authors and associate editors for their time and efforts in preparing this issue.

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