

# Theoretical and Computational Chemistry @BARC

**W**e are extremely happy to showcase this special issue of the BARC Newsletter on the very important occasion of National Science Day. Each year, February 28 is celebrated as National Science Day to commemorate the Nobel Prize-winning work, the 'Raman Effect', discovered by Professor C. V. Raman. We are honored to work on this special issue of BARC Newsletter in the capacity of associate editors. This issue highlights some of the ongoing and important research outcomes in BARC in the field of theoretical and computational chemistry.

Over the years, theoretical and computational chemistry has emerged as an essential and integral part of experimental research not only in chemistry but also in other areas encompassing physical, biological, and engineering sciences. It plays a central role in modern society to design and study new products with important applications in food, healthcare, energy, and environment. Discovering new functional molecules and materials has been accelerated to a great extent with the advent of advanced and sophisticated theoretical and computational chemistry tools and methodologies. Apart from providing an in-depth understanding and rationalization of experimental observations, theoretical and computational studies are also helpful in designing novel molecules and materials with tunable properties. Development and implementation of advanced theories, formulation of fast and accurate simulation techniques, establishing structure-property relations, extending applicability of these techniques in various fields like energy, in particular nuclear energy, environment and healthcare has been the major focus of theoretical and computational research in BARC. With the advent of data mining techniques like artificial intelligence and machine learning, the scope and applicability of theoretical and computational methods to tackle real-life challenges with greater complexity, have expanded manifold.

This newsletter issue comprises 13 articles on varied topics of contemporary theoretical chemistry research-contributed by seasoned scientists from different divisions of BARC. It starts with the interview of Dr. Swapan K. Ghosh, former Head of Theoretical Chemistry Section, BARC, followed by an introductory article on the importance of Theoretical and Computational Chemistry in modern day chemistry research. As this special issue is being published coinciding with the National Science Day events in BARC - to commemorate the great discovery of the 'Raman Effect' - the first technical article of this issue is on the use of experimental Surface-enhanced Raman scattering (SERS) spectroscopy and computational approach in the modern day Raman spectroscopy research. The other articles deal with theoretical chemistry research in varied domains, including nuclear energy, energy conversion and storage, catalysis, exotic chemistry, material properties at extreme conditions and developments of new theoretical and computational methods.

All these articles provide a great deal of knowledge in the respective fields of current theoretical chemistry research at BARC. We hope that the present issue of the BARC newsletter would provide a scientifically stimulating environment for innovative ideas to address current problems in modern society related to food, healthcare, energy, and the environment. On behalf of Theoretical Chemistry Section, Chemistry Division, we sincerely acknowledge and thank all contributors and reviewers of this special issue for their active cooperation and support. We sincerely thank Dr. Swapan K. Ghosh, Dean UM-DAE CEBS for giving his valuable time for the interview. Special thanks to Dr. S. Adhikari, Associate Director, KMG, for giving us the opportunity to serve as the associate editors for this special issue. His novel ideas, encouragement, and support made it possible to bring this issue into a reality in a very short time. We take this opportunity to thank Mr. Manoj Singh, Head, SIRD and the Editorial Team of SIRD, in particular, Mr. Madhav N, Mr. Dinesh J. Vaidya and Smt. Jyoti Panda for their hard work and painstaking efforts in carrying out content curation, design and preparation of proofs of all the articles. We sincerely thank Dr. A. K. Tyagi, Director, Chemistry Group and Director, Bio Science Group for his constant support and encouragement.

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