

Report on CTTC-2020 (held in 2021)

Chemistry Division in association with the Society for Materials Chemistry (SMC) has successfully organised the symposium on the 'Current Trends in Theoretical Chemistry (CTTC-2020)' during 23-25 September 2021 via online mode using the Webex Platform. Dr. A. K. Tyagi, Director Chemistry Group and Dr. T. Bandyopadhyay, Head, Theoretical Chemistry Section acted as the Chairman, CTTC-2020 and Chairman, Local Organising Committee respectively. Primary objective of the symposium has been to provide a vibrant platform for academic interactions and intense discussions on the current trends and future directions in the field of theoretical chemistry. The symposium covered a wide variety of topics that include theoretical formalisms and simulation strategies, electronic structure and spectroscopic properties of molecules, clusters and materials, chemical dynamics, reactivity and catalysis, computational biology, designing new molecules and materials for energy storage and nuclear waste management, machine learning and data mining, etc. The symposium got overwhelming response within a short span of time which clearly indicated the immense research interests in this branch of science in India. More importantly, participants are from a large number of institutes covering the length and breadth of the country with some of the most eminent researchers in the field of theoretical chemistry in India.

The symposium has been launched at 10:00 hrs on 23rd September with the inaugural function followed by an inspiring inaugural address by Prof. R. Chidambaram, DAE Homi Bhabha Chair Professor, on "Theoretical and Computational Chemistry: Synergy with other Disciplines". Plenary Lecture has been delivered by Prof. Rajeev Ahuja, Director, IIT Ropar on "Advanced Modelling of Materials for Clean Energy Applications: Hydrogen Storage Materials and Next-Generation Batteries". During the three days symposium, 23 invited talks, 27 short lectures and 3 technical talks were delivered by the most eminent researchers in the field that include 17 DAE faculty members. It is noteworthy to mention that great importance has been given to the young researchers by arranging large number of short lectures. All the lectures were followed by intense discussions and interaction among the participants. We also arranged online poster presentation where around 100 posters were loaded in the symposium website and all the participants can visit the posters during all the three days. Two dedicated poster sessions were also arranged with short presentations for selected posters along with a summary presentation in each

session and selected posters were awarded with best poster awards. Abstracts of all the invited talks and contributory papers were published as CTTC-2020 conference proceedings. The symposium has been concluded with the concluding session on the final day where many participants applauded the efforts in organising the symposium through online mode. We are confident that the symposium has provided a fertile platform for intense discussions on the recent advancements in the field of theoretical and computational chemistry, generate new ideas and concepts and enhance the knowledge of the young researchers and could lead for interdisciplinary collaborations among the leading research groups in the country. This is also expected to provide an opportunity to bring in new interdisciplinary collaborations among the theoreticians in the country.



