MEETING REPORT

Computational simulations*

A national seminar on computational simulations in polymers, materials and biomolecules was held recently. This programme is the second in the series of 'Seminars on Simulations'. The first one (webinar) was held in August 2021 on 'Recent trends in computational chemistry'.

On day-1, following the inaugural address by V. N. R. Pillai (Vice Chancellor, Somaiya Vidyavihar University (SVU), Mumbai), the keynote lecture by S. Sivaram focused on the importance of simulations and the requirement for knowledge-based, high-quality education. He further emphasized the need for innovative methods of knowledge-based teaching instead of memory-based teaching to improve the quality of education and meet the challenges of the modern world. He also spoke about the advantages of implementing the New Education Policy (NEP) and the initiative of SVU, Mumbai, regarding job-oriented, novel and innovative courses. In the first plenary talk (online), Shridhar R. Gadre (S.P. Pune University, Pune) described the specifics and goals of the seminar as well as the crucial role played by computational simulations in various branches of science.

The first scientific talk delivered by S. Balasubramanian (Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru) was on the indispensability of computational simulations in obtaining insights into supramolecular polymerization. Sourav Pal (Ashoka University, New Delhi) discussed the importance of simulations in addressing future challenges, such as renewable energy, sustainable resources, energy-efficient processes and technologically enabled defense systems, among others.

Intricacies in molecular dynamics (MD) simulations of protein interactions and allosteric reactions from the thermodynamic viewpoint were explained by Suman Chakraborty (S. N. Bose Institute, Kolkata). He further explained the connection between the allosteric reaction and protein interactions employing MD simulations. Durba Sengupta (National Chemical Laboratory (NCL), Pune) gave an informative presentation on biomolecular dynamics utilizing coarse-grained simulations.

Sudip Roy (PreScience In-silico, Bengaluru) presented the key features and the practical applications of the indigenously developed platform for the high throughput AI and physics based drug and materials discovery platform, viz. Prescience in Silico Solution Suite PRINS3. He also highlighted the key challenges in drug and material discovery. Swapan Ghosh (Mumbai University, Mumbai) highlighted the applications of density functional theory to soft condensed matter in different length scales using several simple illustrations from everyday life. The on-line talk by N. Arul Murugan (IIIT New Delhi) dealt with the computational approaches available for drug discovery and the present challenges. He explained the quantum mechanical fragmentation-based data-driven approaches to study the binding affinity in biological systems.

On the second day of the seminar, Swapan Pati (JNCASR, Bengaluru) emphasized the importance of selecting a proper catalyst and thermoelectric materials through various examples. G. S. Sriram (TCS Research, Chennai) mentioned that simulations in the business world are not restricted to matching experimental data. Greater emphasis is placed on the applicability of simulation results to pilot-level or process standardization/optimization levels. Jayant Singh (IIT, Kanpur) described an approach that combines machine learning and computational simulations for designing metal-organic frameworks (MOFs) and separating hydrocarbons. According to him, the strategy can be utilized to address grand challenges such as simulating alkenes from alkanes, CO_2 from dilute emissions, etc.

R. Rajamani (UGC-Department of Atomic Energy Consortium, Indore) discussed the first-principle simulations of bismuth oxides complexes. An automated approach for studying gold clusters, the development of a database and the benchmarking of density functionals was presented by A. Anoop (IIT Kharagpur). Foram Thakkar (Shell India, Bengaluru) discussed MD simulations of carbon molecular sieving membranes. Kumar Vanka (NCL, Pune) presented the density functional theory (DFT)-based simulations of Zeigler–Natta catalysis. Anant D. Kulkarni gave a brief overview of the forthcoming Centre of Computational Studies and Simulations on the SVU campus. He discussed the growth of the global market for computational simulations, focusing on the Asia-Pacific region, and the need for specialized training in computational simulations.

The third session was a poster session dedicated to showcasing the work of young researchers from various institutions across the country. Their research findings were thoroughly discussed and analysed by the experts, who selected the five best ones for ACS poster prizes.

A panel discussion on the 'Future direction in teaching and research in computational simulations' was conducted by Sourav Pal, Jayant Singh, Rajamani, Anoop, Kulkarni and Sriram. The panel discussion ended with probable outcomes and conclusions, as summarized below.

(1) The need for organizing more seminars and training programmes such as workshops and schools for students and young faculty members.

(2) Develop a central pool or repository for 'Made in India' simulation packages, suites and databases, the knowledge base for scientists, faculty members and research scholars.

(3) Importance of teaching and venturing into multiscale simulations augmented with data science-based approaches, namely QSAR/QSPR, AI, ML, etc.

(4) Importance of interdisciplinary teaching and research as well as the development of such curriculum in line with NEP.

On the last day of the seminar, Ramesh Sistla (think Molecular Inc, Bengaluru) comprehensively introduced the Computer Aided Drug Designing methodology and its application to actual drug discovery problems. Sudhir A. Kulkarni (Nova Lead Pharma, Pune) described the experience of going through various phases and critical factors involved in the path from the conceptual design to the successful market launch for a drug for diabetic foot ulcers.

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